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A FUNCTIONAL ANALYTIC FRAMEWORK  
FOR LOCAL ZETA REGULARIZATION AND  
THE SCALAR CASIMIR EFFECT

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Advisor: Prof. Livio Pizzocchero

Coordinator of PhD Studies: Prof. Bert van Geemen

Elaborato Finale di:

Davide Fermi

Matricola: R09931

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Davide Fermi

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Advisor: Prof. L. Pizzocchero  
Coordinator of PhD studies: Prof. Bert van Geemen



# Abstract

It is developed a functional analytic framework allowing to formulate a rigorous implementation of zeta regularization for a canonically quantized scalar field, living on an arbitrary spatial domain and interacting with a classical background potential. This framework relies on the construction of an infinite scale of graded Hilbert spaces associated to the real powers of some given, positive self-adjoint operator. When the latter is a Schrödinger-type differential operator, this formulation provides a natural language to study the integral kernels related to a large class of operators, fulfilling minimal regularity requirements; particular attention is devoted to the regularity of these kernels and to the construction of their analytic continuations with respect to some parameters. Within this framework, complex powers of the elliptic operator giving rise to the Klein-Gordon equation are used to define a zeta-regularized version of the Wightman field whose pointwise evaluation is well-posed. This regularized field determines regularized local observables (such as the stress-energy tensor), whose vacuum expectation values can be expressed in terms of the above mentioned integral kernels. This allows to make contact with the theory of the Casimir effect. Renormalization is achieved by analytic continuation, which is proved to give finite results for the previously mentioned expectation values in most cases of interest. Finally, to exhibit the computational efficiency of the above methods, some explicit examples are discussed.



To my family ...





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# Introduction

In quantum field theory (QFT) there often arises the necessity to give meaning to ill-defined expressions; these appear typically in formal manipulations of distributions that give rise to infinities or divergent quantities when explicit computations are attempted. *Zeta regularization* (ZR) allows to deal with many of these problematic expressions by re-interpreting them as the analytic continuations with respect to a regulator parameter, introduced on purpose, of well-defined integral kernels (or of the corresponding traces) associated to complex powers of the elliptic differential operator appearing in the field equations.

The standard textbook example deals with the sum of positive integers  $\sum_{n=1}^{+\infty} n$ . Of course, this series is divergent in the sense of Cauchy; nevertheless, it can be re-interpreted in terms of the analytic continuation of the Riemann zeta function  $\zeta$ , by introducing the regulator  $s \in \mathbb{C}$  and setting

$$\sum_{n=1}^{+\infty} n \text{ “=” } \left[ \sum_{n=1}^{+\infty} \frac{1}{n^s} \right]_{s=-1} \text{ “=” } [\zeta(s)]_{s=-1} = -\frac{1}{12}. \quad (1)$$

Here the first identity is purely formal, the second one only holds if  $\Re s > 1$  and the third one has to be meant as the evaluation of the analytic continuation at  $s = -1$  (<sup>1</sup>).

The mathematical literature on this topic dates back to the early works of Minakshisundaram and Plejtel [111, 112], and to the subsequent contributions of Seeley [143], Ray and Singer [128].

The first application to QFT was considered in the pioneering work of Dowker and Critchley [51]; soon after a more systematic formulation was developed by Hawking [86] and Wald [152]. Later on, the ZR approach was championed, revisited and widely extended by many authors; among them are, in particular, Cognola, Zerbini and Elizalde [40, 41] (see also [56, 57]), Actor, Svaiter et al. [3, 4, 6, 131, 132] and Moretti et al. [32, 88, 114, 117, 118] (see also the references in the cited works). All the authors mentioned above were mainly interested in the renormalization of local observables, such as the *vacuum expectation value* (VEV) of the stress-energy tensor, having in mind the ultimate purpose of a semi-classical treatment of quantum effects in general relativity (e.g., using the stress-energy VEV as a source in Einstein’s equations).

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<sup>1</sup>The same arguments allow to infer, perhaps even more surprisingly, that  $\sum_{n=1}^{+\infty} n^2 \text{ “=” } 0$ .

On the other hand, the zeta strategy can be applied as well to global observables, such as the VEV of the total energy and of the force on the boundary; in this “global version”, it has become perhaps even more popular than its local counterpart. The literature on global ZR is enormous; here we only cite the classical papers [135, 136] by Zimmerman et al., [22] by Blau, Visser, and Wipf and the monographies of Elizalde et al. [32, 56, 57], of Bordag et al. [24, 25], and of Kirsten [91] (see also the papers [36, 71, 72, 85, 92, 98] by the same author).

Both in the local and in the global versions mentioned above, zeta methods provide a very natural approach to study the theory of the *Casimir effect* (CE): in the present manuscript, with this terminology we refer generically to a class of quite notable physical phenomena which are related to the vacuum state of a quantum field interacting with classical boundaries and/or potentials, possibly living on curved and/or topologically non-trivial background spacetimes. Let us stress that no back-reaction is ever taken into account. The experimental confirmation [28, 93, 113, 147, 148] of these theoretical predictions has shown that operations such as a naive implementation of Wick’s normal ordering (usually interpreted as a simple redefinition of the energy) are highly non-trivial, since they remove a priori the possibility to predict any vacuum effect.

In comparison with the original theoretical derivation of these effects by Casimir [35], and with other methods such as point-splitting [21, 31, 49, 59, 110, 126] (in particular, see [84, 115] for a comparison between point-splitting and the ZR approach) and the algebraic, microlocal approach (see, e.g., [16, 44, 75, 123, 127] and citations therein), the zeta strategy is competitive and, perhaps, more elegant. Nevertheless, in most of the works cited previously ZR is implemented within the framework of Euclidean formulation of QFT, often in connection with expressions which are derived by formal manipulations of functional integrals; moreover, apart from a few exceptions [3, 4, 6, 40, 114, 131, 132] dealing with specific spatial configurations, local aspects are scarcely taken into account when boundaries are also present.

In this manuscript a different, more systematic formulation is proposed for the ZR approach, which can be applied automatically in any specific case. The basic framework under consideration is that of canonical quantization for a Hermitian scalar field, living on an arbitrary spatial subset of Minkowski spacetime; prescribed boundary conditions are also taken into account, as well as the “effective interaction” with a classical, background scalar potential. The attention is mainly focused on the VEV of the stress-energy tensor, of which both the conformal and the non-conformal parts are considered; however, the total energy and boundary forces are also taken into account.

More in detail, the manuscript consists of four chapters, described hereafter.

*Chapter 1* briefly reviews the approach to ZR developed in the previous works [63, 64, 65, 66, 67] (D.F., L. Pizzocchero) where, having in mind a direct application to some specific physical models, the language employed is less formal than the one developed in the subsequent chapters of the present work. Attention is focused on the case of a Hermitian scalar field living on a subset of Minkowski spacetime; time evolution is described by the Klein-Gordon equation with the addition of a classical background potential and suitable

spatial boundary conditions are prescribed. After a brief outline of the classical reference theory, the field is described in second quantization by means of the standard expansion in terms of annihilation and creation operators associated to a complete orthonormal system of eigenfunctions for the elliptic operator defining the “spatial part” of the Klein-Gordon equation. Complex powers of this elliptic operator are used to define a regularized version of the field; in turn, the latter is used to derive a regularized version of the propagator, which is related to the VEVs of many observables (such as the stress-energy tensor). The regularized propagator appears to be connected to the integral kernels associated to complex powers of the elliptic operator mentioned above. In the end, renormalization is defined in terms of the analytic continuation of these kernels.

In *Chapter 2* a more systematic functional analytic framework is developed, allowing to address properly topics such as the integral kernels associated to the complex powers of an elliptic differential operator, their regularity and their analytic continuations (without relying heavily on eigenfunction expansion techniques). This apparatus is conceived to be used in the subsequent Chapter 3 in connection with a more rigorous formulation of the field theory discussed in Chapter 1 and of its regularization. First an abstract framework is described, where a scale of indexed Hilbert spaces is constructed starting from an assigned separable Hilbert space  $\mathcal{H}$  and from a strictly positive, (essentially) self-adjoint operator  $\mathcal{A}$  on it. Next, this abstract framework is employed in the case where  $\mathcal{H}$  is the space of square-summable functions on a given spatial domain  $\Omega \subset \mathbb{R}^d$  and  $\mathcal{A}$  is a Schrödinger-type differential operator; it is shown that the elements of the scale of Hilbert spaces are related to Sobolev spaces and to spaces of differentiable functions. This formalism is used to describe the theory of integral kernels related to a class of suitable operators; regularity and other miscellaneous results are derived for these kernels. Particular attention is dedicated to the Dirichlet kernel (i.e., the kernel related to the complex power  $\mathcal{A}^{-s}$ , for suitable  $s \in \mathbb{C}$ ) and to the heat and cylinder kernels (associated, respectively, to  $e^{-t\mathcal{A}}$  and  $e^{-t\sqrt{\mathcal{A}}}$ , for  $\Re t > 0$ ); it is shown that the first can be expressed in terms of Mellin transforms of the latter. This fact is employed to construct the analytic continuation of the Dirichlet kernel and of its derivatives, by means of three different methods; these rely on suitable assumptions for the heat or cylinder kernels, which are well known to be fulfilled in most cases of interest.

In *Chapter 3* the approach to local ZR discussed in the first chapter is developed within a fully rigorous framework for second quantization, based on Fock space techniques. The starting point is the bosonic Fock space  $\mathfrak{F}^\vee(\mathcal{H})$  on the single particle Hilbert space  $\mathcal{H}$ ; next, for  $h \in \mathcal{H}$ , the Segal field  $\hat{\Phi}_S(h)$  and the conjugate momentum  $\hat{\Pi}_S(h)$  are defined in terms of the annihilation and creation operators (which, in turn, are defined in the standard manner on the dense finite particle subspace of  $\mathfrak{F}^\vee(\mathcal{H})$ ). Assuming  $\mathcal{A}$  to be a strictly positive and self-adjoint operator on  $\mathcal{H}$ , the Wightman field at time zero is described as the unique  $\mathbb{C}$ -linear extension of the  $\mathbb{R}$ -linear map  $h \mapsto \hat{\Phi}_S(\mathcal{A}^{-1/4}h)$  (for  $\bar{h} = h$ ). Time evolution is implemented applying the second quantization map  $\Gamma$  to the strongly continuous, one parameter unitary group  $(e^{-it\sqrt{\mathcal{A}}})_{t \in \mathbb{R}}$  (where  $\sqrt{\mathcal{A}}$  plays the role of the single particle Hamiltonian); it is shown that, under suitable assumptions on  $h$ ,

the time evolved field  $\hat{\varphi}_t(h)$  is differentiable and fulfills a strong form of the Klein-Gordon equation. ZR is implemented using the powers  $\mathcal{A}_\kappa^{-u/4} := (\mathcal{A}/\kappa^2)^{-u/4}$  ( $u \in \mathbb{C}$ ;  $\kappa > 0$  a given mass parameter), to define a family of regularized Dirac deltas  $\delta_{\mathbf{x}}^u := \mathcal{A}_\kappa^{-u/4} \delta_{\mathbf{x}}$  and setting, for  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$ ,

$$\hat{\varphi}^u(x) := \hat{\varphi}_t(\delta_{\mathbf{x}}^u) ; \quad (2)$$

this is shown to be a regular function of  $x$  for  $\Re u$  large enough and it is used to define a zeta-regularized version  $\hat{T}_{\mu\nu}^u(x)$  of the stress-energy tensor operator, by analogy with the corresponding classical observable. Moreover, the VEV of  $\hat{T}_{\mu\nu}^u(x)$  is proven to be an analytic function of  $u$  which can be expressed in terms of the Dirichlet kernel and of its derivatives; the analytic continuation of these kernels can be obtained using one of the methods described in Chapter 2, relating to Mellin transforms. In the end, the renormalized stress-energy VEV is defined by analytic continuation at  $u = 0$ . Related observables, such as the total energy and the pressure on the boundary, are also discussed by similar methods.

In the conclusive *Chapter 4* the framework developed previously is applied to some specific configurations. First of all, some of the results obtained for special cases in our antecedent works [66, 67] are briefly recalled: in particular, attention is focused on the cases of a massless field either interacting with a background harmonic potential or confined within a rectangular box. Next, another case is analyzed which, to the author's knowledge, has never been addressed before using zeta techniques; this is the case of a scalar field confined between two parallel planes  $\pi_0, \pi_a$ , on which a particular type of Robin boundary conditions are prescribed. More precisely, for  $\beta \in \mathbb{R}$ , it is required

$$(1 + \beta \partial_{\mathbf{n}}) \hat{\varphi} \Big|_{\pi_0} = 0 , \quad (1 - \beta \partial_{\mathbf{n}}) \hat{\varphi} \Big|_{\pi_a} = 0 \quad (3)$$

(where  $\partial_{\mathbf{n}}$  indicates the normal derivative at points of  $\pi_0$  and  $\pi_a$ , respectively). To treat this case, an integral representation is derived for the cylinder kernel corresponding to the reduced 1-dimensional problem of a segment with the boundary conditions descending from those in Eq. (3). This integral representation allows to derive an explicit expression for the regularized stress-energy VEV, which can be evaluated explicitly at  $u = 0$ , thus giving the renormalized VEV of the stress-energy tensor.

## Basic notations.

We write  $\mathbb{N}$  for the set of nonnegative integers  $n = 0, 1, 2, \dots$ .

Throughout this manuscript, we indicate with  $\cdot$  and  $|\cdot|$  the standard inner product on  $\mathbb{R}^d$  ( $d \in \{1, 2, 3, \dots\}$ ) and the corresponding norm, respectively. Points of  $\mathbb{R}^d$  are indicated with boldface symbols (such as  $\mathbf{x}, \mathbf{y}, \mathbf{z}$ , etc).

The Lebesgue measure on  $\mathbb{R}^d$  is denoted with  $d\mathbf{x}$  (or  $d\mathbf{y}$ ); we indicate with  $|E|$  the Lebesgue measure of any measurable subset  $E \subset \mathbb{R}^d$ .



We often use  $d$ -dimensional multi-indices, which are sequences  $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ ; the order of any such multi-index is  $|\alpha| := \alpha_1 + \dots + \alpha_d$ . We use the standard notation for partial derivatives and set  $\partial^\alpha := \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d}$ . For functions of two (or more) sets of variables such as  $\psi : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C}$ ,  $(\mathbf{x}, \mathbf{y}) \mapsto \psi(\mathbf{x}, \mathbf{y})$ , given any pair of multi-indices  $\alpha, \beta \in \mathbb{N}^d$ , we use the self-evident notations  $\partial_1^\alpha \partial_2^\beta \psi \equiv \partial_{\mathbf{x}}^\alpha \partial_{\mathbf{y}}^\beta \psi$  to indicate the corresponding partial derivatives.

### About complex powers.

Throughout the present manuscript, the following conventions are employed.

- i.  $\ln : (0, +\infty) \rightarrow \mathbb{R}$  is the elementary logarithm.
- ii. For any  $s \in \mathbb{C}$ , we systematically refer to the standard definition

$$x^s := e^{s \ln x} \quad \text{for all } x \in (0, +\infty) . \quad (4)$$

- iii. For any  $s \in \mathbb{C}$  and for any  $z$  in a convenient subset  $\mathbb{C}^\times$  of the complex plane, we put

$$z^s := e^{s \ln |z| + is \arg z} , \quad (5)$$

where  $\arg : \mathbb{C}^\times \rightarrow \mathbb{R}$  is some determination of the argument; this determination depends on the domain  $\mathbb{C}^\times$  and must be specified in each case of interest. Unless otherwise stated, hereafter we always put

$$\begin{aligned} \mathbb{C}^\times &:= \mathbb{C} \setminus [0, +\infty) ; \\ \arg &:= \text{the unique determination of the argument with values in } (0, 2\pi) . \end{aligned} \quad (6)$$



# Chapter 1

## Motivations and basic ideas

In the present chapter we outline the main heuristic ideas motivating the more rigorous analysis to be discussed in detail throughout the subsequent chapters of this work, where a language more formal and precise from a mathematical point of view is employed. To this purpose, hereafter we briefly recall some results which were first presented more extensively in our previous work [64] (see also [63]). In particular, we consider an approach to ZR which works in the framework of canonical quantization; this makes a major difference in comparison with the more common version of this regularization scheme, which relies substantially on the Euclidean formulation of QFT.

We restrict the attention to the case of a scalar field; this is assumed to live on an assigned spatial domain of arbitrary dimension, to fulfill suitable boundary conditions and, possibly, to interact with a classical background potential (including, in some cases, a mass term). In Section 1.1 we review the reference classical theory, introducing the physical observables of main interest for the subsequent analysis; namely, the stress-energy tensor, the total energy and the pressure on the boundary. In Section 1.2 we consider the canonical quantization of the classical theory described previously; the quantized scalar field is expanded in terms of creation and annihilation operators, using a complete orthonormal set of eigenfunctions of the elliptic operator appearing in the field equations. In the final Section 1.3 we describe the approach to ZR which was first proposed in [63, 64]: the basic idea is to use the complex powers of the previously mentioned elliptic operator to define a regularized version of the field at a point. The latter determines, in turn, a regularized propagator, whose diagonal evaluation is strictly connected to certain integral kernels, to be analyzed in detail in Chapter 2.

In passing, we take the chance to fix some conventions and notations to which we will refer throughout the entire manuscript.

Before proceeding let us stress that, in both the classical and quantum versions of the field theory under analysis, the above mentioned spatial domain, its boundary and the background potential are treated as purely classical objects, which are assigned once and for all and possess no dynamical evolution in time. Therefore, the interaction between these objects and the (quantum) field is described in a purely effective fashion; in particular, no back-reaction is ever taken into account in the analysis to be described in the present Chapter, as well as in the remainder of this work.

## 1.1 The reference classical theory.

We use natural units, so that

$$c = 1 \quad \text{and} \quad \hbar = 1 , \quad (1.1)$$

and work in  $(d + 1)$ -dimensional Minkowski spacetime  $\mathcal{M}_{d+1}$  (with  $d \in \{1, 2, 3, \dots\}$  arbitrary); this is identified with  $\mathbb{R}^{d+1}$  using a set of inertial coordinates

$$x = (x^\mu)_{\mu=0,1,\dots,d} \equiv (x^0, \mathbf{x}) \equiv (t, \mathbf{x}) : \mathcal{M}_{d+1} \rightarrow \mathbb{R}^{d+1} , \quad (1.2)$$

in which the Minkowski metric  $\eta \equiv (\eta_{\mu\nu})$  has coefficients <sup>(1)</sup>

$$(\eta_{\mu\nu}) = \text{diag}(-1, \underbrace{1, \dots, 1}_{d \text{ times}}) . \quad (1.3)$$

We fix a spatial domain  $\Omega \subset \mathbb{R}^d$  and refer to the classical theory of a scalar field

$$\varphi : \mathbb{R} \times \Omega \rightarrow \mathbb{R} , \quad x \mapsto \varphi(x) \equiv \varphi(t, \mathbf{x}) ; \quad (1.4)$$

this is assumed to be at least twice differentiable, to fulfill prescribed conditions (e.g., of Dirichlet, Neumann or Robin type) on the boundary  $\mathbb{R} \times \partial\Omega$  and to decay rapidly at time (and possibly spatial, if  $\Omega$  is unbounded) infinity. Analogous settings are considered, e.g., in [24, 25, 32, 75].

The *action functional* describing the theory under analysis is

$$\mathcal{S}[\varphi] := \int_{\mathbb{R} \times \Omega} dt d\mathbf{x} \frac{1}{2} \left( \partial^\mu \varphi(t, \mathbf{x}) \partial_\mu \varphi(t, \mathbf{x}) + V(\mathbf{x}) \varphi^2(t, \mathbf{x}) \right) , \quad (1.5)$$

where  $V : \Omega \rightarrow \mathbb{R}$ ,  $\mathbf{x} \mapsto V(\mathbf{x})$  is a suitable smooth potential; here and elsewhere, unless otherwise stated, we use *Einstein's summation convention*.

The field time evolution is described by the *Klein-Gordon equation* with external potential

$$0 = (-\partial^\mu \partial_\mu + V) \varphi = (\partial_{tt} - \Delta + V) \varphi \quad (1.6)$$

( $\Delta := \sum_{i=1}^d \partial_{x^i x^i}$  is the  $d$ -dimensional laplacian); of course, initial data for the field and for its time derivative must be provided as well in order to obtain a well-posed evolution differential problem.

The *stress-energy tensor* has components (for  $\mu, \nu \in \{0, \dots, d\}$ )

$$T_{\mu\nu} := (1 - 2\xi) \partial_\mu \varphi \partial_\nu \varphi - \left( \frac{1}{2} - 2\xi \right) \eta_{\mu\nu} (\partial^\lambda \varphi \partial_\lambda \varphi + V \varphi^2) - 2\xi \varphi \partial_{\mu\nu} \varphi ; \quad (1.7)$$

---

<sup>1</sup>Equivalently, the line element corresponding to the Minkowski metric  $\eta$  is assumed to be

$$ds^2 = \eta_{\mu\nu} dx^\mu dx^\nu = -(dx^0)^2 + (dx^1)^2 + \dots + (dx^d)^2 .$$

the parameter  $\xi \in \mathbb{R}$  is fixed arbitrarily. The above mentioned regularity assumptions for the field  $\varphi$  suffice to infer the continuity of the functions  $T_{\mu\nu} : \mathbb{R} \times \Omega \rightarrow \mathbb{R}$ ,  $x \mapsto T_{\mu\nu}(x) \equiv T_{\mu\nu}(t, \mathbf{x})$  (let us stress that all the bilinear expressions in the field in Eq. (1.7) are to be evaluated along the diagonal; so, e.g.,  $(\partial_\mu \varphi \partial_\nu \varphi)(x) = \partial_\mu \varphi(x) \partial_\nu \varphi(x)$ ). The expression in Eq. (1.7) is usually referred to as “improved” stress-energy tensor; this is a well-known modification of the canonical stress-energy tensor (i.e., the conserved Noether current associated with the spacetime translational symmetries of the action functional (1.5)) with an additive term proportional to the real parameter  $\xi$ , that does not alter its divergence (for more details, see Appendix A of [64]). The improved stress-energy tensor was first proposed by Callan, Coleman and Jackiw [34] in order to deal with some pathologies arising in perturbation theory for the corresponding quantized version of the field theory under analysis; later on, this tensor was reinterpreted in terms of the Minkowskian limit for a scalar field coupled to gravity via the curvature scalar [21, 32, 51, 121, 123] (see also the footnote on page 4 of [63]).

Other observables can be defined in terms of the stress-energy tensor. More precisely, the *total energy* at time  $t \in \mathbb{R}$  is the integral over the spatial domain  $\Omega$  of the energy density  $T_{00}(t, \mathbf{x})$ , i.e.,

$$\mathcal{E}(t) := \int_{\Omega} d\mathbf{x} T_{00}(t, \mathbf{x}) ; \quad (1.8)$$

on the other hand, the *pressure* at a point on the boundary of the spatial domain  $\mathbf{x} \in \partial\Omega$  (at times  $t \in \mathbb{R}$ ), is the vector  $\mathbf{p}(x) = (p^i(t, \mathbf{x}))$  ( $i = 1, \dots, d$ ), whose components are

$$p^i(t, \mathbf{x}) := T^i_j(t, \mathbf{x}) n^j(\mathbf{x}) , \quad (1.9)$$

where  $\mathbf{n}(\mathbf{x}) = (n^i(\mathbf{x}))$  is the unit normal to  $\partial\Omega$  at  $\mathbf{x}$ .

## 1.2 Second quantization.

In order to fix some notations, let us now briefly address the second quantization of the classical field theory described in the previous section. Within this framework, we consider the single particle Hilbert space  $\mathcal{H} = L^2(\Omega)$ , with inner product  $\langle | \rangle_{L^2}$ , and the bosonic Fock space  $\mathfrak{F}^\vee(\mathcal{H}) \equiv \mathfrak{F}$  on it, with inner product  $( | )$ .

The classical field  $\varphi : \mathbb{R} \times \Omega \rightarrow \mathbb{R}$  is replaced by the map

$$\hat{\varphi} : \mathbb{R} \times \Omega \rightarrow \mathcal{L}_{sa}(\mathfrak{F}) , \quad x \mapsto \hat{\varphi}(x) \equiv \hat{\varphi}(t, \mathbf{x}) \quad (1.10)$$

(<sup>2</sup>), where we are referring to the space  $\mathcal{L}(\mathfrak{F})$  of linear operators on  $\mathfrak{F}$  and to the subset  $\mathcal{L}_{sa}(\mathfrak{F})$  of self-adjoint operators. Next, let us put

$$\mathcal{A} := -\Delta + V , \quad (1.11)$$

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<sup>2</sup> Of course the notation  $\hat{\varphi} : \mathbb{R} \times \Omega \rightarrow \mathcal{L}_{sa}(\mathfrak{F})$ ,  $(\mathbf{x}, t) \mapsto \hat{\varphi}(\mathbf{x}, t)$  is used here in connection with a *generalized* operator valued function; in fact, as well known,  $\hat{\varphi}$  is an operator valued *distribution*. We defer to Chapter 3 a more rigorous analysis.

intending that the boundary conditions on  $\partial\Omega$  (if any) are accounted for in the above definition; we assume the framework under analysis to grant that  $\mathcal{A}$  is a *strictly positive, selfadjoint* operator on  $\mathcal{H}$ .

To proceed, consider a complete orthonormal set  $(F_k)_{k \in \mathcal{K}}$  of (possibly generalized) eigenfunctions of  $\mathcal{A}$  <sup>(3)</sup>, indexed by an unspecified set of labels  $\mathcal{K}$ , and write the corresponding eigenvalues in the form  $(\omega_k^2)_{k \in \mathcal{K}}$  ( $\omega_k \geq \varepsilon$  for some  $\varepsilon > 0$  and for all  $k \in \mathcal{K}$ ); thus

$$\begin{aligned} F_k : \Omega &\rightarrow \mathbb{C} , & \mathcal{A}F_k &= \omega_k^2 F_k , \\ \langle F_k | F_h \rangle_{L^2} &= \delta(k, h) & \text{for all } k, h &\in \mathcal{K} . \end{aligned} \quad (1.12)$$

Any eigenfunction label  $k \in \mathcal{K}$  can include different parameters, both discrete and continuous. Besides, we generically write  $\int_{\mathcal{K}} dk$  to indicate summation over all labels (i.e., literal summation over discrete parameters and integration over continuous parameters, with respect to a suitable measure);  $\delta(h, k)$  is the Dirac delta function for the label space  $\mathcal{K}$  (this reduces to the Krönecker symbol in the case of discrete parameters).

The set of eigenfunctions described above allows us to derive for the quantized field a normal modes expansion of the form

$$\hat{\varphi}(t, \mathbf{x}) = \int_{\mathcal{K}} \frac{dk}{\sqrt{2\omega_k}} \left[ \hat{a}_k e^{-i\omega_k t} F_k(\mathbf{x}) + \hat{a}_k^\dagger e^{i\omega_k t} \overline{F}_k(\mathbf{x}) \right] \quad (1.13)$$

(with  $\overline{\phantom{x}}$  indicating complex conjugation). Here we are considering the destruction and creation operators  $\hat{a}_k, \hat{a}_k^\dagger \in \mathcal{L}(\mathfrak{F})$  ( $k \in \mathcal{K}$ ) associated to the set of eigenfunctions  $(F_k)_{k \in \mathcal{K}}$ ; these fulfill the canonical commutation relations

$$[\hat{a}_h, \hat{a}_k] = [\hat{a}_h^\dagger, \hat{a}_k^\dagger] = \hat{\mathcal{O}}_{\mathfrak{F}} , \quad [\hat{a}_h, \hat{a}_k^\dagger] = \delta(h, k) \hat{\mathbb{I}}_{\mathfrak{F}} , \quad (1.14)$$

where  $\hat{\mathcal{O}}_{\mathfrak{F}}, \hat{\mathbb{I}}_{\mathfrak{F}} \in \mathcal{L}(\mathfrak{F})$  denote the null and the identity operator on  $\mathfrak{F}$ , respectively. Moreover, indicating with  $\mathbf{v} \in \mathfrak{F}$  the *vacuum state* (of unit norm), there holds the annihilation condition

$$\hat{a}_k \mathbf{v} = \mathbf{o} \quad (1.15)$$

( $\mathbf{o} \in \mathfrak{F}$  is the null element of  $\mathfrak{F}$ , not to be confused with  $\mathbf{v}$ ).

Next let us consider the *propagator*, i.e., the vacuum expectation value (VEV)

$$\langle \mathbf{v} | \hat{\varphi}(x) \hat{\varphi}(y) | \mathbf{v} \rangle \quad (x, y \in \mathbb{R} \times \Omega) ; \quad (1.16)$$

this allows to make connection with the Casimir effect. In fact, one can define second quantized versions of the classical observables mentioned in the previous subsection (such as the stress-energy tensor (1.7)) and compute the corresponding VEVs; all these VEVs can be expressed in terms of the propagator (1.16) and of its derivatives, evaluated along the diagonal  $y = x$ . We defer to Chapter 3 a more detailed analysis.

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<sup>3</sup>For a fully rigorous discussion of generalized eigenfunctions see, e.g., Chapter IV of [78].

The assumption of strict positivity for  $\mathcal{A}$  (granting that  $\omega_k \geq \varepsilon$ , for some  $\varepsilon > 0$  and for all  $k \in \mathcal{K}$ ) excludes the presence of any infrared divergence<sup>4</sup>. On the other hand, the propagator is known to be plagued with ultraviolet divergences, which appear along the diagonal; therefore, expressions such as  $(\mathbf{v} | \hat{\varphi}(x)^2 \mathbf{v}) \equiv (\mathbf{v} | \hat{\varphi}(x) \hat{\varphi}(x) \mathbf{v})$  are merely formal ways to indicate ill-defined quantities.

Our purpose in the next subsection is to redefine the field operator via a suitable regularization scheme, ultimately yielding finite values for the propagator also along the diagonal (and for other related observables).

### 1.3 Zeta regularization.

Let  $\kappa > 0$  denote a parameter, to which we attribute the dimension of a mass (or of an inverse length, since we have fixed  $\hbar = 1$ ). Because of this,  $\kappa$  will be called the *mass scale*; it is introduced for dimensional reasons and it plays the role of a normalization scale. The final, renormalized results appear to depend on  $\kappa$  only when singularities appear in the analytic continuations involved in the following construction. See [22, 32, 56, 88, 114] for further comments regarding this parameter and its presence or absence in the renormalized observables related to the field.

The zeta strategy, in the version proposed in [63, 64] (and employed systematically in [65, 66, 67]), relies on the powers

$$\mathcal{A}_\kappa^{-u/4} := (\mathcal{A}/\kappa^2)^{-u/4}, \quad (1.17)$$

where  $\mathcal{A} = -\Delta + V$  is the operator (1.11) and  $u \in \mathbb{C}$ ; these operators are employed to introduce the *zeta-regularized field operator*

$$\hat{\varphi}^u := \mathcal{A}_\kappa^{-u/4} \hat{\varphi}, \quad (1.18)$$

depending on the complex parameter  $u$  and coinciding with the usual field operator  $\hat{\varphi}$  for  $u = 0$ . We provisionally accept the following heuristic definition of  $\mathcal{A}_\kappa^{-u/4} \hat{\varphi}$ <sup>5</sup>: this is the operator-valued function constructed expanding  $\hat{\varphi}$  as in Eq. (1.13) via a complete orthonormal system of eigenfunctions  $(F_k)_{k \in \mathcal{K}}$  of  $\mathcal{A}$  and letting  $\mathcal{A}_\kappa^{-u/4}$  act on each eigenfunction as  $\mathcal{A}_\kappa^{-u/4} F_k = \kappa^{u/2} \omega_k^{-u/2} F_k$ . In this way, Eq. (1.18) yields

$$\hat{\varphi}^u(t, \mathbf{x}) = \kappa^{u/2} \int_{\mathcal{K}} \frac{dk}{\sqrt{2} \omega_k^{(u+1)/2}} \left[ \hat{a}_k e^{-i\omega_k t} F_k(\mathbf{x}) + \hat{a}_k^\dagger e^{i\omega_k t} \bar{F}_k(\mathbf{x}) \right]. \quad (1.19)$$

Note that, in the limit  $\omega_k \rightarrow +\infty$ , the term  $1/\omega_k^{(u+1)/2}$  in the above integral vanishes rapidly if  $\Re u$  is large; this is a manifestation of the regularizing effect of the operator  $\mathcal{A}_\kappa^{-u/4}$  for large  $\Re u$ .

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<sup>4</sup>In Section 5 of [64], we also considered some variations of the present setting allowing to deal with infrared issues as well.

<sup>5</sup>We defer to Chapter 3 of this manuscript a more rigorous formulation.

The regularized field  $\hat{\varphi}^u$  allows to construct a *regularized propagator*

$$(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) \quad (x, y \in \mathbb{R} \times \Omega) , \quad (1.20)$$

which can be used, in turn, to define regularized versions for the VEV of the other previously mentioned observables as well. In fact, it appears that the regularized propagator (1.20) (along with its derivatives) is regular also along the diagonal  $y = x$  if  $\Re u$  is large enough; this means that the ultraviolet divergences of  $(\mathbf{v} | \hat{\varphi}(x) \hat{\varphi}(y) \mathbf{v})$  have been cured by the regularization scheme described above.

In particular, using the expansion (1.19) along with the commutation relations (1.14), the diagonal regularized propagator  $(\mathbf{v} | (\hat{\varphi}^u(t, \mathbf{x}))^2 \mathbf{v}) \equiv (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(x) \mathbf{v})$  can be computed explicitly. The final result is

$$(\mathbf{v} | (\hat{\varphi}^u(t, \mathbf{x}))^2 \mathbf{v}) = \frac{\kappa^u}{2} \int_{\mathcal{K}} \frac{dk}{\omega_k^{u+1}} F_k(\mathbf{x}) \bar{F}_k(\mathbf{x}) ; \quad (1.21)$$

notice that the right-hand side above does not depend on the time coordinate  $t$ . Moreover, the integral appearing in Eq. (1.21) can be interpreted as the eigenfunction expansion of the integral kernel associated to the complex power  $\mathcal{A}^{-\frac{u+1}{2}}$  evaluated along the diagonal, i.e., as  $\mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{x})$ ; more precisely there holds

$$(\mathbf{v} | (\hat{\varphi}^u(t, \mathbf{x}))^2 \mathbf{v}) = \frac{\kappa^u}{2} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{x}) . \quad (1.22)$$

Typically, the zeta regularized observables derived in the above framework are analytic functions of the parameter  $u$ , for  $\Re u$  sufficiently large. Then, according to the (either restricted or extended) zeta approach described in [64], the renormalized versions of this observables are defined in terms of the analytic continuations (or, rather, of their regular parts) at  $u = 0$  of the regularized counterparts; so, for example, we put

$$(\mathbf{v} | (\hat{\varphi}(t, \mathbf{x}))^2 \mathbf{v})_{ren} := RP \Big|_{u=0} \frac{\kappa^u}{2} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{x}) \quad (1.23)$$

(here  $RP|_{u=0}$  indicates the evaluation in  $u = 0$  of the regular part of the related analytic continuation). As exemplified in Eq. (1.23), the renormalized observables are strictly related to the diagonal values of the integral kernels (and of the corresponding derivatives) associated to complex powers of the differential operator  $\mathcal{A} = -\Delta + V$ .

In view of the above considerations, in order to give a more rigorous and systematic formulation of the approach described above (a formulation to be discussed in Chapter 3), it is first necessary to develop a functional analytic framework allowing to address properly the theory of integral kernels. This topic will be discussed in the forthcoming Chapter 2 where attention is focused, in particular, on the regularity properties of the mentioned kernels and on the methods allowing to construct their analytic continuations.



# Chapter 2

## Functional spaces, operators and kernels

In this chapter we describe the basic functional analytic framework to which we will refer throughout the remainder of the present manuscript. We first recall some well-known facts about distributions, Sobolev spaces and interpolation of Banach spaces. Next, we describe an abstract setting based on a scale of Hilbert spaces associated to the real powers of a given strictly positive, self-adjoint operator. The case where the mentioned operator is an elliptic Schrödinger-type differential operator is then considered in more detail; the results obtained in this setting allow, among else, to give an alternative formulation of the theory of integral kernels related to a suitable type of operators. Finally, we briefly review some results about Mellin transforms and their analytic continuations.

### 2.1 Function spaces.

Throughout the entire manuscript  $\Omega$  denotes a *domain* in  $\mathbb{R}^d$ , meaning that  $\Omega \subset \mathbb{R}^d$  is an open connected subset. We will mainly focus the attention on the settings i) and ii) described hereafter:

i)  $\Omega$  is an arbitrary domain in  $\mathbb{R}^d$ , with no restrictions regarding either regularity or boundedness; in fact,  $\Omega$  could also be unbounded with a boundary which is not even continuous (the case  $\Omega = \mathbb{R}^d$  is not excluded as well).

ii)  $\Omega$  is a bounded domain, with compact boundary  $\partial\Omega$  of class  $C^\infty$ .

In both cases i) and ii),  $\bar{\Omega}$  indicates the closure of  $\Omega$ , i.e.,  $\bar{\Omega} := \Omega \cup \partial\Omega$ .

Possible variations of the above settings are sometimes taken into account as well, in order to hint at simple generalizations of some results to be discussed in the following.

*Remark 2.1.* Unless otherwise stated,  $\Omega$  is always assumed to be as in item i) above.

In the subsequent paragraphs we fix some standards about the main function spaces on  $\Omega$  to be considered in this work.

### Test functions and distributions.

A test function on  $\Omega$  is a smooth, compactly supported function  $f : \Omega \rightarrow \mathbb{C}$ ; these functions form the vector space  $\mathcal{D}(\Omega)$ , which can be equipped with the well known inductive limit topology (see, e.g., [151]). With respect to this topology,  $\mathcal{D}(\Omega)$  is a so-called LF-space, that is a countable, strict inductive limit of Fréchet spaces.

The topological dual space  $\mathcal{D}'(\Omega)$  is the locally convex space of Schwartz distributions on  $\Omega$ ; we write  $\langle f, \varphi \rangle$  for the action of a distribution  $f$  on a test function  $\varphi$ . Unless otherwise stated, all derivatives considered in the sequel are to be understood in the sense of distributions.

### The spaces $L^p(\Omega)$ , $L^p_{\text{loc}}(\Omega)$ .

For any  $p \in (0, +\infty)$ , these spaces consist of measurable functions  $f : \Omega \rightarrow \mathbb{C}$  such that  $|f|^p$  is Lebesgue integrable on  $\Omega$  or (in the local case) on any compact subset of  $\Omega$ . The standard norm on the Banach space  $L^p(\Omega)$  is indicated with  $\|\cdot\|_{L^p}$ ; we regard  $L^2(\Omega)$  as a Hilbert space endowed with the inner product  $\langle f|g \rangle_{L^2} := \int_{\Omega} d\mathbf{x} \overline{f(\mathbf{x})} g(\mathbf{x}) \equiv \int_{\Omega} \overline{f} g$ . We use systematically the embeddings  $L^p(\Omega) \hookrightarrow L^p_{\text{loc}}(\Omega) \hookrightarrow \mathcal{D}'(\Omega)$ .

### Sobolev spaces

Let  $m \in \mathbb{N}$ ; we will often consider the Sobolev space (of  $L^2$  type and) of integer order  $m$

$$H^m(\Omega) := \{f \in \mathcal{D}'(\Omega) \mid \partial^\alpha f \in L^2(\Omega) \text{ for } \alpha \in \mathbb{N}^d, |\alpha| \leq m\} . \quad (2.1)$$

This is a complex Hilbert space with the inner product

$$\langle f|g \rangle_{H^m} := \sum_{\alpha \in \mathbb{N}^d, |\alpha| \leq m} \langle \partial^\alpha f | \partial^\alpha g \rangle_{L^2} , \quad (2.2)$$

inducing the norm  $\|f\|_{H^m} := \sqrt{\langle f|f \rangle_{H^m}}$ ; of course,  $H^0(\Omega) = L^2(\Omega)$ .

Let  $r \in [0, +\infty) \setminus \mathbb{N}$ ; consider the integer part  $[r] \in \mathbb{N}$  and put  $\rho := r - [r] \in (0, 1)$ . The Sobolev space of fractional order  $r$  is

$$H^r(\Omega) := \left\{ f \in \mathcal{D}'(\Omega) \mid \partial^\alpha f \in L^2(\Omega) \text{ for } \alpha \in \mathbb{N}^d, |\alpha| \leq [r], \text{ and} \right. \\ \left. \int_{\Omega \times \Omega} d\mathbf{x} d\mathbf{y} \frac{|\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|^{d+2\rho}} < +\infty \text{ for } \alpha \in \mathbb{N}^d, |\alpha| = [r] \right\} ; \quad (2.3)$$

this is also a complex Hilbert space with the inner product

$$\langle f|g \rangle_{H^r} := \sum_{\alpha \in \mathbb{N}^d, |\alpha| \leq [r]} \langle \partial^\alpha f | \partial^\alpha g \rangle_{L^2} + \sum_{\alpha \in \mathbb{N}^d, |\alpha| = [r]} \int_{\Omega \times \Omega} d\mathbf{x} d\mathbf{y} \frac{(\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})) (\overline{\partial^\alpha g(\mathbf{x}) - \partial^\alpha g(\mathbf{y})})}{|\mathbf{x} - \mathbf{y}|^{d+2\rho}} , \quad (2.4)$$

inducing the norm  $\|f\|_{H^r} := \sqrt{\langle f|f \rangle_{H^r}}$ .

For any  $r \in [0, +\infty)$  (integer or not), we denote with  $H_0^r(\Omega)$  the closure of  $\mathcal{D}(\Omega)$  in the space  $H^r(\Omega)$  (with respect to the associated norm);  $H_0^r(\Omega)$  is itself a Hilbert space with the inner product (2.4) inherited from  $H^r(\Omega)$ . We denote with  $H^{-r}(\Omega)$  its topological dual; so, each  $f \in H^{-r}(\Omega)$  is a continuous linear form on  $H_0^r(\Omega)$  and, by restriction to  $\mathcal{D}(\Omega)$ , it can be identified with a distribution on  $\Omega$ . By the Riesz theorem, there is a unique antilinear isomorphism  $i_r : H_0^r(\Omega) \rightarrow H^{-r}(\Omega)$  such that  $\langle i_r f, g \rangle = \langle f | g \rangle_{H^r}$  for all  $g \in H^r(\Omega)$ ; we define an inner product on  $H^{-r}(\Omega)$  setting

$$\langle f | g \rangle_{H^{-r}} := \langle i_r^{-1} g | i_r^{-1} f \rangle_{H^r} . \quad (2.5)$$

### Poincaré type inequalities.

Two inequalities of this kind will be considered in this work.

i) Assume the (otherwise arbitrary) domain  $\Omega \subset \mathbb{R}^d$  to be bounded along a direction; this means that there exist a unit vector  $\mathbf{n} \in \mathbb{R}^d$  and two constants  $a \in \mathbb{R}$ ,  $h \in (0, +\infty)$  such that  $\Omega$  is contained in the strip  $\{\mathbf{x} \in \mathbb{R}^d \mid a \leq \mathbf{n} \cdot \mathbf{x} \leq a + h\}$  (of course,  $h$  represents the width of the strip). Under these conditions, it is known that there is a constant  $c_\Omega \in (0, +\infty)$  such that

$$\int_\Omega |f|^2 \leq c_\Omega \int_\Omega |\nabla f|^2 \quad \text{for all } f \in H_0^1(\Omega) \quad (2.6)$$

(here  $|\nabla f|^2 := \sum_{i=1}^d |\partial_{x^i} f|^2$ ); as well known (see, e.g., [54, 109]), one can take  $c_\Omega = h^2/2$ .

ii) Another inequality we will refer to involves functions of zero mean (rather than functions vanishing on the boundary of the domain) with domain consisting of any ball  $B(\mathbf{x}_0, r)$  in  $\mathbb{R}^d$  of center  $\mathbf{x}_0$  and radius  $r$ . It is known that there exists a constant  $c_B \in (0, +\infty)$ , depending only on  $d$ , such that for any  $\mathbf{x}_0 \in \mathbb{R}^d$  and  $r \in (0, +\infty)$

$$\int_{B(\mathbf{x}_0, r)} |f|^2 \leq c_B r^2 \int_{B(\mathbf{x}_0, r)} |\nabla f|^2 \quad \text{for all } f \in H^1(B(\mathbf{x}_0, r)) \text{ s.t. } \int_{B(\mathbf{x}_0, r)} f = 0 ; \quad (2.7)$$

one can take  $c_B = 2^{2d}$  (see [79], page 164, Eq. (7.45)).

### Local Sobolev spaces.

For any  $r \in \mathbb{R}$ , we consider the local Sobolev space of order  $r$  (see [38])

$$H_{\text{loc}}^r(\Omega) := \{f \in \mathcal{D}'(\Omega) \mid \varphi f \in H^r(\Omega) \text{ for any } \varphi \in \mathcal{D}(\Omega)\} . \quad (2.8)$$

This carries the locally convex topology induced by the family of seminorms

$$f \mapsto \|\varphi f\|_{H^r} \quad (\varphi \in \mathcal{D}(\Omega)) , \quad (2.9)$$

with  $\|\cdot\|_{H^r}$  indicating the  $H^r$  norm.

### Spaces of differentiable functions and Sobolev embeddings.

Let  $j \in \mathbb{N}$ ; we denote with  $C^j(\Omega)$  the space of functions  $f : \Omega \rightarrow \mathbb{C}$  which are continuous on  $\Omega$  along with all their partial derivatives  $\partial^\alpha f$  of orders  $|\alpha| \leq j$ . We endow  $C^j(\Omega)$  with the Fréchet topology induced by the family of seminorms

$$f \mapsto |f|_{C^j, K} := \max_{\alpha \in \mathbb{N}^d, |\alpha| \leq j} \sup_{\mathbf{x} \in K} |\partial^\alpha f(\mathbf{x})| \quad (K \subset \Omega \text{ compact}) \quad (2.10)$$

(<sup>1</sup>); of course, this family is equivalent to the set of seminorms

$$f \mapsto |f|_{C^j, \varphi} := \max_{\alpha \in \mathbb{N}^d, |\alpha| \leq j} \sup_{\mathbf{x} \in \Omega} |\varphi(\mathbf{x}) \partial^\alpha f(\mathbf{x})| \quad (\varphi \in \mathcal{D}(\Omega)) . \quad (2.11)$$

On the other hand, we indicate with  $C^j(\overline{\Omega})$  the linear subspace of  $C^j(\Omega)$  consisting of functions  $f$  that, along with all their derivatives  $\partial^\alpha f$  of order  $|\alpha| \leq j$ , admit continuous extensions to  $\overline{\Omega}$ ;  $f, \partial^\alpha f$  are often identified with these extensions, which are unique. If  $\Omega$  is bounded,  $C^j(\overline{\Omega})$  is a Banach space with respect to the norm

$$\|f\|_{C^j} := \max_{\alpha \in \mathbb{N}^d, |\alpha| \leq j} \sup_{\mathbf{x} \in \Omega} |\partial^\alpha f(\mathbf{x})| . \quad (2.12)$$

We shall also need the spaces of functions whose derivatives satisfy a Hölder condition for some exponent  $\lambda \in (0, 1]$ . More precisely, we write  $C^{j, \lambda}(\Omega)$  for the space of functions  $f \in C^j(\Omega)$  whose derivatives  $\partial^\alpha f$  of order  $|\alpha| = j$  fulfill, for any compact subset  $K \subset \Omega$ ,

$$\sup_{\mathbf{x}, \mathbf{y} \in K, \mathbf{x} \neq \mathbf{y}} \frac{|\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\lambda} < +\infty ; \quad (2.13)$$

we endow this space with the Fréchet topology induced by family of seminorms

$$|f|_{C^{j, \lambda}, K} := |f|_{C^j, K} + \max_{\alpha \in \mathbb{N}^d, |\alpha| = j} \sup_{\mathbf{x}, \mathbf{y} \in K, \mathbf{x} \neq \mathbf{y}} \frac{|\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\lambda} \quad (K \subset \Omega \text{ compact}) . \quad (2.14)$$

For  $\Omega$  bounded, we indicate with  $C^{j, \lambda}(\overline{\Omega})$  the space of functions  $f \in C^j(\overline{\Omega})$  whose derivatives  $\partial^\alpha f$  of order  $|\alpha| = j$  fulfill

$$\sup_{\mathbf{x}, \mathbf{y} \in \Omega, \mathbf{x} \neq \mathbf{y}} \frac{|\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\lambda} < +\infty ; \quad (2.15)$$

this becomes a Banach space if equipped with the norm

$$\|f\|_{C^{j, \lambda}} := \|f\|_{C^j} + \max_{\alpha \in \mathbb{N}^d, |\alpha| = j} \sup_{\mathbf{x}, \mathbf{y} \in \Omega, \mathbf{x} \neq \mathbf{y}} \frac{|\partial^\alpha f(\mathbf{x}) - \partial^\alpha f(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\lambda} . \quad (2.16)$$

There hold the following well-known results.

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<sup>1</sup>In fact, this family is equivalent to the countable set of seminorms which corresponds to any given sequence of compact subsets  $K_0 \subset K_1 \subset K_2 \subset \dots$  such that  $\Omega = \bigcup_{n \in \mathbb{N}} K_n$ .

**Theorem 2.1.** (Sobolev Embedding) *Let  $r \in \mathbb{R}$  and  $j \in \mathbb{N}$  be such that  $r > j + d/2$ ; then, there hold the following continuous embeddings.*

i) *For any domain  $\Omega \subset \mathbb{R}^d$ , there holds*

$$H_{loc}^r(\Omega) \hookrightarrow C^j(\Omega) ; \quad (2.17)$$

*more precisely, for any  $\lambda \in (0, 1)$  such that  $r > j + d/2 + \lambda$ , it is*

$$H_{loc}^r(\Omega) \hookrightarrow C^{j,\lambda}(\Omega) \hookrightarrow C^j(\Omega) . \quad (2.18)$$

ii) *If  $\Omega \subset \mathbb{R}^d$  is a bounded domain, with compact boundary  $\partial\Omega$  of class  $C^\infty$ , there holds*

$$H^r(\Omega) \hookrightarrow C^j(\overline{\Omega}) ; \quad (2.19)$$

*more precisely, for any  $\lambda \in (0, 1)$  such that  $r > j + d/2 + \lambda$ , it is*

$$H^r(\Omega) \hookrightarrow C^{j,\lambda}(\overline{\Omega}) \hookrightarrow C^j(\overline{\Omega}) . \quad (2.20)$$

*Remark 2.2.* We refer to Proposition 2.13 of [38] and to Corollary 9.1 on page 46 of [97] for the proof of statements i) and ii), respectively. See also [7], Theorems 5.4 and 6.2, for generalizations of the above theorem dealing also with configurations involving unbounded domains whose boundary only fulfill regularity conditions much weaker than the ones in statement ii).

### **The case $\Omega = \mathbb{R}^d$ : tempered distributions, Fourier transforms and another characterization of Sobolev spaces.**

We write  $\mathcal{S}(\mathbb{R}^d)$  for the Schwartz space of smooth functions  $f : \mathbb{R}^d \rightarrow \mathbb{C}$  rapidly decreasing at infinity with all their derivatives; this space has well known topology [151], and its topological dual  $\mathcal{S}'(\mathbb{R}^d)$  is called the space of tempered distributions. Any  $f \in \mathcal{S}'(\mathbb{R}^d)$ , after restriction to the space  $\mathcal{D}(\Omega)$ , can be identified with an element of  $\mathcal{D}'(\Omega)$ . A Fourier transform can be defined

$$\mathfrak{F} : \mathcal{S}'(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d) , \quad f \mapsto \mathfrak{F}f ; \quad (2.21)$$

we use for  $\mathfrak{F}$  the normalization such that

$$(\mathfrak{F}f)(\mathbf{k}) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} d\mathbf{x} f(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \quad (f \in \mathcal{S}(\mathbb{R}^d); \mathbf{k} \in \mathbb{R}^d) . \quad (2.22)$$

For any  $r \in \mathbb{R}$  we have the following, equivalent characterization of the spaces  $H^r(\mathbb{R}^d)$ :

$$H^r(\mathbb{R}^d) = \{f \in \mathcal{S}'(\mathbb{R}^d) \mid (1 + |\mathbf{k}|^2)^{r/2} \mathfrak{F}f \in L^2(\mathbb{R}^d)\} \quad (2.23)$$

(where  $(1 + |\mathbf{k}|^2)^{r/2} \mathfrak{F}f$  indicates multiplication of the Fourier transform  $\mathfrak{F}f$  by the smooth function  $\mathbb{R}^d \rightarrow \mathbb{R}$ ,  $\mathbf{k} \mapsto (1 + |\mathbf{k}|^2)^{r/2}$ ; the quantity

$$\langle f|g \rangle_{H^r(\mathbb{R}^d)} := \langle (1 + |\mathbf{k}|^2)^{r/2} \mathfrak{F}f \mid (1 + |\mathbf{k}|^2)^{r/2} \mathfrak{F}g \rangle_{L^2} \quad (2.24)$$

yields an inner product on  $H^r(\mathbb{R}^d)$  equivalent to the inner products introduced previously for any space  $H^r(\Omega)$  (considering separately the cases  $r \in \mathbb{N}$ ,  $r \in [0, +\infty) \setminus \mathbb{N}$ , and  $r \in (-\infty, 0)$ ). Moreover, there holds the continuous embedding <sup>(2)</sup>

$$H^u(\mathbb{R}^d) \hookrightarrow H^r(\mathbb{R}^d) \quad \text{for } r, u \in \mathbb{R} \text{ with } u \geq r. \quad (2.25)$$

## 2.2 Some known results on Banach spaces.

If  $\mathcal{G}$  is any topological vector space, we write  $\mathcal{G}'$  for the dual vector space, made of the continuous linear forms  $\alpha : \mathcal{G} \rightarrow \mathbb{C}$ ,  $g \mapsto \langle \alpha, g \rangle$ . If  $\mathcal{G}$  is a Banach space with a norm  $\| \cdot \|$ ,  $\mathcal{G}'$  is as well a Banach space with the norm  $\| \alpha \|' := \sup_{g \in \mathcal{G}, g \neq 0} \frac{|\langle \alpha, g \rangle|}{\|g\|}$ ; in particular, for each  $r \in \mathbb{R}$ ,  $(\mathcal{H}^r)'$  is a Banach space with the norm  $\| \cdot \|_r'$  induced by  $\| \cdot \|_r$ .

### Notations for operators. Banach adjoints.

Let  $X, Y$  be any two Banach spaces, endowed with the standard norm topology; we denote with  $X', Y'$  their topological duals, and with  $\langle \cdot, \cdot \rangle$  the bilinear duality pairing between  $X'$  and  $X$  (resp.  $Y'$  and  $Y$ ).

An operator  $\mathcal{B} : \text{Dom}(\mathcal{B}) \subset X \rightarrow Y$  is a linear map whose domain  $\text{Dom}(\mathcal{B})$  is a linear subspace of  $X$ ; if  $\mathcal{B}$  is injective, we write  $\mathcal{B}^{-1}$  for the inverse. We indicate with  $\mathfrak{B}(X, Y)$  the Banach space of continuous (i.e., bounded) operators from  $X$  to  $Y$ ; this is equipped with the standard operator norm  $\| \cdot \|_{\mathfrak{B}(X, Y)}$  (and with the induced topology).

The *Banach adjoint* of a continuous operator  $\mathcal{B} \in \mathfrak{B}(X, Y)$  is the unique continuous operator  $\mathcal{B}^* \in \mathfrak{B}(Y', X')$  such that

$$\langle \mathcal{B}^* g, f \rangle_X = \langle g, \mathcal{B} f \rangle_Y \quad \text{for all } f \in X, g \in Y; \quad (2.26)$$

we refer to the standard theory analyzed, e.g., in [42, 129]. It can be easily proved that the *adjoint map*  $*$  :  $\mathfrak{B}(X, Y) \rightarrow \mathfrak{B}(Y', X')$ ,  $\mathcal{B} \mapsto \mathcal{B}^*$  is an isometric isomorphism <sup>(3)</sup>; moreover, if  $X$  and  $Y$  are reflexive (i.e.,  $X'' = X$  and  $Y'' = Y$ ), any continuous operator  $\mathcal{B} \in \mathfrak{B}(X, Y)$  coincides with its *double adjoint*  $\mathcal{B}^{**} \equiv (\mathcal{B}^*)^* \in \mathfrak{B}(X'', Y'')$ . Given a third Banach space  $Z$  and any two continuous operators  $\mathcal{B} \in \mathfrak{B}(X, Y)$ ,  $\mathcal{C} \in \mathfrak{B}(Y, Z)$ , the *composition*  $\mathcal{C}\mathcal{B} : X \rightarrow Z$  is also continuous and its adjoint  $(\mathcal{C}\mathcal{B})^*$  fulfills  $(\mathcal{C}\mathcal{B})^* = \mathcal{B}^* \mathcal{C}^* \in \mathfrak{B}(Z', X')$ .

We will employ the above mentioned facts in subsection 2.5.

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<sup>2</sup> In fact, using the norm  $\| \cdot \|_{H^r(\mathbb{R}^d)}$  induced by inner product (2.24), for any  $f \in H^u(\mathbb{R}^d)$  one has

$$\|f\|_{H^r(\mathbb{R}^d)}^2 = \|(1 + |\mathbf{k}|^2)^{r/2} \mathfrak{F}f\|_{L^2}^2 \leq \|(1 + |\mathbf{k}|^2)^{u/2} \mathfrak{F}f\|_{L^2}^2 = \|f\|_{H^u(\mathbb{R}^d)}^2.$$

<sup>3</sup>For a proof of this fact, see, e.g., [129], page 186, Theorem VI.2.

### Integration of Banach-valued functions.

Let us consider a real (or complex) Banach space  $X$  and its topological dual  $X'$ , equipped with the standard norm topology; moreover, let  $(\Omega, \mathfrak{M}_\Omega, \mu)$  be a measure space (with  $\mathfrak{M}_\Omega$  a  $\sigma$ -algebra of parts of  $\Omega$ ). A function  $f : \Omega \rightarrow X$  is said to be weakly measurable if, for each  $\alpha \in X'$ , the function  $\langle \alpha, f \rangle : \Omega \rightarrow \mathbb{R}$  (or  $\mathbb{C}$ ),  $\mathbf{x} \mapsto \langle \alpha, f(\mathbf{x}) \rangle$  is measurable in the usual sense. The function  $f$  is said to be weakly integrable (or integrable in the Gelfand-Pettis sense) if it is weakly measurable,  $\langle \alpha, f \rangle$  is Lebesgue integrable for all  $\alpha \in X'$  and there is an element of  $X$ , indicated with  $\int_\Omega f(\mathbf{x}) d\mu(\mathbf{x}) \equiv \int_\Omega f d\mu$ , such that

$$\langle \alpha, \int_\Omega f d\mu \rangle = \int_\Omega \langle \alpha, f \rangle d\mu \quad \text{for all } \alpha \in X'; \quad (2.27)$$

the above element of  $X$  is unique if it exists, and it is called the *integral of  $f$  in the weak (or Gelfand-Pettis) sense*.

In the following developments we will need the forthcoming result.

**Theorem 2.2.** *Let  $X, Y$  be any two real (or complex) Banach spaces,  $f : \Omega \rightarrow X$  a weakly integrable function and let  $\mathcal{B} : X \rightarrow Y$  be a continuous operator; then, the function  $\mathcal{B}f : \Omega \rightarrow Y$ ,  $\mathbf{x} \mapsto (\mathcal{B}f)(\mathbf{x}) \equiv (\mathcal{B}f)(\mathbf{x})$  is weakly integrable and*

$$\mathcal{B} \left( \int_\Omega f d\mu \right) = \int_\Omega (\mathcal{B}f) d\mu . \quad (2.28)$$

See, e.g., [50] and [125] for more details about the topics discussed in the present paragraph (in particular, for the proof of Theorem 2.2).

### Abstract interpolation of complex Banach spaces.

Two complex vector spaces  $X_0, X_1$  are said to be interpolable if their set theoretical intersection  $X_0 \cap X_1$  is a linear subspace of both of them. In this case there exists a vector space  $X_0 + X_1$  that contains  $X_0$  and  $X_1$  as subspaces, and is generated by them;  $X_0 + X_1$  is unique up to linear isomorphisms that preserve the elements of  $X_0$  and  $X_1$ .

Now let us consider two complex Banach spaces  $X_0$  and  $X_1$ , with norms  $\|\cdot\|_{X_0}$  and  $\|\cdot\|_{X_1}$ , respectively; these are said to be interpolable if the underlying vector spaces are so. In this case, both the vector spaces  $X_0 \cap X_1$  and  $X_0 + X_1$  are Banach spaces with respect to the norms  $\|x\|_{X_0 \cap X_1} := \max(\|x\|_{X_0}, \|x\|_{X_1})$  and  $\|x\|_{X_0 + X_1} := \inf\{\|x_0\|_{X_0} + \|x_1\|_{X_1} \mid x_0 \in X_0, x_1 \in X_1, x_0 + x_1 = x\}$ , respectively. It turns out that  $X_0, X_1, X_0 \cap X_1 \hookrightarrow X_0 + X_1$  (continuous embeddings).

To go on, let us consider the strip  $S := \{z \in \mathbb{C} \mid 0 < \Re z < 1\}$  in the complex plane  $\mathbb{C}$ , and its closure  $\bar{S}$  (that is the union of  $S$  with the lines  $s_0 := \{\Re z = 0\}$  and  $s_1 := \{\Re z = 1\}$ ). Let us introduce the function space

$$\mathfrak{F}(X_0, X_1) := \{F \in \text{Hol}(S, X_0 + X_1) \cap C(\bar{S}, X_0 + X_1) \mid (F \upharpoonright s_i) \in C_B(s_i, X_i) \text{ for } i = 0, 1\} , \quad (2.29)$$

where  $\text{Hol}, C, C_B$  mean, respectively, holomorphic, continuous, continuous and bounded.  $\mathfrak{F}(X_0, X_1)$  is a vector space and it becomes a Banach space when it is equipped with the norm

$$\|F\|_{\mathfrak{F}(X_0, X_1)} := \max \left( \sup_{z \in S_0} \|F(z)\|_{X_0}, \sup_{z \in S_1} \|F(z)\|_{X_1} \right). \quad (2.30)$$

For  $\theta \in (0, 1)$ , the interpolation space of order  $\theta$  between  $X_0$  and  $X_1$  is

$$[X_0, X_1]_\theta := \{x \in X_0 + X_1 \mid x = F(\theta) \text{ for some } F \in \mathfrak{F}(X_0, X_1)\}; \quad (2.31)$$

this is a linear subspace of  $X_0 + X_1$ , and it is a Banach space with respect to the norm

$$\|x\|_{[X_0, X_1]_\theta} := \inf \{ \|F\|_{\mathfrak{F}(X_0, X_1)} \mid F \in \mathfrak{F}(X_0, X_1), F(\theta) = x \}. \quad (2.32)$$

It turns out that  $X_0 \cap X_1 \hookrightarrow [X_0, X_1]_\theta \hookrightarrow X_0 + X_1$ . In particular, assume  $X_1 \hookrightarrow X_0$ . Then the two spaces  $X_0, X_1$  are interpolable; in terms of linear structures we have  $X_0 \cap X_1 = X_1$ , and we can take  $X_0 + X_1 = X_0$ . Moreover the norms defined previously for  $X_0 \cap X_1$  and  $X_0 + X_1$  are equivalent to the norms of  $X_1$  and  $X_0$ , respectively. Summing up, in this case,  $X_1 \hookrightarrow [X_0, X_1]_\theta \hookrightarrow X_0$ .

The main theorem in interpolation theory states the following [1, 19, 101]:

**Theorem 2.3.** *Let  $X_0, X_1$  and  $Y_0, Y_1$  be two arbitrary pairs of interpolable Banach spaces and consider two continuous linear operators  $\mathcal{B}_0 : X_0 \rightarrow Y_0$  and  $\mathcal{B}_1 : X_1 \rightarrow Y_1$  such that  $\mathcal{B}_0 \upharpoonright X_0 \cap X_1 = \mathcal{B}_1 \upharpoonright X_0 \cap X_1$ . Let  $\mathcal{B} : X_0 + X_1 \rightarrow Y_0 + Y_1$  be the unique linear map such that  $\mathcal{B} \upharpoonright X_0 = \mathcal{B}_0$  and  $\mathcal{B} \upharpoonright X_1 = \mathcal{B}_1$ . Then, for each  $\theta \in (0, 1)$ ,  $\mathcal{B}_\theta := \mathcal{B} \upharpoonright X_\theta$  maps continuously  $[X_0, X_1]_\theta$  to  $[Y_0, Y_1]_\theta$  and*

$$\|\mathcal{B}_\theta\|_{\mathfrak{B}([X_0, X_1]_\theta, [Y_0, Y_1]_\theta)} \leq (\|\mathcal{B}_0\|_{\mathfrak{B}(X_0, Y_0)})^{1-\theta} (\|\mathcal{B}_1\|_{\mathfrak{B}(X_1, Y_1)})^\theta. \quad (2.33)$$

Many applications of interpolation theory are related to  $L^p$  spaces. More precisely, consider a measure space  $(K, \mathfrak{M}_K, \mu) \equiv K$ , with  $\mu$  a positive measure on some  $\sigma$ -algebra  $\mathfrak{M}_K$  of subsets of  $K$ ; let us write  $\text{Mis}(K)$  for the vector space of complex measurable functions  $K \rightarrow \mathbb{C}$  (or, more precisely, of the equivalence classes of such functions with respect to equality almost everywhere for the measure  $\mu$ ). Let  $p \in [1, +\infty]$ , and  $\omega \in \text{Mis}(K)$  be such that  $\omega(k) > 0$  for almost every (a.e.)  $k \in K$ ; consider the Banach space  $L^p(K, \omega d\mu)$ , made of functions  $f \in \text{Mis}(K)$  which are  $L^p$  with respect to the measure  $\mathfrak{M}_K \ni A \mapsto \int_A \omega d\mu$ . Let  $p_0, p_1 \in [1, +\infty]$  and  $\omega_0, \omega_1 \in \text{Mis}(K)$ , with  $\omega_0, \omega_1 > 0$  almost everywhere. Then, the Banach spaces  $L^{p_0}(K, \omega_0 d\mu)$  and  $L^{p_1}(K, \omega_1 d\mu)$  are both interpolable, and their sum can be realized naturally as a linear subspace of  $\text{Mis}(K)$ ; moreover, for all  $\theta \in (0, 1)$  one has (see [1], Theorem 2.12)

$$[L^{p_0}(K, \omega_0 d\mu), L^{p_1}(K, \omega_1 d\mu)]_\theta = L^p(K, \omega d\mu), \quad (2.34)$$

where  $p \in [1, +\infty]$  and  $\omega \in \text{Mis}(K)$  are defined, respectively, by

$$\frac{1}{p} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}, \quad \omega(k) := \omega_0(k)^{\frac{p}{p_0}(1-\theta)} \omega_1(k)^{\frac{p}{p_1}\theta} \text{ for a.e. } k \in K. \quad (2.35)$$



The equality in Eq. (2.34) must be intended as follows: the left and the right-hand side coincide as vector spaces, and carry the same norm.

A subcase of this result, of interest for us in the sequel, is the one with  $p_0 = p_1 \equiv p$  and  $\omega_0 = w^{r_0}$ ,  $\omega_1 = w^{r_1}$  for some  $w \in \text{Mis}(K)$ , with  $w > 0$  almost everywhere, and  $r_0, r_1 \in \mathbb{R}$ . In this case, Eq.s (2.34) and (2.35) give

$$[L^p(K, w^{r_0} d\mu), L^p(K, w^{r_1} d\mu)]_\theta = L^p(K, w^{(1-\theta)r_0 + \theta r_1} d\mu). \quad (2.36)$$

Standard interpolation results for the Sobolev spaces  $H^n(\mathbb{R}^d)$  can be derived by Eq. (2.36); indeed, for each  $r \in \mathbb{R}$ , the space  $H^r(\mathbb{R}^d)$  of Eq. (2.23) can be identified (via the Fourier transform) with  $L^2(\mathbb{R}^d, w^r d\mathbf{k})$ , where  $w(\mathbf{k}) := 1 + |\mathbf{k}|^2$  and  $d\mathbf{k}$  is the standard Lebesgue measure. So, for all  $r_0, r_1 \in \mathbb{R}$  and  $\theta \in (0, 1)$ , one infers from Eq. (2.36) that

$$[H^{r_0}(\mathbb{R}^d), H^{r_1}(\mathbb{R}^d)]_\theta = H^{(1-\theta)r_0 + \theta r_1}(\mathbb{R}^d). \quad (2.37)$$

A result analogous to Eq. (2.37) holds as well for the Sobolev spaces  $H^r(\Omega)$  ( $r \in \mathbb{R}$ ), under minimal regularity assumptions for the domain  $\Omega \subset \mathbb{R}^d$ ; in particular, if  $\Omega$  is bounded with compact boundary of class  $C^\infty$ , for any  $r_0, r_1 \in \mathbb{R}$  and for any  $\theta \in (0, 1)$  one has <sup>(4)</sup>

$$[H^{r_0}(\Omega), H^{r_1}(\Omega)]_\theta = H^{(1-\theta)r_0 + \theta r_1}(\Omega). \quad (2.38)$$

Let us stress that, contrary to the previous examples (2.34-2.37), the spaces on the two sides of the above equality are in general endowed with distinct norms <sup>(5)</sup>: Eq. (2.38) must be meant to hold algebraically and topologically, in the sense that the mentioned norms are equivalent.

For a more comprehensive analysis of the topics reviewed briefly in the present paragraph, we refer, e.g., to the already cited books [1, 19, 101].

## 2.3 Operators on Hilbert spaces.

In the sequel we consider a complex, separable Hilbert space  $\mathcal{H}$ ; we write  $\langle \cdot | \cdot \rangle$  for the inner product of  $\mathcal{H}$  (antilinear in the left argument, linear in the right one) and  $\| \cdot \|$  for the induced norm.

### Notations for operators.

Similarly to the case of Banach spaces (compare with Section 2.2), an operator on  $\mathcal{H}$  is a linear map  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$ , whose domain  $\text{Dom}(\mathcal{A})$  is a linear subspace of  $\mathcal{H}$ ;  $\mathfrak{B}(\mathcal{H}) \equiv \mathfrak{B}(\mathcal{H}, \mathcal{H})$  is the space of continuous (i.e., bounded) operators from  $\mathcal{H}$  into  $\mathcal{H}$ , and  $\| \cdot \|_{\mathfrak{B}} \equiv \| \cdot \|_{\mathfrak{B}(\mathcal{H}, \mathcal{H})}$  indicates the usual operator norm on this space.

<sup>4</sup>Eq. (2.38) contains a well-known result on Sobolev spaces; see, e.g., Theorem 7.48 of [7], Proposition 2.7 of [96] and Theorem 9.6 of [97] for more details.

<sup>5</sup>In fact, the space  $[H^{r_0}(\Omega), H^{r_1}(\Omega)]_\theta$  carries the interpolation norm defined according to Eq. (2.32) while, if  $r_0, r_1 \geq 0$ ,  $H^{(1-\theta)r_0 + \theta r_1}(\Omega)$  has the standard norm induced by the inner product (2.4).

If  $\text{Dom}(\mathcal{A})$  is dense in  $\mathcal{H}$ , we can define the *Hilbert adjoint* operator  $\mathcal{A}^\dagger$  (see, e.g., [119, 129]). Let us stress that if  $\mathcal{A}$  is continuous and  $\text{Dom}(\mathcal{A}) = \mathcal{H}$  the notion of Banach adjoint defined in Section 2.2 reduces to that of Hilbert adjoint considered here; in fact, viewing  $\mathcal{H}$  as an (anti-)self-dual Banach space, one has  $\mathcal{A}^* = \mathcal{A}^\dagger \in \mathfrak{B}(\mathcal{H})$ . In the remainder of this work, for the sake of brevity, we use the bare adjective “adjoint” as short for “Hilbert adjoint”.

Given a pair of linear operators  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$ ,  $\mathcal{B} : \text{Dom}(\mathcal{B}) \subset \mathcal{H} \rightarrow \mathcal{H}$  and a constant  $c \in \mathbb{C}$ , the operators  $c\mathcal{A}$ ,  $\mathcal{A} + \mathcal{B}$  and  $\mathcal{B}\mathcal{A}$  are obviously defined on the domains  $\text{Dom}(c\mathcal{A}) := \text{Dom}(\mathcal{A})$ ,  $\text{Dom}(\mathcal{A} + \mathcal{B}) := \text{Dom}(\mathcal{A}) \cap \text{Dom}(\mathcal{B})$  and  $\text{Dom}(\mathcal{B}\mathcal{A}) := \{f \in \mathcal{H} \mid f \in \text{Dom}(\mathcal{A}), \mathcal{A}f \in \text{Dom}(\mathcal{B})\}$ . If  $\mathcal{C}$  is another operator on  $\mathcal{H}$  we define  $\mathcal{A} + \mathcal{B} + \mathcal{C} := (\mathcal{A} + \mathcal{B}) + \mathcal{C}$ ,  $\mathcal{C}\mathcal{B}\mathcal{A} := \mathcal{C}(\mathcal{B}\mathcal{A})$ , and so on iteratively. We write  $\mathcal{B} \supset \mathcal{A}$  if  $\mathcal{B}$  is an extension of  $\mathcal{A}$ .

In the sequel we will write  $\sigma(\mathcal{A})$  for the *spectrum* of an operator  $\mathcal{A}$ , defined as in [119, 129].

### The case $\mathcal{H} = L^2(K, \mu)$ . Multiplication operators.

Let us consider again a measure space  $(K, \mathfrak{M}_K, \mu) \equiv (K, \mu)$ , with  $\mu$  a positive measure on some  $\sigma$ -algebra  $\mathfrak{M}_K$  of subsets of  $K$ ; let us recall that we write  $k$  for a generic point of  $K$  and  $\text{Mis}(K)$  for the space of measurable functions on  $K$  (see subsection 2.2). The space  $L^2(K, \mu)$  of complex, square integrable, measurable functions on  $K$  is a Hilbert space with the inner product

$$\langle f | g \rangle := \int_K \bar{f}(k) g(k) d\mu(k) \equiv \int_K \bar{f} g d\mu , \quad (2.39)$$

inducing the norm

$$\|f\|^2 = \int_K |f|^2 d\mu . \quad (2.40)$$

To go on, let us consider a function  $w \in \text{Mis}(K)$ ; the multiplication operator by  $w$  is

$$M_w : \text{Dom}(M_w) \subset L^2(K, \mu) \rightarrow L^2(K, \mu) , \quad f \mapsto M_w f := wf \quad (2.41)$$

with

$$\text{Dom}(M_w) := \{f \in L^2(K, \mu) \mid wf \in L^2(K, \mu)\} . \quad (2.42)$$

This is a linear operator with dense domain, whose adjoint is

$$(M_w)^\dagger = M_{\bar{w}} ; \quad (2.43)$$

in particular,  $M_w$  is self-adjoint if  $w$  is real valued. The operator  $M_w$  is defined on the whole space  $L^2(K, \mu)$  and bounded (i.e.,  $M_w \in \mathfrak{B}(L^2(K, \mu))$ ) if and only if  $w$  is essentially bounded (i.e., bounded up to sets of zero  $\mu$  measure); in this case

$$\|M_w\|_{\mathfrak{B}} = \text{ess sup}_{k \in K} |w(k)| . \quad (2.44)$$

For any given  $w \in \text{Mis}(K)$ , the spectrum of  $M_w$  is as follows:

$$\sigma(M_w) = \text{EssIm } w , \quad (2.45)$$

where the right-hand side indicates the essential image of  $w$ , defined by

$$\text{EssIm } w := \{\lambda \in \mathbb{C} \mid \mu(w^{-1}(B(\lambda, \epsilon))) > 0 \text{ for each } \epsilon > 0\} \quad (2.46)$$

(with  $B(\lambda, \epsilon) := \{\lambda' \in \mathbb{C} \mid |\lambda' - \lambda| < \epsilon\}$ ).

If  $w$  is real valued, in which case  $M_w$  is self-adjoint, one infers from Eq. (2.45) that, for all  $a \in \mathbb{R}$ ,

$$w \geq a \text{ } \mu\text{-almost everywhere} \Leftrightarrow \sigma(M_w) \subset [a, +\infty) . \quad (2.47)$$

Given any pair of functions  $v, w \in \text{Mis}(K)$  one has

$$M_{v+w} \supset M_w + M_v , \quad M_{vw} \supset M_v M_w , \quad (2.48)$$

with  $\supset$  replaced by  $=$  if  $v$  and  $w$  are essentially bounded. Moreover, for  $c \in \mathbb{C} \setminus \{0\}$ , it is

$$M_{cw} = c M_w , \quad (2.49)$$

while  $M_{0 \cdot w} \supset 0 \cdot M_w$ .

### Spectral theorem and functional calculus for self-adjoint operators.

Let us consider an abstract, separable Hilbert space  $\mathcal{H}$  and a self-adjoint operator  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$ . The ‘‘multiplication operator version’’ of the spectral theorem (see [129]) states that there exist a measure space  $(K, \mu)$ , a measurable function  $w : K \rightarrow \mathbb{R}$  and a Hilbertian isomorphism  $\mathcal{I} : \mathcal{H} \rightarrow L^2(K, \mu)$  such that

$$\mathcal{A} = \mathcal{I}^{-1} M_w \mathcal{I} . \quad (2.50)$$

Obviously enough,  $\mathcal{I}^{-1} M_w \mathcal{I}$  indicates the linear operator  $f \mapsto \mathcal{I}^{-1} M_w \mathcal{I} f$  with domain  $\mathcal{I}^{-1}(\text{Dom}(M_w))$ . The set  $(K, \mu, w, \mathcal{I})$  is not uniquely determined by  $\mathcal{A}$ , but this is no cause of concern for the relevant constructions associated to this representation and, in particular, for the functional calculus described hereafter. For future use, we mention that one can choose  $(K, \mu)$  so that  $\mu(K) < +\infty$  (see [129], page 260, Theorem VIII.4).

Now, let us consider a measurable function

$$\phi : \sigma(\mathcal{A}) \subset \mathbb{R} \rightarrow \mathbb{C} . \quad (2.51)$$

As well known, the *functional calculus* for self-adjoint operators allows to associate to  $\phi$  an operator  $\phi(\mathcal{A}) : \text{Dom}(\phi(\mathcal{A})) \subset \mathcal{H} \rightarrow \mathcal{H}$  with dense domain, which is everywhere defined and bounded if  $\phi$  is bounded; this has adjoint  $\phi(\mathcal{A})^\dagger = \overline{\phi}(\mathcal{A})$  where  $\overline{\phi} : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  is the complex conjugate function. If  $(K, \mu, w, \mathcal{I})$  is a set as above, the composition  $\phi \circ w \in \text{Mis}(K)$  makes sense, because  $w(k) \in \sigma(\mathcal{A})$  for  $\mu$ -a.e.  $k \in K$ ; it turns out that

$$\phi(\mathcal{A}) = \mathcal{I}^{-1} M_{\phi \circ w} \mathcal{I} : \mathcal{I}^{-1}(\text{Dom}(M_{\phi \circ w})) \subset \mathcal{H} \rightarrow \mathcal{H} \quad (2.52)$$

<sup>(6)</sup>. As an example, for  $z \in \mathbb{C}$ ,  $e^{-z\mathcal{A}}$  is defined as above choosing  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ ,  $\phi(\lambda) := e^{-z\lambda}$ ; this operator is self-adjoint if  $z \in \mathbb{R}$ , and  $e^{-z\mathcal{A}} \in \mathfrak{B}(\mathcal{H})$  if  $\sigma(\mathcal{A}) \subset [0, +\infty)$  and  $\Re z \geq 0$ .

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<sup>6</sup>As a matter of fact, one could define  $\phi(\mathcal{A})$  as the unique operator on  $\mathcal{H}$  fulfilling Eq. (2.52), for each  $(K, \mu, w, \mathcal{I})$ . The previously mentioned condition of boundedness for  $\phi(\mathcal{A})$  and the expression given for its adjoint are made evident by the representation (2.52).

**Complex powers of a strictly positive, self-adjoint operator.**

In the rest of this paragraph we consider a self-adjoint operator  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$ , assuming

$$\sigma(\mathcal{A}) \subset [\varepsilon, +\infty) \quad \text{for some } \varepsilon > 0 . \quad (2.53)$$

Up to Hilbertian isomorphisms, it can be assumed that

$$\mathcal{H} = L^2(K, \mu) , \quad (2.54)$$

and that  $\mathcal{A}$  is the multiplication operator by a measurable function <sup>(7)</sup>

$$w : K \rightarrow [\varepsilon, +\infty) ; \quad (2.55)$$

so,

$$\text{Dom}(\mathcal{A}) = \{f \in L^2(K, \mu) \mid wf \in L^2(K, \mu)\} , \quad \mathcal{A}f = wf . \quad (2.56)$$

Now, let  $s \in \mathbb{C}$  and consider the operator  $\mathcal{A}^{-s}$ , which can be defined applying the standard functional calculus with  $\phi(\lambda) := \lambda^{-s}$ .

In the realization (2.54-2.56) of  $\mathcal{H}$  and  $\mathcal{A}$ , assumed as a standard in the sequel, for any  $s \in \mathbb{C}$  one has

$$\text{Dom}(\mathcal{A}^{-s}) = \{f \in L^2(K, \mu) \mid w^{-s}f \in L^2(K, \mu)\} , \quad \mathcal{A}^{-s}f = w^{-s}f . \quad (2.57)$$

If  $\Re s \geq 0$ , one has  $|w^{-s}| = w^{-\Re s} \leq \varepsilon^{-\Re s}$ ; so,

$$\Re s \geq 0 \quad \Rightarrow \quad \mathcal{A}^{-s} \in \mathfrak{B}(\mathcal{H}) \quad \text{and} \quad \|\mathcal{A}^{-s}\|_{\mathfrak{B}} \leq \varepsilon^{-\Re s} . \quad (2.58)$$

One readily checks that  $\mathcal{A}^0 = \mathbb{I}$  (with  $\mathbb{I}$  the identity operator on  $\mathcal{H}$ ), that  $\mathcal{A}^1 = \mathcal{A}$  and that  $\mathcal{A}^{-1}$  coincides with the inverse of the injective operator  $\mathcal{A}$ ; for  $n \in \mathbb{N}$  one has

$$\mathcal{A}^n = \underbrace{\mathcal{A} \dots \mathcal{A}}_{n \text{ times}} , \quad \mathcal{A}^{-n} = \underbrace{\mathcal{A}^{-1} \dots \mathcal{A}^{-1}}_{n \text{ times}} . \quad (2.59)$$

**Trace class and Hilbert-Schmidt operators.**

Let  $\mathcal{C} \in \mathfrak{B}(\mathcal{H})$  be any nonnegative self-adjoint operator (so that, in particular,  $\langle f | \mathcal{C} f \rangle \geq 0$  for all  $f \in \mathcal{H}$ ). The trace of  $\mathcal{C}$  is

$$\text{Tr } \mathcal{C} := \sum_{n \in \mathbb{N}} \langle u_n | \mathcal{C} u_n \rangle \in [0, +\infty] , \quad (2.60)$$

where  $(u_n)_{n \in \mathbb{N}}$  is any orthonormal basis of  $\mathcal{H}$ ; the trace is in fact independent of the basis.

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<sup>7</sup>Indeed, the assumptions made on  $\sigma(\mathcal{A})$  ensure that  $\mathcal{A}$  can be realized as the multiplication by a real function  $w$  such that  $w(k) \geq \varepsilon$  for a.e.  $k \in K$ . Redefining  $w$  on a set of measure zero, if necessary, we obtain  $w(k) \geq \varepsilon$  for all  $k$ .

Given any  $\mathcal{C} \in \mathfrak{B}(\mathcal{H})$ , we can associate to it the nonnegative self-adjoint operator  $|\mathcal{C}| := \sqrt{\mathcal{C}^\dagger \mathcal{C}}$  <sup>(8)</sup>. As well known,  $\mathcal{C}$  is said to be of *trace class* if  $\text{Tr } |\mathcal{C}| < +\infty$ ; in this case we can define

$$\text{Tr } \mathcal{C} := \sum_{n \in \mathbb{N}} \langle u_n | \mathcal{C} u_n \rangle \in \mathbb{C} , \quad (2.61)$$

where  $(u_n)_{n \in \mathbb{N}}$  is any orthonormal basis of  $\mathcal{H}$  (the above series is shown to converge, with a sum independent of the basis). In the sequel, we indicate with  $\mathfrak{B}_1(\mathcal{H})$  the set of trace class operators on  $\mathcal{H}$ , which is found to be a two-sided ideal of  $\mathfrak{B}(\mathcal{H})$ .

Let us also recall that an operator  $\mathcal{B} \in \mathfrak{B}(\mathcal{H})$  is said to be *Hilbert-Schmidt* if  $\text{Tr}(\mathcal{B}^\dagger \mathcal{B}) < +\infty$ ; the set  $\mathfrak{B}_2(\mathcal{H})$  of these operators is a two-sided ideal of  $\mathfrak{B}(\mathcal{H})$ , and  $\mathfrak{B}_2(\mathcal{H}) \supset \mathfrak{B}_1(\mathcal{H})$ . To go on we assume the Hilbert space to be  $\mathcal{H} = L^2(K, \mu)$ , with  $\mu$  a  $\sigma$ -finite, separable measure on  $K$ . Then, as well known (see, e.g., [119]),  $\mathfrak{B}_2(\mathcal{H})$  can be identified isomorphically with the Hilbert space  $L^2(K \times K, \mu \otimes \mu)$ ; in particular, this means that for any  $\mathcal{B} \in \mathfrak{B}_2(\mathcal{H})$  there exists a unique *integral kernel*  $\mathcal{B}(, ) \in L^2(\Omega \times \Omega)$  such that, for any  $f \in \mathcal{H}$ ,

$$(\mathcal{B}f)(h) = \int_K d\mu(k) \mathcal{B}(h, k) f(k) \quad (\text{for } \mu\text{-a.e. } k \in K) . \quad (2.62)$$

Moreover, for any given orthonormal basis  $(u_n)_{n \in \mathbb{N}}$  of  $\mathcal{H}$  (recall that  $\mathcal{H}$  is assumed to be separable), there holds the  $L^2$ -convergent expansion

$$\mathcal{B}(h, k) = \sum_{n, m \in \mathbb{N}} \langle u_m | \mathcal{B} u_n \rangle u_m(h) \overline{u_n(k)} \quad (\text{for } \mu\text{-a.e. } h, k \in K) . \quad (2.63)$$

## 2.4 Conjugations and Hilbert spaces

### Generalities

Let us consider a complex vector space  $\mathcal{H}$ ; a *conjugation* on  $\mathcal{H}$  is an antilinear, involutive map  $\mathcal{J} : \mathcal{H} \rightarrow \mathcal{H}$ ; so, for all  $\alpha, \beta \in \mathbb{C}$  and for all  $f, g \in \mathcal{H}$ , there hold

$$\mathcal{J}(\alpha f + \beta g) = \bar{\alpha} \mathcal{J}f + \bar{\beta} \mathcal{J}g , \quad \mathcal{J}^2 f = f , \quad (2.64)$$

(where  $\bar{\phantom{x}}$  indicates the usual complex conjugation). Given the conjugation  $\mathcal{J}$ , we can introduce the sets

$$\mathcal{H}_\pm := \{f \in \mathcal{H} \mid \mathcal{J}f = \pm f\} ; \quad (2.65)$$

for obvious reasons, the elements of  $\mathcal{H}_+$  and  $\mathcal{H}_-$  are called, respectively, the  $\mathcal{J}$ -real and the  $\mathcal{J}$ -imaginary vectors of  $\mathcal{H}$ . One readily checks that  $\mathcal{H}_\pm$  are real vector subspaces of  $\mathcal{H}$ , and that

$$\mathcal{H}_\mp = i \mathcal{H}_\pm ; \quad (2.66)$$

moreover, one finds that

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \quad (2.67)$$

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<sup>8</sup>This is, the power of exponent 1/2 of the nonnegative self-adjoint operator  $\mathcal{C}^\dagger \mathcal{C}$ .

(direct sum of real vector spaces) and that the projections  $\mathcal{P}_\pm : \mathcal{H} \rightarrow \mathcal{H}_\pm$  corresponding to the above decomposition are given by

$$\mathcal{P}_+ := \frac{\mathbb{I} + \mathcal{J}}{2}, \quad \mathcal{P}_- := \frac{\mathbb{I} - \mathcal{J}}{2} \quad (2.68)$$

(of course  $\mathcal{P}_\pm \mathcal{P}_\mp = \mathbb{O}$  and  $\mathcal{P}_+ + \mathcal{P}_- = \mathbb{I}$ , with  $\mathbb{O}$  and  $\mathbb{I}$  indicating the null and the identity operators on  $\mathcal{H}$ , respectively). Let us also mention that, for all  $f \in \mathcal{H}$ , there hold the following identities:

$$\mathcal{P}_\pm(i f) = i \mathcal{P}_\mp f, \quad f = \mathcal{P}_+ f + i \mathcal{P}_+(-i f). \quad (2.69)$$

Now, let us consider a ( $\mathbb{C}$ -linear) operator  $\mathcal{B} : \text{Dom}(\mathcal{B}) \subset \mathcal{H} \rightarrow \mathcal{H}$ , with domain on a (complex) vector subspace;  $\mathcal{B}$  is said to be  *$\mathcal{J}$ -real* if [138, 155]

$$\mathcal{J}\text{Dom}(\mathcal{B}) \subset \text{Dom}(\mathcal{B}) \quad \text{and} \quad \mathcal{J}\mathcal{B}f = \mathcal{B}\mathcal{J}f \text{ for all } f \in \text{Dom}(\mathcal{B}). \quad (2.70)$$

Since  $\mathcal{J}$  is in particular an involution, the second relation in Eq. (2.70) can be restated as follows, for all  $f \in \text{Dom}(\mathcal{B})$ :

$$\mathcal{J}\mathcal{B}\mathcal{J}^{-1}f = \mathcal{B}f. \quad (2.71)$$

To conclude, we stipulate the following: a conjugation on a complex *topological* vector space  $\mathcal{H}$ ; is a conjugation on  $\mathcal{H}$  as a vector space, which is also a homeomorphism in the given topology. In this case, the subspaces  $\mathcal{H}_\pm$  defined as before are closed subsets of  $\mathcal{H}$ .

### Conjugations on a Hilbert space.

A conjugation on a complex *Hilbert* space  $\mathcal{H}$  (equipped with inner product  $\langle \cdot | \cdot \rangle$ ) is a conjugation  $\mathcal{J}$  in the vector space  $\mathcal{H}$  with the additional property

$$\langle \mathcal{J}f | \mathcal{J}g \rangle = \overline{\langle f | g \rangle} \quad (2.72)$$

for all  $f, g \in \mathcal{H}$ ; this indicates that  $\mathcal{J}$  is an antiunitary operator. One easily checks that condition (2.72) has the equivalent formulation

$$\langle \mathcal{J}f | g \rangle = \overline{\langle f | \mathcal{J}g \rangle}, \quad (2.73)$$

sometimes used in the sequel <sup>(9)</sup>.

When a conjugation  $\mathcal{J}$  is given on the Hilbert space  $\mathcal{H}$ , we can then introduce the real vector subspaces  $\mathcal{H}_\pm$ , defined as in the previous subsection, and check that (2.72) implies  $\langle f | g \rangle \in \mathbb{R}$  if  $f, g$  are both in  $\mathcal{H}_+$  or both in  $\mathcal{H}_-$ .

To go on, let us consider a self-adjoint operator  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$  and recall that (for  $\mathcal{H}$  separable) the spectral theorem ensures the existence of a Hilbertian isomorphism  $\mathcal{I} : \mathcal{H} \rightarrow L^2(K, \mu)$  such that  $\mathcal{I}\mathcal{A}\mathcal{I}^{-1}$  is the multiplication operator by a measurable

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<sup>9</sup>Applying Eq. (2.72) with  $g$  replaced by  $\mathcal{J}g$ , and using  $\mathcal{J}^2g = g$ , one infers (2.73). One uses similar arguments to infer (2.72) from (2.73)

function  $w : K \rightarrow \mathbb{R}$ . In addition let us assume that  $\mathcal{A}$  is  $\mathcal{J}$ -real, in the sense of the previous subsection (see Eq. (2.70)); then, the system  $(K, \mu, w, \mathcal{I})$  mentioned before can be chosen so that

$$\mathcal{I}\mathcal{J}\mathcal{I}^{-1} = \bar{\phantom{x}}, \quad (2.74)$$

where  $\bar{\phantom{x}} : L^2(K, \mu) \rightarrow L^2(K, \mu)$ ,  $f \mapsto \bar{f}$  is the usual pointwise complex conjugation <sup>(10)</sup>. Let us also mention the relation

$$\mathcal{J}\phi(\mathcal{A})\mathcal{J}^{-1} = \bar{\phi}(\mathcal{A}) \quad (2.75)$$

holding for each measurable function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ : this is self-evident if we represent  $\mathcal{A}$  as a multiplication operator using a system  $(K, \mu, w, \mathcal{I})$  with the property (2.74).

## 2.5 Scale of Hilbert spaces associated to a positive self-adjoint operator.

Let us consider an abstract Hilbert space  $(\mathcal{H}, \langle \cdot | \cdot \rangle) \equiv \mathcal{H}$  and let  $\mathcal{A} : \text{Dom}(\mathcal{A}) \subset \mathcal{H} \rightarrow \mathcal{H}$  be a self-adjoint operator on it with spectrum as in Eq. (2.53) (i.e.,  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$  for some  $\varepsilon > 0$ ). Unless otherwise stated,  $\mathcal{H}$  is endowed with no further structure.

In the present section we assume that, when a normed space  $X$  is a linear subspace of another normed space  $Y$ , their completions are realized so that  $\bar{X}$  is a linear subspace of  $\bar{Y}$  (such a realization is always possible).

### Finite order spaces.

Hereafter we introduce a family of spaces, associated to the real powers of  $\mathcal{A}$ , i.e., to the operators  $\mathcal{A}^r$  for  $r \in \mathbb{R}$ .

**Proposition 2.4.** *For any  $r \in \mathbb{R}$ , the following statements hold.*

i) Define  $\langle \cdot | \cdot \rangle_r : \text{Dom}(\mathcal{A}^{r/2}) \times \text{Dom}(\mathcal{A}^{r/2}) \rightarrow \mathbb{C}$  and  $\|\cdot\|_r : \text{Dom}(\mathcal{A}^{r/2}) \rightarrow [0, +\infty)$  by

$$\langle g|f \rangle_r := \langle \mathcal{A}^{r/2}g | \mathcal{A}^{r/2}f \rangle, \quad \|f\|_r^2 := \|\mathcal{A}^{r/2}f\|^2. \quad (2.76)$$

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<sup>10</sup>This statement is derived reconsidering the standard proof of the “multiplication operator form” for the spectral theorem on self-adjoint operators, as given in [129]; one must perform a rather simple adaptation of the argument to the case where  $\mathcal{H}$  carries a conjugation  $\mathcal{J}$  and the operator  $\mathcal{A}$  is  $\mathcal{J}$ -real. The main points in this adaptation are the following:

i) the spectral measure  $P$  of  $\mathcal{A}$  is as well  $\mathcal{J}$ -real:  $\mathcal{J}P(M)\mathcal{J}^{-1} = P(M)$  for each Borel subset of the spectrum of  $\mathcal{A}$ . Due to this, for each measurable function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  one has  $\mathcal{J}\phi(\mathcal{A})\mathcal{J}^{-1} = \bar{\phi}(\mathcal{A})$  where  $\bar{\phi}$  is the usual complex conjugate;

ii) In the standard proof of the “multiplication operator” theorem, one lets the functions of  $\mathcal{A}$  act on a maximal family of cyclic vectors of  $\mathcal{H}$ , whose existence is proved via the Zorn lemma. In the present adaptation one must use a maximal family of  $\mathcal{J}$ -real cyclic vectors, whose existence is again established by Zornication.

Then,  $\langle | \rangle_r$  is an inner product and  $\| \cdot \|_r$  is the induced norm; moreover, in the realization (2.54-2.56) of  $\mathcal{H}$  and  $\mathcal{A}$ , one has

$$\langle g|f \rangle_r = \int_K w^r \bar{g} f d\mu , \quad \|f\|_r^2 = \int_K w^r |f|^2 d\mu . \quad (2.77)$$

ii) Let us denote with  $\mathcal{H}^r$  the Hilbert space obtained completing  $(\text{Dom}(\mathcal{A}^{r/2}), \langle | \rangle_r)$ . If  $\mathcal{H}$  and  $\mathcal{A}$  are realized as in (2.54-2.56), this Hilbert space can be represented as

$$\mathcal{H}^r = \{f \in \text{Mis}(K, \mu) \mid w^{r/2} f \in L^2(K, \mu)\} ; \quad (2.78)$$

its inner product and norm, denoted again with  $\langle | \rangle_r$  and  $\| \cdot \|_r$ , can be expressed as in Eq. (2.77) for all  $f, g \in \mathcal{H}^r$ . In other terms

$$\mathcal{H}^r = L^2(K, w^r d\mu) . \quad (2.79)$$

iii) There holds

$$\mathcal{H}^r = \text{Dom}(\mathcal{A}^{r/2}) \quad \text{for } r \in \mathbb{R}, r \geq 0 . \quad (2.80)$$

iv) Consider the linear subspace  $\text{Dom}(e^{\mathcal{A}}) \subset \mathcal{H}$  that, in the realization (2.54-2.56) of  $\mathcal{H}$  and  $\mathcal{A}$ , is given by

$$\text{Dom}(e^{\mathcal{A}}) = \{f \in L^2(K, \mu) \mid e^w f \in L^2(K, \mu)\} \subset \mathcal{H} . \quad (2.81)$$

For all  $r \in \mathbb{R}$  there holds

$$\text{Dom}(e^{\mathcal{A}}) \subset \text{Dom}(\mathcal{A}^{r/2}) \subset \mathcal{H}^r , \quad (2.82)$$

and  $\text{Dom}(e^{\mathcal{A}})$  is dense in  $(\mathcal{H}^r, \| \cdot \|_r)$ .

*Proof.* Point i) is obvious. Now, provisionally regard  $\mathcal{H}^r$  to be *defined* by Eq. (2.78), and intend  $\langle | \rangle_r : \mathcal{H}^r \times \mathcal{H}^r \rightarrow \mathbb{C}$  to be defined as in Eq. (2.77); due to (2.79), it is evident that  $\mathcal{H}^r$  is a Hilbert space with this inner product and that the norm induced by this inner product, denoted with  $\| \cdot \|_r$ , can be expressed as in Eq. (2.77). As well, it appears that  $\mathcal{H}^r \supset \text{Dom}(\mathcal{A}^{r/2})$  and that the inner product  $\langle | \rangle_r$  of  $\mathcal{H}^r$  extends the inner product on  $\text{Dom}(\mathcal{A}^{r/2})$  of item i). In the sequel we will prove in order points iii), iv) and finally ii).

iii) For any  $f \in \mathcal{H}^r$  ( $r \geq 0$ ) one has

$$+\infty > \int_K w^r |f|^2 d\mu \geq \varepsilon^r \int_{\mathcal{H}} |f|^2 d\mu ,$$

whence  $f \in L^2(K, \mu)$ . By comparison with the representation of Eq. (2.57), one concludes that  $f \in \text{Dom}(\mathcal{A}^{r/2})$ , so that iii) follows.

iv) For any  $r \in \mathbb{R}$ , there exists a constant  $C_r > 0$  such that  $x^r \leq C_r e^x$  for all  $x \in \mathbb{R}$  such that  $x \geq \varepsilon$ ; this implies  $w^r \leq C_r e^w$  so that, for any  $f \in \text{Dom}(e^{\mathcal{A}})$ , one has

$$\int_K w^r |f|^2 d\mu \leq C_r \int_K e^w |f|^2 d\mu < +\infty ,$$



and the inclusions in Eq. (2.82) follow.

Let us now pass to prove the density of  $\text{Dom}(e^A)$  in  $\mathcal{H}^r$ , choosing arbitrarily  $f \in \mathcal{H}^r$  and constructing a sequence  $(f_n)_{n \in \mathbb{N}}$  in  $\text{Dom}(e^A)$  such that  $\|f - f_n\|_r \rightarrow 0$  for  $n \rightarrow +\infty$ . Define

$$f_n := (\chi_{[0,n]} \circ w)^{1/2} f ,$$

where  $\chi_{[0,n]} : \mathbb{R} \rightarrow \mathbb{R}$  is the indicator function of the interval  $[0, n]$  (<sup>11</sup>); we will prove that

$$f_n \in \text{Dom}(e^A) \quad \text{for all } n \in \mathbb{N} . \quad (2.83)$$

Let us first show that  $f_n \in L^2(K, \mu)$  for all  $n \in \mathbb{N}$ . In fact, for  $r \geq 0$  it is  $\mathcal{H}^r = \text{Dom}(\mathcal{A}^{r/2}) \subset L^2(K, \mu)$ ; thus  $f \in L^2(K, \mu)$ , and the obvious inequality  $|f_n| \leq |f|$  implies  $f_n \in L^2(K, \mu)$ . For  $r < 0$ , from the definition of  $f_n$  it follows that  $|f_n| \leq (w/n)^{r/2} |f|$ , so that

$$\int_K |f_n|^2 d\mu \leq \frac{1}{n^r} \int_K w^r |f|^2 d\mu = \frac{1}{n^r} \|f\|_r^2 < +\infty ;$$

thus,  $f_n \in L^2(K, \mu)$  for all  $n \in \mathbb{N}$ . Now note that  $e^w |f_n| \leq e^n |f_n|$ , whence

$$\int_K e^{2w} |f_n|^2 d\mu \leq e^{2n} \int_K |f_n|^2 d\mu < +\infty ,$$

so that Eq. (2.83) is proven.

Let us pass to evaluate the quantity

$$\|f - f_n\|_r^2 = \int_K w^r |f - f_n|^2 d\mu .$$

By construction, we have  $f_n(k) \rightarrow f(k)$  for a.e.  $k \in K$  in the limit  $n \rightarrow +\infty$ , whence  $w^r |f - f_n|^2 \rightarrow 0$   $\mu$ -almost everywhere. Moreover  $w^r |f - f_n|^2 = w^r (1 - (\chi_{[0,n]} \circ w)^{1/2})^2 |f|^2 \leq w^r |f|^2 \in L^1(K, \mu)$  so, by Lebesgue's theorem on dominated convergence (see, e.g., [47], page 417, Theorem 2.1),

$$\int_K w^r |f - f_n|^2 d\mu \rightarrow 0 \quad \text{for } n \rightarrow +\infty .$$

Summing up, we have proven that  $\text{Dom}(e^A)$  is dense in  $\mathcal{H}^r$  for any  $r \in \mathbb{R}$ .

ii) For any  $r \in \mathbb{R}$ , to state that  $\mathcal{H}^r$  is the completion of  $\text{Dom}(\mathcal{A}^{r/2})$ , one has to prove that  $\text{Dom}(\mathcal{A}^{r/2})$  is dense in  $\mathcal{H}^r$ . For  $r \geq 0$  this holds trivially, since  $\text{Dom}(\mathcal{A}^{r/2}) = \mathcal{H}^r$  by point iii); for  $r < 0$  the thesis follows from the density of  $\text{Dom}(e^A) \subset \text{Dom}(\mathcal{A}^{r/2})$  in  $\mathcal{H}^r$  (see point iv)).  $\square$

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<sup>11</sup>For any subset  $J \subset \mathbb{R}$ , the indicator function is

$$\chi_J : \mathbb{R} \rightarrow \{0, 1\}, \quad t \mapsto \chi_J(t) := \begin{cases} 1 & \text{for } t \in J \\ 0 & \text{for } t \notin J \end{cases} .$$

*Remark 2.3.* In the sequel we will keep the notations  $\mathcal{H}^r$ ,  $\langle \cdot | \cdot \rangle_r$ , and so on for the spaces considered in the previous proposition. Of course, since  $\mathcal{A}^0 = \mathbb{I}$  we have  $\mathcal{H}^0 = \mathcal{H}$  and  $\langle \cdot | \cdot \rangle_0 = \langle \cdot | \cdot \rangle$ .

**Proposition 2.5.** *Let  $r, r' \in \mathbb{R}$  with  $r' \geq r$ ; then the following statements hold, showing in particular that  $\mathcal{H}^{r'} \xrightarrow{\text{dense}} \mathcal{H}^r$ .*

i)  $\text{Dom}(\mathcal{A}^{r'/2})$  (resp.  $\mathcal{H}^{r'}$ ) is a linear subspace of  $\text{Dom}(\mathcal{A}^{r/2})$  (resp.,  $\mathcal{H}^r$ ) and

$$\|f\|_r \leq \varepsilon^{-(r'-r)/2} \|f\|_{r'} \quad \text{for all } f \in \mathcal{H}^{r'} ; \quad (2.84)$$

so, the continuous embedding  $\mathcal{H}^{r'} \hookrightarrow \mathcal{H}^r$  holds.

ii)  $\mathcal{H}^{r'}$  is dense in  $\mathcal{H}^r$ .

*Proof.* i) All the above statements follow easily using representations of the form (2.57) for  $\text{Dom}(\mathcal{A}^{r'/2})$ ,  $\text{Dom}(\mathcal{A}^{r/2})$ , (2.78) for  $\mathcal{H}^{r'}$ ,  $\mathcal{H}^r$ , and (2.77) for  $\|\cdot\|_{r'}$ ,  $\|\cdot\|_r$ ; it must be taken into account that  $w^r = w^{r'}/w^{r'-r} \leq w^{r'}/\varepsilon^{r'-r}$ , as well.

ii) It has already been proved that  $\text{Dom}(e^{\mathcal{A}}) \subset \mathcal{H}^{r'}$  is dense in  $\mathcal{H}^r$ ; of course, this suffices to grant the density of  $\mathcal{H}^{r'}$  in  $\mathcal{H}^r$ .  $\square$

**Proposition 2.6.** *Let  $r_0, r_1 \in \mathbb{R}$ ,  $\theta \in (0, 1)$ , and consider the interpolation space  $[\mathcal{H}^{r_0}, \mathcal{H}^{r_1}]_\theta$ ; then*

$$[\mathcal{H}^{r_0}, \mathcal{H}^{r_1}]_\theta = \mathcal{H}^{(1-\theta)r_0 + \theta r_1} . \quad (2.85)$$

*Proof.* It suffices to use the realization  $\mathcal{H}^r = L^2(K, w^r d\mu)$  of Eq. (2.79), for each  $r \in \mathbb{R}$ , and to recall the identity in Eq. (2.36).  $\square$

## Infinite order spaces.

Let us now pass to discuss two natural spaces: the first one is contained in all the spaces  $\mathcal{H}^r$  ( $r \in \mathbb{R}$ ) and the second one contains them all.

**Definition 2.7.** We put

$$\mathcal{H}^{+\infty} := \bigcap_{r \in \mathbb{R}} \mathcal{H}^r , \quad (2.86)$$

and equip this linear space with the locally convex topology  $\mathcal{T}^{+\infty}$  induced by the family of norms  $\|\cdot\|_r$  ( $r \in \mathbb{R}$ ).

*Remark 2.4.* i) The topological space  $(\mathcal{H}^{+\infty}, \mathcal{T}^{+\infty})$  is complete, due to the completeness of each space  $\mathcal{H}^r$  in the corresponding norm topology induced by  $\|\cdot\|_r$ .

ii) For any  $r \in \mathbb{R}$ , there exists an  $n \in \mathbb{N}$  such that  $n \geq r$  so that, by Proposition 2.5,  $\|\cdot\|_r \leq \varepsilon^{-(n-r)/2} \|\cdot\|_n$ ; therefore, the topology induced on  $\mathcal{H}^{+\infty}$  by the family  $(\|\cdot\|_r)_{r \in \mathbb{R}}$  coincides with the topology induced by the countable subfamily  $(\|\cdot\|_n)_{n \in \mathbb{N}}$ . In conclusion,  $\mathcal{T}^{+\infty}$  is a Fréchet topology.

**Proposition 2.8.** *For each  $r \in \mathbb{R}$  there holds  $\mathcal{H}^{+\infty} \xrightarrow{\text{dense}} \mathcal{H}^r$ .*

*Proof.* By construction, it is  $\mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^r$ . The density follows from the fact that  $\text{Dom}(e^A)$  is contained in  $\mathcal{H}^{+\infty}$  and dense in  $\mathcal{H}^r$ .  $\square$

**Definition 2.9.** We put

$$\mathcal{H}^{-\infty} := \bigcup_{r \in \mathbb{R}} \mathcal{H}^r, \quad (2.87)$$

and equip this linear space with the inductive limit topology  $\mathcal{T}^{-\infty}$  corresponding to the family of normed subspaces  $(\mathcal{H}^r, \|\cdot\|_r)$  ( $r \in \mathbb{R}$ ).

*Remark 2.5.* i) For a general definition of inductive limit topologies, see e.g. [42]. In few words,  $\mathcal{T}^{-\infty}$  is the finest locally convex topology on  $\mathcal{H}^{-\infty}$  such that  $\mathcal{H}^r \hookrightarrow \mathcal{H}^{-\infty}$  for all  $r \in \mathbb{R}$ .

For any given locally convex space  $(\mathcal{Y}, \mathcal{T}_{\mathcal{Y}})$ , a linear operator  $\mathcal{B} : \mathcal{H}^{-\infty} \rightarrow \mathcal{Y}$  is continuous in the topologies  $\mathcal{T}^{-\infty}$  and  $\mathcal{T}_{\mathcal{Y}}$  if and only if the restriction  $\mathcal{B} \upharpoonright \mathcal{H}^r$  is continuous in the topologies  $\mathcal{T}^r$  and  $\mathcal{T}_{\mathcal{Y}}$  for each  $r \in \mathbb{R}$  (see, again, [42]).

ii) Let  $\mathbb{L}$  denote any subset of  $\mathbb{R}$  such that  $\inf \mathbb{L} = -\infty$  (e.g.,  $\mathbb{L} := \{-1, -2, -3, \dots\}$ ). Then, for each  $r \in \mathbb{R}$ , there is an  $\ell \in \mathbb{L}$  such that  $\mathcal{H}^r \hookrightarrow \mathcal{H}^{\ell}$  (just take any  $\ell$  such that  $r \geq \ell$ ); of course, it also holds that for each  $\ell \in \mathbb{L}$  there is  $r \in \mathbb{R}$  such that  $\mathcal{H}^{\ell} \hookrightarrow \mathcal{H}^r$  (just take  $r = \ell$ ). Due to these facts we have

$$\mathcal{H}^{-\infty} = \bigcup_{\ell \in \mathbb{L}} \mathcal{H}^{\ell} \quad (2.88)$$

and the topology  $\mathcal{T}^{-\infty}$  coincides with the inductive limit topology on  $\mathcal{H}^{-\infty}$  given by the family of normed subspaces  $(\mathcal{H}^{\ell}, \|\cdot\|_{\ell})$  ( $\ell \in \mathbb{L}$ ) <sup>(12)</sup>.

**Proposition 2.10.**  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$  is a Hausdorff space.

*Proof.* Choose representations of  $\mathcal{H}$  and  $\mathcal{A}$  as in Eq.s (2.54-2.56) such that the measure space  $(K, \mu)$  satisfies  $\mu(K) < +\infty$  (we already mentioned that such a representation always exists); then

$$\mathcal{H}^{-\infty} = \{f \in \text{Mis}(K) \mid w^{r/2}f \in L^2(K, \mu) \text{ for some } r \in \mathbb{R}\}. \quad (2.89)$$

Now, for each measurable subset  $M \subset K$ , let us put

$$\alpha_M : \mathcal{H}^{-\infty} \rightarrow \mathbb{C}, \quad f \mapsto \langle \alpha_M, f \rangle := \int_M e^{-w} f d\mu.$$

The integral defining  $\langle \alpha_M, f \rangle$  exists for any  $f \in \mathcal{H}^{-\infty}$ ; in fact, if  $r \in \mathbb{R}$  is such that  $w^{r/2}f \in L^2(K, \mu)$ , it follows that

$$\begin{aligned} \int_M |e^{-w} f| d\mu &= \int_M e^{-w} w^{-r/2} w^{r/2} |f| d\mu \leq \\ &\sqrt{\int_M e^{-2w} w^{-r} d\mu} \sqrt{\int_M w^r |f|^2 d\mu} \leq \sqrt{C_r \mu(M)} \sqrt{\int_K w^r |f|^2 d\mu} < +\infty, \end{aligned}$$

<sup>12</sup>Concerning the last statement, see e.g. [42], page 118, Proposition 5.8.

where we have put  $C_r := \sup_{\lambda \in [\epsilon, +\infty)} e^{-2\lambda} \lambda^{-r}$  (so that  $e^{-2w} w^{-r} \leq C_r$ ). Clearly,  $\alpha_M$  is a linear form on  $\mathcal{H}^{-\infty}$ ; moreover, for each  $r \in \mathbb{R}$ , the previous manipulations also imply  $|\langle \alpha_M, f \rangle| \leq \sqrt{C_r \mu(M)} \|f\|_r$  for all  $f \in \mathcal{H}^r$ , so that  $\alpha_M \upharpoonright \mathcal{H}^r$  is continuous. In conclusion,  $\alpha_M$  is a continuous linear form on  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$  (see the comments in Remark 2.5).

Now observe that, for each  $f \in \mathcal{H}^{-\infty}$ ,

$$\begin{aligned} \langle \alpha_M, f \rangle = 0 \quad \text{for any measurable subset } M \subset K &\Rightarrow \\ \Rightarrow e^{-w} f = 0 \quad \text{a.e. in } K &\Rightarrow f = 0 \quad \text{a.e. in } K . \end{aligned}$$

To go on, let  $f, g \in \mathcal{H}^{-\infty}$  and  $f \neq g$ ; then there is a measurable subset  $M \subset K$  such that  $\delta := |\langle \alpha_M, f - g \rangle| > 0$  (otherwise we would have  $f - g = 0$ ). Put  $\mathcal{U}_f := \{f' \in \mathcal{H}^{-\infty} \mid |\langle \alpha_M, f' - f \rangle| < \delta/3\}$  and  $\mathcal{U}_g := \{g' \in \mathcal{H}^{-\infty} \mid |\langle \alpha_M, g' - g \rangle| < \delta/3\}$ ; then, it appears that  $\mathcal{U}_f$  and  $\mathcal{U}_g$  are open subsets of  $\mathcal{H}^{-\infty}$  containing  $f$  and  $g$ , respectively, and  $\mathcal{U}_f \cap \mathcal{U}_g = \emptyset$ .  $\square$

*Remark 2.6.* The spaces  $\mathcal{H}^r$  ( $r \in \mathbb{R}$ ) and  $\mathcal{H}^{+\infty}$  are also Hausdorff for obvious reasons; this fact follows trivially from Proposition 2.10 since  $\mathcal{H}^{+\infty} \subset \mathcal{H}^r \subset \mathcal{H}^{-\infty}$  and any subset of a Hausdorff space is itself Hausdorff (see, e.g., [26], page 77). Summing up,  $\mathcal{H}^r$  is a Hausdorff space for any  $r \in [-\infty, +\infty]$ .

**Proposition 2.11.** *Each one of the sets  $\text{Dom}(e^A)$ ,  $\text{Dom}(\mathcal{A}^{r/2})$  and  $\mathcal{H}^r$  ( $r \in \mathbb{R}$ ) is dense in  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$ .*

*Proof.* Since the chain of inclusions  $\text{Dom}(e^A) \subset \text{Dom}(\mathcal{A}^{r/2}) \subset \mathcal{H}^r$  holds, it suffices to prove the density of  $\text{Dom}(e^A)$  in  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$ ; to this purpose, let us consider any  $f \in \mathcal{H}^{-\infty}$  and prove that there exists a sequence  $(f_n)_{n \in \mathbb{N}}$  of elements of  $\text{Dom}(e^A)$  such that  $f_n \rightarrow f$  for  $n \rightarrow +\infty$  in  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$ . Indeed, let  $r$  be such that  $f \in \mathcal{H}^r$ ; then, due to Proposition 2.4, there is a sequence  $(f_n)_{n \in \mathbb{N}}$  in  $\text{Dom}(e^A)$  such that  $f_n \rightarrow f$  in  $(\mathcal{H}^r, \|\cdot\|_r)$  for  $n \rightarrow +\infty$ . From here and from  $\mathcal{H}^r \hookrightarrow \mathcal{H}^{-\infty}$  it follows that  $f_n \rightarrow f$  in  $(\mathcal{H}^{-\infty}, \mathcal{T}^{-\infty})$  for  $n \rightarrow +\infty$ .  $\square$

**Proposition 2.12.** *Let  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  be a measurable function and assume that, for some  $b \in \mathbb{R}$ ,*

$$\sup_{\lambda \in \sigma(\mathcal{A})} \lambda^b |\phi(\lambda)| < +\infty . \quad (2.90)$$

*Then, the following statements hold:*

*i) The operator  $\phi(\mathcal{A}) : \text{Dom}(\phi(\mathcal{A})) \subset \mathcal{H} \rightarrow \mathcal{H}$  has a unique continuous linear extension, denoted with the same symbol,  $\phi(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ .*

ii) Let  $r, r' \in \mathbb{R}$  be such that  $r' - r \geq -2b$ . Then, the extension  $\phi(\mathcal{A})$  sends continuously  $\mathcal{H}^{r'}$  into  $\mathcal{H}^r$ ; moreover, for all  $f \in \mathcal{H}^{r'}$  one has <sup>(13)</sup>

$$\|\phi(\mathcal{A})f\|_r \leq Q_{rr'} \|f\|_{r'} , \quad Q_{rr'} := \sup_{\lambda \in \sigma(\mathcal{A})} \lambda^{-(r'-r)/2} |\phi(\lambda)| < +\infty . \quad (2.91)$$

iii) In particular assume that, for some  $b \in \mathbb{R}$ , it is

$$|\phi(\lambda)| = \lambda^{-b} \quad \text{for all } \lambda \in \sigma(\mathcal{A}) ; \quad (2.92)$$

then the extension  $\phi(\mathcal{A})$  of item i) is a Hilbertian isomorphism between  $\mathcal{H}^r$  and  $\mathcal{H}^{r+2b}$  for each  $r \in \mathbb{R}$ .

*Proof.* i) ii) First of all, let us prove that the mentioned continuous extension is unique, assuming it to exist. In fact, consider two distinct continuous extensions  $\phi(\mathcal{A}), \phi'(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ . By construction,  $\phi(\mathcal{A})$  and  $\phi'(\mathcal{A})$  coincide on the set  $\text{Dom}(\phi(\mathcal{A}))$  which is dense in  $\mathcal{H}$  and, consequently, in  $\mathcal{H}^{-\infty}$  (see Proposition 2.11); so  $\phi(\mathcal{A}) = \phi'(\mathcal{A})$  everywhere on  $\mathcal{H}^{-\infty}$  by continuity.

In order to prove the existence of the continuous linear extension, represent  $\mathcal{H}^{-\infty}$  as in Eq. (2.89) and define

$$\phi(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty} , \quad f \mapsto \phi(\mathcal{A})f := (\phi \circ w)f \quad (2.93)$$

(recalling that  $w(k) \in \sigma(\mathcal{A}) = \text{Dom}(\phi)$  for a.e.  $k \in K$ , so that  $\phi \circ w$  is defined almost everywhere in  $K$ ). Let us prove that the map (2.93) is well defined. To this purpose, let  $f \in \mathcal{H}^{-\infty}$ ; then  $f \in \mathcal{H}^{r'}$  for some  $r' \in \mathbb{R}$ . If we consider any  $r \in \mathbb{R}$  such that  $r' - r \geq -2b$ , writing (almost everywhere in  $K$ )

$$w^{r/2} \phi(\mathcal{A})f = w^{-(r'-r)/2} (\phi \circ w) w^{r'/2} f ,$$

we infer

$$w^{r/2} |\phi(\mathcal{A})f| \leq Q_{rr'} w^{r'/2} |f| , \quad (2.94)$$

with  $Q_{rr'}$  as in Eq. (2.91). From Eq. (2.94) and from  $w^{r'/2} f \in L^2(K, \mu)$  it follows that  $w^{r/2} \phi(\mathcal{A})f \in L^2(K, \mu)$ , which amounts to state that  $\phi(\mathcal{A})f \in \mathcal{H}^r \hookrightarrow \mathcal{H}^{-\infty}$ .

Summing up, we have shown that the map in Eq. (2.93) actually sends  $\mathcal{H}^{-\infty}$  into  $\mathcal{H}^{-\infty}$ ; the linearity of this map is evident. The previous argument also indicates that  $\phi(\mathcal{A})\mathcal{H}^{r'} \subset \mathcal{H}^r$  for  $r' - r \geq -2b$ ; moreover, the inequality in Eq. (2.94) can be used to infer the norm inequality in Eq. (2.91). This also implies the continuity of  $\phi(\mathcal{A})$  as a map  $\mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ .

iii) The thesis is almost evident; the main point in the proof is the (obvious) identity  $w^{r/2+b} |\phi(\mathcal{A})f| = w^{r/2} f$ .  $\square$

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<sup>13</sup>Note that the supremum defining  $Q_{rr'}$  is finite. In fact, for any  $\lambda \in \sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ , we have

$$\begin{aligned} \lambda^{-(r'-r)/2} |\phi(\lambda)| &= \varepsilon^{-(r'-r)/2} (\lambda/\varepsilon)^{-(r'-r)/2} |\phi(\lambda)| \leq \\ &\leq \varepsilon^{-(r'-r)/2} (\lambda/\varepsilon)^b |\phi(\lambda)| = \varepsilon^{-(r'-r+2b)/2} \lambda^b |\phi(\lambda)| , \end{aligned}$$

and Eq. (2.90) gives the thesis.

**Corollary 2.13.** *i) For any  $s \in \mathbb{C}$ , the operator  $\mathcal{A}^{-s} : \text{Dom}(\mathcal{A}^{-s}) \subset \mathcal{H}^{-\infty} \rightarrow \mathcal{H} \subset \mathcal{H}^{-\infty}$  has a unique, continuous linear extension (indicated with the same symbol)  $\mathcal{A}^{-s} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ .*

*ii) The extension of item i) is such that, for any  $r \in \mathbb{R}$ ,*

$$\mathcal{A}^{-s}(\mathcal{H}^r) = \mathcal{H}^{r+2\Re s}, \quad \|\mathcal{A}^{-s}f\|_{r+2\Re s} = \|f\|_r \quad \text{for all } f \in \mathcal{H}^r. \quad (2.95)$$

*iii) Concerning the continuous extensions to  $\mathcal{H}^{-\infty}$ , the following statements hold:  $\mathcal{A}^0 = \mathbb{I}_{\mathcal{H}^{-\infty}}$ ,  $\mathcal{A}^{-(s+s')} = \mathcal{A}^{-s}\mathcal{A}^{-s'}$  for any  $s, s' \in \mathbb{C}$ , and  $\mathcal{A}^s$  is the inverse operator of  $\mathcal{A}^{-s}$  for any  $s \in \mathbb{C}$ .*

*Proof.* i) ii) The thesis follows by statements i) and iii) of Proposition 2.12. Indeed, for any  $s \in \mathbb{C}$ , the map  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ ,  $\lambda \mapsto \lambda^{-s}$  is measurable and fulfills Eq. (2.92) for  $b = \Re s$ .

iii) All these statements follow easily noting that, for any  $s \in \mathbb{C}$ , the linear continuous extension  $\mathcal{A}^{-s} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  in item i) is defined according to Eq. (2.93), so that  $\mathcal{A}^{-s}f = w^{-s}f$  for all  $f \in \mathcal{H}^{-\infty}$ .  $\square$

**Corollary 2.14.** *i) For any  $\mathbf{t} \in \mathbb{C}$  with  $\Re \mathbf{t} \geq 0$  consider the operators  $e^{-\mathbf{t}\mathcal{A}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})$  mapping the respective domains  $\text{Dom}(e^{-\mathbf{t}\mathcal{A}})$ ,  $\text{Dom}(e^{-\mathbf{t}\sqrt{\mathcal{A}}})$ ,  $\text{Dom}(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}) \subset \mathcal{H} \subset \mathcal{H}^{-\infty}$  into  $\mathcal{H} \subset \mathcal{H}^{-\infty}$ . Each of them admits a unique continuous linear extension (indicated with the same symbol)*

$$e^{-\mathbf{t}\mathcal{A}}, e^{-\mathbf{t}\sqrt{\mathcal{A}}}, \frac{e^{-\mathbf{t}\sqrt{\mathcal{A}}}}{\sqrt{\mathcal{A}}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}. \quad (2.96)$$

*ii) Assume  $\Re \mathbf{t} > 0$  and consider the extensions of item i); these are such that, for any  $r, r' \in \mathbb{R}$ , and for all  $f \in \mathcal{H}^{r'}$ , one has*

$$\|e^{-\mathbf{t}\mathcal{A}}f\|_r \leq \begin{cases} \left(\frac{r-r'}{2e\Re \mathbf{t}}\right)^{(r-r')/2} \|f\|_{r'} & \text{for } 0 < \Re \mathbf{t} \leq \frac{r-r'}{2\varepsilon} \\ \varepsilon^{(r-r')/2} e^{-\varepsilon \Re \mathbf{t}} \|f\|_{r'} & \text{for } \Re \mathbf{t} > \frac{r-r'}{2\varepsilon} \end{cases}, \quad (2.97)$$

$$\|e^{-\mathbf{t}\sqrt{\mathcal{A}}}f\|_r \leq \begin{cases} \left(\frac{r-r'}{e\Re \mathbf{t}}\right)^{r-r'} \|f\|_{r'} & \text{for } 0 < \Re \mathbf{t} \leq \frac{r-r'}{\sqrt{\varepsilon}} \\ \varepsilon^{(r-r')/2} e^{-\sqrt{\varepsilon} \Re \mathbf{t}} \|f\|_{r'} & \text{for } \Re \mathbf{t} > \frac{r-r'}{\sqrt{\varepsilon}} \end{cases}, \quad (2.98)$$

$$\|(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})f\|_r \leq \begin{cases} \left(\frac{r-r'-1}{e\Re \mathbf{t}}\right)^{r-r'-1} \|f\|_{r'} & \text{for } 0 < \Re \mathbf{t} \leq \frac{r-r'-1}{\sqrt{\varepsilon}} \\ \varepsilon^{(r-r'-1)/2} e^{-\sqrt{\varepsilon} \Re \mathbf{t}} \|f\|_{r'} & \text{for } \Re \mathbf{t} > \frac{r-r'-1}{\sqrt{\varepsilon}} \end{cases}. \quad (2.99)$$

Moreover, each of the extensions  $e^{-\mathbf{t}\mathcal{A}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})$  maps continuously  $\mathcal{H}^{-\infty}$  into  $\mathcal{H}^{+\infty}$ .

*iii) Assume  $\Re \mathbf{t} = 0$ , so that  $\mathbf{t} = it$  for some  $t \in \mathbb{R}$ . Then the extensions  $e^{-it\mathcal{A}}$ ,  $e^{-it\sqrt{\mathcal{A}}}$  of item i) are Hilbertian automorphism of  $\mathcal{H}^r$ , for each  $r \in \mathbb{R}$ ; in particular, there holds*

$$\|e^{-it\mathcal{A}}f\|_r = \|e^{-it\sqrt{\mathcal{A}}}f\|_r = \|f\|_r. \quad (2.100)$$

Moreover, the extension  $e^{-it\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$  is an Hilbertian isomorphism of  $\mathcal{H}^r$  into  $\mathcal{H}^{r+1}$ , for any  $r \in \mathbb{R}$ ; in particular,

$$\|(e^{-it\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})f\|_r = \|f\|_{r+1} . \quad (2.101)$$

*Proof.* Hereafter we report the proof only for the operator  $e^{-t\mathcal{A}}$ ; the proofs of the analogous statements for the other two operators  $e^{-t\sqrt{\mathcal{A}}}$ ,  $e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$  can be derived by similar arguments.

i) ii) The thesis follows by items i) and ii) of Proposition 2.12. Indeed, for any  $t \in \mathbb{C}$  with  $\Re t > 0$ , the map  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ ,  $\lambda \mapsto e^{-\lambda t}$  is measurable and fulfills Eq. (2.91) with

$$Q_{rr'} = \sup_{\lambda \in \sigma(\mathcal{A})} \lambda^{-(r'-r)/2} e^{-\lambda \Re t} = \begin{cases} \left(\frac{r-r'}{2e\Re t}\right)^{(r-r')/2} & \text{for } 0 < \Re t \leq \frac{r-r'}{2\varepsilon} \\ \varepsilon^{(r-r')/2} e^{-\varepsilon \Re t} & \text{for } \Re t > \frac{r-r'}{2\varepsilon} \end{cases} .$$

Moreover, for all  $f \in \mathcal{H}^{-\infty}$ , there exists an  $r' \in \mathbb{R}$  such that  $f \in \mathcal{H}^{r'}$ ; then, by Item ii), for any  $t \in \mathbb{C}$  with  $\Re t > 0$ , one has  $e^{-t\mathcal{A}}f \in \mathcal{H}^r$  for all  $r \in \mathbb{R}$ ; thus  $e^{-t\mathcal{A}}f \in \mathcal{H}^{+\infty}$ , that is the thesis. The continuity of  $e^{-t\mathcal{A}}$  from  $\mathcal{H}^{-\infty}$  to  $\mathcal{H}^{+\infty}$  is proved by similar arguments.

iv) Consider the elementary identities  $|e^{-it\lambda}| = |e^{-it\sqrt{\lambda}}| = 1$  and  $|e^{-it\sqrt{\lambda}}/\sqrt{\lambda}| = \lambda^{-1/2}$ , for  $\lambda \in \sigma(\mathcal{A})$ ; then, the thesis follows straightforwardly from item iii) of Proposition 2.12.  $\square$

## Duality relations.

In the present paragraph we discuss duality relations holding for both the finite ( $\mathcal{H}^r$ ,  $r \in \mathbb{R}$ ) and infinite order ( $\mathcal{H}^{\pm\infty}$ ) spaces considered in the two previous subsections.

**Definition 2.15.** We consider the set

$$\mathcal{H}^{(2)} := \bigcup_{r \in \mathbb{R}} \mathcal{H}^{-r} \times \mathcal{H}^r . \quad (2.102)$$

*Remark 2.7.* Note that the space  $\mathcal{H}^{(2)}$  contains, in particular,  $\mathcal{H} \times \mathcal{H} = \mathcal{H}^0 \times \mathcal{H}^0$ .

**Proposition 2.16.** The inner product  $\langle | \rangle$  of  $\mathcal{H}$  has a unique extension

$$\langle | \rangle : \mathcal{H}^{(2)} \rightarrow \mathbb{C} \quad (2.103)$$

that is continuous when restricted to any of the products  $\mathcal{H}^{-r} \times \mathcal{H}^r$  ( $r \in \mathbb{R}$ )<sup>14</sup>. For each  $r \in \mathbb{R}$ , the map (2.103) restricted to  $\mathcal{H}^{-r} \times \mathcal{H}^r$  is a sesquilinear Hermitian form; moreover, for all  $f \in \mathcal{H}^{-r}$  and all  $g \in \mathcal{H}^r$ , it fulfills

$$|\langle f|g \rangle| \leq \|f\|_{-r} \|g\|_r . \quad (2.104)$$

<sup>14</sup>Of course,  $\mathcal{H}^{-r} \times \mathcal{H}^r$  ( $r \in \mathbb{R}$ ) is equipped with the product topology.

*Proof.* Let us first prove that the extension  $\langle | \rangle$  with the above requirements, if it exists, is unique; to this purpose, it suffices to show that any extension with the above properties is uniquely determined on any product  $\mathcal{H}^{-r} \times \mathcal{H}^r$  ( $r \in \mathbb{R}$ ). In fact, if  $r \geq 0$ ,  $\mathcal{H}^r \times \mathcal{H}^r$  is dense in  $\mathcal{H}^{-r} \times \mathcal{H}^r$  and the extension must agree with the usual inner product of  $\mathcal{H}$  on  $\mathcal{H}^r \times \mathcal{H}^r$  ( $\subset \mathcal{H} \times \mathcal{H}$ ); similar arguments hold if  $r < 0$  considering the space  $\mathcal{H}^{-r} \times \mathcal{H}^{-r}$  in place of  $\mathcal{H}^r \times \mathcal{H}^r$ .

To prove existence of the extension (2.103), consider the realization of  $\mathcal{H}$  and  $\mathcal{A}$  given in Eq.s (2.54-2.56) and define

$$\langle f|g \rangle := \int_K \bar{f}g \, d\mu \quad \text{for all } (f, g) \in \mathcal{H}^{(2)}. \quad (2.105)$$

The above integral exists; in fact, if  $r \in \mathbb{R}$  is such that  $(f, g) \in \mathcal{H}^{-r} \times \mathcal{H}^r$ , we have

$$\begin{aligned} \int_K |\bar{f}g| \, d\mu &= \int_K w^{-r/2}|f| w^{r/2}|g| \, d\mu \leq \\ &\leq \sqrt{\int_K w^{-r}|f|^2 \, d\mu} \sqrt{\int_K w^r|g|^2 \, d\mu} = \|f\|_{-r} \|g\|_r < +\infty. \end{aligned} \quad (2.106)$$

It is clear that (2.105) defines an extension of the inner product on  $\mathcal{H} \times \mathcal{H}$ . For all  $r \in \mathbb{R}$ , the map (2.105) is a sesquilinear Hermitian form on  $\mathcal{H}^{-r} \times \mathcal{H}^r$ ; moreover, due to the estimate in Eq. (2.106), it fulfills the inequality (2.104), which implies its continuity.  $\square$

In the sequel we keep the notation  $\langle | \rangle$  for the extension (2.103) of the inner product on  $\mathcal{H}$ . In the forthcoming Proposition 2.18 this extension is used to prove that  $\mathcal{H}^{-r}$  can be identified isomorphically with the dual of the Banach space  $\mathcal{H}^r$ ; in the subsequent Proposition 2.20 it is shown that  $\mathcal{H}^{-\infty}$  can be identified with the dual of the Fréchet space  $\mathcal{H}^{+\infty}$ , as well.

**Definition 2.17.** For  $r \in \mathbb{R}$ , we define the map

$$\mathcal{I}^r : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)' , \quad f \mapsto \mathcal{I}^r f \quad \text{such that} \quad \langle \mathcal{I}^r f, g \rangle := \langle f|g \rangle \quad \text{for all } g \in \mathcal{H}^r. \quad (2.107)$$

**Proposition 2.18.** *The following statements hold.*

i) *The map  $\mathcal{I}^r$  in Eq. (2.107) is well defined, antilinear, bijective and fulfills*

$$\|\mathcal{I}^r f\|'_r = \|f\|_{-r} \quad \text{for all } f \in \mathcal{H}^{-r}. \quad (2.108)$$

(and thus, summing up, it is an antilinear isomorphism of Banach spaces).

ii) *Let  $r, r' \in \mathbb{R}$  with  $r' \geq r$ , so that  $\mathcal{H}^{r'} \hookrightarrow \mathcal{H}^r$  and  $\mathcal{H}^{-r} \hookrightarrow \mathcal{H}^{-r'}$ ; then*

$$\mathcal{I}^{r'} f = \mathcal{I}^r f \upharpoonright \mathcal{H}^{r'} \quad \text{for all } f \in \mathcal{H}^{-r}. \quad (2.109)$$



*Proof.* i) Fix  $r \in \mathbb{R}$ ; due to Proposition 2.16 it appears that, for each  $f \in \mathcal{H}^{-r}$ , the element  $\mathcal{I}^r f$  defined in Eq. (2.107) is a continuous linear form on  $\mathcal{H}^r$ , with the norm bound (recall Eq. (2.104))

$$\|\mathcal{I}^r f\|'_r \leq \|f\|_{-r}. \quad (2.110)$$

It is evident as well that  $\mathcal{I}^r$  is a continuous antilinear map from  $\mathcal{H}^{-r}$  to  $(\mathcal{H}^r)'$ . In the sequel we use again the representations (2.54-2.56) for  $\mathcal{H}$  and  $\mathcal{A}$ , so that

$$\langle \mathcal{I}^r f, g \rangle = \int_K \bar{f} g d\mu \quad \text{for all } f \in \mathcal{H}^{-r}, g \in \mathcal{H}^r. \quad (2.111)$$

Let us prove Eq. (2.108), for a given  $f \in \mathcal{H}^{-r}$ . To this purpose, put  $g = w^{-r} f$ ; then  $\int_K w^r |g|^2 d\mu = \int_K w^{-r} |f|^2 d\mu$ , which implies  $g \in \mathcal{H}^r$  and  $\|g\|_r = \|f\|_{-r}$ . For this  $g$  it is  $\langle \mathcal{I}^r f, g \rangle = \int_K w^{-r} |f|^2 d\mu = \|f\|_{-r} \|f\|_{-r} = \|f\|_{-r} \|g\|_r$ , whence  $\|\mathcal{I}^r f\|'_r \geq \|f\|_{-r}$ . From here and from Eq. (2.110) the thesis (2.108) follows.

To conclude, let us prove that  $\mathcal{I}^r$  is bijective between  $\mathcal{H}^{-r}$  and  $\mathcal{H}^r$ . Due to Eq. (2.108),  $\mathcal{I}^r$  has zero kernel, so it is injective. To prove surjectivity, let  $\alpha \in (\mathcal{H}^r)'$ ; since  $\mathcal{H}^r$  is a Hilbert space with the inner product  $\langle \cdot | \cdot \rangle_r$ , by the Riesz theorem there exists an  $h \in \mathcal{H}^r$  such that

$$\langle \alpha, g \rangle = \langle h | g \rangle_r = \int_K w^r \bar{h} g d\mu \quad \text{for all } g \in \mathcal{H}^r. \quad (2.112)$$

Put  $f := w^r h$ ; then  $\int_K w^{-r} |f|^2 d\mu = \int_K w^r |h|^2 d\mu < +\infty$ , so that  $f \in \mathcal{H}^{-r}$ . Moreover, Eq. (2.112) implies  $\langle \alpha, g \rangle = \int_K \bar{f} g d\mu = \langle \mathcal{I}^r f, g \rangle$  for all  $g \in \mathcal{H}^r$ ; this means  $\alpha = \mathcal{I}^r f$ , thus the surjectivity of  $\mathcal{I}^r$  is proved.

ii) The thesis follows immediately from the definitions of  $\mathcal{I}^r$  and  $\mathcal{I}^{r'}$ .  $\square$

Consider now  $(\mathcal{H}^{+\infty})'$ , the topological dual of the space  $\mathcal{H}^{+\infty}$ . Recall that the topology on the Fréchet space  $\mathcal{H}^{+\infty}$  is induced by the family of norms  $\|\cdot\|_r \upharpoonright \mathcal{H}^r$  ( $r \in \mathbb{R}$ ); so, a linear form  $\alpha : \mathcal{H}^{+\infty} \rightarrow \mathbb{C}$  is continuous if and only if there exist  $r \in \mathbb{R}$  and  $C_r \in [0, +\infty)$  such that  $|\langle \alpha, f \rangle| \leq C_r \|f\|_r$  for all  $f \in \mathcal{H}^{+\infty}$ . This condition is equivalent to state that  $\alpha$  is the restriction of a continuous linear form on  $\mathcal{H}^r$ ; this form on  $\mathcal{H}^r$  is unique, due to the density of  $\mathcal{H}^{+\infty}$  in  $\mathcal{H}^r$ . Therefore, by identifying the elements of  $(\mathcal{H}^{+\infty})'$  with their restrictions to  $\mathcal{H}^r$ , one has

$$(\mathcal{H}^{+\infty})' = \bigcup_{r \in \mathbb{R}} (\mathcal{H}^r)'. \quad (2.113)$$

**Definition 2.19.** From now on,  $(\mathcal{H}^{+\infty})'$  will be equipped with the inductive limit topology corresponding to the family of Banach spaces  $((\mathcal{H}^r)', \|\cdot\|'_r)$ .

*Remark 2.8.* The above topology is the finest locally convex topology on  $(\mathcal{H}^{+\infty})'$  that makes continuous the injection of each space  $((\mathcal{H}^r)', \|\cdot\|'_r)$  in  $(\mathcal{H}^{+\infty})'$ .

The following statement is easily proved using, where necessary, the already known facts on the Banach anti-isomorphisms  $\mathcal{I}^r : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)'$ .

**Proposition 2.20.**  $\mathcal{H}^{-\infty} \times \mathcal{H}^{+\infty}$  is contained in the set  $\mathcal{H}^{(2)}$  defined in Eq. (2.102); let us put

$$\mathcal{I}^\infty : \mathcal{H}^{-\infty} \rightarrow (\mathcal{H}^{+\infty})', \quad f \mapsto \mathcal{I}^\infty f \quad \text{such that} \quad \langle \mathcal{I}^\infty f, g \rangle := \langle f | g \rangle \quad \text{for all } g \in \mathcal{H}^{+\infty}. \quad (2.114)$$

The map  $\mathcal{I}^\infty$  is well defined, antilinear and bijective; it is a homeomorphism with respect to the inductive limit topologies of  $\mathcal{H}^{-\infty}$  and  $(\mathcal{H}^{+\infty})'$  introduced in the Definitions 2.9 and 2.19. For any  $r \in \mathbb{R}$  and any  $f \in \mathcal{H}^{-r}$ , there holds

$$\mathcal{I}^\infty f = \mathcal{I}^r f \upharpoonright \mathcal{H}^{+\infty}. \quad (2.115)$$

*Proof.* Let  $(f, g) \in \mathcal{H}^{-\infty} \times \mathcal{H}^{+\infty}$ ; then  $f \in \mathcal{H}^{-r}$  for some  $r \in [0, +\infty)$ . Since  $g \in \mathcal{H}^r$ , we have  $(f, g) \in \mathcal{H}^{-r} \times \mathcal{H}^r \subset \mathcal{H}^{(2)}$ ; this proves the inclusion  $\mathcal{H}^{-\infty} \times \mathcal{H}^{+\infty} \subset \mathcal{H}^{(2)}$ .

Now, let  $f \in \mathcal{H}^{-\infty}$ , and define  $\mathcal{I}^\infty f : \mathcal{H}^r \rightarrow \mathbb{C}$  following (2.114). Clearly,  $\mathcal{I}^\infty f$  is a linear map. If  $r \in \mathbb{R}$  is such that  $f \in \mathcal{H}^{-r}$ , it is evident that  $\mathcal{I}^\infty f = \mathcal{I}^r f \upharpoonright \mathcal{H}^{+\infty}$ , and this restriction is continuous on  $\mathcal{H}^{+\infty}$  since  $\mathcal{I}^r f$  is continuous on  $\mathcal{H}^r$  and  $\mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^r$ .

In conclusion  $\mathcal{I}^\infty f \in (\mathcal{H}^{+\infty})'$  and we have a well defined map  $\mathcal{I}^\infty : \mathcal{H}^{-\infty} \rightarrow (\mathcal{H}^{+\infty})'$ ,  $f \mapsto \mathcal{I}^\infty f$ . The antilinearity of this map is self-evident; hereafter we show that  $\mathcal{I}^\infty$  is bijective.

Indeed, let  $f, f' \in \mathcal{H}^{-\infty}$  be such that  $\mathcal{I}^\infty f = \mathcal{I}^\infty f'$ . There exists  $r \in \mathbb{R}$  such that  $f, f' \in \mathcal{H}^{-r}$ ; this implies  $\mathcal{I}^r f \upharpoonright \mathcal{H}^{+\infty} = \mathcal{I}^r f' \upharpoonright \mathcal{H}^{+\infty}$  which gives (by the density of  $\mathcal{H}^{+\infty}$  in  $\mathcal{H}^r$ )  $\mathcal{I}^r f = \mathcal{I}^r f'$ . Thus, we infer that  $f = f'$ , which proves the injectivity of  $\mathcal{I}^\infty$ .

To prove surjectivity, let us take  $\alpha \in (\mathcal{H}^{+\infty})'$  and show that  $\alpha = \mathcal{I}^\infty f$  for some  $f \in \mathcal{H}^{-\infty}$ . Indeed, there are  $r \in \mathbb{R}$  and  $\alpha_r \in (\mathcal{H}^r)'$  such that  $\alpha = \alpha_r \upharpoonright \mathcal{H}^{+\infty}$ ; if  $f \in \mathcal{H}^{-r}$  is such that  $\alpha_r = \mathcal{I}^r f$ , we have  $\mathcal{I}^\infty f = \mathcal{I}^r f \upharpoonright \mathcal{H}^{+\infty} = \alpha$ .

To infer that  $\mathcal{I}^\infty$  is in fact a homeomorphism (i.e., continuous with continuous inverse), one can use the continuity of the maps  $\mathcal{I}^r : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)'$  ( $r \in \mathbb{R}$ ) (see Proposition 2.18), recalling the fundamental properties of the inductive limit topologies on  $\mathcal{H}^{-\infty}$  and on  $(\mathcal{H}^{+\infty})'$  <sup>(15)</sup>.  $\square$

## Banach adjoints of continuous operators.

Consider the scale of spaces  $\mathcal{H}^r$  ( $r \in \mathbb{R}$ ) discussed previously in this section; even though each of these spaces is in fact a Hilbert space (with inner product  $\langle | \rangle_r$ ; see Proposition 2.4), in the present subsection we shall only consider the underlying Banach space structure. In particular, hereafter we discuss the notion of adjoint for a continuous operator acting between any two of the Banach spaces  $\mathcal{H}^r$  ( $r \in \mathbb{R}$ ).

Recall that for any  $r \in \mathbb{R}$  (or  $r = +\infty$ ) the topological dual of the Banach space  $\mathcal{H}^r$ , i.e.  $(\mathcal{H}^r)'$ , is anti-linearly isomorphic  $\mathcal{H}^{-r}$  (see Proposition 2.18); moreover, the duality pairing

<sup>15</sup>For example, recall that the map  $\mathcal{I}^\infty : \mathcal{H}^{-\infty} \rightarrow (\mathcal{H}^{+\infty})'$  is continuous if and only if its restriction  $\mathcal{I}^\infty \upharpoonright \mathcal{H}^{-r} : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)'$  is so, for all  $r \in \mathbb{R}$ ; on the other hand, the continuity of  $\mathcal{I}^\infty \upharpoonright \mathcal{H}^{-r}$  can be inferred noting that  $\mathcal{I}^\infty \upharpoonright \mathcal{H}^{-r} \equiv \mathcal{I}^r : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)'$  (which is continuous) and that the embedding  $(\mathcal{H}^r)' \hookrightarrow (\mathcal{H}^{+\infty})'$  is continuous, since  $(\mathcal{H}^{+\infty})'$  is endowed with the inductive limit topology.

between these spaces is described by the restriction to  $\mathcal{H}^{-r} \times \mathcal{H}^r$  of the map  $\langle | \rangle : \mathcal{H}^{(2)} \rightarrow \mathbb{C}$ , introduced in Proposition 2.16. In view of these facts, the notion of Banach adjoint of a continuous operator (see Section 2.2) can be rephrased as follows within the framework under analysis.

**Definition 2.21.** Let  $r, r' \in \mathbb{R}$  and consider a continuous linear operator  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{r'}$ . The *Banach adjoint* of  $\mathcal{B}$  is the unique continuous operator  $\mathcal{B}^* : \mathcal{H}^{-r'} \rightarrow \mathcal{H}^{-r}$  such that

$$\langle \mathcal{B}^* g | f \rangle = \langle g | \mathcal{B} f \rangle \quad \text{for all } f \in \mathcal{H}^r, g \in \mathcal{H}^{-r'}. \quad (2.116)$$

*Remark 2.9.* Let us point out a few facts concerning the above definition.

i) The symbol  $\langle | \rangle$  on the left-hand side of Eq. (2.116) is used to indicate the restriction of the map (2.103) to  $\mathcal{H}^{-r} \times \mathcal{H}^r$ ; on the other hand, the same symbol is used on the right-hand side of the cited equation to denote the restriction of the map (2.103) to  $\mathcal{H}^{-r'} \times \mathcal{H}^{r'}$ .

ii) Recall that the map  $\langle | \rangle : \mathcal{H}^{(2)} \rightarrow \mathbb{C}$  of Proposition 2.16 is an extension of the inner product on  $\mathcal{H}$ ; thus, given a continuous operator  $\mathcal{B} : \mathcal{H} \rightarrow \mathcal{H}$  ( $\mathcal{H} \equiv \mathcal{H}^0$ ), the corresponding Banach adjoint  $\mathcal{B}^* : \mathcal{H} \rightarrow \mathcal{H}$  (defined according to Eq. (2.116)) does in fact coincide with the standard Hilbert adjoint  $\mathcal{B}^\dagger$ . On the other hand, despite the fact that  $\mathcal{H}^r$  and  $\mathcal{H}^{r'}$  are also Hilbert spaces, the adjoint of an operator  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{r'}$  described above is different from the notion of Hilbert adjoint with respect to the inner products  $\langle | \rangle_r$  (of  $\mathcal{H}^r$ ) and  $\langle | \rangle_{r'}$  (of  $\mathcal{H}^{r'}$ ). Within the present manuscript Hilbert adjoints with respect to the products  $\langle | \rangle_r$  and  $\langle | \rangle_{r'}$  will *never* be considered.

iii) Let  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{+\infty}$  be a continuous operator (for some  $r \in \mathbb{R}$ ); due to the results of Proposition 2.20, we can generalize the Definition 2.21 of adjoint operator to include this case. In analogy to Definition 2.21, we say that the adjoint of  $\mathcal{B}$  is the unique continuous operator  $\mathcal{B}^* : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-r}$  fulfilling Eq. (2.116) for all  $f \in \mathcal{H}^{-\infty}$  and for all  $g \in \mathcal{H}^r$ ; of course, the expression in the right-hand side of the cited equation must be intended here in terms of the isomorphism  $\mathcal{I}^\infty : \mathcal{H}^{-\infty} \rightarrow (\mathcal{H}^{+\infty})'$  introduced in Eq. (2.114).<sup>(16)</sup>

The results on Banach adjoints already mentioned in Section 2.2 can be straightforwardly translated in the present framework; we enumerate them in the subsequent Lemma.

**Lemma 2.22.** Let  $r, r', r'' \in \mathbb{R}$ ; then, there hold the following results.

i) The adjoint map

$$* : \mathfrak{B}(\mathcal{H}^r, \mathcal{H}^{r'}) \rightarrow \mathfrak{B}(\mathcal{H}^{-r'}, \mathcal{H}^{-r}), \quad \mathcal{B} \mapsto \mathcal{B}^* \quad (2.117)$$

is an isometric anti-isomorphism<sup>(17)</sup>.

ii) Any continuous operator  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{r'}$  coincides with its double adjoint  $\mathcal{B}^{**} \equiv (\mathcal{B}^*)^* : \mathcal{H}^r \rightarrow \mathcal{H}^{r'}$ , that is

$$\mathcal{B}^{**} = \mathcal{B}. \quad (2.118)$$

<sup>16</sup>On the contrary, it is not so easy to extend the notion of adjoint operator to the case of a continuous operator  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{-\infty}$  ( $r \in \mathbb{R}$ ) within this context since, in general, there only holds the strict inclusion  $(\mathcal{H}^{-\infty})' \supset \mathcal{H}^{+\infty}$  (and not the equality).

<sup>17</sup>Recall that, for any pair of Banach spaces  $X$  and  $Y$ ,  $\mathfrak{B}(X, Y)$  indicates the Banach space of linear continuous operators from  $X$  to  $Y$ .

iii) Let  $\mathcal{B} : \mathcal{H}^r \rightarrow \mathcal{H}^{r'}$  and  $\mathcal{C} : \mathcal{H}^{r'} \rightarrow \mathcal{H}^{r''}$  be any pair of continuous operators and consider their composition  $\mathcal{CB} : \mathcal{H}^r \rightarrow \mathcal{H}^{r''}$ ; this is also a continuous operator and its adjoint  $(\mathcal{CB})^* : \mathcal{H}^{-r''} \rightarrow \mathcal{H}^{-r}$  fulfills

$$(\mathcal{CB})^* = \mathcal{B}^* \mathcal{C}^* . \quad (2.119)$$

*Proof.* All the statements in the present Lemma are obtained as trivial reformulations of well-known results on Banach adjoint operators in the framework under analysis.  $\square$

**Proposition 2.23.** Let  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  be any measurable function fulfilling the assumption (2.90) for some  $b \in \mathbb{R}$ ; for any pair  $r, r' \in \mathbb{R}$  with  $r' - r \geq -2b$ , consider the continuous extension  $\phi(\mathcal{A}) : \mathcal{H}^{r'} \rightarrow \mathcal{H}^r$  introduced in Proposition 2.12. Then, the corresponding adjoint operator  $\phi(\mathcal{A})^* : \mathcal{H}^{-r} \rightarrow \mathcal{H}^{-r'}$  is given by

$$\phi(\mathcal{A})^* = \overline{\phi}(\mathcal{A}) \quad (2.120)$$

( $\overline{\phi} : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  denotes the complex conjugate of the function  $\phi$ ; in the right-hand side of Eq. (2.120) we are considering the extension of  $\overline{\phi}(\mathcal{A})$  to a continuous map  $\mathcal{H}^{-r} \rightarrow \mathcal{H}^{-r'}$ , which exists since  $(-r) - (-r') = r' - r \geq -2b$ ).

*Remark 2.10.* In the case where  $\phi(\mathcal{A})$  maps  $\mathcal{H}^{-r}$  into  $\mathcal{H}^r$  continuously, for some given  $r \in \mathbb{R}$  with  $r \leq b$ , using the previous results with  $r' = -r$  we infer

$$\phi(\mathcal{A})^* = \overline{\phi}(\mathcal{A}) \in \mathfrak{B}(\mathcal{H}^{-r}, \mathcal{H}^r) . \quad (2.121)$$

In particular, if  $\phi$  is real-valued it follows that

$$\phi(\mathcal{A})^* = \phi(\mathcal{A}) ; \quad (2.122)$$

then, in analogy with the theory of operators on Hilbert spaces, we refer to  $\phi(\mathcal{A})$  as a *generalized self-adjoint operator*.

*Proof.* Consider the representations of  $\mathcal{H}$  and  $\mathcal{A}$  given in Eq.s (2.54-2.56); in particular, recall that the sesquilinear form  $\langle \cdot | \cdot \rangle : \mathcal{H}^{-r} \times \mathcal{H}^r \rightarrow \mathbb{C}$  (for all  $r \in \mathbb{R}$ ) can be expressed as in Eq. (2.105) and that  $\phi(\mathcal{A})$  coincides with the multiplication operator  $M_{\phi(w)} : \mathcal{H} \rightarrow \mathcal{H}$ ,  $f \mapsto M_{\phi(w)} f := \phi(w)f$  (which also defines a unique continuous extension  $\phi(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  according to the prescription (2.93)). Using the basic identity (2.116) for adjoint operators we infer, for all  $g \in \mathcal{H}^{-r}$  and all  $f \in \mathcal{H}^{r'}$ ,

$$\langle \phi(\mathcal{A})^* g | f \rangle = \langle g | \phi(\mathcal{A}) f \rangle = \int_K d\mu \bar{g}(\phi(w)f) = \int_K d\mu \overline{(\phi(w)g)} f = \langle \overline{\phi}(\mathcal{A}) g | f \rangle ;$$

due to the arbitrariness of  $f$  and  $g$ , the above chain of equalities implies the thesis.  $\square$

**Corollary 2.24.** *There hold the following results.*

i) Let  $r \in \mathbb{R}$ ,  $s \in \mathbb{C}$  and consider the continuous operator  $\mathcal{A}^{-s} : \mathcal{H}^r \rightarrow \mathcal{H}^{r+2\Re s}$ ; its adjoint is the continuous operator

$$(\mathcal{A}^{-s})^* = (\mathcal{A}^{-\bar{s}} \upharpoonright \mathcal{H}^{-(r+2\Re s)}) : \mathcal{H}^{-(r+2\Re s)} \rightarrow \mathcal{H}^{-r} . \quad (2.123)$$

ii) Let  $r \in \mathbb{R}$ ,  $\mathbf{t} \in \mathbb{C}$  with  $\Re \mathbf{t} > 0$  and consider the restriction of the continuous operator  $e^{-\mathbf{t}\mathcal{A}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{+\infty}$  to the space  $\mathcal{H}^r$ ; its adjoint is the continuous operator

$$(e^{-\mathbf{t}\mathcal{A}})^* = e^{-\bar{\mathbf{t}}\mathcal{A}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-r} . \quad (2.124)$$

If  $\Re \mathbf{t} = 0$ , so that  $\mathbf{t} = it$  for some  $t \in \mathbb{R}$ , the adjoint of the continuous operator  $e^{-it\mathcal{A}} : \mathcal{H}^r \rightarrow \mathcal{H}^r$  is

$$(e^{-it\mathcal{A}})^* = (e^{it\mathcal{A}} \upharpoonright \mathcal{H}^{-r}) : \mathcal{H}^{-r} \rightarrow \mathcal{H}^{-r} . \quad (2.125)$$

Analogous results hold for the exponential operators  $e^{-t\sqrt{\mathcal{A}}}$  and  $e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$ .

*Proof.* Both items i) and ii) follow straightforwardly from Proposition 2.23; in particular, for ii) recall the considerations in Remarks 2.10.  $\square$

## The case of a Hilbert space with conjugation

Let us now assume that the basic Hilbert space  $\mathcal{H}$  is endowed with a *conjugation*  $\mathcal{J} : \mathcal{H} \rightarrow \mathcal{H}$  (see Section 2.4 and, especially, the second paragraph therein); moreover, let us assume that the operator  $\mathcal{A}$  used in the previous subsections to construct the scale of spaces  $\mathcal{H}^r$  ( $r \in [-\infty, +\infty]$ ) is  $\mathcal{J}$ -real (so that  $\mathcal{A}$  and  $\mathcal{J}$  commute).

**Proposition 2.25.** *The map  $\mathcal{J} : \mathcal{H} \rightarrow \mathcal{H}$  has a unique continuous extension to the topological vector space  $\mathcal{H}^{-\infty}$ . This extension, denoted from now on with  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ , possesses the following properties:*

- i)  $\mathcal{J}$  is a conjugation on the topological vector space  $\mathcal{H}^{-\infty}$ ;
- ii)  $\mathcal{J}(\mathcal{H}^r) = \mathcal{H}^r$  for all  $r \in [-\infty, +\infty]$ ;
- iii) for all  $f \in \mathcal{H}^{-\infty}$  and  $g \in \mathcal{H}^{+\infty}$  one has

$$\langle \mathcal{J}f | \mathcal{J}g \rangle = \overline{\langle f | g \rangle} \quad (2.126)$$

or, equivalently,

$$\langle \mathcal{J}f | g \rangle = \overline{\langle f | \mathcal{J}g \rangle} \quad (2.127)$$

(where  $\langle | \rangle$  is the extension (2.103) of the inner product of  $\mathcal{H}$ );

iv) for each  $r \in \mathbb{R}$ ,  $\mathcal{J} \upharpoonright \mathcal{H}^r$  is a conjugation on the Hilbert space  $\mathcal{H}^r$ :

$$\langle \mathcal{J}f | \mathcal{J}g \rangle_r = \overline{\langle f | g \rangle_r} . \quad (2.128)$$

v) let  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  be a measurable function fulfilling the assumption (2.90) for some  $b \in \mathbb{R}$  and consider the continuous extension  $\phi(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  introduced in Proposition 2.12 and the analogous map  $\bar{\phi}(\mathcal{A}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ . Then, the relation

$$\mathcal{J}\phi(\mathcal{A})\mathcal{J}^{-1} = \bar{\phi}(\mathcal{A}) \quad (2.129)$$

holds in the space of operators from  $\mathcal{H}^{-\infty}$  to  $\mathcal{H}^{-\infty}$ .

*Proof.* The continuous extension of  $\mathcal{J}$  to  $\mathcal{H}^{-\infty}$ , if it exists, is unique due to the density of  $\mathcal{H}$  in  $\mathcal{H}^{-\infty}$ . In the sequel we prove that such a continuous extension exists and fulfills statements i)-v).

To this purpose, let us recall the formulation of the spectral theorem given in the second paragraph of Section 2.4 for a  $\mathcal{J}$ -real self-adjoint operator; due to this formulation, it suffices to prove existence and i)-v) when  $\mathcal{H} = L^2(K, \mu)$ ,  $\mathcal{A}$  is the multiplication operator by measurable function  $w : K \rightarrow [\varepsilon, +\infty)$  and  $\mathcal{J} : L^2(K, \mu) \rightarrow L^2(K, \mu)$  is the usual complex conjugation:  $\mathcal{J}f = \bar{f}$ . In this case, let us define

$$\mathcal{J}f := \bar{f} \quad \text{for all } f \in \mathcal{H}^{-\infty} \subset \text{Mis}(K) ; \quad (2.130)$$

then, one readily checks that  $\mathcal{J}$  maps  $\mathcal{H}^{-\infty}$  to  $\mathcal{H}^{-\infty}$  extending continuously the conjugation of  $\mathcal{H} = L^2(K, \mu)$ , and that all statements i)-v) hold.  $\square$

**Corollary 2.26.** *Consider the map  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  defined by Proposition 2.25 and the operators  $\mathcal{A}^{-s}, \mathcal{A}^{-\bar{s}}, e^{\mathbf{t}\mathcal{A}}, e^{-\bar{\mathbf{t}}\mathcal{A}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  for any  $s \in \mathbb{C}$ ,  $\mathbf{t} \in \mathbb{C}$  with  $\Re \mathbf{t} \geq 0$ ; then*

$$\mathcal{J}\mathcal{A}^{-s}\mathcal{J}^{-1} = \mathcal{A}^{-\bar{s}} , \quad (2.131)$$

$$\mathcal{J}e^{-\mathbf{t}\mathcal{A}}\mathcal{J}^{-1} = e^{-\bar{\mathbf{t}}\mathcal{A}} , \quad (2.132)$$

and analogous results hold for the exponential operators  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}, e^{-\bar{\mathbf{t}}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ .

*Proof.* Use item v) of the Proposition 2.25 with  $\phi(\lambda) := \lambda^{-s}$ ,  $\phi(\lambda) := e^{-\mathbf{t}\lambda}$  and so on.  $\square$

### Further results on the complex powers of $\mathcal{A}$ .

Let us keep all the assumptions and the notations of the previous subsections; in particular, we consider the (extensions of the) powers  $\mathcal{A}^{-s} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ , for  $s \in \mathbb{C}$ . Moreover, for any fixed  $r \in \mathbb{R}$ , let us define the strip

$$\Sigma_r := \{s \in \mathbb{C} \mid \Re s > r\} . \quad (2.133)$$

**Lemma 2.27.** *Let  $r_1, r_2 \in \mathbb{R}$ ; for all  $s \in \Sigma_{(r_1+r_2)/2}$ , the operator  $\mathcal{A}^{-s}$  maps continuously  $\mathcal{H}^{-r_1}$  into  $\mathcal{H}^{r_2}$ .*

*Proof.* Recall that, for any  $s \in \mathbb{C}$ ,  $\mathcal{A}^{-s}$  maps continuously  $\mathcal{H}^{-r_1}$  to  $\mathcal{H}^{-r_1+2\Re s}$  (see Corollary 2.13). Moreover, for any  $s \in \Sigma_{(r_1+r_2)/2}$ , we have  $-r_1 + 2\Re s > r_2$  so that  $\mathcal{H}^{-r_1+2\Re s} \hookrightarrow \mathcal{H}^{r_2}$ ; this suffices to infer the thesis.  $\square$

Let us recall once more that, for any  $r_1, r_2 \in \mathbb{R}$ ,  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  indicates the Banach space of continuous linear operators from  $\mathcal{H}^{-r_1}$  to  $\mathcal{H}^{r_2}$ , with the usual operator norm.

**Proposition 2.28.** *For any  $r_1, r_2 \in \mathbb{R}$ , the following function is holomorphic:*

$$\Sigma_{(r_1+r_2)/2} \rightarrow \mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2}) , \quad s \mapsto \mathcal{A}^{-s} \upharpoonright \mathcal{H}^{-r_1} . \quad (2.134)$$

*Proof.* Let us fix  $s_0 \in \Sigma_{(r_1+r_2)/2}$  arbitrarily. For any  $s \in \Sigma_{(r_1+r_2)/2}$ ,  $\mathcal{A}^{-s}$  can be represented as the multiplication operator by the function  $w^{-s} : K \rightarrow \mathbb{C}$ ; the latter can be re-expressed, in turn, as follows:

$$\begin{aligned} w^{-s} &= w^{-s_0} w^{-(s-s_0)} = w^{-s_0} e^{-(s-s_0) \ln w} = \\ &= w^{-s_0} \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} (-\ln w)^n = \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} w^{-s_0} (-\ln w)^n . \end{aligned}$$

Hereafter we will prove the following statements, yielding the thesis.

- i) For each  $n \in \mathbb{N}$ , the operator  $\mathcal{A}^{-s_0}(-\ln \mathcal{A})^n$  maps  $\mathcal{H}^{-r_1}$  into  $\mathcal{H}^{r_2}$ , and  $\mathcal{C}_n := \mathcal{A}^{-s_0}(-\ln \mathcal{A})^n \upharpoonright \mathcal{H}^{-r_1}$  is continuous from  $\mathcal{H}^{-r_1}$  to  $\mathcal{H}^{r_2}$ .
  - ii) The series  $\sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n$  is convergent in  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  for all  $s$  inside the disc  $D(s_0, \Re s_0 - (r_1+r_2)/2) \subset \Sigma_{(r_1+r_2)/2}$ .
  - iii) For all  $s \in D(s_0, \Re s_0 - (r_1+r_2)/2)$ , the sum of the series in item ii) equals  $\mathcal{A}^{-s} \upharpoonright \mathcal{H}^{-r_1}$ .
- These statements are proved in the following Steps 1, 2 and 3.

*Step 1 - Statement i) holds and, for each  $n \in \mathbb{N}$ , the operator  $\mathcal{C}_n$  has norm*

$$\|\mathcal{C}_n\|_{\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})} \leq \max \left( \varepsilon^{-(\Re s_0 - \frac{r_1+r_2}{2})} |\ln \varepsilon|^n , \left( \frac{n}{e} \right)^n \left( \Re s_0 - \frac{r_1+r_2}{2} \right)^{-n} \right) . \quad (2.135)$$

Let us fix  $n \in \mathbb{N}$ ; moreover, let  $f \in \mathcal{H}^{-r_1}$  so that  $w^{-r_1/2} f \in L^2(K, \mu)$ . Then

$$w^{r_2/2} [w^{-s_0}(-\ln w)^n] f = [w^{-(s_0 - \frac{r_1+r_2}{2})}(-\ln w)^n] w^{-r_1/2} f ,$$

so that we have  $w^{-s_0}(-\ln w)^n f \in \mathcal{H}^{r_2}$  if the function  $w^{-(s_0 - \frac{r_1+r_2}{2})}(-\ln w)^n$  is essentially bounded on  $K$ . To go on, recall that  $\Re s_0 - (r_1+r_2)/2 > 0$  (since  $s_0 \in \Sigma_{(r_1+r_2)/2}$ ) and that  $w(k) \geq \varepsilon$  for a.e.  $k \in K$ ; then, analyzing by elementary means the function  $F_n : [\varepsilon, +\infty) \rightarrow \mathbb{R}$ ,  $z \mapsto F_n(z) := z^{-(\Re s_0 - \frac{r_1+r_2}{2})} |\ln z|^n$ , we obtain

$$\begin{aligned} \operatorname{ess\,sup}_K \left| w^{-(s_0 - \frac{r_1+r_2}{2})}(-\ln w)^n \right| &\leq \sup_{z \in [\varepsilon, +\infty)} F_n(z) = \max \left( F_n(\varepsilon) , F_n(e^{n/(\Re s_0 - \frac{r_1+r_2}{2})}) \right) = \\ &= \max \left( \varepsilon^{-(\Re s_0 - \frac{r_1+r_2}{2})} |\ln \varepsilon|^n , \left( \frac{n}{e} \right)^n \left( \Re s_0 - \frac{r_1+r_2}{2} \right)^{-n} \right) < +\infty . \end{aligned}$$

Summing up, we have shown that  $\mathcal{A}^{-s_0}(-\ln \mathcal{A})^n f = w^{-s_0}(-\ln w)^n f \in \mathcal{H}^{r_2}$ , and that  $\mathcal{C}_n := \mathcal{A}^{-s_0}(-\ln \mathcal{A})^n \upharpoonright \mathcal{H}^{-r_1} : \mathcal{H}^{-r_1} \rightarrow \mathcal{H}^{r_2}$  fulfills

$$\|\mathcal{C}_n f\|_{r_2} \leq \max \left( \varepsilon^{-(\Re s_0 - \frac{r_1+r_2}{2})} |\ln \varepsilon|^n , \left( \frac{n}{e} \right)^n \left( \Re s_0 - \frac{r_1+r_2}{2} \right)^{-n} \right) \|f\|_{-r_1} ,$$

for all  $f \in \mathcal{H}^{-r_1}$ ; so,  $\mathcal{C}_n$  is continuous with norm fulfilling Eq. (2.135).

*Step 2 - Statement ii) holds.* The convergence radius of the series  $\sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n$  in the Banach space  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  is  $\rho \in [0, +\infty]$ , where

$$\frac{1}{\rho} := \limsup_{n \rightarrow +\infty} \left( \frac{1}{n!} \|\mathcal{C}_n\|_{\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})} \right)^{1/n} .$$

Let us show that  $\rho \geq \Re s_0 - (r_1 + r_2)/2$ ; in fact, due to Eq. (2.135) we have

$$\frac{1}{\rho} \leq \max \left( \lim_{n \rightarrow +\infty} \left( \frac{1}{n!} \varepsilon^{-(\Re s_0 - \frac{r_1 + r_2}{2})} |\ln \varepsilon|^n \right)^{1/n}, \lim_{n \rightarrow +\infty} \left( \frac{1}{n!} \left( \frac{n}{e} \right)^n \left( \Re s_0 - \frac{r_1 + r_2}{2} \right)^{-n} \right)^{1/n} \right) \\ = \frac{1}{\Re s_0 - \frac{r_1 + r_2}{2}}$$

(to compute the above limits, we have used the Stirling formula  $n! = (n/e)^n \sqrt{2\pi n} u_n$ , with  $u_n \rightarrow 1$  for  $n \rightarrow +\infty$ ).

*Step 3 - Proof of statement iii).* Let  $s \in D(s_0, \Re s_0 - (r_1 + r_2)/2)$ ; for all  $f \in \mathcal{H}^{-r_1}$ , the convergence of the series  $\sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n$  in the space  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  and the definition of  $\mathcal{C}_n$  imply the following

$$\left( \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n \right) f = \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n f = \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} w^{-s_0} (-\ln w)^n f,$$

and the last series converges in  $\mathcal{H}^{r_2}$ . On the other hand, it can be checked that the series  $\sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} w^{-s_0} (-\ln w)^n$  converges in  $L^\infty(K, \mu)$  to the function  $w^{-s}$ ; in conclusion,

$$\left( \sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n \right) f = w^{-s} f$$

for all  $f \in \mathcal{H}^{-r_1}$ , that is,  $\sum_{n=0}^{+\infty} \frac{(s-s_0)^n}{n!} \mathcal{C}_n = \mathcal{A}^{-s} \upharpoonright \mathcal{H}^{-r_1}$ .  $\square$

**Proposition 2.29.** *For any  $r_1, r_2 \in \mathbb{R}$ , the following maps are holomorphic:*

$$\Sigma_0 \rightarrow \mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2}), \quad \mathbf{t} \mapsto e^{-\mathbf{t}\mathcal{A}} \upharpoonright \mathcal{H}^{-r_1}, \quad e^{-\mathbf{t}\sqrt{\mathcal{A}}} \upharpoonright \mathcal{H}^{-r_1}, \quad (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}) \upharpoonright \mathcal{H}^{-r_1}. \quad (2.136)$$

*Proof.* We report the proof only for the map  $\mathbf{t} \mapsto e^{-\mathbf{t}\mathcal{A}}$ ; the derivation of same results for the other exponential functions is analogous. We move along the same lines as in the proof of the previous Proposition 2.28.

So, let  $r_1, r_2 \in \mathbb{R}$  and let us fix  $\mathbf{t}_0 \in \Sigma_0$ . Recall that, for all  $\mathbf{t} \in \Sigma_0$ ,  $e^{-\mathbf{t}\mathcal{A}}$  can be represented as the multiplication operator by the function  $e^{-\mathbf{t}w} : K \rightarrow \mathbb{C}$ ; the latter can be re-expressed, in turn, as

$$e^{-\mathbf{t}w} = e^{-\mathbf{t}_0 w} e^{-(\mathbf{t}-\mathbf{t}_0)w} = \\ = e^{-\mathbf{t}_0 w} \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} (-w)^n = \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} e^{-\mathbf{t}_0 w} (-w)^n.$$

Hereafter we will prove the following statements, yielding the thesis.

i) For each  $n \in \mathbb{N}$  and for any  $r_1, r_2 \in \mathbb{R}$ ,  $e^{-\mathbf{t}_0 \mathcal{A}} (-\mathcal{A})^n$  maps  $\mathcal{H}^{-r_1}$  into  $\mathcal{H}^{r_2}$  and  $\mathcal{C}_n := e^{-\mathbf{t}_0 \mathcal{A}} (-\mathcal{A})^n \upharpoonright \mathcal{H}^{-r_1}$  is continuous from  $\mathcal{H}^{-r_1}$  to  $\mathcal{H}^{r_2}$ .



ii) The series  $\sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n$  converges in  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  for all  $\mathbf{t}$  belonging to the disc  $D(\Re \mathbf{t}_0, \Re \mathbf{t}_0) \subset \Sigma_0$ .

iii) The sum of the series in item ii) equals  $e^{-\mathbf{t}\mathcal{A}} \upharpoonright \mathcal{H}^{-r_1}$ , for all  $\mathbf{t} \in D(\Re \mathbf{t}_0, \Re \mathbf{t}_0)$ .

These statements are proved in the following Steps 1, 2 and 3.

*Step 1 - Statement i) holds and, for each  $n \in \mathbb{N}$  and for any  $r_1, r_2 \in \mathbb{R}$ , the operator  $\mathcal{C}_n$  has norm*

$$\|\mathcal{C}_n\|_{\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})} \leq \max \left( \varepsilon^{n+\frac{r_1+r_2}{2}} e^{-\Re \mathbf{t}_0 \varepsilon}, \left( \frac{n+\frac{r_1+r_2}{2}}{e \Re \mathbf{t}_0} \right)^{n+\frac{r_1+r_2}{2}} \right). \quad (2.137)$$

Let us fix  $n \in \mathbb{N}$  and let  $f \in \mathcal{H}^{-r_1}$ , so that  $w^{-r_1/2} f \in L^2(K, \mu)$ ; then

$$w^{r_2/2} [e^{-\mathbf{t}_0 w} (-w^n)] f = \left[ e^{-\mathbf{t}_0 w} (-1)^n w^{n+\frac{r_1+r_2}{2}} \right] w^{-r_1/2} f.$$

Therefore, it suffices to show that the function  $e^{-\mathbf{t}_0 w} w^{n+\frac{r_1+r_2}{2}}$  is essentially bounded on  $K$  to infer that  $e^{-\mathbf{t}_0 w} (-w)^n f \in \mathcal{H}^{r_2}$ . To this purpose, let us first recall that  $\Re \mathbf{t}_0 > 0$  (since  $\mathbf{t}_0 \in \Sigma_0$ ) and that  $w(k) \geq \varepsilon$  for a.e.  $k \in K$ ; then, analyzing by elementary means the function  $F_n : [\varepsilon, +\infty) \rightarrow \mathbb{R}$ ,  $z \mapsto F_n(z) := e^{-\mathbf{t}_0 z} z^{n+\frac{r_1+r_2}{2}}$ , we obtain

$$\begin{aligned} \operatorname{ess\,sup}_K |e^{-\mathbf{t}_0 w} (-1)^n w^{n+\frac{r_1+r_2}{2}}| &\leq \sup_{z \in [\varepsilon, +\infty)} F_n(z) = \\ &= \max \left( F_n(\varepsilon), F_n \left( \frac{n+\frac{r_1+r_2}{2}}{2} \right) \right) = \max \left( e^{-\Re \mathbf{t}_0 \varepsilon} \varepsilon^{n+\frac{r_1+r_2}{2}}, \left( \frac{n+\frac{r_1+r_2}{2}}{e \Re \mathbf{t}_0} \right)^{n+\frac{r_1+r_2}{2}} \right) < +\infty. \end{aligned}$$

As stated above, this implies that  $e^{-\mathbf{t}_0 \mathcal{A}} (-\mathcal{A})^n f = e^{-\mathbf{t}_0 w} (-w)^n f \in \mathcal{H}^{r_2}$  which also ensures that the operator  $\mathcal{C}_n := e^{-\mathbf{t}_0 \mathcal{A}} (-\mathcal{A})^n \upharpoonright \mathcal{H}^{-r_1}$  maps  $\mathcal{H}^{-r_1}$  to  $\mathcal{H}^{r_2}$ . Moreover, the arguments employed also give

$$\|\mathcal{C}_n f\|_{r_2} \leq \max \left( e^{-\Re \mathbf{t}_0 \varepsilon} \varepsilon^{n+\frac{r_1+r_2}{2}}, \left( \frac{n+\frac{r_1+r_2}{2}}{e \Re \mathbf{t}_0} \right)^{n+\frac{r_1+r_2}{2}} \right) \|f\|_{-r_1},$$

for all  $f \in \mathcal{H}^{-r_1}$ ; so,  $\mathcal{C}_n$  is continuous with norm fulfilling Eq. (2.137).

*Step 2 - Statement ii) holds.* Indeed, the convergence radius of the series  $\sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n$  in the Banach space  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  is  $\rho \in [0, +\infty]$ , where

$$\frac{1}{\rho} := \limsup_{n \rightarrow +\infty} \left( \frac{1}{n!} \|\mathcal{C}_n\|_{\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})} \right)^{1/n}.$$

Next note that, due to Eq. (2.137), we have

$$\frac{1}{\rho} \leq \max \left( \lim_{n \rightarrow +\infty} \left( \frac{1}{n!} e^{-\Re \mathbf{t}_0 \varepsilon} \varepsilon^{n+\frac{r_1+r_2}{2}} \right)^{1/n}, \lim_{n \rightarrow +\infty} \left( \frac{1}{n!} \left( \frac{n+\frac{r_1+r_2}{2}}{e \Re \mathbf{t}_0} \right)^{n+\frac{r_1+r_2}{2}} \right)^{1/n} \right) = \frac{1}{\Re \mathbf{t}_0}$$

(the above limits have been computed using again the Stirling formula  $n! = (n/e)^n \sqrt{2\pi n} u_n$ , with  $u_n \rightarrow 1$  for  $n \rightarrow +\infty$ ); so,  $\rho \geq \Re \mathbf{t}_0$ .

*Step 3 - Proof of statement iii).* Let  $\mathbf{t} \in D(\mathfrak{R}\mathbf{t}_0, \mathfrak{R}\mathbf{t}_0)$ . For all  $f \in \mathcal{H}^{-r_1}$ , the convergence of the series  $\sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n$  in the space  $\mathfrak{B}(\mathcal{H}^{-r_1}, \mathcal{H}^{r_2})$  and the definition of  $\mathcal{C}_n$  imply the following

$$\left( \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n \right) f = \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n f = \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} e^{-\mathbf{t}_0 w} (-w)^n f ;$$

the last series converges in  $\mathcal{H}^{r_2}$ . On the other hand, it can be checked that the series  $\sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} e^{-\mathbf{t}_0 w} (-w)^n$  converges in  $L^\infty(K, \mu)$  to the function  $e^{-\mathbf{t}w}$ ; summing up, we have shown that

$$\left( \sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n \right) f = e^{-\mathbf{t}w} f$$

for all  $f \in \mathcal{H}^{-r_1}$ , that is,  $\sum_{n=0}^{+\infty} \frac{(\mathbf{t}-\mathbf{t}_0)^n}{n!} \mathcal{C}_n = e^{-\mathbf{t}\mathcal{A}} \upharpoonright \mathcal{H}^{-r_1}$ .  $\square$

**Proposition 2.30.** *For any  $r \in \mathbb{R}$  and for any  $n \in \mathbb{N}$ , the following maps are of class  $C^n$ :*

$$\begin{aligned} \mathbb{R} &\rightarrow \mathfrak{B}(\mathcal{H}^{r+2(n+1)}, \mathcal{H}^r), & t &\mapsto e^{-it\mathcal{A}} \upharpoonright \mathcal{H}^{r+2(n+1)}, \\ \mathbb{R} &\rightarrow \mathfrak{B}(\mathcal{H}^{r+n+1}, \mathcal{H}^r), & t &\mapsto e^{-it\sqrt{\mathcal{A}}} \upharpoonright \mathcal{H}^{r+n+1}, \\ \mathbb{R} &\rightarrow \mathfrak{B}(\mathcal{H}^{r+n}, \mathcal{H}^r), & t &\mapsto (e^{-it\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}) \upharpoonright \mathcal{H}^{r+n}. \end{aligned} \quad (2.138)$$

*Proof.* As an example, we consider the map  $t \mapsto e^{-it\mathcal{A}}$  and show the existence and continuity of its first derivative (arguments similar to those presented hereafter can be employed to discuss the higher order derivatives). Let us stress that, in view of the identity  $e^{-it\mathcal{A}} = e^{-it_0\mathcal{A}} e^{-i(t-t_0)\mathcal{A}}$  and of the fact that  $e^{-it_0\mathcal{A}}$  is an Hilbertian isomorphism on  $\mathcal{H}^r$  (for any  $t_0 \in \mathbb{R}$  and for any  $r \in \mathbb{R}$ ), it suffices to discuss the differentiability in  $t = 0$ . Therefore, to infer the existence of  $\frac{d}{dt} e^{-it\mathcal{A}}$ , it suffices to show that

$$\frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} \rightarrow 0 \quad \text{in } \mathfrak{B}(\mathcal{H}^{r+4}, \mathcal{H}^r) \text{ for } t \rightarrow 0. \quad (2.139)$$

Notice that, by definition, there holds

$$\left\| \frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} \right\|_{\mathfrak{B}(\mathcal{H}^{r+4}, \mathcal{H}^r)} = \sup_{f \in \mathcal{H}^{r+4}} \frac{\| \frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} f \|_r}{\|f\|_{r+4}} ;$$

moreover, using representations of  $\mathcal{H}$  and  $\mathcal{A}$  as in Eq.s (2.54-2.56), for any  $f \in \mathcal{H}^{r+2(n+1)}$  we have

$$\begin{aligned} \left\| \frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} f \right\|_r^2 &= \int_K d\mu w^r \left| \frac{e^{-itw} - 1 + iw t}{t} f \right|^2 = \\ &= \int_K d\mu w^r \frac{2}{t^2} \left( 1 - \cos(wt) - tw \sin(wt) + \frac{1}{2} w^2 t^2 \right) |f|^2. \end{aligned}$$

On the other hand, it can be proved by elementary means that  $\frac{2}{t^2}(1 - \cos(wt) - tw \sin(wt) + \frac{1}{2}w^2t^2) \leq \frac{1}{4}w^4t^2$  for  $|t|$  small enough; this allows to infer

$$\left\| \frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} f \right\|_r^2 \leq \frac{t^2}{4} \int_K d\mu w^{r+4} |f|^2 = \frac{t^2}{4} \|f\|_{r+4}^2 .$$

Summing up, the above considerations imply

$$\left\| \frac{e^{-it\mathcal{A}} - 1 + it\mathcal{A}}{t} \right\|_{\mathfrak{B}(\mathcal{H}^{r+4}, \mathcal{H}^r)} \leq \frac{1}{2} |t| ,$$

which, in view of Eq. (2.139), proves the existence of the map  $\mathbb{R} \rightarrow \mathfrak{B}(\mathcal{H}^{r+4}, \mathcal{H}^r)$ ,  $t \mapsto \frac{d}{dt} e^{-it\mathcal{A}} = -i\mathcal{A} e^{-it\mathcal{A}}$ . The latter can also be shown to be continuous by arguments analogous to those employed above, thus yielding the thesis.  $\square$

Before moving on, let us prove the following proposition, relating the complex powers  $\mathcal{A}^{-s}$  ( $s \in \mathbb{C}$ ) to the Mellin transforms of the exponential operators  $e^{-t\mathcal{A}}, e^{-t\sqrt{\mathcal{A}}}, e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$ .

**Proposition 2.31.** *Let  $\mathbf{t} \in (0, +\infty)$  and consider the operators  $e^{-t\mathcal{A}}, e^{-t\sqrt{\mathcal{A}}}, e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{+\infty}$  defined in Corollary 2.14; besides, let  $r_1, r_2 \in \mathbb{R}$  be such that  $r_1 + r_2 > 0$ . Then, for all  $f \in \mathcal{H}^{-r_1}$  and all  $s \in \Sigma_{(r_1+r_2)/2}$  the following relations hold in  $\mathcal{H}^{r_2}$ :*

$$\mathcal{A}^{-s} f = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \mathbf{t}^{s-1} e^{-t\mathcal{A}} f , \quad (2.140)$$

$$\mathcal{A}^{-s} f = \frac{1}{\Gamma(2s)} \int_0^{+\infty} dt \mathbf{t}^{2s-1} e^{-t\sqrt{\mathcal{A}}} f , \quad (2.141)$$

$$\mathcal{A}^{-s} f = \frac{1}{\Gamma(2s-1)} \int_0^{+\infty} dt \mathbf{t}^{2s-2} (e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}) f . \quad (2.142)$$

In the above, all integrals are intended in the Gelfand-Pettis sense and involve functions from  $(0, +\infty)$  to  $\mathcal{H}^{r_2}$  (in fact, according to Corollary 2.14,  $e^{-t\mathcal{A}}f, e^{-t\sqrt{\mathcal{A}}}f, (e^{-t\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})f \in \mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^{r_2}$ ).

*Proof.* We report the proof only for the operator  $e^{-t\mathcal{A}}$  (the proof for the other operators is analogous). Fix  $r_1, r_2 \in \mathbb{R}$  with  $r_1 + r_2 > 0$ ; for any  $s \in \Sigma_{(r_1+r_2)/2}$  and any  $f \in \mathcal{H}^{-r_1}$ , one has  $\mathcal{A}^{-s} f \in \mathcal{H}^{2\Re s - r_1} \hookrightarrow \mathcal{H}^{r_2}$  (see Corollary 2.13). Next, recall that all linear forms on  $\mathcal{H}^{r_2}$  have the form  $\langle g | \cdot \rangle$ , for some  $g \in \mathcal{H}^{-r_2}$  (with  $\langle | \cdot \rangle$  denoting the extended inner product of Proposition 2.16). Then, by the definition of the Gelfand-Pettis integral, proving Eq. (2.140) amounts to showing the following: for any  $g \in \mathcal{H}^{-r_2}$ , the function  $\mathbf{t} \mapsto \mathbf{t}^{s-1} \langle g | e^{-t\mathcal{A}} f \rangle$  is integrable and

$$\langle g | \mathcal{A}^{-s} f \rangle = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \mathbf{t}^{s-1} \langle g | e^{-t\mathcal{A}} f \rangle . \quad (2.143)$$

Now, consider the representation (2.54-2.56) for  $\mathcal{H}$  and  $\mathcal{A}$ ; then,  $\mathcal{A}^{-s}$  and  $e^{-\mathbf{t}\mathcal{A}}$  correspond to the multiplication operators by the functions  $w^{-s} : K \rightarrow \mathbb{C}$  and  $e^{-\mathbf{t}w} : K \rightarrow \mathbb{R}$ , respectively. So, Eq. (2.143) (to be proved) can be rephrased as

$$\int_K d\mu w^{-s} \bar{g} f = \frac{1}{\Gamma(s)} \int_0^{+\infty} d\mathbf{t} \mathbf{t}^{s-1} \int_K d\mu e^{-\mathbf{t}w} \bar{g} f. \quad (2.144)$$

Indeed, recall that  $w(k) \in [\varepsilon, +\infty)$  for a.e.  $k \in K$  and that  $\Re s > 0$ , since  $s \in \Sigma_{(r_1+r_2)/2}$  and  $r_1+r_2 > 0$ ; in consequence of this, we have (see [122], page 139, Eq. 5.9.1)  $w(k)^{-s} = \frac{1}{\Gamma(s)} \int_0^{+\infty} d\mathbf{t} \mathbf{t}^{s-1} e^{-\mathbf{t}w(k)}$  for a.e.  $k \in K$ . Therefore Eq. (2.144) is, in turn, equivalent to

$$\frac{1}{\Gamma(s)} \int_K d\mu \left( \int_0^{+\infty} d\mathbf{t} \mathbf{t}^{s-1} e^{-\mathbf{t}w} \right) \bar{g} f = \frac{1}{\Gamma(s)} \int_0^{+\infty} d\mathbf{t} \mathbf{t}^{s-1} \left( \int_K d\mu e^{-\mathbf{t}w} \bar{g} f \right).$$

Summing up, the thesis follows if we can show that the order of integration on  $K$  and  $(0, +\infty)$  can be interchanged; this statement is ensured by the Fubini-Tonelli theorem [134] if

$$I := \int_{(0,+\infty) \times K} d\mathbf{t} \otimes d\mu \left| \mathbf{t}^{s-1} e^{-\mathbf{t}w} \bar{g} f \right| < +\infty. \quad (2.145)$$

To prove Eq. (2.145), first re-express the integral therein as

$$I = \int_{(0,+\infty) \times K} d\mathbf{t} \otimes d\mu \mathbf{t}^{\Re s-1} (e^{-\mathbf{t}w} w^{\frac{r_1+r_2}{2}}) |w^{-r_2/2} g| |w^{-r_1/2} f|.$$

Then, consider the function  $F : (0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto F(\mathbf{t}) := \sup_{w \in [\varepsilon, +\infty)} |w^{\frac{r_1+r_2}{2}} e^{-\mathbf{t}w}|$ ; by elementary methods, we obtain

$$F(\mathbf{t}) = \left( \frac{r_1+r_2}{2e\mathbf{t}} \right)^{\frac{r_1+r_2}{2}} \chi_{(0, (r_1+r_2)/(2\varepsilon)]}(\mathbf{t}) + \left( \varepsilon^{\frac{r_1+r_2}{2}} e^{-\varepsilon\mathbf{t}} \right) \chi_{((r_1+r_2)/(2\varepsilon), +\infty)}(\mathbf{t})$$

(where  $\chi$  denotes the indicator function; see the footnote 11 of page 29). It follows that

$$I \leq \left( \int_0^{+\infty} d\mathbf{t} \mathbf{t}^{\Re s-1} F(\mathbf{t}) \right) \left( \int_K d\mu |w^{-r_2/2} g| |w^{-r_1/2} f| \right). \quad (2.146)$$

On the one hand, due to Hölder's inequality we have  $\int_K d\mu |w^{-r_2/2} g| |w^{-r_1/2} f| \leq \|g\|_{-r_2} \|f\|_{-r_1}$ , so that the second integral in Eq. (2.146) is finite. On the other hand, concerning the first integral in the same equation, we have

$$\int_0^{+\infty} d\mathbf{t} \mathbf{t}^{\Re s-1} F(\mathbf{t}) = \left( \frac{r_1+r_2}{2e} \right)^{\frac{r_1+r_2}{2}} \int_0^{\frac{r_1+r_2}{2\varepsilon}} d\mathbf{t} \mathbf{t}^{\Re s - \frac{r_1+r_2}{2} - 1} + \varepsilon^{\frac{r_1+r_2}{2}} \int_{\frac{r_1+r_2}{2\varepsilon}}^{+\infty} d\mathbf{t} \mathbf{t}^{\Re s-1} e^{-\mathbf{t}\varepsilon};$$

both the integrals on the right-hand side are finite since  $s \in \Sigma_{(r_1+r_2)/2}$  and  $\varepsilon > 0$ . Summing up, Eq. (2.146) proves Eq. (2.145), thus yielding the thesis.  $\square$

## 2.6 Schrödinger-type operators: regularity and self-adjointness.

So far, we have been considering an abstract framework where  $\mathcal{A}$  was some self-adjoint operator acting on a given Hilbert space  $\mathcal{H}$ . In this section we analyze more in detail the case where the basic Hilbert space is  $\mathcal{H} = L^2(\Omega)$ , with  $\Omega \subset \mathbb{R}^d$  a suitable domain, and  $\mathcal{A}$  is determined by some differential operator on it.

### Regularity results for elliptic differential operators.

#### Local results.

Let us first assume that  $\Omega$  is an arbitrary domain in  $\mathbb{R}^d$  and let us choose a “potential”

$$V \in C^\infty(\Omega, \mathbb{R}) ; \quad (2.147)$$

we will make more specific hypotheses on  $\Omega$  and  $V$  when necessary. Moreover, let us consider the second-order, proper (see [38, 107, 156]) elliptic differential operator of Schrödinger type

$$A := -\Delta + V : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega) \quad (2.148)$$

(recall that  $\Delta$  stands for the  $d$ -dimensional Laplacian, i.e.,  $\Delta := \sum_{i=1}^d \partial_{x^i x^i}$ ). For any  $n \in \mathbb{N}$  and any  $r \in \mathbb{R}$ , it is easily checked that

$$A^n H_{\text{loc}}^{r+2n}(\Omega) \subset H_{\text{loc}}^r(\Omega) \quad (2.149)$$

and that  $A^n \upharpoonright H_{\text{loc}}^{r+2n}(\Omega)$  maps continuously  $H_{\text{loc}}^{r+2n}(\Omega)$  into  $H_{\text{loc}}^r(\Omega)$  (see [38], page 98, Proposition 2.13). Furthermore, the standard theory of local regularity for elliptic differential operators allows to derive the following result.

**Theorem 2.32.** *For  $n \in \mathbb{N}$ , the following statements hold.*

*i) One has*

$$H_{\text{loc}}^{2n}(\Omega) = \{f \in \mathcal{D}'(\Omega) \mid A^m f \in L_{\text{loc}}^2(\Omega) \text{ for } m = 0, \dots, n\} . \quad (2.150)$$

*ii) Consider the standard topology of  $H_{\text{loc}}^{2n}(\Omega)$ , based on the family of seminorms  $f \mapsto \|\varphi f\|_{H^{2n}}$  ( $\varphi \in \mathcal{D}(\Omega)$ ). This coincides with the topology induced by the family of seminorms*

$$f \mapsto \|\varphi A^m f\|_{L^2} \quad (\varphi \in \mathcal{D}(\Omega), m \in \{0, \dots, n\}) . \quad (2.151)$$

*Proof.* We give the proof of the statements i) and ii) in several steps.

*Step 1 - Proof of i).* Let us provisionally denote with  $\mathcal{H}^{2n}(\Omega)$  the right-hand side of Eq. (2.150); it is evident that  $H_{\text{loc}}^{2n}(\Omega) \subset \mathcal{H}^{2n}(\Omega)$ . The proof of the reverse inclusion relies on the following well-known result:

$$m \in \mathbb{N}, r \in \mathbb{R}, f \in \mathcal{D}'(\Omega), A^m f \in H_{\text{loc}}^r(\Omega) \quad \Rightarrow \quad f \in H_{\text{loc}}^{r+2m}(\Omega) \quad (2.152)$$

(see, e.g., [141] and Theorem 3.2 of [97]). Now, let  $f \in \mathcal{H}^{2n}(\Omega)$ ; the condition in Eq. (2.150) with  $m = n$  reads  $A^n f \in L^2_{\text{loc}}(\Omega) \equiv H^0_{\text{loc}}(\Omega)$  and this implies  $f \in H^{2n}_{\text{loc}}(\Omega)$ .

*Step 2 - An inequality.* For any  $\ell \in \mathbb{Z}$  and any compact subset  $K \subset \Omega$ , let us define the set  $H^\ell_K(\Omega) := \{f \in H^\ell(\Omega) \mid \text{supp } f \subset K\}$ ; then  $AH^{\ell+2}_K(\Omega) \subset H^\ell_K(\Omega)$ . Since  $A$  is a proper elliptic operator of degree 2 in the sense of [38] (see also [107, 156]), for each  $\ell \in \mathbb{Z}$  and each compact subset  $K \subset \Omega$  there exists a constant  $C_{\ell,K} > 0$  such that

$$\|f\|_{H^{\ell+2}} \leq C_{\ell,K} (\|Af\|_{H^\ell} + \|f\|_{L^2}) \quad \text{for all } f \in H^{\ell+2}_K(\Omega) \quad (2.153)$$

(see [38], Theorem 8.11; the inequality written above follows from Eq. (8.11.3) therein, setting  $m = 2$  and  $t = 0$  <sup>(18)</sup>).

*Step 3 - Another inequality.* Let  $\ell \in \mathbb{Z}$ ,  $\varphi \in \mathcal{D}(\Omega)$ . We claim there is a constant  $C_{\ell,\varphi}$  such that, for all  $f \in H^{\ell+2}_{\text{loc}}(\Omega)$ ,

$$\|\varphi f\|_{H^{\ell+2}} \leq C_{\ell,\varphi} \left( \|\varphi(Af)\|_{H^\ell} + \sum_{i=1}^d \|(\partial_{x^i}\varphi)f\|_{H^{\ell+1}} + \|(\Delta\varphi)f\|_{H^\ell} + \|\varphi f\|_{L^2} \right). \quad (2.154)$$

Indeed, let  $\ell, \varphi$  be as above, and set  $K := \text{supp } \varphi$ ; in the sequel, “const.” indicates a positive constant, depending only on  $\ell$  and  $\varphi$ . Let  $f \in H^{\ell+2}_{\text{loc}}(\Omega)$ ; then  $\varphi f \in H^{\ell+2}_K(\Omega)$  and the inequality in Eq. (2.153) for this function gives

$$\|\varphi f\|_{H^{\ell+2}} \leq \text{const.} (\|A(\varphi f)\|_{H^\ell} + \|\varphi f\|_{L^2}). \quad (2.155)$$

On the other hand  $A(\varphi f) = \varphi(Af) - 2 \sum_{i=1}^d \partial_{x^i} [(\partial_{x^i}\varphi)f] + (\Delta\varphi)f$ , which allows to infer

$$\|A(\varphi f)\|_{H^\ell} \leq \|\varphi(Af)\|_{H^\ell} + \text{const.} \sum_{i=1}^d \|(\partial_{x^i}\varphi)f\|_{H^{\ell+1}} + \|(\Delta\varphi)f\|_{H^\ell}. \quad (2.156)$$

Moreover, recall that  $\varphi$  is smooth and has compact support. These facts and the inequalities in Eq.s (2.155) (2.156) yield the thesis (2.154).

*Step 4 - Proof of ii).* Let us show that each of the topologies based respectively on the family of seminorms  $f \mapsto \|\varphi A^m f\|_{L^2}$  and  $f \mapsto \|\varphi f\|_{H^{2n}}$  ( $\varphi \in \mathcal{D}(\Omega)$ ) is finer than the other. To this purpose we will prove that, for all  $\varphi \in \mathcal{D}(\Omega)$  and for all  $n \in \mathbb{N}$ , there exist two constants  $C_{n,\varphi}, C'_{n,\varphi} > 0$  and two finite sets  $I_n, I'_{n,\varphi}$  such that

$$\|\varphi f\|_{H^{2n}} \leq C_{n,\varphi} \sum_{(m,\alpha) \in I_n} \|(\partial^\alpha \varphi) A^m f\|_{L^2}, \quad (2.157)$$

---

<sup>18</sup>As a matter of fact, the cited Eq. (8.11.3) of [38] is stated for functions in  $C^\infty(\Omega)$  with support in a given compact subset, but can be readily extended to functions in  $H^{\ell+2}_K(\Omega)$  by elementary density arguments.

$$\|\varphi A^n f\|_{L^2} \leq C'_{n,\varphi} \sum_{\psi \in I'_{n,\varphi}} \|\psi f\|_{H^{2n}} . \quad (2.158)$$

The set  $I_n$  appearing above has elements of the form  $(m, \alpha)$ , where  $m \in \{0, \dots, n\}$  and  $\alpha$  a multi-index with  $|\alpha| \leq 2n$ ; on the contrary,  $I'_{n,\varphi}$  is a subset of  $\mathcal{D}(\Omega)$ .

Let us begin proving Eq. (2.157). By Eq. (2.154) in Step 3 of the present proof (here employed with  $\ell = 2(n-1)$ ), for all  $f \in H_{\text{loc}}^{2n}(\Omega)$  one has

$$\|\varphi f\|_{H^{2n}} \leq C_{2(n-1),\varphi} \left( \|\varphi(Af)\|_{H^{2(n-1)}} + \sum_{i=1}^d \|(\partial_{x^i}\varphi)f\|_{H^{2n-1}} + \|(\Delta\varphi)f\|_{H^{2(n-1)}} + \|\varphi f\|_{L^2} \right) ;$$

note that all the terms on the right-hand side of this inequality are of the form  $\|(\partial^\alpha\varphi)v\|_{H^k}$  for some multi-index  $\alpha$  of order  $|\alpha| \leq 2$  and some  $v \in H_{\text{loc}}^k(\Omega)$  ( $k \in \mathbb{N}$ ,  $k < 2n$ ). Each of these terms can be estimated in the same way, employing once more Eq. (2.154) (with  $\varphi$  replaced by  $\partial^\alpha\varphi$ ). This procedure can be iterated  $n$  times, until only norms of order 0 or less are left on the right-hand side; clearly, each term remaining is of the form  $\|(\partial^\alpha\varphi)A^m f\|_{H^k}$  for some  $m \in \{0, \dots, n\}$ ,  $k \in \{-1, 0\}$  and  $\alpha$  a multi-index with  $|\alpha| \leq 2n$ . Then, the inequality (2.157) follows since  $\|v\|_{H^{-1}} \leq \text{const.} \|v\|_{H^0} = \text{const.} \|v\|_{L^2}$  for all  $v \in L^2(\Omega)$  with compact support<sup>19</sup>.

Let us now pass to justify Eq. (2.158); indeed, this inequality is a just a reformulation of an already mentioned fact, i.e., the continuity of the differential operator  $(A^n \upharpoonright H_{\text{loc}}^{2n}(\Omega)) : H_{\text{loc}}^{2n}(\Omega) \rightarrow L^2_{\text{loc}}(\Omega)$  (let us recall again reference [38]).  $\square$

### Global results.

Making stricter assumptions on the domain  $\Omega$ , on its boundary  $\partial\Omega$  and on the regularity of the potential  $V$  defining the elliptic operator  $A$  of Eq. (2.148), one can infer stronger versions of Theorem 2.32 which allow to deal with the behaviour of the functions under analysis up to the boundary of  $\Omega$ .

For example, from here to the end of this paragraph, let us consider the case where

$$\begin{aligned} \Omega \subset \mathbb{R}^d \text{ is a bounded domain with compact boundary } \partial\Omega \text{ of class } C^\infty \\ \text{and } V : \Omega \rightarrow \mathbb{R} \text{ has a } C^\infty \text{ extension } V : \bar{\Omega} = \Omega \cup \partial\Omega \rightarrow \mathbb{R} ; \end{aligned} \quad (2.159)$$

these hypotheses suffice to infer the continuity of the differential operator  $(A^n \upharpoonright H^{\ell+2n}(\Omega)) : H^{\ell+2n}(\Omega) \rightarrow H^\ell(\Omega)$  for any  $n \in \mathbb{N}$  and any  $\ell \in \mathbb{Z}$  (compare with Eq. (2.149)).

In this situation, it is natural to consider the behaviour of functions on the boundary of  $\Omega$ . As well known (see, e.g., [109]) there is a linear, continuous operation of *trace*

$$H^1(\Omega) \rightarrow L^2(\partial\Omega) , \quad f \mapsto f \upharpoonright \partial\Omega \quad (2.160)$$

<sup>19</sup>See [97], Chapter 2, Section 3, pages 121–122.

that coincides with the usual operation of restriction to  $\partial\Omega$  on any function  $f \in C^1(\overline{\Omega})$ ; moreover the space  $H_0^1(\Omega)$  (defined, we recall it, as the closure of  $\mathcal{D}(\Omega)$  in  $H^1(\Omega)$ ) admits in the present case the representation

$$H_0^1(\Omega) = \{f \in H^1(\Omega) \mid f \upharpoonright \partial\Omega = 0\} . \quad (2.161)$$

The prescription  $f \upharpoonright \partial\Omega = 0$  is a *Dirichlet boundary condition*; in the sequel we will be especially interested in analysing the differential operator  $A$  (and its powers) with these boundary conditions, indicated by the symbol  $\mathfrak{D}$ . In view of this, following [109] (see pages 228–229), we introduce the following space:

**Definition 2.33.** For  $n \in \mathbb{N}$  we put

$$H_{\mathfrak{D}}^{2n}(\Omega) := \{f \in H^{2n}(\Omega) \mid (A^m f) \upharpoonright \partial\Omega = 0 \text{ for } m = 0, \dots, n-1\} . \quad (2.162)$$

*Remark 2.11.* If  $f \in H^{2n}(\Omega)$  and  $m \in \{0, \dots, n-1\}$ , then  $A^m f \in H^{2n-2m}(\Omega) \subset H^1(\Omega)$ , so it makes sense to speak of the trace  $(A^m f) \upharpoonright \partial\Omega$ . Elementary considerations related to the linearity and continuity of the operators  $A^m, \upharpoonright \partial\Omega$  ensure that  $H_{\mathfrak{D}}^{2n}(\Omega)$  is a closed linear subspace of  $H^{2n}(\Omega)$  and, in particular, it is itself a Banach space with the norm  $\|\cdot\|_{H^{2n}}$ ; furthermore, it appears that  $\mathcal{D}(\Omega)$  and, consequently, its closure  $H_0^{2n}(\Omega)$  are linear subspaces of  $H_{\mathfrak{D}}^{2n}(\Omega)$ .

In analogy to Theorem 2.32, one can infer the forthcoming result.

**Theorem 2.34.** For  $n \in \mathbb{N}$ , the following statements hold.

i) One has

$$H_{\mathfrak{D}}^{2n}(\Omega) = \left\{ f \in \mathcal{D}'(\Omega) \mid \begin{array}{l} A^n f \in L^2(\Omega) \text{ and} \\ A^m f \in H_0^1(\Omega) \text{ for } m = 0, \dots, n-1 \end{array} \right\} . \quad (2.163)$$

ii) The standard topology of  $H_{\mathfrak{D}}^{2n}(\Omega)$ , inherited from  $H^{2n}(\Omega)$ , coincides with the topology induced by the norm

$$f \mapsto \sum_{m=0}^n \|A^m f\|_{L^2} . \quad (2.164)$$

*Proof.* The thesis can be proved moving along the same lines as in the proof of Theorem 2.32; hereafter we only point out the main steps.

The essential argument is the following, well-known result of regularity (see [62] page 323, Theorem 5):

$$\begin{aligned} k \in \mathbb{N}, \quad g \in H_0^1(\Omega), \quad Ag \in H^k(\Omega) &\Rightarrow \\ g \in H^{k+2}(\Omega) \quad \text{and} \quad \|g\|_{H^{k+2}} \leq \text{const.} (\|Ag\|_{H^k} + \|g\|_{L^2}) . & \end{aligned} \quad (2.165)$$

In order to show statement i), let us temporarily indicate with  $\mathcal{H}_{\mathfrak{D}}^{2n}(\Omega)$  the space in the right-hand side of Eq. (2.163); of course,  $H_{\mathfrak{D}}^{2n}(\Omega) \subset \mathcal{H}_{\mathfrak{D}}^{2n}(\Omega)$ . On the other hand, for any  $f \in \mathcal{H}_{\mathfrak{D}}^{2n}(\Omega)$ , we have  $A(A^{n-1}f) = A^n f \in L^2(\Omega)$  and  $A^{n-1}f \in H_0^1(\Omega)$ ; by (2.165) with



$g = A^{n-1}f$  and  $k = 0$ , this implies that  $A^{n-1}f \in H^2(\Omega)$ . Iterating these arguments one obtains  $A^{n-\ell}f \in H^{2\ell}(\Omega)$  for  $\ell = 0, \dots, n$  and, in particular,  $f \in H^{2n}(\Omega)$ , which proves the inclusion  $\mathcal{H}_{\mathcal{D}}^{2n}(\Omega) \subset H_{\mathcal{D}}^{2n}(\Omega)$ .

Next, since  $\Omega$  is bounded and the potential  $V$  is smooth up to the boundary (whence, bounded along with its derivatives), it can be easily checked that there exists a positive constant “const.” such that, for all  $f \in H_{\mathcal{D}}^{2n}(\Omega)$ ,

$$\sum_{m=0}^n \|A^m f\|_{L^2} \leq \text{const.} \|f\|_{H^{2n}} ; \quad (2.166)$$

on the other hand for  $f \in H_{\mathcal{D}}^{2n}(\Omega)$ , repeated use of the inequality in (2.165) gives  $\|f\|_{H^{2n}} \leq \text{const.} (\|Af\|_{H^{2n-2}} + \|f\|_{L^2}) \leq \text{const.} (\|A^2f\|_{H^{2n-4}} + \|Af\|_{L^2} + \|f\|_{L^2})$  and, more generally,  $\|f\|_{H^{2n}} \leq \text{const.} (\|A^\ell f\|_{H^{2n-2\ell}} + \sum_{m=0}^{\ell} \|A^m f\|_{L^2})$  for  $\ell = 0, \dots, n$ ; in particular, with  $\ell = n$  we have

$$\|f\|_{H^{2n}} \leq \text{const.} \sum_{m=0}^n \|A^m f\|_{L^2} . \quad (2.167)$$

Summing up, Eq.s (2.166) (2.167) prove statement ii).  $\square$

### Some possible generalizations.

Results analogous to those discussed in the previous Theorems 2.32 and 2.34 can be derived under more general hypotheses for the differential operator  $A$ , for the domain  $\Omega$  and for the boundary conditions on  $\partial\Omega$ . The proofs of these results closely resemble those of the cited theorems, and do in fact rely on essentially the same arguments; for this reason, these proofs will not be reported in this manuscript. We will limit ourself to simply mention some variations of Theorems 2.32, 2.34 and to hint at some of their possible, further generalizations. Let us notice that, as a matter of fact, some of these generalizations are not of direct interest for the physical applications to be considered in Chapter 3 of this work. Nevertheless, they are likely to have an interest of their own and in connection with other topics, which are not dealt with in the present manuscript; for these reasons we report them here anyway for completeness.

First of all, let us stress that if  $A$  is any second order, formally self-adjoint, proper elliptic differential operator <sup>(20)</sup>

$$A := \sum_{|\alpha| \leq 2} a_\alpha \partial^\alpha : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega) \quad (2.168)$$

---

<sup>20</sup>Formal self-adjointness of the operator  $A$  in (2.168) means that  $A$  coincides with its *Lagrange adjoint* [39]

$$A^\dagger := \sum_{|\alpha| \leq 2} (-\partial)^\alpha \bar{a}_\alpha : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega) .$$

We refer again to [38, 107, 156] for the definition of proper differential operator.

for some smooth coefficients  $a_\alpha : \Omega \rightarrow \mathbb{C}$  ( $\alpha \in \mathbb{N}^d$ ,  $|\alpha| \leq 2$ ), then the results of Theorem 2.32 continue to hold, understanding  $A$  to be as in Eq. (2.168); similarly, if the domain  $\Omega$  and its boundary are as in Eq. (2.159), assuming that  $a_\alpha \in C^\infty(\bar{\Omega})$  and that Dirichlet boundary conditions are prescribed on  $\partial\Omega$  one can infer statements analogous to those of Theorem 2.34 <sup>(21)</sup>.

Next, let us note that one could make weaker assumptions on the regularity of the boundary  $\partial\Omega$  and of the coefficients defining the differential operator  $A$ . For example, let us consider the case where  $A$  is as in Eq. (2.168) with  $a_\alpha \in C^{2j}(\Omega)$  for some  $j \in \mathbb{N}$ ; then, Theorem 2.32 continues to hold for all  $n \in \mathbb{N}$  with  $n \leq j$ . On the other hand, Theorem 2.34 is still valid for the same values of  $n$ , if  $\Omega$  is bounded with boundary  $\partial\Omega$  of class  $C^{2j+2}$  and if  $a_\alpha \in C^{2j}(\bar{\Omega})$  ( $|\alpha| \leq 2$ ).

Finally, let us draw the attention to the fact that boundary conditions different from those of Dirichlet type could be taken into account, as well. To this purpose, let us consider the case described in Eq. (2.159), where  $\Omega$  is bounded with boundary of class  $C^\infty$  and  $A = -\Delta + V$  with  $V \in C^\infty(\bar{\Omega})$ ; hereafter we briefly analyze as examples the cases where either *Neumann* or *Robin boundary conditions* (respectively indicated with the symbols  $\mathfrak{N}$  and  $\mathfrak{R}$ ) are imposed on  $\partial\Omega$ . Following the Definition 2.33 of  $H_{\mathfrak{D}}^{2n}(\Omega)$  ( $n \in \mathbb{N}$ ), we consider the spaces described hereafter (see again [109], pages 228–229).

**Definition 2.35.** For any  $n \in \mathbb{N}$ , we introduce the spaces (compare with Eq. (2.162))

$$H_{\mathfrak{N}}^{2n}(\Omega) := \{f \in H^{2n}(\Omega) \mid \partial_{\mathbf{n}}(A^m f) \upharpoonright \partial\Omega = 0 \text{ for } m = 0, \dots, n-1\}, \quad (2.169)$$

$$H_{\mathfrak{R}}^{2n}(\Omega) := \{f \in H^{2n}(\Omega) \mid (h + \partial_{\mathbf{n}})(A^m f) \upharpoonright \partial\Omega = 0 \text{ for } m = 0, \dots, n-1\}; \quad (2.170)$$

here  $\mathbf{n} : \partial\Omega \rightarrow \mathbb{R}^d$  is the outer normal versor,  $\partial_{\mathbf{n}} = \sum_{i=1}^d n^i \partial_i$  indicates the normal derivative at points of  $\partial\Omega$  and  $h : \partial\Omega \rightarrow \mathbb{C}$  is an assigned function of class  $C^\infty$  <sup>(22)</sup>.

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<sup>21</sup> In fact, results analogous to Theorems 2.32 and 2.34 can be derived for any proper elliptic differential operator of arbitrary order  $p \in \mathbb{N}$ , with smooth coefficients  $a_\alpha$  ( $|\alpha| \leq p$ ):

$$A := \sum_{|\alpha| \leq p} a_\alpha \partial^\alpha : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\Omega).$$

For example, in place of Eq. (2.150) it can be proved that

$$H_{\text{loc}}^{pn}(\Omega) = \{f \in \mathcal{D}'(\Omega) \mid A^m f \in L_{\text{loc}}^2(\Omega) \text{ for all } m \in \{0, \dots, n\}\}$$

and that the topology determined by the family of seminorms  $f \mapsto \|\varphi A^m f\|_{L^2}$  ( $\varphi \in \mathcal{D}(\Omega)$ ,  $m \in \{0, \dots, n\}$ ) is equivalent to the usual one of  $H_{\text{loc}}^{pn}(\Omega)$ . Moreover, results analogous to those of Theorem 2.34 could be derived assuming that  $\Omega$  is bounded with smooth boundary  $\partial\Omega$  and that the coefficients  $a_\alpha$  ( $|\alpha| \leq 2p$ ) are of class  $C^\infty$  on  $\bar{\Omega}$ . Nevertheless, the case of a differential operator  $A$  of order different from  $p = 2$  mentioned within this footnote is not strictly relevant for the purposes of the present work; therefore, it will never be considered in the remainder of this manuscript.

<sup>22</sup>For  $m = 0, \dots, n-1$ , the above prescriptions on the normal derivatives of  $A^m f$  make sense because (for  $i = 1, \dots, d$ ) one has  $\partial_i(A^m f) \in H^1(\Omega)$ , which allows to define the trace of this function on  $\partial\Omega$ .

Let us assume that  $\mathbf{n}, h$  have extensions  $\mathbf{n} \in C^\infty(\bar{\Omega}, \mathbb{R}^d)$ ,  $h \in C^\infty(\bar{\Omega}, \mathbb{C})$  (allowing to define  $\partial_{\mathbf{n}} := \sum_{i=1}^d n^i \partial_i$  and  $h + \partial_{\mathbf{n}}$  everywhere on  $\Omega$ ). Then, in analogy to Theorem 2.34, one can easily infer the forthcoming result, which we report here without proof.

**Theorem 2.36.** *For  $n \in \mathbb{N}$ , the following statements hold.*

i) *One has*

$$H_{\mathfrak{R}}^{2n}(\Omega) := \left\{ f \in \mathcal{D}'(\Omega) \mid \begin{array}{l} A^n f \in L^2(\Omega) \text{ and} \\ \partial_{\mathbf{n}}(A^m f) \in H_0^1(\Omega) \text{ for } m = 0, \dots, n-1 \end{array} \right\}, \quad (2.171)$$

$$H_{\mathfrak{R}}^{2n}(\Omega) := \left\{ f \in \mathcal{D}'(\Omega) \mid \begin{array}{l} A^n f \in L^2(\Omega) \text{ and} \\ (h + \partial_{\mathbf{n}})(A^m f) \in H_0^1(\Omega) \text{ for } m = 0, \dots, n-1 \end{array} \right\}. \quad (2.172)$$

ii) *The topology of induced by  $H^{2n}(\Omega)$  on  $H_{\mathfrak{R}}^{2n}(\Omega)$  and  $H_{\mathfrak{R}}^{2n}(\Omega)$  coincides with the one determined by the norm  $f \mapsto \sum_{m=0}^n \|A^m f\|_{L^2}$ .*

*Remark 2.12.* As a matter of fact, most of the results to be derived in the remainder of the present Chapter 2 continue to hold under more general assumptions; for brevity, this fact will not be restated every once in a while, although it is implicitly understood most of the times.

In order to avoid misunderstandings, let us stress that in the following we will always assume  $A$  to be the differential operator of Eq. (2.148). Moreover, we will generically speak of *suitable boundary conditions* (*s.b.c.* for short) when the prescribed conditions on  $\partial\Omega$  are of Dirichlet, Neumann or Robin type; in fact, we will typically consider boundary conditions of Dirichlet type, even though most of the results presented in the following continue to hold if Dirichlet conditions are replaced with s.b.c. (also of Neumann or Robin type).

### The general notion of admissible operator. Some examples.

Let us consider the Schrödinger-type differential operator  $A := -\Delta + V$  introduced in Eq. (2.148), where  $V \in C^\infty(\Omega)$ . The definition that follows will be referred to systematically in the sequel.

**Definition 2.37.** Consider a linear subspace  $\mathcal{D}_{\mathcal{A}}$  of the Hilbert space  $L^2(\Omega)$ . We say that  $\mathcal{D}_{\mathcal{A}}$  is an *admissible domain* for  $A$  if:

i)  $A \mathcal{D}_{\mathcal{A}} \subset L^2(\Omega)$  and the operator

$$\mathcal{A} := (A \upharpoonright \mathcal{D}_{\mathcal{A}}) : \mathcal{D}_{\mathcal{A}} \subset L^2(\Omega) \rightarrow L^2(\Omega) \quad (2.173)$$

is self-adjoint;

ii)  $\sigma(\mathcal{A}) \subset (0, +\infty)$  (strict inclusion), where  $\sigma(\mathcal{A})$  indicates the spectrum of  $\mathcal{A}$ .

Under the above conditions,  $\mathcal{A}$  will be referred to as an *admissible operator*.

Herefter we review some known cases where  $\mathcal{D}_{\mathcal{A}}$  verifies the admissibility conditions. In these examples  $\mathcal{D}_{\mathcal{A}}$  is contained in  $H_0^1(\Omega)$  which means that, if  $\partial\Omega \neq \emptyset$ , Dirichlet boundary conditions are being considered.

Given  $\mathcal{D}_A$  and  $V$  with suitable features, the propositions reviewed hereafter contain sufficient conditions for the self-adjointness of  $\mathcal{A}$  and also localize the spectrum  $\sigma(\mathcal{A})$  within proper intervals, thus allowing to prove in certain cases that  $\sigma(\mathcal{A}) \subset (0, +\infty)$ .

It would not be difficult to extend our list of examples considering cases where the boundary conditions are of either Neumann or Robin type (see the comments at the end of the previous subsection).

**Proposition 2.38.** *i) Assume*

$$\begin{aligned} \Omega \subset \mathbb{R}^d \text{ to be an arbitrary domain,} \\ V(\mathbf{x}) \geq W \text{ for all } \mathbf{x} \in \Omega \text{ (} W \in \mathbb{R} \text{)} \end{aligned} \quad (2.174)$$

and define

$$\mathcal{D}_A := \{f \in H_0^1(\Omega) \mid Af \in L^2(\Omega)\} . \quad (2.175)$$

Then  $\mathcal{A} := A \upharpoonright \mathcal{D}_A$  is self-adjoint and

$$\sigma(\mathcal{A}) \subset [W, +\infty) . \quad (2.176)$$

In particular,  $\mathcal{A}$  is an admissible operator if  $W > 0$ .

ii) In the particular case  $\Omega = \mathbb{R}^d$ , the definition (2.175) of  $\mathcal{D}_A$  is equivalent to

$$\mathcal{D}_A := \{f \in L^2(\mathbb{R}^d) \mid Af \in L^2(\mathbb{R}^d)\} . \quad (2.177)$$

*Proof.* i) Assume first  $W = 0$ ; in this case  $\mathcal{A}$  is  $m$ -accretive (see [89], Theorem I). Since  $\mathcal{A}$  is symmetric, this is equivalent to say that  $\mathcal{A}$  is self-adjoint and  $\sigma(\mathcal{A}) \subset [0, +\infty)$  (see [90], page 279, Problem 3.32).

Consider now the case of an arbitrary  $W \in \mathbb{R}$ . Let  $\tilde{V}(\mathbf{x}) := V(\mathbf{x}) - W$ , and  $\tilde{A}$ ,  $\text{Dom}(\tilde{A})$ ,  $\tilde{\mathcal{A}}$  be defined respectively as  $A$ ,  $\mathcal{D}_A$  and  $\mathcal{A}$  replacing  $V$  with  $\tilde{V}$ ; since  $\tilde{V}(\mathbf{x}) \geq 0$ , the result proved above for  $W = 0$  implies that  $\tilde{\mathcal{A}}$  is self-adjoint and  $\sigma(\tilde{\mathcal{A}}) \subset [0, +\infty)$ . On the other hand, one easily checks that  $\mathcal{D}_A = \text{Dom}(\tilde{\mathcal{A}})$  and that  $\mathcal{A} = \tilde{\mathcal{A}} + W\mathbb{I}$  (with  $\mathbb{I}$  indicating the identity operator on  $L^2(\Omega)$ ), whence the thesis about  $\mathcal{A}$ .

ii) Let  $\Omega = \mathbb{R}^d$  and recall that  $H_0^1(\mathbb{R}^d) = H^1(\mathbb{R}^d)$  (see [7], page 56, Corollary 3.19); to get the thesis, it must be shown that  $f \in L^2(\mathbb{R}^d)$  and  $Af \in L^2(\mathbb{R}^d)$  imply  $f \in H^1(\mathbb{R}^d)$ . Indeed, the assumptions on  $f$  and Proposition (2.32) give  $f \in H_{loc}^2(\mathbb{R}^d)$ , so the first and second distributional derivatives of  $f$  are ordinary functions of class  $L_{loc}^2(\mathbb{R}^d)$ . To prove that  $f \in H^1(\mathbb{R}^d)$  it remains to show that  $\int_{\mathbb{R}^d} |\nabla f|^2 = \sum_{i=1}^d \int_{\mathbb{R}^d} |\partial_i f|^2 < +\infty$ ; let us only sketch the argument, based on the manipulations reported hereafter and on the remark that  $V - W \geq 0$ :

$$+\infty > \int_{\mathbb{R}^d} \bar{f}(-\Delta f + Vf) - W \int_{\mathbb{R}^d} |f|^2 = \int_{\mathbb{R}^d} |\nabla f|^2 + \int_{\mathbb{R}^d} (V - W)|f|^2 \geq \int_{\mathbb{R}^d} |\nabla f|^2 .$$

□

**Proposition 2.39.** *Assume*

$$\begin{aligned} \Omega \subset \mathbb{R}^d \text{ to be a domain bounded along a direction ,} \\ V(\mathbf{x}) \geq W \text{ for all } \mathbf{x} \in \Omega \text{ (} W \in \mathbb{R} \text{)} \end{aligned} \quad (2.178)$$

and consider the self-adjoint operator  $\mathcal{A}$  with domain  $\mathcal{D}_{\mathcal{A}}$  as in Eq. (2.175). Then

$$\sigma(\mathcal{A}) \subset \left[ \frac{1}{c_{\Omega}} + W, +\infty \right) , \quad (2.179)$$

where  $c_{\Omega} > 0$  is a constant fulfilling the Poincaré inequality of Eq. (2.6). In particular,  $\mathcal{A}$  is an admissible operator whenever  $W > -1/c_{\Omega}$ .

*Proof.* It suffices to show that

$$\langle f | \mathcal{A}f \rangle_{L^2} \geq \left( \frac{1}{c_{\Omega}} + W \right) \|f\|_{L^2}^2 \quad \text{for all } f \in \mathcal{D}_{\mathcal{A}} . \quad (2.180)$$

In fact, given  $f \in \mathcal{D}_{\mathcal{A}}$  we have

$$\langle f | \mathcal{A}f \rangle_{L^2} = \int_{\Omega} \bar{f}(-\Delta f + Vf) = \int_{\Omega} |\nabla f|^2 + \int_{\Omega} V|f|^2 \geq \frac{1}{c_{\Omega}} \int_{\Omega} |f|^2 + W \int_{\Omega} |f|^2 ,$$

whence the thesis of Eq. (2.180).  $\square$

**Proposition 2.40.** *Let*

$$\Omega = \mathbb{R}^d , \quad V(\mathbf{x}) \geq W \text{ for all } \mathbf{x} \in \mathbb{R}^d \text{ (} W \in \mathbb{R} \text{)} , \quad (2.181)$$

and consider the self-adjoint operator  $\mathcal{A}$  with domain  $\mathcal{D}_{\mathcal{A}}$  as in Eq. (2.177). Besides, assume that there exist  $r_0 \in (0, +\infty)$ ,  $p \in (1, +\infty)$  and  $a, b \in (0, +\infty)$  (depending on  $V$ ) such that, for all  $\mathbf{x}_0 \in \mathbb{R}^d$ ,

$$\frac{1}{|B(\mathbf{x}_0, r_0)|} \int_{B(\mathbf{x}_0, r_0)} (V - W) \geq a , \quad (2.182)$$

$$\left( \frac{1}{|B(\mathbf{x}_0, r_0)|} \int_{B(\mathbf{x}_0, r_0)} (V - W)^p \right)^{\frac{1}{p}} \leq \frac{b}{|B(\mathbf{x}_0, r_0)|} \int_{B(\mathbf{x}_0, r_0)} (V - W) ; \quad (2.183)$$

finally, let  $c_B \in (0, +\infty)$  denote a constant fulfilling the Poincaré-type inequality of Eq. (2.7). Then

$$\sigma(\mathcal{A}) \subset [F + W, +\infty) , \quad F := \frac{a}{2^{2d}(2c_B^2 a b^{\frac{p}{p-1}} r_0^2 + 1) \max(2, 2^{\frac{1}{p-1}})} > 0 . \quad (2.184)$$

In particular,  $\mathcal{A}$  is an admissible operator if  $W > -F$ .

*Proof.* In the case  $W = 0$ , the thesis is proved in [145] (see Theorem A of this work; the constants  $c_i$ ,  $i = 1, 2, 3, 4$ , mentioned therein satisfy  $c_1 = c_B$ ,  $c_2 = 2^d$ ,  $c_3 \geq a$ ,  $c_4 = b$ ). The case of an arbitrary  $W \in \mathbb{R}$  is treated applying the results of [145] with  $V$  replaced by  $\tilde{V} := V - W$ ; then, as in the proof of the Proposition 2.38, one must note that the operator  $\tilde{\mathcal{A}}$  corresponding to  $\tilde{V}$  has the same domain  $\mathcal{D}_{\tilde{\mathcal{A}}}$  as  $\mathcal{A}$  and is related to it by  $\mathcal{A} = \tilde{\mathcal{A}} + W\mathbb{I}$  (again, recall that  $\mathbb{I}$  is the identity operator on  $L^2(\Omega)$ ).  $\square$

Let us add to the previous examples a statement on the integer powers  $\mathcal{A}^n$  ( $n \in \mathbb{N}$ ) of a suitable admissible operator  $\mathcal{A}$ ; let us recall that by item iii) in Proposition 2.4, the space  $\text{Dom}(\mathcal{A}^n)$  coincides with the abstract space  $\mathcal{H}^{2n}$  associated to  $\mathcal{A}$ ; the latter carries the Hilbertian norm  $\|f\|_{2n} := \|\mathcal{A}^n f\|_{L^2}$ .

**Proposition 2.41.** *Assume  $\mathcal{A}$  to be an admissible operator with domain  $\mathcal{D}_{\mathcal{A}} = \{f \in H_0^1(\Omega) \mid Af \in L^2(\Omega)\}$ . Then the following statements i) and ii) hold.*

i) For all  $n \in \mathbb{N}$

$$\text{Dom}(\mathcal{A}^n) = \{f \in \mathcal{D}'(\Omega) \mid A^m f \in H_0^1(\Omega) \text{ for } m = 0, \dots, n-1, A^n f \in L^2(\Omega)\}. \quad (2.185)$$

ii) If in addition the assumptions (2.159) are fulfilled (so that  $H_0^1(\Omega) = \{f \in H^1(\Omega) \mid f \upharpoonright \partial\Omega = 0\}$  and  $\mathcal{D}_{\mathcal{A}}$  can be interpreted in terms of Dirichlet boundary conditions), then, for all  $n \in \mathbb{N}$ ,

$$\text{Dom}(\mathcal{A}^n) = \{f \in H^{2n}(\Omega) \mid A^m f \upharpoonright \partial\Omega = 0 \text{ for } m = 0, \dots, n-1\}; \quad (2.186)$$

$\text{Dom}(\mathcal{A}^n)$  is a closed subspace of  $H^{2n}(\Omega)$ , and the topology that it inherits from  $H^{2n}(\Omega)$  coincides with the one induced by the norm  $\|f\|_{2n} = \|\mathcal{A}^n f\|_{L^2}$ .

*Proof.* i) This statement follows by a simple verification by recurrence, based on the definition  $\text{Dom}(\mathcal{A}^{n+1}) = \{f \in \text{Dom}(\mathcal{A}^n) \mid \mathcal{A}^n f \in \mathcal{D}_{\mathcal{A}}\}$ .

ii) To prove the representation (2.186) of  $\text{Dom}(\mathcal{A}^n)$ , we must show that the right-hand sides of Eq.s (2.185) and (2.186) coincide; in fact, we already know this from subsection 2.6 (see Definition 2.33 and Theorem 2.34). In the cited subsection we have already noted that the space described by (2.186) is a closed subspace of  $H^{2n}(\Omega)$ , and we have shown that the topology that it inherits from  $H^{2n}(\Omega)$  agrees with the one given by the norm  $f \mapsto \sum_{m=0}^n \|\mathcal{A}^m f\|_{L^2}$  (see again Theorem 2.34). In the present case where admissibility requires  $\text{Dom}(\mathcal{A}) \subset [\varepsilon, +\infty)$  for some  $\varepsilon > 0$ , we have  $\|\mathcal{A}^m f\|_{L^2} \leq \varepsilon^{-(n-m)} \|\mathcal{A}^n f\|_{L^2}$  for  $m = 0, \dots, n$  (see Eq. (2.84)), so that  $\|\mathcal{A}^n f\|_{L^2}$  is a norm equivalent to  $\sum_{m=0}^n \|\mathcal{A}^m f\|_{L^2}$ .  $\square$

### Embedding results for the scale of Hilbert spaces.

Assume again  $\Omega \subset \mathbb{R}^d$  to be an arbitrary domain and  $A$  to be a Schrödinger-type operator as in Eq. (2.148). Let  $\mathcal{D}_{\mathcal{A}} \subset L^2(\Omega)$  denote any admissible domain for  $A$  and consider the spaces  $(\mathcal{H}^r, \|\cdot\|_r)$  associated to the admissible operator  $\mathcal{A}$  (see Proposition 2.4). Recall that  $\|f\|_r = \|\mathcal{A}^{r/2} f\|_{L^2}$ , for  $f \in \text{Dom}(\mathcal{A}^{r/2})$ ; besides,  $\mathcal{H}^r$  coincides with  $\text{Dom}(\mathcal{A}^{r/2})$  for  $r \geq 0$ , and it is its completion for  $r < 0$ .

**Proposition 2.42.** *Let  $r \in [0, +\infty)$ ; then  $\mathcal{H}^r$  is a linear subspace of  $H_{\text{loc}}^r(\Omega)$ , and there holds the continuous embedding*

$$\mathcal{H}^r \hookrightarrow H_{\text{loc}}^r(\Omega) . \quad (2.187)$$

*Proof.* The proof is divided in several steps.

*Step 1 - The thesis holds in the case  $r = 2n$ , for any  $n \in \mathbb{N}$ .* Let  $f \in \mathcal{H}^{2n} = \text{Dom}(\mathcal{A}^n)$ ; then  $A^m f \in L^2(\Omega) \subset L_{\text{loc}}^2(\Omega)$  for all  $m \in \{0, \dots, n\}$ . This implies  $f \in H_{\text{loc}}^{2n}(\Omega)$ , due to item i) of Theorem 2.32. On the one hand, by item ii) of the same theorem, the topology of  $H_{\text{loc}}^{2n}(\Omega)$  is induced by the family of seminorms  $f \mapsto \|\varphi A^m f\|_{L^2}$ , for  $\varphi \in \mathcal{D}(\Omega)$  and  $m \in \{0, \dots, n\}$ . On the other hand, for such  $\varphi, m$  and for all  $f \in \mathcal{H}^{2n}$ , one has

$$\begin{aligned} \|\varphi A^m f\|_{L^2} &= \|\varphi \mathcal{A}^m f\|_{L^2} \leq \\ &\leq \left( \sup_{\Omega} |\varphi| \right) \|\mathcal{A}^m f\|_{L^2} = \left( \sup_{\Omega} |\varphi| \right) \|f\|_{2m} \leq \left( \sup_{\Omega} |\varphi| \right) \varepsilon^{-(n-m)} \|f\|_{2n} \end{aligned}$$

(see Proposition 2.5 for the last inequality); this proves the continuity of the embedding  $\mathcal{H}^{2n} \hookrightarrow H_{\text{loc}}^{2n}(\Omega)$ .

*Step 2 - Reformulation of the statement to be proved, for arbitrary  $r$ .* For each  $\varphi \in \mathcal{D}(\Omega)$ , let us introduce the linear operator of multiplication  $M_{\varphi} : \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\mathbb{R}^d)$ ,  $f \mapsto M_{\varphi} f := \varphi f$ . Consider any  $r \in [0, +\infty)$ ; then, the definition of  $H_{\text{loc}}^r(\Omega)$  can be rephrased as  $H_{\text{loc}}^r(\Omega) = \{f \in \mathcal{D}'(\Omega) \mid M_{\varphi} f \in H^r(\mathbb{R}^d) \text{ for all } \varphi \in \mathcal{D}(\Omega)\}$ . Recall that the topology of  $H_{\text{loc}}^r(\Omega)$  is, by construction, the initial topology with respect to the family of maps  $M_{\varphi} : H_{\text{loc}}^r(\Omega) \rightarrow H^r(\mathbb{R}^d)$  ( $\varphi \in \mathcal{D}(\Omega)$ ). Then, due to the characteristic property of the initial topology, the statement  $\mathcal{H}^r \hookrightarrow H_{\text{loc}}^r(\Omega)$  is equivalent to the following: “for each  $\varphi \in \mathcal{D}(\Omega)$ ,  $M_{\varphi}$  maps continuously  $\mathcal{H}^r$  into  $H^r(\mathbb{R}^d)$ ”.

*Step 3 - Proof of the thesis for arbitrary  $r \in [0, +\infty)$ .* Given such an  $r$ , let  $n$  denote the unique natural number such that  $2n < r < 2n + 2$ ; then there is a unique  $\theta \in (0, 1)$  such that  $r = 2n(1 - \theta) + (2n + 2)\theta$ . Due to Step 1, we know that  $\mathcal{H}^{2n} \hookrightarrow H_{\text{loc}}^{2n}(\Omega)$  and  $\mathcal{H}^{2n+2} \hookrightarrow H_{\text{loc}}^{2n+2}(\Omega)$ ; so, due to Step 2, for each  $\varphi \in \mathcal{D}(\Omega)$  the operator  $M_{\varphi}$  maps continuously  $\mathcal{H}^{2n}$  into  $H^{2n}(\mathbb{R}^d)$ , and  $\mathcal{H}^{2n+2}$  into  $H^{2n+2}(\mathbb{R}^d)$ . By the fundamental theorem of interpolation (Theorem 2.3), for each  $\varphi$  the operator  $M_{\varphi}$  maps continuously  $[\mathcal{H}^{2n}, \mathcal{H}^{2n+2}]_{\theta}$  into  $[H^{2n}(\mathbb{R}^d), H^{2n+2}(\mathbb{R}^d)]_{\theta}$ ; however, using Eq.s (2.37) (2.85) with  $r_0 = 2n$ ,  $r_1 = 2n + 2$ , we obtain  $[\mathcal{H}^{2n}, \mathcal{H}^{2n+2}]_{\theta} = \mathcal{H}^r$  and  $[H^{2n}(\mathbb{R}^d), H^{2n+2}(\mathbb{R}^d)]_{\theta} = H^r(\mathbb{R}^d)$ . In conclusion, for any  $\varphi \in \mathcal{D}(\Omega)$  the operator  $M_{\varphi}$  maps continuously  $\mathcal{H}^r$  to  $H^r(\mathbb{R}^d)$ ; due to Step 2, this proves that  $\mathcal{H}^r \hookrightarrow H_{\text{loc}}^r(\Omega)$ .  $\square$

**Corollary 2.43.** *Let  $r \in \mathbb{R}$  and  $j \in \mathbb{N}$  be such that  $r > j + d/2$ ; then there holds the continuous inclusion*

$$\mathcal{H}^r \hookrightarrow C^j(\Omega) . \quad (2.188)$$

*More precisely,  $\mathcal{H}^r \hookrightarrow C^{j,\lambda}(\Omega) \hookrightarrow C^j(\Omega)$  for each  $\lambda \in (0, 1)$  such that  $r > j + d/2 + \lambda$ .*

*Proof.* In fact  $\mathcal{H}^r \hookrightarrow H_{\text{loc}}^r(\Omega)$ , (for  $r \geq 0$ ) by the previous proposition, and  $H_{\text{loc}}^r(\Omega) \hookrightarrow C^{j,\lambda}(\Omega) \hookrightarrow C^j(\Omega)$  by the Sobolev embedding theorem (see Theorem 2.1 of page 17).  $\square$

Similarly to the analysis performed in subsection 2.6, hereafter we are going to show that stronger versions of Proposition 2.42 and of the related Corollary 2.43 can be derived making stricter hypotheses on the regularity of the domain  $\Omega$ , of its boundary  $\partial\Omega$  and of the Schrödinger-type operator  $A = -\Delta + V$ .

For example, let us make the assumptions described in Eq. (2.159), so that  $\Omega$  is a bounded domain with boundary of class  $C^\infty$  and  $A = -\Delta + V$  with  $V \in C^\infty(\bar{\Omega})$ , and consider the Sobolev spaces  $H^r(\Omega)$  ( $r \in \mathbb{R}$ ). Then, there hold the following results.

**Proposition 2.44.** *Let the assumptions (2.159) hold with Dirichlet boundary conditions prescribed on  $\partial\Omega$ ; then, for any  $r \in [0, +\infty)$ ,  $\mathcal{H}^r$  is a linear subspace of  $H^r(\Omega)$  and there holds the continuous embedding*

$$\mathcal{H}^r \hookrightarrow H^r(\Omega) . \quad (2.189)$$

*Proof.* The proof closely resembles that of Proposition 2.42, and it is divided in several steps likewise.

*Step 1 - The thesis holds in the case  $r = 2n$ , for any  $n \in \mathbb{N}$ .* This is granted by item ii) of Proposition 2.41, dealing with  $\text{Dom}(\mathcal{A}^n) = \mathcal{H}^{2n}$ .

*Step 2 - Proof of the thesis for arbitrary  $r \in [0, +\infty)$ .* Let  $n \in \mathbb{N}$  be such that  $2n < r < 2n + 2$ ; then, there exists a unique  $\theta \in (0, 1)$  such that  $r = 2n(1 - \theta) + (2n + 2)\theta$ . Due to the interpolation relations (2.85) and (2.38), we have  $[\mathcal{H}^{2n}, \mathcal{H}^{2n+2}]_\theta = \mathcal{H}^r$  and  $[H^{2n}(\Omega), H^{2n+2}(\Omega)]_\theta = H^r(\Omega)$ . on the other hand, due to Step 1, we already know that the identity maps linearly and continuously  $\mathcal{H}^{2n}$  into  $H^{2n}(\Omega)$  and  $\mathcal{H}^{2n+2}$  into  $H^{2n+2}(\Omega)$ . So, by the fundamental theorem of interpolation (see Theorem 2.3), the identity maps linearly and continuously  $\mathcal{H}^r$  into  $H^r(\Omega)$ .  $\square$

**Corollary 2.45.** *Let the assumptions (2.159) hold with Dirichlet boundary conditions prescribed on  $\partial\Omega$ ; moreover, let  $r \in \mathbb{R}$  and  $j \in \mathbb{N}$  be such that  $r > j + d/2$ . Then there holds the continuous inclusion*

$$\mathcal{H}^r \hookrightarrow C^j(\bar{\Omega}) . \quad (2.190)$$

*More precisely,  $\mathcal{H}^r \hookrightarrow C^{j,\lambda}(\bar{\Omega}) \hookrightarrow C^j(\bar{\Omega})$  for each  $\lambda \in (0, 1)$  such that  $r > j + d/2 + \lambda$ .*

*Proof.* In fact  $\mathcal{H}^r \hookrightarrow H^r(\Omega)$  (for  $r \geq 0$ ) by the previous proposition, and  $H^r(\Omega) \hookrightarrow C^{j,\lambda}(\bar{\Omega}) \hookrightarrow C^j(\bar{\Omega})$  by the Sobolev embedding (2.19) of Theorem 2.1.  $\square$

## Dirac delta functions.

### The Dirac delta at interior points.

Let once more  $\Omega$  be an arbitrary domain and let  $V : \Omega \rightarrow \mathbb{R}$  be a smooth potential on it; we indicate with  $\mathbf{x}$  an arbitrary point in the interior of  $\Omega$ , i.e.,

$$\mathbf{x} \in \Omega . \quad (2.191)$$

Corollary 2.43, discussed in the previous subsection, has the following implications.



**Proposition 2.46.** *Let  $\mathbf{x} \in \Omega$ ; then, there hold the subsequent statements.*

i) *There exists a unique element  $\delta_{\mathbf{x}} \in \mathcal{H}^{-\infty}$  such that, for all  $r > d/2$ ,  $\delta_{\mathbf{x}} \in \mathcal{H}^{-r}$  and*

$$\langle \delta_{\mathbf{x}} | f \rangle = f(\mathbf{x}) \quad \text{for all } f \in \mathcal{H}^r . \quad (2.192)$$

ii) *Let  $\alpha$  denote a multi-index of order  $|\alpha|$ ; then, there exists a unique element  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-\infty}$  such that, for all  $r > |\alpha| + \frac{d}{2}$ ,  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-r}$  and*

$$\langle \partial^\alpha \delta_{\mathbf{x}} | f \rangle = (-1)^{|\alpha|} \partial^\alpha f(\mathbf{x}) \quad \text{for all } f \in \mathcal{H}^r . \quad (2.193)$$

*Remark 2.13.* Let us stress that the left-hand sides of Eq.s (2.192) (2.193) both contain the extension (2.103) of the inner product  $\langle | \rangle$  on  $\mathcal{H} \equiv L^2(\Omega)$ . To define the right-hand side of Eq. (2.192), notice that  $\mathcal{H}^r \hookrightarrow C^0(\Omega)$  for any  $r > d/2$  and evaluate at  $\mathbf{x}$  the continuous function  $f$ ; on the other hand, recall that  $\mathcal{H}^r \hookrightarrow C^j(\Omega)$  for  $r > j + d/2$ , so that the the right-hand side of Eq. (2.193) can be interpreted in terms of the  $\alpha$ -th derivative at  $\mathbf{x}$  of the  $C^j$  function  $f$  (for any  $|\alpha| \leq j$ ).

*Proof.* i) First note that the evaluation map

$$e_{\mathbf{x}} : C^0(\Omega) \rightarrow \mathbb{C} , \quad f \mapsto \langle e_{\mathbf{x}}, f \rangle := f(\mathbf{x})$$

is a continuous linear form. Now, let us fix  $r > d/2$  arbitrarily; since  $\mathcal{H}^r \hookrightarrow C^0(\Omega)$ ,  $e_{\mathbf{x}}|_{\mathcal{H}^r}$  is an element of the topological dual  $(\mathcal{H}^r)'$ . Then, by Proposition 2.18 there is a unique element of  $\mathcal{H}^{-r}$ , which we denote provisionally with  $\delta_{\mathbf{x}}^r$ , such that  $\langle \delta_{\mathbf{x}}^r | f \rangle = \langle e_{\mathbf{x}}, f \rangle = f(\mathbf{x})$  for all  $f \in \mathcal{H}^r$ .

To go on, note that  $\delta_{\mathbf{x}}^s = \delta_{\mathbf{x}}^r$  for all  $s, r \in \mathbb{R}$  such that  $s \geq r > d/2$ ; in fact, for any such  $s$  and  $r$ , one has  $\delta_{\mathbf{x}}^s \in \mathcal{H}^{-s}$ ,  $\delta_{\mathbf{x}}^r \in \mathcal{H}^{-r} \subset \mathcal{H}^{-s}$  and  $\langle \delta_{\mathbf{x}}^s | f \rangle = f(\mathbf{x}) = \langle \delta_{\mathbf{x}}^r | f \rangle$  for all  $f \in \mathcal{H}^s \subset \mathcal{H}^r$ , so that  $\delta_{\mathbf{x}}^s$  and  $\delta_{\mathbf{x}}^r$  are the same element of  $\mathcal{H}^{-s}$ .

In conclusion, all the elements  $\delta_{\mathbf{x}}^r$  ( $r > d/2$ ) are copies of a same element, that we indicate with  $\delta_{\mathbf{x}}$ ; this element belongs to  $\mathcal{H}^{-r}$  for any  $r > d/2$ , and it fulfills Eq. (2.192) by construction. Finally, it is easy to check that an element of  $\mathcal{H}^{-\infty}$  possessing the same properties coincides with this  $\delta_{\mathbf{x}}$ , thus granting its uniqueness.

ii) The proof follows by arguments similar to the ones employed to show statement i) for the special case  $|\alpha| = 0$ . For any  $j \in \mathbb{N}$  and for any multi-index  $\alpha$  of order  $\leq j$ , one uses the continuity of the linear form

$$e_{\mathbf{x}}^\alpha : C^j(\Omega) \rightarrow \mathbb{C} , \quad f \mapsto \langle e_{\mathbf{x}}^\alpha, f \rangle := (\partial^\alpha f)(\mathbf{x}) \quad (2.194)$$

together with the continuous embedding  $\mathcal{H}^r \hookrightarrow C^j(\Omega)$  for  $r > j + d/2$ ; the element  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-\infty}$  is the one corresponding to the linear form  $(-1)^{|\alpha|} e_{\mathbf{x}}^\alpha$ .  $\square$

Apart from the use of the spaces  $\mathcal{H}^r$  (for  $r > j + d/2$ ), Eq.s (2.192) and (2.193) closely resemble the definitions given in the standard theory of Schwartz distributions for the Dirac delta function at a point  $\mathbf{x}$  and for its derivatives, respectively; this justifies the following definition.

**Definition 2.47.** In the sequel,  $\delta_{\mathbf{x}}$  and  $\partial^\alpha \delta_{\mathbf{x}}$  will be referred to as the *Dirac delta* at  $\mathbf{x}$  and its  $\alpha$ -th derivative, respectively.

**Proposition 2.48.** Let  $j \in \mathbb{N}$  and  $r \in \mathbb{R}$  be such that  $r > j + d/2$ ; consider the map

$$\delta : \Omega \rightarrow \mathcal{H}^{-r} \quad \mathbf{x} \mapsto \delta_{\mathbf{x}} . \quad (2.195)$$

This map is of class  $C^j$  from  $\Omega$  to the Banach space  $\mathcal{H}^{-r}$ ; more precisely,  $\delta \in C^{j,\lambda}(\Omega, \mathcal{H}^{-r})$  for any  $\lambda \in (0, 1)$  such that  $r > j + d/2 + \lambda$ .

Moreover, for any multi-index  $\alpha$  of order  $\leq j$ , the corresponding partial derivative of  $\delta$  at a point  $\mathbf{x} \in \Omega$  is given by

$$(\partial^\alpha \delta)(\mathbf{x}) = (-1)^{|\alpha|} \partial^\alpha \delta_{\mathbf{x}} . \quad (2.196)$$

*Proof.* In this proof, for any locally convex space  $X$ , the topological dual space  $X'$  is equipped with the strong topology (i.e., with the topology of uniform convergence on the bounded subsets of  $X$ ); this topology is induced by the family of seminorms  $p_{\mathcal{B}}$  ( $\mathcal{B} \subset X$  bounded) where, for each  $\lambda \in X'$ , we set

$$p_{\mathcal{B}}(\lambda) := \sup_{x \in \mathcal{B}} |\langle \lambda, x \rangle| . \quad (2.197)$$

In particular, if  $X$  is a Banach space, the strong topology on  $X'$  is just the usual norm topology. The rest of the proof is divided in several steps.

*Step 1 - The maps  $e^\alpha$  on  $C^{j,\lambda}(\Omega)$ .* Let  $j \in \mathbb{N}$ ,  $\lambda \in (0, 1)$ , and consider a multi-index  $\alpha$  of order  $\leq j$ . For each  $\mathbf{x} \in \Omega$  we put

$$e_{\mathbf{x}}^\alpha : C^{j,\lambda}(\Omega) \rightarrow \mathbb{C}, \quad f \mapsto \langle e_{\mathbf{x}}^\alpha, f \rangle := (\partial^\alpha f)(\mathbf{x}) ;$$

in particular, let us stress that

$$e_{\mathbf{x}}^0 \equiv e_{\mathbf{x}}$$

is the usual evaluation map on  $C^{0,\lambda}(\Omega)$ . Clearly,  $e_{\mathbf{x}}^\alpha \in (C^{j,\lambda}(\Omega))'$ ; so, we have the map

$$e^\alpha : \Omega \rightarrow (C^{j,\lambda}(\Omega))', \quad \mathbf{x} \mapsto e_{\mathbf{x}}^\alpha . \quad (2.198)$$

*Step 2 - Let  $j \in \mathbb{N}$ ,  $\lambda \in (0, 1)$  and consider a multi-index  $\alpha$  of order  $\leq j$ . Then the map (2.198) is of class  $C^{0,1}$  (i.e., locally Lipschitz, hence continuous) if  $|\alpha| < j$  and of class  $C^{0,\lambda}$  (hence continuous) if  $|\alpha| = j$ .* For the sake of brevity, hereafter we put

$$\tilde{\lambda} := \begin{cases} 1 & \text{if } |\alpha| < j \\ \lambda & \text{if } |\alpha| = j \end{cases} .$$

Let us consider any compact subset  $K \subset \Omega$ . If  $f \in C^{j,\lambda}(\Omega)$  and  $\mathbf{x}, \mathbf{y} \in K$  (with  $\mathbf{y} \neq \mathbf{x}$ ) we have

$$\langle e_{\mathbf{y}}^\alpha - e_{\mathbf{x}}^\alpha, f \rangle = \partial^\alpha f(\mathbf{y}) - \partial^\alpha f(\mathbf{x}) = \frac{\partial^\alpha f(\mathbf{y}) - \partial^\alpha f(\mathbf{x})}{|\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}}} |\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}}$$

that implies

$$|\langle e_{\mathbf{y}}^{\alpha} - e_{\mathbf{x}}^{\alpha}, f \rangle| \leq |f|_K^{\alpha, \tilde{\lambda}} |\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}} \quad \text{for } \mathbf{x}, \mathbf{y} \in K, \quad |f|_K^{\alpha, \tilde{\lambda}} := \sup_{\mathbf{x}, \mathbf{y} \in K, \mathbf{y} \neq \mathbf{x}} \frac{|\partial^{\alpha} f(\mathbf{y}) - \partial^{\alpha} f(\mathbf{x})|}{|\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}}} \quad (2.199)$$

(if  $|\alpha| < j$ , so that  $\tilde{\lambda} = 1$ , the finiteness of  $|f|_K^{\alpha, \tilde{\lambda}}$  follows from the fact that  $\partial^{\alpha} f$  is a  $C^1$  function). For any bounded subset  $\mathcal{B}$  of  $C^{j, \lambda}(\Omega)$ , let us put

$$M_{K, \mathcal{B}}^{\alpha, \tilde{\lambda}} := \sup_{f \in \mathcal{B}} |f|_K^{\alpha, \tilde{\lambda}} < +\infty$$

(the sup over  $\mathcal{B}$  is finite, because  $f \mapsto |f|_K^{\alpha, \tilde{\lambda}}$  is a continuous seminorm on  $C^{j, \lambda}(\Omega)$ ; compare with Eq. (2.14)). Returning to Eq. (2.199) we see that

$$|\langle e_{\mathbf{y}}^{\alpha} - e_{\mathbf{x}}^{\alpha}, f \rangle| \leq M_{K, \mathcal{B}}^{\alpha, \tilde{\lambda}} |\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}} \quad \text{for } \mathbf{x}, \mathbf{y} \in K, f \in \mathcal{B};$$

therefore, if  $p_{\mathcal{B}}$  is the seminorm on  $(C^{j, \lambda}(\Omega))'$  defined by Eq. (2.197), we have

$$p_{\mathcal{B}}(e_{\mathbf{y}}^{\alpha} - e_{\mathbf{x}}^{\alpha}) \leq M_{K, \mathcal{B}}^{\alpha, \tilde{\lambda}} |\mathbf{y} - \mathbf{x}|^{\tilde{\lambda}} \quad \text{for } \mathbf{x}, \mathbf{y} \in K .$$

Since the above relation holds for any bounded subset  $\mathcal{B} \subset C^{j, \lambda}(\Omega)$ , we have proved that  $e^{\alpha}$  is of class  $C^{0, \tilde{\lambda}}$ .

*Step 3 - Let  $j \in \mathbb{N}$ ,  $\lambda \in (0, 1)$ . The map*

$$e : \Omega \rightarrow (C^{j, \lambda}(\Omega))', \quad \mathbf{x} \mapsto e_{\mathbf{x}}$$

*is of class  $C^{j, \lambda}$ ; for each multi-index  $\alpha$  of order  $\leq j$  and each  $\mathbf{x} \in \Omega$ , the  $\alpha$ -th partial derivative of the map  $e$  at  $\mathbf{x}$  is*

$$(\partial^{\alpha} e)(\mathbf{x}) = e_{\mathbf{x}}^{\alpha} . \quad (2.200)$$

To exemplify the necessary arguments, hereafter we give the proof for  $j = 1$ ; so, our purpose is to prove that

$$e : \Omega \rightarrow (C^{1, \lambda}(\Omega))', \quad \mathbf{x} \mapsto e_{\mathbf{x}}$$

is of class  $C^{1, \lambda}$  with partial derivatives

$$(\partial_i e)(\mathbf{x}) = e_{\mathbf{x}}^i \quad (i = 1, \dots, d; \langle e_{\mathbf{x}}^i, f \rangle := \partial_i f(\mathbf{x}) \text{ for each } f \in C^{1, \lambda}(\Omega)) .$$

Due to Step 1, we already know that the maps  $e^i : \Omega \rightarrow C^{1, \lambda}(\Omega)$ ,  $\mathbf{x} \mapsto e_{\mathbf{x}}^i$  are of class  $C^{0, \lambda}$ ; therefore, to get the thesis it suffices to prove the following, at each  $\mathbf{x} \in \Omega$ :

$$\frac{e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i}{|\mathbf{y} - \mathbf{x}|} \rightarrow 0 \quad \text{in } (C^{1, \lambda}(\Omega))' \quad \text{for } \mathbf{y} \in \Omega, \mathbf{y} \rightarrow \mathbf{x} . \quad (2.201)$$

Let us fix  $\mathbf{x} \in \Omega$ ; for  $f \in C^{1,\lambda}(\Omega)$  and  $\mathbf{y} \in \Omega$  we have

$$\langle e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i, f \rangle = f(\mathbf{y}) - f(\mathbf{x}) - \sum_{i=1}^d (y^i - x^i) (\partial_i f)(\mathbf{x}). \quad (2.202)$$

To go on, we let us consider a radius  $\rho > 0$  such that  $\overline{B(\mathbf{x}, \rho)} \subset \Omega$ . Then, for  $\mathbf{y} \in \overline{B(\mathbf{x}, \rho)}$  we can write

$$f(\mathbf{y}) - f(\mathbf{x}) = \sum_{i=1}^d (y^i - x^i) \int_0^1 d\tau (\partial_i f)(\mathbf{x} + \tau(\mathbf{y} - \mathbf{x}));$$

inserting this result into Eq. (2.202) we easily obtain

$$\langle e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i, f \rangle = \sum_{i=1}^d (y^i - x^i) \int_0^1 d\tau [(\partial_i f)(\mathbf{x} + \tau(\mathbf{y} - \mathbf{x})) - (\partial_i f)(\mathbf{x})]. \quad (2.203)$$

On the other hand, for  $\mathbf{y} \in \overline{B(\mathbf{x}, \rho)}$  and  $\tau \in [0, 1]$  we have

$$\left| (\partial_i f)(\mathbf{x} + \tau(\mathbf{y} - \mathbf{x})) - (\partial_i f)(\mathbf{x}) \right| \leq |f|_{\mathbf{x}, \rho}^{i, \lambda} |\mathbf{y} - \mathbf{x}|^\lambda, \quad |f|_{\mathbf{x}, \rho}^{i, \lambda} := \sup_{\mathbf{z}, \mathbf{w} \in \overline{B(\mathbf{x}, \rho)}, \mathbf{z} \neq \mathbf{w}} \frac{|\partial_i f(\mathbf{z}) - \partial_i f(\mathbf{w})|}{|\mathbf{z} - \mathbf{w}|^\lambda}. \quad (2.204)$$

From here and from Eq. (2.203) we obtain

$$\begin{aligned} \left| \langle e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i, f \rangle \right| &\leq \left( \sum_{i=1}^d |y^i - x^i| |f|_{\mathbf{x}, \rho}^{i, \lambda} \right) |\mathbf{y} - \mathbf{x}|^\lambda \\ &\leq \sqrt{\sum_{i=1}^d (|f|_{\mathbf{x}, \rho}^{i, \lambda})^2} |\mathbf{y} - \mathbf{x}|^{1+\lambda} \quad \text{for } f \in C^{1,\lambda}(\Omega), \mathbf{y} \in \overline{B(\mathbf{x}, \rho)}. \end{aligned}$$

To go on, for any bounded subset  $\mathcal{B}$  of  $C^{1,\lambda}(\Omega)$ , let us put

$$M_{\mathbf{x}, \rho}^{\mathcal{B}, 1, \lambda} := \sup_{f \in \mathcal{B}} \sqrt{\sum_{i=1}^d (|f|_{\mathbf{x}, \rho}^{i, \lambda})^2} < +\infty.$$

Returning to Eq. (2.204) we see that

$$\left| \langle e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i, f \rangle \right| \leq M_{\mathbf{x}, \rho}^{\mathcal{B}, 1, \lambda} |\mathbf{y} - \mathbf{x}|^{1+\lambda} \quad \text{for } \mathbf{y} \in \overline{B(\mathbf{x}, \rho)}, f \in \mathcal{B};$$

therefore, if  $p_{\mathcal{B}}$  is the seminorm on  $(C^{1,\lambda}(\Omega))'$  defined by Eq. (2.197), we have

$$p_{\mathcal{B}} \left( e_{\mathbf{y}} - e_{\mathbf{x}} - \sum_{i=1}^d (y^i - x^i) e_{\mathbf{x}}^i \right) \leq M_{\mathbf{x}, \rho}^{\mathcal{B}, 1, \lambda} |\mathbf{y} - \mathbf{x}|^{1+\lambda} \quad \text{for } \mathbf{y} \in \overline{B(\mathbf{x}, \rho)}. \quad (2.205)$$

By the arbitrariness of the bounded subset  $\mathcal{B} \subset C^{1,\lambda}(\Omega)$ , this suffices to obtain the thesis (2.201).

*Step 4 - Let  $r \in \mathbb{R}$ ,  $j \in \mathbb{N}$  and  $\lambda \in (0, 1)$  be such that  $r > j + d/2 + \sigma$ . Then the map (2.195)  $\delta : \Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto \delta_{\mathbf{x}}$  is of class  $C^{j,\lambda}$  and its derivatives are as in Eq. (2.196), for each multi-index  $\alpha$  of order  $\leq j$  and each  $\mathbf{x} \in \Omega$ . First of all let us recall the embedding  $\mathcal{H}^r \hookrightarrow C^{j,\lambda}(\Omega)$ ; this induces a continuous linear map*

$$\mathcal{R}^r : (C^{j,\lambda}(\Omega))' \rightarrow (\mathcal{H}^r)' , \quad \alpha \mapsto \mathcal{R}^r \alpha := \alpha \upharpoonright \mathcal{H}^r . \quad (2.206)$$

Let us also recall that there is a Banach antilinear isomorphism  $\mathcal{I}^r : \mathcal{H}^{-r} \rightarrow (\mathcal{H}^r)'$  such that  $\langle \mathcal{I}^r g, f \rangle := \langle g|f \rangle$  for  $g \in \mathcal{H}^{-r}$ ,  $f \in \mathcal{H}^r$ .

Now, for any  $\mathbf{x} \in \Omega$ ,  $e_{\mathbf{x}} \in (C^{j,\lambda}(\Omega))'$  and  $\delta_{\mathbf{x}} \in \mathcal{H}^{-r}$  are such that

$$\langle e_{\mathbf{x}}, f \rangle = f(\mathbf{x}) \text{ for } f \in C^{j,\lambda}(\Omega) , \quad \langle \delta_{\mathbf{x}}|f \rangle = f(\mathbf{x}) \text{ for } f \in \mathcal{H}^r$$

(recall Step 1 and Eq. (2.192)). Therefore  $\mathcal{R}^r e_{\mathbf{x}} = \mathcal{I}^r \delta_{\mathbf{x}}$ , i.e.,

$$\delta_{\mathbf{x}} = (\mathcal{I}^r)^{-1} \mathcal{R}^r e_{\mathbf{x}} . \quad (2.207)$$

The map  $(\mathcal{I}^r)^{-1} \mathcal{R}^r : (C^{j,\lambda}(\Omega))' \rightarrow \mathcal{H}^r$  is antilinear and continuous, and  $e : \mathbf{x} \in \Omega \mapsto e_{\mathbf{x}} \in (C^{j,\lambda}(\Omega))'$  is of class  $C^{j,\lambda}$  according to Step 3; therefore  $\delta : \mathbf{x} \in \Omega \mapsto \delta_{\mathbf{x}} \in \mathcal{H}^r$  is also of class  $C^{j,\lambda}$ . Moreover, for  $|\alpha| \leq j$  and  $\mathbf{x} \in \Omega$  we have

$$(\partial^\alpha \delta)(\mathbf{x}) = (\mathcal{I}^r)^{-1} \mathcal{R}^r (\partial^\alpha e)(\mathbf{x}) = (\mathcal{I}^r)^{-1} \mathcal{R}^r e_{\mathbf{x}}^\alpha \quad (2.208)$$

where the last equality is again due to Step 3. Summing up, for each  $f \in \mathcal{H}^r$  we have

$$\langle (\partial^\alpha \delta)(\mathbf{x})|f \rangle = \langle e_{\mathbf{x}}^\alpha, f \rangle = (\partial^\alpha f)(\mathbf{x}),$$

and comparing this result with the relation (2.193)  $\langle \partial^\alpha \delta_{\mathbf{x}}|f \rangle = (-1)^{|\alpha|} (\partial^\alpha f)(\mathbf{x})$  we finally obtain Eq. (2.196), i.e., the thesis.  $\square$

### Extension of the previous results up to the boundary.

Let us remark that so far in this subsection we have always assumed  $\mathbf{x}$  to be a point in the interior of the open set  $\Omega$  (see Eq. (2.191)). Nonetheless, it appears from the proofs of Propositions 2.46 and 2.48 that, making stronger regularity assumptions, the same results stated in these propositions continue to hold as well for points on the boundary  $\partial\Omega$ .

For example, let us make the stricter hypotheses (2.159), so that  $\Omega$  is a bounded domain with boundary of class  $C^\infty$  and  $\mathcal{A} = -\Delta + V$  with  $V \in C^\infty(\bar{\Omega})$ ; moreover, assume Dirichlet boundary conditions are imposed for the operator  $\mathcal{A}$ , which is also supposed to be strictly positive. Thus,

$$\begin{aligned} \text{Dom}(\mathcal{A}) \equiv \mathcal{D}_{\mathcal{A}} &= \{f \in H_0^1(\Omega) \mid (-\Delta + V)f \in L^2(\Omega)\} , \\ \sigma(\mathcal{A}) &\subset [\varepsilon, +\infty) \text{ for some } \varepsilon > 0 . \end{aligned} \quad (2.209)$$

Throughout the present paragraph,  $\mathbf{x}$  denotes any point in the closure  $\overline{\Omega}$  of the domain  $\Omega$ , that is

$$\mathbf{x} \in \overline{\Omega} = \Omega \cup \partial\Omega . \quad (2.210)$$

In this situation, we have the continuous embeddings  $\mathcal{H}^r \hookrightarrow C^{j,\lambda}(\overline{\Omega}) \hookrightarrow C^j(\overline{\Omega})$  for  $r \in \mathbb{R}$ ,  $j \in \mathbb{N}$ ,  $\lambda \in (0, 1)$  s.t.  $r > j + d/2 + \lambda$ . This yields the following variants of Propositions 2.46 and 2.48, that are easily proved replacing  $C^j(\Omega)$  with  $C^j(\overline{\Omega})$ , and  $C^{j,\lambda}(\Omega)$  with  $C^{j,\lambda}(\overline{\Omega})$ .

**Proposition 2.49.** *Under the assumptions (2.159) and (2.209), both statements i) and ii) of Proposition 2.46 hold for any  $\mathbf{x} \in \overline{\Omega}$ , allowing to define  $\delta_{\mathbf{x}}$  and  $\partial^\alpha \delta_{\mathbf{x}}$  even for  $\mathbf{x} \in \partial\Omega$ .*

**Proposition 2.50.** *Consider the assumptions (2.159) and (2.209); moreover, let  $j \in \mathbb{N}$ ,  $r \in \mathbb{R}$  be such that  $r > j + d/2$ . Then, the map*

$$\delta : \Omega \rightarrow \mathcal{H}^{-r} \quad \mathbf{x} \mapsto \delta_{\mathbf{x}} , \quad (2.211)$$

*is of class  $C^j(\overline{\Omega}, \mathcal{H}^{-r})$ ; more precisely, it is of class  $C^{j,\lambda}(\overline{\Omega}, \mathcal{H}^{-r})$  for each  $\lambda \in (0, 1)$  s.t.  $r > j + d/2 + \lambda$ . The continuous extension of (2.211) to  $\overline{\Omega}$  is the map  $\mathbf{x} \mapsto \delta_{\mathbf{x}}$  defined according to Proposition 2.49; furthermore, for any multi-index  $\alpha$  of order  $\leq j$ , the (continuous extension to  $\overline{\Omega}$  of the) partial derivative  $\partial^\alpha \delta$  fulfills Eq. (2.196) at all points  $\mathbf{x} \in \overline{\Omega}$ .*

### Weak integrability of Dirac delta functions.

Let us return to the case where  $\Omega$  is an arbitrary domain. The statement that follows refers to the notion of weak integrability for Banach valued functions (see the paragraph in Section 2.2; we refer, in particular, to Theorem 2.2).

**Proposition 2.51.** *Let  $r \in \mathbb{R}$ ,  $r > d/2$  and  $f \in L^2(\Omega)$ . Then the map  $\Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto f(\mathbf{x}) \delta_{\mathbf{x}}$  is weakly measurable and integrable with respect to the Lebesgue measure  $d\mathbf{x}$ ; moreover,*

$$\int_{\Omega} d\mathbf{x} f(\mathbf{x}) \delta_{\mathbf{x}} = f . \quad (2.212)$$

*Remark 2.14.* The integral in Eq. (2.212) should produce an element of  $\mathcal{H}^{-r}$ ; in fact,  $f \in L^2(\Omega) \equiv \mathcal{H}^0 \subset \mathcal{H}^{-r}$ .

*Proof.* Considerations about weak measurability and weak integrability involve the dual space of  $\mathcal{H}^{-r}$ , which is antilinearly isomorphic to  $\mathcal{H}^r$  via the map  $\mathcal{H}^r \rightarrow (\mathcal{H}^{-r})'$ ,  $g \mapsto \langle g | \cdot \rangle$  (as usual,  $\langle | \cdot \rangle$  indicates the extension (2.103) of the inner product of  $\mathcal{H} \equiv L^2(\Omega)$  to  $\mathcal{H}^{(2)}$ ). Let us now fix  $g \in \mathcal{H}^r$  arbitrarily. Then, for a.e.  $\mathbf{x} \in \Omega$  we have  $\langle g | f(\mathbf{x}) \delta_{\mathbf{x}} \rangle = f(\mathbf{x}) \overline{\langle \delta_{\mathbf{x}} | g \rangle} = f(\mathbf{x}) \overline{g(\mathbf{x})}$ , i.e., the map  $\Omega \rightarrow \mathbb{C}$ ,  $\mathbf{x} \mapsto \langle g | f(\mathbf{x}) \delta_{\mathbf{x}} \rangle$  coincides a.e. with  $f \overline{g}$ ; this map is clearly measurable and integrable (since  $f \in L^2(\Omega)$  and  $g \in \mathcal{H}^r \hookrightarrow \mathcal{H} \equiv L^2(\Omega)$ ). Therefore, the map  $\Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto f(\mathbf{x}) \delta_{\mathbf{x}}$  is weakly measurable; moreover, for all  $g \in \mathcal{H}^r$ , it is  $\int_{\Omega} d\mathbf{x} \langle g | f(\mathbf{x}) \delta_{\mathbf{x}} \rangle = \int_{\Omega} d\mathbf{x} f(\mathbf{x}) \overline{g(\mathbf{x})} = \langle g | f \rangle$ . This means that  $\mathbf{x} \mapsto f(\mathbf{x}) \delta_{\mathbf{x}}$  is weakly integrable, with integral  $f$ .  $\square$

### Complex conjugate of Dirac delta functions.

Let us consider the general framework outlined in subsection 2.5 for an abstract Hilbert space  $\mathcal{H}$  with a conjugation  $\mathcal{J}$ . Of course, in the setting considered in the present section, there is a natural conjugation on the basic Hilbert space  $\mathcal{H} = L^2(\Omega)$ : namely, the complex conjugation

$$\mathcal{J} : L^2(\Omega) \rightarrow L^2(\Omega) , \quad f \mapsto \mathcal{J}f := \bar{f} . \quad (2.213)$$

Needless to say, in this case the projectors  $\mathcal{P}_+$  and  $\mathcal{P}_-$  (see Eq. (2.68)) associated to  $\mathcal{J}$  are simply the maps associating to any given complex function  $f : \Omega \rightarrow \mathbb{C}$  its real part  $\Re f$  and its imaginary part  $\Im f$  multiplied by the imaginary unit, respectively; so,

$$\mathcal{P}_+ f = \Re f , \quad \mathcal{P}_- f = i \Im f . \quad (2.214)$$

Furthermore, it appears that  $\mathcal{J}$  commutes with the admissible operator  $\mathcal{A}$  associated to any given Schrödinger operator  $A := -\Delta + V$  ( $V : \Omega \rightarrow \mathbb{R}$ ); i.e.,  $\mathcal{A}$  is  $\mathcal{J}$ -real or, briefly, *real*. Therefore, we can consider the corresponding extension  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ , defined according to Proposition 2.25.

There holds the following result concerning the Dirac delta, which will be useful for the physical applications to be discussed in the next chapter.

**Lemma 2.52.** *Let  $\mathbf{x} \in \Omega$ . Then, for any multi-index  $\alpha$ , the  $\alpha$ -th derivative of the Dirac delta  $\partial^\alpha \delta_{\mathbf{x}}$  ( $\in \mathcal{H}^{-r}$ , for  $r > |\alpha| + d/2$ ) is invariant under the extended complex conjugation  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ , i.e.,*

$$\mathcal{J} \partial^\alpha \delta_{\mathbf{x}} = \partial^\alpha \delta_{\mathbf{x}} . \quad (2.215)$$

*Proof.* Let us choose  $j \in \mathbb{N}$ ,  $r \in \mathbb{R}$  such that  $|\alpha| \leq j$  and  $r > j + d/2$ ; then  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-r}$ . Let us recall that the extension  $\mathcal{J}$  can be characterized as follows: for each  $g \in \mathcal{H}^{-r}$ ,  $\mathcal{J}g$  is the unique element of  $\mathcal{H}^{-r}$  such that  $\langle \mathcal{J}g | f \rangle = \overline{\langle g | \mathcal{J}f \rangle}$  for all  $f \in \mathcal{H}^r$ . On the other hand, for any  $f \in \mathcal{H}^r \hookrightarrow C^j(\Omega)$ , one has

$$\langle \mathcal{J} \partial^\alpha \delta_{\mathbf{x}} | f \rangle = \overline{\langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{J}f \rangle} = \overline{(-1)^{|\alpha|} \partial^\alpha \bar{f}(\mathbf{x})} = (-1)^{|\alpha|} \partial^\alpha f(\mathbf{x}) = \langle \partial^\alpha \delta_{\mathbf{x}} | f \rangle ,$$

which suffices to infer the thesis. □

*Remark 2.15.* Lemma 2.52 continues to hold as well for points on the boundary  $\partial\Omega$  whenever the stricter assumptions (2.159) and (2.209) are met.

## 2.7 Integral kernels.

Let us consider the framework of the previous section; in particular, let  $\mathcal{D}_{\mathcal{A}} \subset L^2(\Omega)$  denote any admissible domain for the differential operator  $A = -\Delta + V$ , and consider the spaces  $(\mathcal{H}^r, \|\cdot\|_r)$  associated to the admissible operator  $\mathcal{A}$  (see Proposition 2.4). Next, let us consider a linear operator

$$\mathcal{B} : \text{Dom}(\mathcal{B}) \subset \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty} ; \quad (2.216)$$

in the sequel of this work we will be mainly interested in the case where  $\mathcal{B}$  fulfills the following condition, for some  $j \in \mathbb{N}$ :

$$\begin{aligned} &\text{there exists } \vartheta \in (0, +\infty) \text{ such that, for all } j_1, j_2 \in \mathbb{N} \text{ with } j_1 + j_2 \leq j, \\ &\mathcal{B} \text{ maps continuously } \mathcal{H}^{-(j_2+d/2+\vartheta)} \text{ to } \mathcal{H}^{j_1+d/2+\vartheta} \end{aligned} \quad (2.217)$$

(<sup>23</sup>). We refer to the above equation as *condition (2.217)<sub>j</sub>*.

*Remark 2.16.* i) Since  $\mathcal{H}^{j-j_2+d/2+\vartheta} \hookrightarrow \mathcal{H}^{j_1+d/2+\vartheta}$  for all  $j_1, j_2$  as in Eq. (2.217)<sub>j</sub>, it appears that this condition is equivalent to the following one:

$$\begin{aligned} &\text{there exists } \vartheta \in (0, +\infty) \text{ such that, for all } j_2 \in \mathbb{N} \text{ with } j_2 \leq j, \\ &\mathcal{B} \text{ maps continuously } \mathcal{H}^{-(j_2+d/2+\vartheta)} \text{ to } \mathcal{H}^{j-j_2+d/2+\vartheta}. \end{aligned} \quad (2.218)$$

ii) In particular, condition (2.217)<sub>0</sub> reads

$$\begin{aligned} &\text{there exists } \vartheta \in (0, +\infty) \text{ such that} \\ &\mathcal{B} \text{ maps continuously } \mathcal{H}^{-(d/2+\vartheta)} \text{ to } \mathcal{H}^{d/2+\vartheta}. \end{aligned} \quad (2.219)$$

iii) Of course, (2.217)<sub>j</sub> implies (2.217)<sub>i</sub> for all  $i \in \{0, \dots, j\}$ .

**Definition 2.53.** If the condition (2.217)<sub>0</sub> holds, the *integral kernel* associated to the operator  $\mathcal{B}$  is the map

$$\mathcal{B}(\cdot, \cdot) : \Omega \times \Omega \rightarrow \mathbb{C}, \quad (\mathbf{x}, \mathbf{y}) \mapsto \mathcal{B}(\mathbf{x}, \mathbf{y}) := \langle \delta_{\mathbf{x}} | \mathcal{B} \delta_{\mathbf{y}} \rangle \quad (2.220)$$

(where  $\langle \cdot | \cdot \rangle$  indicates the extension (2.103) of the inner product on  $\mathcal{H}$ . Note that, for  $\vartheta$  as in (2.217)<sub>0</sub>, one has  $\delta_{\mathbf{x}}, \delta_{\mathbf{y}} \in \mathcal{H}^{-(d/2+\vartheta)}$  and  $\mathcal{B}\delta_{\mathbf{y}} \in \mathcal{H}^{d/2+\vartheta}$ ).

Shortly afterwards, we will prove that the function (2.220) is continuous on  $\Omega \times \Omega$ , and even more regular if  $\mathcal{B}$  fulfills condition (2.217)<sub>j</sub> for some  $j > 0$  ( $j \in \mathbb{N}$ ). The following Lemma will be useful for the sequel.

**Lemma 2.54.** *Suppose  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  is a measurable function fulfilling condition (2.90) (i.e.,  $\sup_{\lambda \in \sigma(\mathcal{A})} \lambda^b |\phi(\lambda)| < +\infty$ ) for some  $b \in \mathbb{R}$ . If  $b > (j+d)/2$  for some  $j \in \mathbb{N}$ , then the operator  $\mathcal{B} := \phi(\mathcal{A})$  (extended to  $\mathcal{H}^{-\infty}$ ) fulfills condition (2.217)<sub>j</sub>.*

*Proof.* The thesis follows by an elementary application of Proposition 2.12.  $\square$

In the forthcoming subsection 2.7, we present a series of results describing some notable features of the integral kernels associated to a suitable class of operators. For brevity we choose to discuss these results only in the general setting corresponding to an arbitrary domain  $\Omega$  with  $V$  a smooth potential on it. Nonetheless, it appears from the related proofs that, whenever the stricter hypotheses (2.159) are fulfilled and suitable boundary

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<sup>23</sup>Let us stress that, within the general setting considered within the present work, there holds  $\mathcal{H}^{j_1+d/2+\vartheta} \hookrightarrow C^{j_1}(\Omega)$  (see Corollary 2.43); on the other hand, under the stricter assumptions (2.159), one can infer the stronger result  $\mathcal{H}^{j_1+d/2+\vartheta} \hookrightarrow C^{j_1}(\overline{\Omega})$  (see Corollary 2.45).



conditions (see, e.g., Eq. (2.209)) are prescribed, the results to be presented in the sequel can be easily generalized to describe the behaviour of the integral kernels up to the boundary. We refer to the subsequent subsection 2.7 for more details and further results related to this case.

### General results on integral kernels.

Let us present several results for the integral kernels associated to operators fulfilling condition (2.217)<sub>j</sub> (for some  $j \in \mathbb{N}$ ). These results apply, in particular, to operators of the form  $\mathcal{B} = \phi(\mathcal{A})$  as in Lemma 2.54.

**Lemma 2.55.** *Let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$ . Then,  $\mathcal{B}(\cdot, \cdot) \in C^j(\Omega \times \Omega)$ ; moreover, for any pair of multi-indices  $\alpha, \beta$  such that  $|\alpha| + |\beta| \leq j$  and for all  $\mathbf{x}, \mathbf{y} \in \Omega$ , one has*

$$\partial_1^\alpha \partial_2^\beta \mathcal{B}(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B} \partial^\beta \delta_{\mathbf{y}} \rangle \quad (2.221)$$

(where  $\partial_1$  and  $\partial_2$  represent derivatives with respect to the first and second argument, respectively).

*Proof.* First notice that each derivative of order  $\leq j$  of the kernel  $\mathcal{B}(\cdot, \cdot)$  involves (in an arbitrary order) differentiating  $\alpha_i$  times with respect to  $x^i$  and  $\beta_i$  times with respect to  $y^i$  (for  $i = 1, \dots, d$ ), where  $\alpha = (\alpha_1, \dots, \alpha_d)$  and  $\beta = (\beta_1, \dots, \beta_d)$  are such that  $|\alpha| + |\beta| \leq j$ . We generically write  $\partial^\gamma \mathcal{B}(\cdot, \cdot)$  for such a derivative. The thesis holds if we can show that  $\partial^\gamma \mathcal{B}(\cdot, \cdot) : \Omega \times \Omega \rightarrow \mathbb{C}$  exists, is continuous and has the explicit expression in the right-hand side of Eq. (2.221).

To this purpose, let us recall that both the extended inner product  $\langle \cdot | \cdot \rangle$  and the (linear) operator  $\mathcal{B}$  are continuous on the corresponding domains of definition; so, by linearity  $\partial^\gamma \mathcal{B}(\cdot, \cdot)$  exists and, for all  $(\mathbf{x}, \mathbf{y}) \in \Omega \times \Omega$ , we can write

$$\partial^\gamma \mathcal{B}(\mathbf{x}, \mathbf{y}) = \langle (\partial^\alpha \delta)(\mathbf{x}) | \mathcal{B}(\partial^\beta \delta)(\mathbf{y}) \rangle . \quad (2.222)$$

In consequence of this, the function  $\partial^\gamma \mathcal{B}(\cdot, \cdot)$  can be viewed as the composition of the maps

$$\begin{aligned} \delta^{(\alpha, \beta)} : \Omega \times \Omega &\rightarrow \mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{-(|\beta|+d/2+\vartheta)} , & (\mathbf{x}, \mathbf{y}) &\mapsto ((\partial^\alpha \delta)(\mathbf{x}), (\partial^\beta \delta)(\mathbf{y})) , \\ \mathfrak{B}^{(\alpha, \beta)} : \mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{-(|\beta|+d/2+\vartheta)} &\rightarrow \mathbb{C} , & (f, g) &\mapsto \langle f | \mathcal{B} g \rangle \end{aligned}$$

for some  $\vartheta \in (0, +\infty)$  such that Eq. (2.217) holds<sup>(24)</sup>. On the one hand, since the map  $\Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto \delta_{\mathbf{x}}$  is of class  $C^{j_0}$  for all  $r > j_0 + d/2$  (see Propositions 2.46 and 2.48), it appears that  $\delta^{(\alpha, \beta)}$  is continuous. On the other hand, let us recall that the operator  $\mathcal{B} : \mathcal{H}^{-(|\beta|+d/2+\vartheta)} \rightarrow \mathcal{H}^{|\alpha|+d/2+\vartheta}$  and the bilinear map  $\langle \cdot | \cdot \rangle : \mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{|\alpha|+d/2+\vartheta} \rightarrow \mathbb{C}$  are both continuous; this suffices to infer that  $\mathfrak{B}^{(\alpha, \beta)}$  is continuous as well. Summing

<sup>24</sup>Of course,  $\mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$  is equipped with the product of the Banach topologies of its factors.

up, the above considerations show that  $\partial^\gamma \mathcal{B}(\cdot, \cdot)$  is continuous since it is given by the composition of continuous functions.

To conclude, let us notice that Eq. (2.222) and the identity (2.196) for the derivatives  $(\partial^\alpha \delta)(\mathbf{x})$ ,  $(\partial^\beta \delta)(\mathbf{y})$  yield for  $\partial^\gamma \mathcal{B}(\cdot, \cdot)$  the expression in the right-hand side of Eq. (2.221), thus proving the thesis.  $\square$

**Proposition 2.56.** *Let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$  and let  $\alpha, \beta$  be any two multi-indices, each one of order  $\leq j$ .*

*i) Let  $f \in L^2(\Omega)$  and consider the  $(C^j)$  map  $\mathcal{B}f : \Omega \rightarrow \mathbb{C}$ . Then, for any  $\mathbf{x} \in \Omega$ , the map  $\Omega \rightarrow \mathbb{C}$ ,  $\mathbf{y} \mapsto \partial^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y})$  is integrable and*

$$(\partial^\alpha \mathcal{B}f)(\mathbf{x}) = \int_{\Omega} d\mathbf{y} (\partial_1^\alpha \mathcal{B})(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) ; \quad (2.223)$$

*in particular, if  $\alpha = \emptyset$ , this gives*

$$(\mathcal{B}f)(\mathbf{x}) = \int_{\Omega} d\mathbf{y} \mathcal{B}(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) . \quad (2.224)$$

*ii) For any fixed  $\mathbf{x} \in \Omega$ , consider the (continuous) map  $\partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) : \Omega \rightarrow \mathbb{C}$ ,  $\mathbf{y} \mapsto \partial_1^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y})$ ; then  $\partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) \in L^2(\Omega)$ .*

*iii) For any fixed  $\mathbf{y} \in \Omega$ , consider the (continuous) map  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) : \Omega \rightarrow \mathbb{C}$ ,  $\mathbf{x} \mapsto \partial_2^\beta \mathcal{B}(\mathbf{x}, \mathbf{y})$ ; this is given by*

$$\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) = (-1)^{|\beta|} \mathcal{B} \partial^\beta \delta_{\mathbf{y}} . \quad (2.225)$$

*Moreover, there exists  $\vartheta \in (0, +\infty)$  such that  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) \in \mathcal{H}^{j-|\beta|+d/2+\vartheta}$ .*

*Remark 2.17.* The last statement in item iii) of the above proposition allows to infer, in particular, that  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) \in L^2(\Omega)$  and  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) \in C^{j-|\beta|}(\Omega)$ . Furthermore, if  $j - |\beta| + d/2 + \vartheta \geq 2$ , there holds  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y}) \in \mathcal{H}^2 = \text{Dom}(\mathcal{A})$ , so that  $\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y})$  fulfills (at least in weak sense) the possible boundary conditions included in the definition of  $\mathcal{A}$  (see, e.g., Eq. (2.209)); we will return to this topic in subsection 2.7, where stricter assumptions are made for the domain  $\Omega$  and for the potential  $V$ .

*Proof.* In the sequel we always assume  $\vartheta \in (0, +\infty)$  and  $j \in \mathbb{N}$  to be as in Eq. (2.217).

i) Let  $f \in L^2(\Omega)$ . Due to Proposition 2.51 (here employed with  $r = d/2 + \vartheta > d/2$ ), the map  $\Omega \rightarrow \mathcal{H}^{-(d/2+\vartheta)}$ ,  $\mathbf{y} \mapsto f(\mathbf{y}) \delta_{\mathbf{y}}$  is weakly integrable and  $f = \int_{\Omega} d\mathbf{y} f(\mathbf{y}) \delta_{\mathbf{y}}$ . From here and from the continuity of  $\mathcal{B}$  between  $\mathcal{H}^{-(d/2+\vartheta)}$  and  $\mathcal{H}^{j+d/2+\vartheta}$ , we infer the weak integrability of the map  $\Omega \rightarrow \mathcal{H}^{j+d/2+\vartheta}$ ,  $\mathbf{y} \mapsto f(\mathbf{y}) \mathcal{B} \delta_{\mathbf{y}}$  and the relation  $\mathcal{B}f = \int_{\Omega} d\mathbf{y} f(\mathbf{y}) \mathcal{B} \delta_{\mathbf{y}}$  proved in Theorem 2.2. Now, fix a point  $\mathbf{x} \in \Omega$  and a multi-index  $\alpha$  of order  $\leq j$ . Since  $\langle \partial^\alpha \delta_{\mathbf{x}} | \cdot \rangle$  is a continuous linear form on  $\mathcal{H}^{j+d/2+\vartheta}$ , it follows that the map  $\Omega \rightarrow \mathbb{C}$ ,  $\mathbf{y} \mapsto f(\mathbf{y}) \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B} \delta_{\mathbf{y}} \rangle$  is integrable, and  $\langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B}f \rangle = \int_{\Omega} d\mathbf{y} f(\mathbf{y}) \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B} \delta_{\mathbf{y}} \rangle$ . Making explicit the definitions of  $\partial^\alpha \delta_{\mathbf{x}}$  and  $\partial_1^\alpha \mathcal{B}(\cdot, \cdot)$ , we can say that the map  $\Omega \rightarrow \mathbb{C}$ ,  $\mathbf{y} \mapsto \partial_1^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})$  is integrable, and that Eq. (2.224) holds.

ii) From item i) we know that  $\partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) f$  is integrable for each  $f \in L^2(\Omega)$ . The considerations in the proof of item i) also show that the map  $L^2(\Omega) \rightarrow \mathbb{C}$ ,  $f \mapsto \int_{\Omega} d\mathbf{y} \partial_1^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y}) f(\mathbf{y})$

is continuous (because  $\mathcal{B} \upharpoonright L^2(\Omega) : L^2(\Omega) \hookrightarrow \mathcal{H}^{-(d/2+\vartheta)} \rightarrow \mathcal{H}^{j+d/2+\vartheta}$  is continuous); so,  $\partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) \in L^2(\Omega)$  due to the Riesz representation theorem.

iii) First recall that  $\partial^\beta \delta_{\mathbf{y}} \in \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$  and  $\mathcal{B} : \mathcal{H}^{-(|\beta|+d/2+\vartheta)} \rightarrow \mathcal{H}^{j-|\beta|+d/2+\vartheta}$ , so that  $\mathcal{B}\partial^\beta \delta_{\mathbf{y}} \in \mathcal{H}^{j-|\beta|+d/2+\vartheta}$ . On the other hand, due to Eq. (2.221) and to the definition of  $\delta_{\mathbf{x}}$ , for all  $\mathbf{x} \in \Omega$  we have  $\partial_2^\beta \mathcal{B}(\mathbf{x}, \mathbf{y}) = (-1)^{|\beta|} \langle \delta_{\mathbf{x}} | \mathcal{B}\partial^\beta \delta_{\mathbf{y}} \rangle = (-1)^{|\beta|} (\mathcal{B}\partial^\beta \delta_{\mathbf{y}})(\mathbf{x})$ , whence the thesis (2.225).  $\square$

**Corollary 2.57.** *Let  $\mathcal{B}$  fulfill the condition (2.217)<sub>j</sub> for some  $j \in \mathbb{N}$  and assume  $\mathcal{B}_{\mathcal{H}} := (\mathcal{B} \upharpoonright \mathcal{H}) : \mathcal{H} \rightarrow \mathcal{H}$  to be of Hilbert-Schmidt type, i.e.,  $\mathcal{B}_{\mathcal{H}} \in \mathfrak{B}_2(\mathcal{H})$  <sup>(25)</sup>; moreover, let  $\mathcal{B}_{\mathcal{H}}(\cdot, \cdot)$  and  $\mathcal{B}(\cdot, \cdot)$  denote, respectively, the corresponding Hilbert-Schmidt kernel and the integral kernel introduced in Eq. (2.220). Then, there holds*

$$\mathcal{B}(\mathbf{x}, \mathbf{y}) = \mathcal{B}_{\mathcal{H}}(\mathbf{x}, \mathbf{y}) \quad \text{for a.e. } \mathbf{x}, \mathbf{y} \in \Omega. \quad (2.226)$$

*Proof.* First of all, let us recall that the Hilbert-Schmidt kernel  $\mathcal{B}_{\mathcal{H}}(\cdot, \cdot) \in L^2(\Omega \times \Omega)$  of  $\mathcal{B}_{\mathcal{H}}$  is the unique function such that, for all  $f \in \mathcal{H}$ , there holds (see Eq. (2.62))

$$(\mathcal{B}_{\mathcal{H}}f)(\mathbf{x}) = \int_{\Omega} d\mathbf{y} \mathcal{B}_{\mathcal{H}}(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) \quad (\text{for a.e. } \mathbf{x} \in \Omega).$$

Then, the thesis follows easily from the above relation and from Eq. (2.224) of Proposition 2.56, by the arbitrariness of  $f \in \mathcal{H}$  in both these identities.  $\square$

*Remark 2.18.* The above Corollary states that the usual notion of integral kernel for Hilbert-Schmidt operators and the different definition we introduced previously (using the Dirac delta elements  $\delta_{\mathbf{x}}, \delta_{\mathbf{y}} \in \mathcal{H}^{-r}$ ) do in fact coincide when both are well-defined.

**Proposition 2.58.** *Let  $\mathcal{B}$  be a linear continuous operator fulfilling the assumption (2.217)<sub>j</sub> for some  $j \in \mathbb{N}$  and some  $\vartheta \in (0, +\infty)$ . Consider a linear operator  $\mathcal{C} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  and assume that, for all  $j_1 \in \mathbb{N}$  with  $j_1 \leq j$ , there exists  $\vartheta' \in (0, +\infty)$  such that  $\mathcal{C}$  sends continuously  $\mathcal{H}^{j_1+d/2+\vartheta}$  into  $\mathcal{H}^{j_1+d/2+\vartheta'}$ . Then, for any multi-index  $\beta$  of order  $\leq j$  and for all  $\mathbf{y} \in \Omega$ , there holds*

$$\mathcal{C}(\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y})) = \partial_2^\beta (\mathcal{C}\mathcal{B})(\cdot, \mathbf{y}) \quad (2.227)$$

(this identity is meant to hold in  $\mathcal{H}^{j-|\beta|+d/2+\vartheta'} \hookrightarrow C^{j-|\beta|}(\Omega)$ ).

*Proof.* Eq. (2.227) can be formally derived by the following chain of equalities

$$\mathcal{C}(\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y})) = (-1)^{|\beta|} \mathcal{C}\mathcal{B}\partial^\beta \delta_{\mathbf{y}} = \partial_2^\beta (\mathcal{C}\mathcal{B})(\cdot, \mathbf{y}),$$

where the fundamental relation (2.225) has been used in both passages (for  $|\beta| \leq j_2$  and  $j_1 + j_2 \leq j$ ). More precisely, if  $\vartheta' > \vartheta$  one must consider the integral kernels corresponding to the continuous operators  $\mathcal{B} : \mathcal{H}^{-j_2+d/2+\vartheta} \rightarrow \mathcal{H}^{j_1+d/2+\vartheta}$  and  $\mathcal{C}\mathcal{B} : \mathcal{H}^{-(j_2+d/2+\vartheta)}$

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<sup>25</sup>Here, we are referring to the general theory reviewed in the final paragraph of Section 2.3, on page 24.

$\rightarrow (\mathcal{H}^{j_1+d/2+\vartheta'} \hookrightarrow) \mathcal{H}^{j_1+d/2+\vartheta}$ ; on the other hand, if  $\vartheta' < \vartheta$  one must use the identity (2.225) for the restrictions  $(\mathcal{B} \upharpoonright \mathcal{H}^{-j_2+d/2+\vartheta'}) : \mathcal{H}^{-(j_2+d/2+\vartheta')} (\hookrightarrow \mathcal{H}^{-(j_2+d/2+\vartheta)}) \rightarrow (\mathcal{H}^{j_1+d/2+\vartheta} \hookrightarrow) \mathcal{H}^{j_1+d/2+\vartheta'}$  and  $(\mathcal{CB} \upharpoonright \mathcal{H}^{-j_2+d/2+\vartheta'}) : \mathcal{H}^{-(j_2+d/2+\vartheta')} \rightarrow \mathcal{H}^{j_1+d/2+\vartheta'}$ .  $\square$

From now on, given any operator  $\mathcal{B} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  fulfilling condition (2.217)<sub>j</sub> for some  $j \in \mathbb{N}$  and some  $\vartheta \in (0, +\infty)$ , we always consider its restriction (indicated with the same symbol)  $\mathcal{B} \equiv \mathcal{B} \upharpoonright \mathcal{H}^{-(j+d/2+\vartheta)}$ ; this restriction sends continuously  $\mathcal{H}^{-(j+d/2+\vartheta)}$  into  $\mathcal{H}^{d/2+\vartheta}$ . Then, following the general considerations of subsection 2.5, we can consider the (Banach) adjoint of  $\mathcal{B}$ , i.e.,

$$\mathcal{B}^* : \mathcal{H}^{-(j+d/2+\vartheta)} \rightarrow \mathcal{H}^{d/2+\vartheta} . \quad (2.228)$$

The forthcoming Propositions 2.59 and 2.60 refer to this operator and to its kernel.

**Proposition 2.59.** *Let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$ ; then there hold the following results.*

- i) *The adjoint operator  $\mathcal{B}^*$  (see Eq. (2.228)) also fulfills the condition (2.217)<sub>j</sub>; therefore, Lemma 2.55 and Proposition 2.56 continue to hold with  $\mathcal{B}$  replaced by  $\mathcal{B}^*$ .*
- ii) *Let  $\alpha, \beta$  be any pair of multi-indices with  $|\alpha| + |\beta| \leq j$  and consider the kernels  $\mathcal{B}(\cdot, \cdot)$  and  $\mathcal{B}^*(\cdot, \cdot)$ ; then, for all  $\mathbf{x}, \mathbf{y} \in \Omega$ , there holds*

$$\partial_1^\alpha \partial_2^\beta \mathcal{B}^*(\mathbf{x}, \mathbf{y}) = \overline{\partial_1^\beta \partial_2^\alpha \mathcal{B}(\mathbf{y}, \mathbf{x})} . \quad (2.229)$$

*Proof.* i) Let  $\vartheta$  be as in Eq. (2.217); for any  $j_1, j_2 \in \mathbb{N}$  with  $j_1 + j_2 \leq j$ , we can consider the restrictions  $\mathcal{B} \upharpoonright \mathcal{H}^{-(j_2+d/2+\vartheta)}$  sending continuously  $\mathcal{H}^{-(j_2+d/2+\vartheta)}$  into  $\mathcal{H}^{j_1+d/2+\vartheta}$ . By definition, the corresponding Banach adjoints  $(\mathcal{B} \upharpoonright \mathcal{H}^{-(j_2+d/2+\vartheta)})^*$  send  $\mathcal{H}^{-(j_1+d/2+\vartheta)}$  into  $\mathcal{H}^{j_2+d/2+\vartheta}$ ; moreover, by construction, these maps coincide with the restrictions of the Banach adjoint (2.228)  $\mathcal{B}^* \upharpoonright \mathcal{H}^{-(j_1+d/2+\vartheta)}$ . This suffices to infer the thesis.

ii) As pointed out above, due to statement i) in the present proposition, Lemma 2.55 also holds for the kernel  $\mathcal{B}^*(\cdot, \cdot)$ ; in particular, the general identity (2.221) implies both  $\partial_1^\alpha \partial_2^\beta \mathcal{B}^*(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B}^* \partial^\beta \delta_{\mathbf{y}} \rangle$  and  $\partial_1^\beta \partial_2^\alpha \mathcal{B}(\mathbf{y}, \mathbf{x}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\beta \delta_{\mathbf{y}} | \mathcal{B} \partial^\alpha \delta_{\mathbf{x}} \rangle$ . Next, let us recall that the bilinear form  $\langle \cdot | \cdot \rangle$  is hermitian, so that  $\langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B}^* \partial^\beta \delta_{\mathbf{y}} \rangle = \overline{\langle \mathcal{B}^* \partial^\beta \delta_{\mathbf{y}} | \partial^\alpha \delta_{\mathbf{x}} \rangle}$ . The thesis follows noting that the basic relation (2.116) for the adjoint operator implies  $\langle \mathcal{B}^* \partial^\beta \delta_{\mathbf{y}} | \partial^\alpha \delta_{\mathbf{x}} \rangle = \langle \partial^\beta \delta_{\mathbf{y}} | \mathcal{B} \partial^\alpha \delta_{\mathbf{x}} \rangle$ .  $\square$

**Proposition 2.60.** *Let  $\mathcal{B}$  and  $\mathcal{C}$  be two operators both fulfilling the assumption (2.217)<sub>j</sub> for some given  $j \in \mathbb{N}$ , and consider the corresponding integral kernels. Then, for any pair of multi-indices  $\alpha, \beta$  with  $|\alpha| + |\beta| \leq j$  and for all  $\mathbf{x}, \mathbf{y} \in \Omega$ , there hold the following identities:*

$$\langle \partial_2^\alpha \mathcal{B}(\cdot, \mathbf{x}) | \partial_2^\beta \mathcal{C}(\cdot, \mathbf{y}) \rangle = \partial_1^\alpha \partial_2^\beta (\mathcal{B}^* \mathcal{C})(\mathbf{x}, \mathbf{y}) , \quad (2.230)$$

$$\langle \partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) | \partial_1^\beta \mathcal{C}(\mathbf{y}, \cdot) \rangle = \partial_2^\alpha \partial_1^\beta (\mathcal{CB}^*)(\mathbf{y}, \mathbf{x}) . \quad (2.231)$$

*Remark 2.19.* i) Due to Proposition 2.56, the functions  $\partial_2^\alpha \mathcal{B}(\cdot, \mathbf{x})$ ,  $\partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot)$ ,  $\partial_2^\alpha \mathcal{C}(\cdot, \mathbf{x})$ ,  $\partial_1^\alpha \mathcal{C}(\mathbf{x}, \cdot)$  (for any fixed  $\mathbf{x} \in \Omega$ ) all belong to  $L^2(\Omega)$ ; so, the expressions  $\langle \cdot | \cdot \rangle$  in the left-hand sides of Eq.s (2.230) (2.231) can both to be intended as usual inner products in  $L^2(\Omega)$ .

ii) Let us point out that the expressions in the right-hand sides of Eq.s (2.230) (2.231) does in fact make sense under the weaker assumption that the operator  $\mathcal{B}^* \mathcal{C}$  (or  $\mathcal{CB}^*$ )

possesses the property (2.217)<sub>j</sub>. This fact can be used to give meaning to the left-hand sides of the cited equations also for less regular operators  $\mathcal{B}, \mathcal{C}$ ; we will return on this topic in the following (see Remark 2.20).

*Proof.* Let us first prove Eq. (2.230); to this purpose, note that due to item iii) of Proposition 2.56 there holds

$$\langle \partial_2^\alpha \mathcal{B}(\cdot, \mathbf{x}) | \partial_2^\beta \mathcal{C}(\cdot, \mathbf{y}) \rangle = (-1)^{|\alpha|+|\beta|} \langle \mathcal{B} \partial^\alpha \delta_{\mathbf{x}} | \mathcal{C} \partial^\beta \delta_{\mathbf{y}} \rangle. \quad (2.232)$$

Now, consider the assumption (2.217)<sub>j</sub> for  $\mathcal{B}$  and  $\mathcal{C}$ ; for any  $i_1, i_2, j_1, j_2 \in \mathbb{N}$  with  $i_1 + i_2 \leq j$  and  $j_1 + j_2 \leq j$ , this assumption grants the existence of some  $\vartheta \in (0, +\infty)$  such that the maps  $\mathcal{B} : \mathcal{H}^{-(i_2+d/2+\vartheta)} \rightarrow \mathcal{H}^{i_1+d/2+\vartheta}$  ( $\hookrightarrow \mathcal{H}^{-(j_1+d/2+\vartheta)}$ ) and  $\mathcal{C} : \mathcal{H}^{-(j_2+d/2+\vartheta)} \rightarrow \mathcal{H}^{j_1+d/2+\vartheta}$  ( $\hookrightarrow \mathcal{H}^{-(j_2+d/2+\vartheta)}$ ) are both continuous <sup>(26)</sup>.

Due to the above considerations, the expression  $\langle | \rangle$  in the right-hand side of Eq. (2.232) can be interpreted in terms of the extension (2.103) of the inner product on  $\mathcal{H}$  (see Proposition 2.16) acting on  $\mathcal{H}^{-(j_1+d/2+\vartheta)} \times \mathcal{H}^{j_1+d/2+\vartheta}$ . Then, recalling that  $\mathcal{B} = \mathcal{B}^{**} \equiv (\mathcal{B}^*)^*$  (see item ii) of Lemma 2.22) and using the basic identity (2.116) for adjoint operators, it follows that

$$\langle \mathcal{B} \partial^\alpha \delta_{\mathbf{x}} | \mathcal{C} \partial^\beta \delta_{\mathbf{y}} \rangle = \langle (\mathcal{B}^*)^* \partial^\alpha \delta_{\mathbf{x}} | \mathcal{C} \partial^\beta \delta_{\mathbf{y}} \rangle = \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B}^* \mathcal{C} \partial^\beta \delta_{\mathbf{y}} \rangle. \quad (2.233)$$

Next, note that  $\mathcal{B}^* \mathcal{C} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  also fulfills the assumption (2.217)<sub>j</sub>: in fact,  $\mathcal{B}^* \mathcal{C}$  sends continuously  $\mathcal{H}^{-(j_2+d/2+\vartheta)}$  into  $\mathcal{H}^{j_1+d/2+\vartheta}$  for all  $j_1 + j_2 \leq j$  <sup>(27)</sup>. So, the last expression in Eq. (2.233) can be reformulated in terms of integral kernels giving

$$\langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B}^* \mathcal{C} \partial^\beta \delta_{\mathbf{y}} \rangle = (-1)^{|\alpha|+|\beta|} \partial_1^\alpha \partial_2^\beta (\mathcal{B}^* \mathcal{C})(\mathbf{x}, \mathbf{y}). \quad (2.234)$$

Summing up, Eq.s (2.232-2.234) yield Eq. (2.230).

In order to prove Eq. (2.231) let us first notice that, explicitating the inner product in  $L^2(\Omega)$  and using the identity (2.229) of Proposition 2.59, one infers

$$\begin{aligned} \langle \partial_1^\alpha \mathcal{B}(\mathbf{x}, \cdot) | \partial_1^\beta \mathcal{C}(\cdot, \mathbf{y}) \rangle &= \int_{\Omega} d\mathbf{z} \overline{\partial_1^\alpha \mathcal{B}(\mathbf{x}, \mathbf{z})} \partial_1^\beta \mathcal{C}(\mathbf{y}, \mathbf{z}) = \\ &= \int_{\Omega} d\mathbf{z} \partial_2^\alpha \mathcal{B}^*(\mathbf{z}, \mathbf{x}) \overline{\partial_2^\beta \mathcal{C}^*(\mathbf{z}, \mathbf{y})} = \langle \partial_2^\beta \mathcal{C}^*(\cdot, \mathbf{y}) | \partial_2^\alpha \mathcal{B}^*(\cdot, \mathbf{x}) \rangle. \end{aligned} \quad (2.235)$$

Then, the thesis follows using the previously discussed identity (2.230), making obvious substitutions and recalling that  $\mathcal{C}^{**} = \mathcal{C}$ .  $\square$

<sup>26</sup>Of course, the embeddings indicated within round brackets hold since they involve spaces of positive and negative orders on the left and right-hand sides respectively. Let us also point out that  $\mathcal{B}$  and  $\mathcal{C}$  may fulfill condition (2.217)<sub>j</sub> for different parameters  $\theta_{\mathcal{B}} \neq \theta_{\mathcal{C}} \in (0, +\infty)$ ; in this case, it suffices to put  $\theta := \min\{\theta_{\mathcal{B}}, \theta_{\mathcal{C}}\}$  in the previous considerations.

<sup>27</sup>To prove this statement, recall once more that the maps  $\mathcal{C} : \mathcal{H}^{-(j_2+d/2+\vartheta)} \rightarrow \mathcal{H}^{j_1+d/2+\vartheta}$  and  $\mathcal{B}^* : \mathcal{H}^{-(i_1+d/2+\vartheta)} \rightarrow \mathcal{H}^{i_2+d/2+\vartheta}$  are continuous and that there holds the continuous embedding  $\mathcal{H}^{j_1+d/2+\vartheta} \hookrightarrow \mathcal{H}^{-(j_2+d/2+\vartheta)}$  for all  $i_1, i_2, j_1, j_2 \in \mathbb{N}$  as above.

Let us now consider the extension  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  of the complex conjugation  $\mathcal{J} : \mathcal{H} \rightarrow \mathcal{H}$ ,  $f \mapsto \mathcal{J}f := \overline{f}$  (see Proposition 2.25). Then, there holds the following result, which we report here only for completeness.

**Lemma 2.61.** *Let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$ . Then, for any multi-index  $\beta$  of order  $\leq j$  and for all  $\mathbf{y} \in \Omega$ , there holds*

$$\overline{\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y})} = \partial_2^\beta (\mathcal{J}\mathcal{B}\mathcal{J}^{-1})(\cdot, \mathbf{y}) \quad (2.236)$$

(of course, also in this case this identity is meant to hold in  $\mathcal{H}^{j-|\beta|+d/2+\vartheta} \hookrightarrow C^{j-|\beta|}(\Omega)$ ; see below Eq. (2.227)).

*Proof.* The thesis follows straightforwardly from the chain of equalities

$$\overline{\partial_2^\beta \mathcal{B}(\cdot, \mathbf{y})} = (-1)^{|\beta|} \mathcal{J}\mathcal{B}\mathcal{J}^{-1} \mathcal{J} \partial_2^\beta \delta_{\mathbf{y}} = (-1)^{|\beta|} \mathcal{J}\mathcal{B}\mathcal{J}^{-1} \partial_2^\beta \delta_{\mathbf{y}} = \partial_2^\beta (\mathcal{J}\mathcal{B}\mathcal{J}^{-1})(\cdot, \mathbf{y})$$

which can be easily derived recalling the properties of the extended complex conjugation  $\mathcal{J}$ , along with the results of Proposition 2.56 and of Lemma 2.52.  $\square$

## The Dirichlet kernel. The heat, cylinder and modified cylinder kernels.

Let us keep all the notations of the previous sections; for any  $r \in \mathbb{R}$ ,  $\Sigma_r$  denotes again the strip  $\{s \in \mathbb{C} \mid \Re s > r\}$  (see Eq. (2.133)). Note that, for any  $s \in \Sigma_{d/2}$  there exists  $\vartheta > 0$  such that  $\Re s > d/2 + \vartheta$ , so that the operator  $\mathcal{A}^{-s}$  maps continuously  $\mathcal{H}^{-(d/2+\vartheta)}$  to  $\mathcal{H}^{d/2+\vartheta}$ . Then, the results obtained previously in the present section allow us to define the kernel

$$\mathcal{A}^{-s}(\cdot, \cdot) \in C^0(\Omega \times \Omega), \quad (\mathbf{x}, \mathbf{y}) \mapsto \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) := \langle \delta_{\mathbf{x}} | \mathcal{A}^{-s} \delta_{\mathbf{y}} \rangle. \quad (2.237)$$

**Definition 2.62.** For  $s \in \Sigma_{d/2}$ , the function  $\mathcal{A}^{-s}(\cdot, \cdot)$  is referred to as the *Dirichlet kernel* of  $\mathcal{A}$  of order  $s$ .

Next, let  $\mathbf{t} \in (0, +\infty)$ ; each of the operators  $e^{-\mathbf{t}\mathcal{A}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$  and  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$  maps continuously  $\mathcal{H}^{-(d/2+\vartheta)}$  to  $\mathcal{H}^{d/2+\vartheta}$  for any  $\vartheta \in \mathbb{R}$  (in particular, for  $\vartheta > 0$ ). Again, the previous results of this section allow us to define the kernels

$$e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot), e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\cdot, \cdot), (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\cdot, \cdot) \in C^0(\Omega \times \Omega); \quad (2.238)$$

these are such that, for example,

$$e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) := \langle \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle \quad \text{for all } \mathbf{x}, \mathbf{y} \in \Omega. \quad (2.239)$$

**Definition 2.63.** Let  $\mathbf{t} \in (0, +\infty)$ .  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\cdot, \cdot)$  and  $(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\cdot, \cdot)$  are referred to, respectively, as the *heat*, *cylinder* (or Poisson) and *modified cylinder kernel* of  $\mathcal{A}$  at  $\mathbf{t}$ .

Let us point out some properties of the above kernels.

**Proposition 2.64.** (Properties of the Dirichlet kernel). *Let  $j \in \mathbb{N}$  and let  $\alpha, \beta$  be any pair of multi-indices such that  $|\alpha| + |\beta| \leq j$ .*

*i) For all  $s \in \Sigma_{(j+d)/2}$ , the kernel  $\mathcal{A}^{-s}(\cdot, \cdot)$  is in  $C^j(\Omega \times \Omega)$  and there hold all the statements of Proposition 2.56. Moreover, for any  $\mathbf{x}, \mathbf{y} \in \Omega$ , one has*

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-\bar{s}}(\mathbf{x}, \mathbf{y}) = \partial_1^\beta \partial_2^\alpha \mathcal{A}^{-\bar{s}}(\mathbf{y}, \mathbf{x}) = \overline{\partial_1^\beta \partial_2^\alpha \mathcal{A}^{-s}(\mathbf{y}, \mathbf{x})}; \quad (2.240)$$

*ii) Let  $\vartheta \in (0, +\infty)$  and put*

$$r_{(\alpha\beta, \vartheta)} := \frac{|\alpha| + |\beta| + d}{2} + \vartheta; \quad (2.241)$$

*then, for all  $s \in \Sigma_{(j+d)/2+\vartheta}$ , there holds the pointwise bound (for  $\mathbf{x}, \mathbf{y} \in \Omega$ )*

$$|\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})| \leq \varepsilon^{-(\Re s - r_{(\alpha\beta, \vartheta)})} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)}. \quad (2.242)$$

*iii) Let  $s_1 \in \Sigma_{(j+d)/2}$ , so that  $\mathcal{A}^{-s_1}$  fulfills the assumption (2.217)<sub>j</sub> for some  $\vartheta \in (0, +\infty)$ ; moreover, let  $s_2 \in \Sigma_{-\vartheta/2}$ . Then, for any fixed  $\mathbf{y} \in \Omega$ , there holds*

$$\mathcal{A}^{-s_2}(\partial_2^\beta \mathcal{A}^{-s_1}(\cdot, \mathbf{y})) = \partial_2^\beta \mathcal{A}^{-(s_1+s_2)}(\cdot, \mathbf{y}) \quad (2.243)$$

*(for any  $\vartheta' \in (0, +\infty)$ , Eq. (2.243) can be meant to hold in  $\mathcal{H}^{j-|\beta|+d/2+\vartheta'} \hookrightarrow C^{j-|\beta|}(\Omega)$ ).*

*iv) For all  $s_1, s_2 \in \Sigma_{(j+d)/2}$  and for all  $\mathbf{x}, \mathbf{y} \in \Omega$ ,  $\partial_1^\alpha \mathcal{A}^{-s_1}(\mathbf{x}, \cdot), \partial_2^\beta \mathcal{A}^{-s_1}(\cdot, \mathbf{y}) \in L^2(\Omega)$  and*

$$\langle \partial_2^\alpha \mathcal{A}^{-s_1}(\cdot, \mathbf{x}) | \partial_2^\beta \mathcal{A}^{-s_2}(\cdot, \mathbf{y}) \rangle_{L^2} = \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-(\bar{s}_1+s_2)}(\mathbf{x}, \mathbf{y}), \quad (2.244)$$

$$\langle \partial_1^\alpha \mathcal{A}^{-s_1}(\mathbf{x}, \cdot) | \partial_1^\beta \mathcal{A}^{-s_2}(\mathbf{y}, \cdot) \rangle_{L^2} = \partial_2^\alpha \partial_1^\beta \mathcal{A}^{-(\bar{s}_1+s_2)}(\mathbf{y}, \mathbf{x}). \quad (2.245)$$

*v) For any fixed  $\mathbf{x}, \mathbf{y} \in \Omega$ , the map*

$$\Sigma_{(j+d)/2} \rightarrow \mathbb{C}, \quad s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \quad (2.246)$$

*is analytic. Moreover, for any  $n \in \mathbb{N}$  and  $s \in \Sigma_{(j+d)/2}$ , the kernel  $(\partial_s^n \mathcal{A}^{-s})(\cdot, \cdot) \equiv (\mathcal{A}^{-s}(-\ln \mathcal{A})^n)(\cdot, \cdot)$  belongs to  $C^j(\Omega \times \Omega)$  and*

$$\partial_1^\alpha \partial_2^\beta (\partial_s^n \mathcal{A}^{-s})(\mathbf{x}, \mathbf{y}) = \partial_s^n \left( \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \right). \quad (2.247)$$

*vi) Let  $s \in \Sigma_{(j+d)/2}$  and  $\beta$  be a multi-index of order  $\leq j$  such that  $j - |\beta| + d/2 > 2$ ; then, for any fixed  $\mathbf{y} \in \Omega$ ,  $\partial_2^\beta \mathcal{A}^{-s}(\cdot, \mathbf{y}) \in \text{Dom}(\mathcal{A})$  <sup>(28)</sup>.*

*Remark 2.20.* Regarding the statements of item iv), recall the general considerations of item ii) in Remark 2.19; in the present setting, the right-hand sides of both Eq.s (2.244) (2.245) do also make sense under the assumption  $s_1, s_2 \in \mathbb{C}$  with  $s_1 + s_2 \in \Sigma_{(j+d)/2}$ , which is weaker than the hypothesis  $s_1, s_2 \in \Sigma_{(j+d)/2}$ . This fact and other analogous considerations will be used in the following applications to construct the analytic continuation of certain expressions which can be represented in the form (2.244) (2.245); see Chapter 3.

<sup>28</sup>In particular, this allows to infer that the map  $\Omega \rightarrow \mathbb{C}, \mathbf{x} \mapsto \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})$  fulfills (in weak sense) the possible boundary conditions included in the definition of  $\mathcal{A}$ .

*Proof.* i) Let  $s \in \Sigma_{(j+d)/2}$ ; then, there exists  $\vartheta \in (0, +\infty)$  such that  $s > (j+d)/2 + \vartheta$  which also implies  $s > (j_1 + j_2 + d)/2 + \vartheta$  for all  $j_1, j_2 \in \mathbb{N}$  with  $j_1 + j_2 \leq j$ . Since  $\mathcal{A}^{-s}$  maps continuously  $\mathcal{H}^{-(j_2+d/2+\vartheta)}$  into  $\mathcal{H}^{j_1+d/2+\vartheta}$  for all  $j_1 + j_2 \leq j$ , Lemma 2.55 and Proposition 2.56 yield the first part of the thesis. On the other hand, the first identity in Eq. (2.240) follows straightforwardly from Proposition 2.59 and Corollary 2.24; the second identity in the cited equation follows from Corollary 2.26 and from Lemma 2.61, in view of the regularity of the kernels involved.

ii) Let again  $s, \vartheta$  be as in the proof of item i). Recall that due to Lemma 2.55, there holds  $\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{A}^{-s} \partial^\beta \delta_{\mathbf{y}} \rangle$ ; keeping in mind that the bilinear form  $\langle | \rangle : \mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{|\alpha|+d/2+\vartheta} \rightarrow \mathbb{C}$  is continuous (see Eq. (2.104)), this allows to infer

$$\begin{aligned} & |\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})| \\ & \leq \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\mathcal{A}^{-s} \partial^\beta \delta_{\mathbf{y}}\|_{|\alpha|+d/2+\vartheta} = \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{|\alpha|+d/2+\vartheta-2\Re s}, \end{aligned}$$

where the last equality can be derived using the second relation in Eq. (2.95). Then, the thesis follows using the bound (2.84) of Proposition 2.5.

iii) For all  $j_1 \in \mathbb{N}$  with  $j_1 \leq j$ , item i) of Corollary 2.13 implies  $\mathcal{A}^{-s_2}(\mathcal{H}^{j_1+d/2+\vartheta}) = \mathcal{H}^{j_1+d/2+\vartheta+2\Re s_2}$ . Furthermore, the hypothesis on  $s_2$  grants that  $\vartheta + 2\Re s_2 > \vartheta'$  for some  $\vartheta' > 0$ , so that  $\mathcal{H}^{j_1+d/2+\vartheta+2\Re s_2} \hookrightarrow \mathcal{H}^{j_1+d/2+\vartheta'}$ ; this allows to infer that the map  $\mathcal{A}^{-s_2} : \mathcal{H}^{j_1+d/2+\vartheta} \rightarrow \mathcal{H}^{j_1+d/2+\vartheta'}$  is continuous. Then, the thesis follows straightforwardly from Proposition 2.58.

iv) The statement  $\partial_1^\alpha \mathcal{A}^{-s_1}(\mathbf{x}, \cdot), \partial_2^\beta \mathcal{A}^{-s_1}(\cdot, \mathbf{y}) \in L^2(\Omega)$  follows from items ii) and iii) of Proposition 2.56, while Eq.s (2.244) (2.245) can be derived using Proposition 2.60.

v) It suffices to show that the map  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})$  is analytic on the strip  $\Sigma_{(j+d)/2+\vartheta}$  for each  $\vartheta \in (0, +\infty)$ . Recall that  $\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{A}^{-s} \partial^\beta \delta_{\mathbf{y}} \rangle$ , with  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-(|\alpha|+d/2+\vartheta)}$  and  $\partial^\beta \delta_{\mathbf{y}} \in \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$  (see item ii) of the present proof). So, the map  $\Sigma_{(j+d)/2} \ni s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})$  can be represented as the composition of the map  $\Sigma_{(|\alpha|+|\beta|+d)/2+\vartheta} \rightarrow \mathfrak{B}(\mathcal{H}^{-(|\beta|+d/2+\vartheta)}, \mathcal{H}^{|\alpha|+d/2+\vartheta}), s \mapsto \mathcal{A}^{-s} \upharpoonright \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$ , which is analytic due to Proposition 2.28, with the linear (continuous) form  $\mathfrak{B}(\mathcal{H}^{-(|\beta|+d/2+\vartheta)}, \mathcal{H}^{|\alpha|+d/2+\vartheta}) \rightarrow \mathbb{C}, \mathcal{B} \mapsto \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B} \partial^\beta \delta_{\mathbf{y}} \rangle$ ; this is sufficient to infer the thesis.

vi) The thesis follows easily from item iii) of Proposition 2.56 and from the considerations of the related Remark 2.17, noting that  $\partial_2^\beta \mathcal{A}^{-s}(\cdot, \mathbf{y}) \in \mathcal{H}^{j-|\beta|+d/2+\vartheta}$  for some  $\vartheta \in (0, +\infty)$ .  $\square$

**Proposition 2.65.** (Properties of the exponential kernels). *Let  $j \in \mathbb{N}$  and let  $\alpha, \beta$  be any two multi-indices with  $|\alpha| + |\beta| \leq j$ .*

i) *For all  $\mathbf{t} \in \Sigma_0$ , the kernel  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  is in  $C^\infty(\Omega \times \Omega)$  and there hold all the statements of Proposition 2.56 for any  $j \in \mathbb{N}$ ; moreover, for any  $\mathbf{x}, \mathbf{y} \in \Omega$ , one has*

$$\partial_1^\alpha \partial_2^\beta e^{-\bar{\mathbf{t}}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \partial_1^\beta \partial_2^\alpha e^{-\bar{\mathbf{t}}\mathcal{A}}(\mathbf{y}, \mathbf{x}) = \overline{\partial_1^\beta \partial_2^\alpha e^{-\mathbf{t}\mathcal{A}}(\mathbf{y}, \mathbf{x})}. \quad (2.248)$$

ii) *Let  $\vartheta \in (0, +\infty)$  and put again (see Eq. (2.241))*

$$r_{(\alpha, \beta, \vartheta)} := \frac{|\alpha| + |\beta| + d}{2} + \vartheta;$$



then, there holds the pointwise bound (for  $\mathbf{x}, \mathbf{y} \in \Omega$ )

$$|\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})| \leq \begin{cases} \left( \frac{r(\alpha, \vartheta)}{e^{\Re \mathbf{t}}} \right)^{r(\alpha, \vartheta)} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } 0 < \Re \mathbf{t} \leq \frac{r(\alpha, \vartheta)}{\varepsilon} \\ \varepsilon^{r(\alpha, \vartheta)} e^{-\varepsilon \Re \mathbf{t}} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } \Re \mathbf{t} > \frac{r(\alpha, \vartheta)}{\varepsilon} \end{cases}. \quad (2.249)$$

iii) For all  $\mathbf{t}_1, \mathbf{t}_2 \in \Sigma_0$  and for all fixed  $\mathbf{y} \in \Omega$ , there holds

$$e^{-\mathbf{t}_2 \mathcal{A}}(\partial_2^\beta e^{-\mathbf{t}_1 \mathcal{A}}(\cdot, \mathbf{y})) = \partial_2^\beta e^{-(\mathbf{t}_1 + \mathbf{t}_2) \mathcal{A}}(\cdot, \mathbf{y}). \quad (2.250)$$

iv) For all  $\mathbf{t}_1, \mathbf{t}_2 \in \Sigma_0$  and for all  $\mathbf{x}, \mathbf{y} \in \Omega$ ,  $\partial_1^\alpha e^{-\mathbf{t}_1 \mathcal{A}}(\mathbf{x}, \cdot), \partial_2^\beta e^{-\mathbf{t}_1 \mathcal{A}}(\cdot, \mathbf{y}) \in L^2(\Omega)$  and

$$\langle \partial_2^\alpha e^{-\mathbf{t}_1 \mathcal{A}}(\cdot, \mathbf{x}) | \partial_2^\beta e^{-\mathbf{t}_2 \mathcal{A}}(\cdot, \mathbf{y}) \rangle = \partial_1^\alpha \partial_2^\beta e^{-(\bar{\mathbf{t}}_1 + \mathbf{t}_2) \mathcal{A}}(\mathbf{x}, \mathbf{y}), \quad (2.251)$$

$$\langle \partial_1^\alpha e^{-\mathbf{t}_1 \mathcal{A}}(\mathbf{x}, \cdot) | \partial_1^\beta e^{-\mathbf{t}_2 \mathcal{A}}(\mathbf{y}, \cdot) \rangle = \partial_2^\alpha \partial_1^\beta e^{-(\bar{\mathbf{t}}_1 + \mathbf{t}_2) \mathcal{A}}(\mathbf{y}, \mathbf{x}). \quad (2.252)$$

v) For any fixed  $\mathbf{x}, \mathbf{y} \in \Omega$ , the map

$$\Sigma_0 \rightarrow \mathbb{C}, \quad \mathbf{t} \mapsto \partial_1^\alpha \partial_2^\beta (e^{-\mathbf{t}\mathcal{A}})(\mathbf{x}, \mathbf{y}) \quad (2.253)$$

is analytic.

vi) Let  $\mathbf{t} \in \Sigma_0$  and  $\beta$  be a multi-index; then, for any fixed  $\mathbf{y} \in \Omega$ ,  $\partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\cdot, \mathbf{y}) \in \text{Dom}(\mathcal{A})$  <sup>(29)</sup>.

Analogous results also hold for the kernels  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\cdot, \cdot), (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\cdot, \cdot)$ . In particular, in place of Eq. (2.249), for  $\mathbf{x}, \mathbf{y} \in \Omega$  there hold

$$|\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y})| \leq \quad (2.254)$$

$$\begin{cases} \left( \frac{2r(\alpha, \vartheta)}{e^{\Re \mathbf{t}}} \right)^{2r(\alpha, \vartheta)} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } 0 < \Re \mathbf{t} \leq \frac{2r(\alpha, \vartheta)}{\sqrt{\varepsilon}} \\ \varepsilon^{r(\alpha, \vartheta)} e^{-\sqrt{\varepsilon} \Re \mathbf{t}} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } \Re \mathbf{t} > \frac{2r(\alpha, \vartheta)}{\sqrt{\varepsilon}} \end{cases};$$

$$|\partial_1^\alpha \partial_2^\beta (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\mathbf{x}, \mathbf{y})| \leq \quad (2.255)$$

$$\begin{cases} \left( \frac{2r(\alpha, \vartheta) - 1}{e^{\Re \mathbf{t}}} \right)^{2r(\alpha, \vartheta) - 1} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } 0 < \Re \mathbf{t} \leq \frac{2r(\alpha, \vartheta) - 1}{\sqrt{\varepsilon}} \\ \varepsilon^{r(\alpha, \vartheta) - 1/2} e^{-\sqrt{\varepsilon} \Re \mathbf{t}} \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } \Re \mathbf{t} > \frac{2r(\alpha, \vartheta) - 1}{\sqrt{\varepsilon}} \end{cases}.$$

<sup>29</sup>In particular, this allows to infer that the map  $\Omega \rightarrow \mathbb{C}, \mathbf{x} \mapsto \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$  fulfills (in weak sense) the possible boundary conditions included in the definition of  $\mathcal{A}$ .

*Proof.* i) Fix  $\mathbf{t} \in (0, +\infty)$  and  $j \in \mathbb{N}$  arbitrarily; the operator  $e^{-\mathbf{t}\mathcal{A}}$  maps continuously  $\mathcal{H}^{-(j_2+d/2+\vartheta)}$  into  $\mathcal{H}^{j_1+d/2+\vartheta}$  for each  $\vartheta \in (0, +\infty)$  and for all  $j_1, j_2 \in \mathbb{N}$  (in particular, if  $j_1 + j_2 \leq j$ ). So, the integral kernel  $(e^{-\mathbf{t}\mathcal{A}})(\cdot, \cdot)$  is of class  $C^j$  by Lemma 2.55, and Proposition 2.56 holds for such  $j$ . Then, the first part of the thesis (i.e.,  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot) \in C^\infty(\Omega \times \Omega)$ ) follows from the arbitrariness of  $j \in \mathbb{N}$ . The first identity in Eq. (2.248) can be easily proved using Lemma 2.59 and Corollary 2.24; also in this case, the second identity in the cited equation follows from Corollary 2.26 and from Lemma 2.61, in view of the regularity of the kernels involved.

ii) First recall that, due to Lemma 2.55, we have  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \partial^\beta \delta_{\mathbf{y}} \rangle$ ; due to Eq. (2.104) for the bilinear form  $\langle \cdot | \cdot \rangle : \mathcal{H}^{-(|\alpha|+d/2+\vartheta)} \times \mathcal{H}^{|\alpha|+d/2+\vartheta} \rightarrow \mathbb{C}$  for any  $\vartheta \in (0, +\infty)$ , we have

$$|\partial_1^\alpha \partial_2^\beta (e^{-\mathbf{t}\mathcal{A}})(\mathbf{x}, \mathbf{y})| \leq \|\partial^\alpha \delta_{\mathbf{x}}\|_{-(|\alpha|+d/2+\vartheta)} \|e^{-\mathbf{t}\mathcal{A}} \partial^\beta \delta_{\mathbf{y}}\|_{|\alpha|+d/2+\vartheta}.$$

The thesis (2.249) follows easily noting that the bound (2.97) of Corollary 2.14 gives (with  $r_{(\alpha, \beta, \vartheta)}$  as in Eq. (2.241))

$$\|e^{-\mathbf{t}\mathcal{A}} \partial^\beta \delta_{\mathbf{y}}\|_{|\alpha|+d/2+\vartheta} \leq \begin{cases} \left(\frac{r_{(\alpha, \beta, \vartheta)}}{e^{\Re \mathbf{t}}}\right)^{r_{(\alpha, \beta, \vartheta)}} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } 0 < \Re \mathbf{t} \leq \frac{r_{(\alpha, \beta, \vartheta)}}{\varepsilon} \\ \varepsilon^{\frac{|\alpha|+|\beta|+d}{2}+\vartheta} e^{-\varepsilon \Re \mathbf{t}} \|\partial^\beta \delta_{\mathbf{y}}\|_{-(|\beta|+d/2+\vartheta)} & \text{for } \Re \mathbf{t} > \frac{|\alpha|+|\beta|+d+2\vartheta}{2\varepsilon} \end{cases}$$

iii) The thesis follows from Proposition 2.58 since  $e^{-\mathbf{t}\mathcal{A}}(\mathcal{H}^{-\infty}) = \mathcal{H}^{+\infty}$  for all  $\mathbf{t} \in \Sigma_0$  (see Corollary 2.14) and  $\mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^r$  for any  $r \in \mathbb{R}$  (see Proposition 2.8).

iv) Once more, the square-integrability of  $\partial_1^\alpha e^{-\mathbf{t}_1 \mathcal{A}}(\mathbf{x}, \cdot)$  and  $\partial_2^\beta e^{-\mathbf{t}_2 \mathcal{A}}(\cdot, \mathbf{y})$  follows from items ii) and iii) of Proposition 2.56, while Eq.s (2.251)–(2.252) can be derived using Proposition 2.60.

v) Due to item ii) of the present proof we have  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = (-1)^{|\alpha|+|\beta|} \langle \partial^\alpha \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \partial^\beta \delta_{\mathbf{y}} \rangle$ , with  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-(|\alpha|+d/2+\vartheta)}$ ,  $\partial^\beta \delta_{\mathbf{y}} \in \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$  for any  $r > j + d/2$ . So, the map  $\mathbf{t} \mapsto \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$  can be viewed as the composition of the map  $\Sigma_0 \rightarrow \mathfrak{B}(\mathcal{H}^{-(|\beta|+d/2+\vartheta)}, \mathcal{H}^{|\alpha|+d/2+\vartheta})$ ,  $\mathbf{t} \mapsto e^{-\mathbf{t}\mathcal{A}} \upharpoonright \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$ , which is analytic due to Proposition 2.29, with the linear (continuous) form  $\mathfrak{B}(\mathcal{H}^{-(|\beta|+d/2+\vartheta)}, \mathcal{H}^{|\alpha|+d/2+\vartheta}) \rightarrow \mathbb{C}$ ,  $\mathcal{B} \mapsto \langle \partial^\alpha \delta_{\mathbf{x}} | \mathcal{B} \partial^\beta \delta_{\mathbf{y}} \rangle$ ; this is sufficient to infer the thesis.

vi) Also in this case, the thesis follows noting that  $\partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\cdot, \mathbf{y}) \in \mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^2 \equiv \text{Dom}(\mathcal{A})$  (see, again, item iii) of Proposition 2.56 and Remark 2.17).  $\square$

## Heat and cylinder kernels as solutions of differential problems.

Assume again  $\Omega \subset \mathbb{R}^d$  to be an arbitrary domain and let  $\mathcal{A}$  be the admissible operator obtained restricting the differential operator  $A = -\Delta + V$  ( $V \in C^\infty(\Omega)$ ) to an admissible domain  $\mathcal{D}_{\mathcal{A}} \equiv \text{Dom}(\mathcal{A}) \subset L^2(\Omega)$  <sup>(30)</sup>. In the following, we will consider differential equations where more than one variable appear at the same time (namely,  $\mathbf{x}$  and  $\mathbf{y} \in \Omega$ );

<sup>30</sup>As a matter of fact, the results to be discussed in the present subsection continue to hold also if  $A$  is an otherwise generic, elliptic differential operator with smooth coefficients as in the footnote 21 of page 54.

in order to avoid confusion, we specify the variable to which the differential operator  $A$  is referred to by introducing the notation

$$A_{\mathbf{x}} := -\Delta_{\mathbf{x}} + V(\mathbf{x}) \quad (\mathbf{x} \in \Omega) \quad (2.256)$$

where, of course,  $\Delta_{\mathbf{x}}$  indicates the laplacian involving derivatives with respect to  $\mathbf{x}$ . Now, consider the heat and cylinder kernels which were introduced in the previous subsection as the integral kernels associated to the exponential operators  $e^{-\mathbf{t}\mathcal{A}}$  and  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$  (for  $\mathbf{t} \in (0, +\infty)$ ).

**Definition 2.66.** For any fixed  $\mathbf{y} \in \Omega$ , let us define the maps

$$K_{\mathbf{y}} : (0, +\infty) \times \Omega \rightarrow \mathbb{R}, \quad (\mathbf{t}, \mathbf{x}) \mapsto K_{\mathbf{y}}(\mathbf{t}; \mathbf{x}) := e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}), \quad (2.257)$$

$$T_{\mathbf{y}} : (0, +\infty) \times \Omega \rightarrow \mathbb{R}, \quad (\mathbf{t}, \mathbf{x}) \mapsto T_{\mathbf{y}}(\mathbf{t}; \mathbf{x}) := e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y}). \quad (2.258)$$

*Remark 2.21.* For any  $\mathbf{t} \in (0, +\infty)$ , there hold the following identities:

$$K_{\mathbf{y}}(\mathbf{t}; \cdot) = e^{-\mathbf{t}\mathcal{A}}\delta_{\mathbf{y}}, \quad T_{\mathbf{y}}(\mathbf{t}; \cdot) = e^{-\mathbf{t}\sqrt{\mathcal{A}}}\delta_{\mathbf{y}}; \quad (2.259)$$

note that the expressions on the right-hand sides of the above relations are, in fact, elements of  $\mathcal{H}^{+\infty} \hookrightarrow C^\infty(\Omega)$ . The fact that  $K_{\mathbf{y}}(\mathbf{t}; \cdot), T_{\mathbf{y}}(\mathbf{t}; \cdot) \in \mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^2 = \text{Dom}(\mathcal{A})$  also indicates that these functions fulfill the boundary conditions encoded in the definition of  $\text{Dom}(\mathcal{A})$ .

**Proposition 2.67.** Fix  $\mathbf{y} \in \Omega$ . Then,  $K_{\mathbf{y}}$  and  $T_{\mathbf{y}}$  possess the following properties:

$$\left\{ \begin{array}{ll} (\partial_{\mathbf{t}} + A_{\mathbf{x}}) K_{\mathbf{y}}(\mathbf{t}; \mathbf{x}) = 0 & \text{for } (\mathbf{t}, \mathbf{x}) \in (0, +\infty) \times \Omega \\ \lim_{\mathbf{t} \rightarrow 0^+} K_{\mathbf{y}}(\mathbf{t}; \cdot) = \delta_{\mathbf{y}} \text{ in } \mathcal{H}^{-d/2+\vartheta} & \text{for any } \vartheta \in (0, +\infty) \end{array} \right. ; \quad (2.260)$$

$$\left\{ \begin{array}{ll} (\partial_{\mathbf{t}\mathbf{t}} + A_{\mathbf{x}}) T_{\mathbf{y}}(\mathbf{t}; \mathbf{x}) = 0 & \text{for } (\mathbf{t}, \mathbf{x}) \in (0, +\infty) \times \Omega \\ \lim_{\mathbf{t} \rightarrow 0^+} T_{\mathbf{y}}(\mathbf{t}; \cdot) = \delta_{\mathbf{y}} \text{ in } \mathcal{H}^{-d/2+\vartheta} & \text{for any } \vartheta \in (0, +\infty) \end{array} \right. . \quad (2.261)$$

*Remark 2.22.* Let us stress that the first equations in both Eq.s (2.260) and (2.261) can be meant to hold pointwisely, since both the kernels  $K_{\mathbf{y}}$  and  $T_{\mathbf{y}}$  are smooth for  $(\mathbf{t}, \mathbf{x}) \in (0, +\infty) \times \Omega$  (see Remark 2.21 along with Proposition 2.65).

*Proof.* We are going to prove the equations in (2.260) (the proof of the analogous relations in (2.261) is similar and will not be reported here). We refer to Remark 2.21 for the proof of the second equation. On the other hand, let us fix  $\vartheta \in (0, +\infty)$  arbitrarily; then the first equation follows if we can rigorously justify the following chain of (formal) equalities

$$\begin{aligned} \partial_{\mathbf{t}} K_{\mathbf{y}}(\mathbf{t}; \mathbf{x}) &= \partial_{\mathbf{t}} \langle \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle \stackrel{1)}{=} \langle \delta_{\mathbf{x}} | \partial_{\mathbf{t}} e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle \stackrel{2)}{=} -\langle \delta_{\mathbf{x}} | \mathcal{A} e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle = \\ &\stackrel{3)}{=} -A_{\mathbf{x}} \langle \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle = -A_{\mathbf{x}} K_{\mathbf{y}}(\mathbf{t}; \mathbf{x}). \end{aligned}$$

As in the proof of statement ii) of Proposition 2.65, notice that for any fixed  $\mathbf{x}, \mathbf{y} \in \Omega$  the map  $\Sigma_0 \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto \langle \delta_{\mathbf{x}} | e^{-\mathbf{t}\mathcal{A}} \delta_{\mathbf{y}} \rangle$  can be interpreted as the composition of the analytic function  $\Sigma_0 \rightarrow \mathfrak{B}(\mathcal{H}^{-(d/2+\vartheta)}, \mathcal{H}^{d/2+\vartheta})$ ,  $\mathbf{t} \mapsto e^{-\mathbf{t}\mathcal{A}}$  with the linear form  $\mathfrak{B}(\mathcal{H}^{-(d/2+\vartheta)}, \mathcal{H}^{d/2+\vartheta}) \rightarrow \mathbb{C}$ ,  $\mathcal{B} \mapsto \langle \delta_{\mathbf{x}} | \mathcal{B} \delta_{\mathbf{y}} \rangle$ ; then, 1) follows by the linearity and by the continuity of the second map. Equality 2) follows easily from Proposition 2.29. To prove equality 3), just notice that for any  $f \in \mathcal{H}^{2+d/2+\vartheta} \hookrightarrow C^2(\Omega)$  there holds  $\langle \delta_{\mathbf{x}} | \mathcal{A}f \rangle = (\mathcal{A}f)(\mathbf{x}) = (Af)(\mathbf{x}) = A_{\mathbf{x}}f(\mathbf{x}) = A_{\mathbf{x}}\langle \delta_{\mathbf{x}} | f \rangle$ ; then, the thesis follows since  $e^{-\mathbf{t}\mathcal{A}}\delta_{\mathbf{y}} \in \mathcal{H}^{+\infty} \hookrightarrow \mathcal{H}^{2+d/2+\vartheta}$  (for any  $\mathbf{t} \in (0, +\infty)$ ).  $\square$

## Asymptotic behaviours of the heat and cylinder kernels.

Hereafter we report some facts on the asymptotic behaviour of the heat and cylinder kernels  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\cdot, \cdot)$  in the limits of small and large values of the parameter  $\mathbf{t} \in (0, +\infty)$ . Some of these facts can be easily inferred within the framework presented in this manuscript, in view of the results proved in the previous subsection 2.7. Moreover, we also take the chance to point out some more properties of the above mentioned kernels, which in the literature are well-known to hold and are closely related to the interpretation of  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  and  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\cdot, \cdot)$  as solutions of the differential problems (2.260)–(2.261) discussed previously in Proposition 2.67.

First of all, recall the bounds reported in Eq.s (2.249), (2.254) and (2.255).

The cited equations state the well-known exponential decay for  $\Re \mathbf{t} \rightarrow +\infty$  of the heat, cylinder and modified cylinder kernels, respectively. As a matter of fact, by a slight generalization of Proposition 2.65, the same behaviour can be easily proved to hold for both the spatial and  $t$ -derivatives of the kernels cited above.

The equations cited above also give bounds on the small- $t$  behaviour of the exponential kernels; these bounds have been derived using only the abstract functional analytic tools developed in the previous sections for the self-adjoint operator  $\mathcal{A}$ . As a matter of fact, since  $\mathcal{A}$  is a Schrödinger type differential operator  $-\Delta + V$ , acting in a (sufficiently regular) domain  $\Omega \subset \mathbb{R}^d$  (and, possibly, with suitable boundary conditions on  $\partial\Omega$ ), much more can be said about the asymptotic behaviour of the heat kernel for  $t \rightarrow 0^+$ . We refer to the monographies by Berline et al. [20], Calin et al. [33], Chavel [37], Davies [46], Gilkey [80] and Grigor'yan [82] (and to the works cited therein) for a complete and throughout analysis of this topic.

In the sequel we limit ourself to consider a particular case of Theorem 2.4 on page 39 in [32] (see also Lemma 2.1 in [116]): we focus the attention to the configurations described by the assumptions (2.159) and (2.209).

**Theorem 2.68.** *Let the assumptions (2.159) and (2.209) be fulfilled (so that Dirichlet boundary conditions are taken into account). Then, there exists a unique sequence of real-valued (smooth) functions  $a_n : \Omega \times \Omega \rightarrow \mathbb{R}$  ( $n \in \mathbb{N}$ ;  $a_0(\mathbf{x}, \mathbf{y}) \equiv 1$ ) such that, in the limit*

$\mathbf{t} \rightarrow 0^+$  for all  $\mathbf{x}, \mathbf{y} \in \Omega$ , there holds

$$\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}A}(\mathbf{x}, \mathbf{y}) = \partial_1^\alpha \partial_2^\beta \left( \frac{1}{(4\pi\mathbf{t})^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\mathbf{t}}} \sum_{n=1}^N a_n(\mathbf{x}, \mathbf{y}) \mathbf{t}^n \right) + \frac{e^{-\frac{\eta|\mathbf{x}-\mathbf{y}|^2}{4\mathbf{t}}}}{(4\pi\mathbf{t})^{d/2}} \mathbf{t}^{N-|\alpha|-|\beta|} O_{\eta,N}^{(\alpha,\beta)}(\mathbf{t}; \mathbf{x}, \mathbf{y}) \quad (2.262)$$

for any pair of multi-indices  $\alpha, \beta$ ,  $N \in \mathbb{N}$  with  $N > 2(|\alpha| + |\beta|) + d/2$ ,  $\eta \in (0, 1)$  and for some continuous function  $O_{\eta,N}^{(\alpha,\beta)} : [0, +\infty) \times \Omega \times \Omega \rightarrow \mathbb{C}$ .

*Remark 2.23.* i) The coefficients  $a_n$  ( $n \in \mathbb{N}$ ) introduced in the above theorem are usually referred to as *HMDS coefficients*, which is short for Hadamard-Minakshisundaram-DeWitt-Seeley after the authors who gave the earliest and most significant contributions to the study of the asymptotic behaviour of the heat kernel.

ii) Let us stress that the expression

$$K_0(\mathbf{t}; \mathbf{x}, \mathbf{y}) := \frac{1}{(4\pi\mathbf{t})^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\mathbf{t}}} \quad (2.263)$$

in Eq. (2.262) is just the heat kernel associated to the laplacian on the whole space  $\mathbb{R}^d$ .

iii) In view of points i) and v) of Proposition 2.65, Theorem 2.68 suggests the existence of a smooth function  $H : [0, +\infty) \times \Omega \times \Omega \rightarrow \mathbb{R}$  such that

$$e^{-\mathbf{t}A}(\mathbf{x}, \mathbf{y}) = \frac{1}{(4\pi\mathbf{t})^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\mathbf{t}}} H(\mathbf{t}; \mathbf{x}, \mathbf{y}) \quad \text{for all } \mathbf{t} \in (0, +\infty), \mathbf{x}, \mathbf{y} \in \Omega. \quad (2.264)$$

This actually occurs in many interesting examples. In the sequel, when necessary, we will assume existence of such a smooth  $H$ .

iv) Following [32], we refer to [152] and [37] for some generalizations of this theorem, also dealing with some settings involving unbounded domains and configurations where  $\Omega$  is a (curved) Riemannian manifold.

The corresponding small- $\mathbf{t}$  analysis for the cylinder kernel is more involved and less well-known. Starting from the expansion (2.262) for the heat kernel, Fulling [60, 73, 74, 76] (see also [13]) proved by means of Riesz summation methods the following result.

**Theorem 2.69.** *Let the assumptions (2.159) and (2.209) be fulfilled (so that Dirichlet boundary conditions are being considered). Then, there exists a unique pair of sequences of real-valued functions  $e_n, f_n : \Omega \rightarrow \mathbb{R}$  ( $n \in \mathbb{N}$ ) such that for any  $N \in \mathbb{N}$ , in the limit  $\mathbf{t} \rightarrow 0^+$  ( $\mathbf{t} \in (0, +\infty)$ ),  $\mathbf{x}, \mathbf{y} \in \Omega$  interior points), there holds*

$$e^{-\mathbf{t}\sqrt{A}}(\mathbf{x}, \mathbf{x}) = \frac{1}{\mathbf{t}^d} \left( \sum_{n=0}^N e_n(\mathbf{x}) \mathbf{t}^n + \sum_{\substack{n=d+1 \\ n-d \text{ odd}}}^N f_n(\mathbf{x}) \mathbf{t}^n \ln \mathbf{t} + O(\mathbf{t}^{N+1} \ln \mathbf{t}) \right). \quad (2.265)$$

Before proceeding, let us mention that the heat and cylinder kernels often admit asymptotic expansions of the forms (2.262), (2.265), even under assumptions weaker than those made in corresponding Theorems 2.68, 2.69. For these reason, in the following, expressions of the form (2.262) and (2.265) will often be assumed to hold as hypotheses.

## Integral representations of the Dirichlet kernel in terms of the exponential kernels.

Consider the Dirichlet kernel along with the heat, cylinder and modified cylinder kernels. Hereafter we use the methods developed in the previous subsections to give an alternative derivation of some identities known in the literature, relating  $\mathcal{A}^{-s}(\cdot, \cdot)$  to some integral transforms of the exponential kernels  $e^{-tA}(\cdot, \cdot)$ ,  $e^{-t\sqrt{A}}(\cdot, \cdot)$ ,  $(e^{-t\sqrt{A}}/\sqrt{A})(\cdot, \cdot)$ . More precisely, there holds the following proposition.

**Proposition 2.70.** *Let  $j \in \mathbb{N}$ ; then, for all  $s \in \Sigma_{(j+d)/2}$  and for any pair of multi-indices  $\alpha, \beta$  with  $|\alpha| + |\beta| \leq j$ , the following relations hold pointwisely for all  $\mathbf{x}, \mathbf{y} \in \Omega$  :*

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \, t^{s-1} \partial_1^\alpha \partial_2^\beta e^{-tA}(\mathbf{x}, \mathbf{y}) , \quad (2.266)$$

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(2s)} \int_0^{+\infty} dt \, t^{2s-1} \partial_1^\alpha \partial_2^\beta e^{-t\sqrt{A}}(\mathbf{x}, \mathbf{y}) , \quad (2.267)$$

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(2s-1)} \int_0^{+\infty} dt \, t^{2s-2} \partial_1^\alpha \partial_2^\beta (e^{-t\sqrt{A}}/\sqrt{A})(\mathbf{x}, \mathbf{y}) . \quad (2.268)$$

*Proof.* The thesis follows easily from Proposition 2.31 and from the relation (2.221) of Lemma 2.55, recalling that  $\partial^\alpha \delta_{\mathbf{x}} \in \mathcal{H}^{-(|\alpha|+d/2+\vartheta)}$  and  $\partial^\beta \delta_{\mathbf{x}} \in \mathcal{H}^{-(|\beta|+d/2+\vartheta)}$  for any pair of multi-indices  $\alpha, \beta$  with  $|\alpha| + |\beta| \leq j$  and any  $\vartheta \in (0, +\infty)$ .  $\square$

*Remark 2.24.* The above proposition allows to express the Dirichlet kernel and its spatial derivatives in terms of the Mellin transforms of the exponential kernels and of the corresponding derivatives. We review the theory of Mellin transforms and the methods allowing to construct their analytic continuations in the following Section 2.8.

## The case of a compact domain with smooth boundary.

In this subsection we restrict the attention to settings which fulfill the stronger regularity hypotheses (2.159), so that  $\Omega$  is bounded with boundary of class  $C^\infty$  and  $A = -\Delta + V$  with  $V \in C^\infty(\overline{\Omega})$ ; moreover, we assume (2.209) to hold, so that Dirichlet conditions are prescribed on the boundary  $\partial\Omega$ .

Let  $\mathcal{B} : \text{Dom}(\mathcal{B}) \subset \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  be an operator fulfilling the condition (2.217) $_j$ , for some  $j \in \mathbb{N}$ , so that

there exists  $\vartheta \in (0, +\infty)$  such that, for all  $j_1, j_2 \in \mathbb{N}$  with  $j_1 + j_2 \leq j$ ,  
 $\mathcal{B}$  maps continuously  $\mathcal{H}^{-(j_2+d/2+\vartheta)}$  to  $\mathcal{H}^{j_1+d/2+\vartheta}$ .

Keeping in mind the results discussed in the previous Section 2.6 for configurations of the above type, it can be easily proved that in this case the integral kernel  $\mathcal{B}(\cdot, \cdot)$  can be extended up to the boundary  $\partial\Omega$  of the domain  $\Omega$ ; more precisely, one can consider the map (compare with Eq. (2.220))

$$\mathcal{B}(\cdot, \cdot) : \overline{\Omega} \times \overline{\Omega} \rightarrow \mathbb{C} , \quad (\mathbf{x}, \mathbf{y}) \mapsto \mathcal{B}(\mathbf{x}, \mathbf{y}) := \langle \delta_{\mathbf{x}} | \mathcal{B} \delta_{\mathbf{y}} \rangle . \quad (2.269)$$

Moreover, all the regularity results derived in subsection 2.7 can be easily generalized to analogous formulations describing the boundary behaviour of the kernel (2.269). In particular, we have the following variant of Lemma 2.55.

**Lemma 2.71.** *Let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$ . Then,  $\mathcal{B}(\cdot, \cdot) \in C^j(\overline{\Omega} \times \overline{\Omega})$  (and Eq. (2.221) for the derivatives of  $\mathcal{B}(\cdot, \cdot)$ ) holds everywhere on  $\Omega$ .*

Other results on the integral kernel  $\mathcal{B}(\cdot, \cdot)$  are reported in the subsequent paragraphs.

### Boundary conditions.

Recall the results stated in item iii) of Proposition 2.56 and the facts mentioned in the related Remark 2.17. We mentioned therein that, generally, the kernel  $\mathcal{B}(\cdot, \cdot)$  fulfills in weak sense the possible boundary conditions which are taken into account in the definition of the domain  $\text{Dom}(\mathcal{A})$ .

The forthcoming Proposition 2.72 and the subsequent Remark 2.25 show that the the boundary conditions prescribed on  $\partial\Omega$  are, in fact, satisfied pointwisely.

**Proposition 2.72.** *Let the assumptions (2.159) and (2.209) hold; moreover, let (2.217)<sub>j</sub> hold for some  $j \in \mathbb{N}$ . Then, for any multi-index  $\alpha$  of order  $\leq j$  and for any  $\mathbf{y} \in \overline{\Omega}$ , there hold*

$$\partial_2^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{x} \in \partial\Omega} = 0 \quad \text{and} \quad \partial_1^\alpha \mathcal{B}(\mathbf{y}, \mathbf{x}) \Big|_{\mathbf{x} \in \partial\Omega} = 0. \quad (2.270)$$

*Proof.* First of all note that, in view of the symmetry relation (2.229), it suffices to prove the first identity in Eq. (2.270). So, let us consider the expression  $\partial_2^\alpha \mathcal{B}(\cdot, \mathbf{y})$  and notice that, due to Proposition 2.56 (see, in particular, Eq. (2.225)), there holds  $\partial_2^\alpha \mathcal{B}(\cdot, \mathbf{y}) = (-1)^{|\alpha|} \mathcal{B} \partial^\alpha \delta_{\mathbf{y}}$  for any  $\mathbf{y} \in \overline{\Omega}$ . On the other hand, recall that  $\partial^\alpha \delta_{\mathbf{y}} \in \mathcal{H}^{-(|\alpha|+d/2+\vartheta)}$  for any  $\vartheta > 0$ ; this, along with the assumption (2.217)<sub>j</sub>, allows to infer that  $\partial_2^\alpha \mathcal{B}(\cdot, \mathbf{y}) \in \mathcal{H}^{j-|\alpha|+d/2+\vartheta} \hookrightarrow \mathcal{H}^{d/2+\vartheta}$ . Then, the thesis follows recalling that  $\mathcal{H}^{d/2+\vartheta} \hookrightarrow H^{d/2+\vartheta}(\Omega) \hookrightarrow C^0(\overline{\Omega})$  (see Proposition 2.44 and the related Corollary 2.45), along with the results of item iii) of Proposition 2.56 (see also the related Remark 2.17).  $\square$

*Remark 2.25.* Analogous results can be derived for other kind of boundary conditions. More precisely, if Neumann conditions are prescribed on  $\partial\Omega$ , for any multi-index  $\alpha$  of order  $\leq j-1$  and for any  $\mathbf{y} \in \overline{\Omega}$ , there holds

$$\partial_{\mathbf{n}(\mathbf{x})} \partial_2^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{x} \in \partial\Omega} = 0 \quad \text{and} \quad \partial_{\mathbf{n}(\mathbf{x})} \partial_1^\alpha \mathcal{B}(\mathbf{y}, \mathbf{x}) \Big|_{\mathbf{x} \in \partial\Omega} = 0, \quad (2.271)$$

where  $\partial_{\mathbf{n}(\mathbf{x})}$  indicates the normal derivative at  $\mathbf{x} \in \partial\Omega$ .

On the other hand, when Robin boundary conditions are imposed on  $\partial\Omega$  (for some given smooth function  $h : \partial\Omega \rightarrow \mathbb{R}$ ), for any multi-index  $\alpha$  of order  $\leq j-1$  and for any  $\mathbf{y} \in \overline{\Omega}$ , there holds

$$\begin{aligned} (h(\mathbf{x}) + \partial_{\mathbf{n}(\mathbf{x})} \partial_2^\alpha \mathcal{B}(\mathbf{x}, \mathbf{y})) \Big|_{\mathbf{x} \in \partial\Omega} &= 0 \quad \text{and} \\ (h(\mathbf{x}) + \partial_{\mathbf{n}(\mathbf{x})} \partial_1^\alpha \mathcal{B}(\mathbf{y}, \mathbf{x})) \Big|_{\mathbf{x} \in \partial\Omega} &= 0. \end{aligned} \quad (2.272)$$

### Eigenfunction expansions and traces.

Let us first consider the topic *eigenfunction expansions*; to this purpose, let us recall that the notions of Hilbert-Schmidt kernel and of integral kernel introduced previously (using the Dirac delta elements), associated to a given suitable operator, do in fact coincide when both are well-defined (see Corollary 2.57). On the other hand, the kernels related to Hilbert-Schmidt operators can be expanded as in Eq. (2.63) using any assigned orthonormal basis of  $L^2(\Omega)$ . In the present setting it is natural to choose this basis as a set of eigenfunctions of  $\mathcal{A}$ . In fact, since  $\Omega$  is bounded and suitable boundary conditions (e.g., of Dirichlet, Neumann or Robin type) are prescribed on  $\partial\Omega$ , the operator  $\mathcal{A} := -\Delta + V$  has purely discrete spectrum and possesses such a basis of eigenfunctions. For the sake of definiteness, hereafter we will perform our analysis in the case of Dirichlet conditions; thus, from here to the end of the paragraph, besides boundedness of the domain  $\Omega$  and smoothness of its boundary  $\partial\Omega$ , we assume  $\mathcal{A}$  to have the features (2.209):

$$\begin{aligned} \text{Dom}(\mathcal{A}) &\equiv \mathcal{D}_{\mathcal{A}} = \{f \in H_0^1(\Omega) \mid (-\Delta + V)f \in L^2(\Omega)\} , \\ \sigma(\mathcal{A}) &\subset [\varepsilon, +\infty) \text{ for some } \varepsilon > 0 . \end{aligned}$$

In this case,  $\mathcal{A}$  is known to admit a complete orthonormal system of eigenfunctions  $(F_n)_{n \in \mathbb{N}}$  with positive eigenvalues, denoted with  $\omega_n^2$  where  $\omega_n > 0$ :

$$\mathcal{A}F_n = \omega_n^2 F_n . \quad (2.273)$$

The eigenvalues can be ordered so that

$$0 < \omega_0 \leq \omega_1 \leq \omega_2 \leq \dots \quad \text{and} \quad \lim_{n \rightarrow +\infty} \omega_n = +\infty , \quad (2.274)$$

where some of the inequalities in the first relation could in fact be equalities in order to deal with degenerate eigenvalues (see, e.g., [138], page 94, Proposition 5.12).

In this situation  $\sigma(\mathcal{A}) = \{\omega_n^2 \mid n \in \mathbb{N}\}$ . For each function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  (which is automatically measurable),  $\phi(\mathcal{A})$  is the operator with eigenfunctions  $F_n$  and eigenvalues  $\phi(\omega_n^2)$  defined on the linear subspace of  $L^2(\Omega)$  on which the eigenfunction expansion converges; more precisely,

$$\begin{aligned} \text{Dom}(\phi(\mathcal{A})) &= \left\{ f \in L^2(\Omega) \mid \sum_{n=0}^{+\infty} |\phi(\omega_n^2)|^2 |\langle F_n | f \rangle|^2 < +\infty \right\} , \\ \phi(\mathcal{A})f &= \sum_{n=0}^{+\infty} \phi(\omega_n^2) \langle F_n | f \rangle F_n \quad \text{for } f \in \text{Dom}(\phi(\mathcal{A})) \text{ (} L^2 \text{ convergence)} \end{aligned} \quad (2.275)$$

<sup>(31)</sup>. As a matter of fact, much more can be said about the eigenfunctions and eigenvalues of the admissible operator  $\mathcal{A}$ .

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<sup>31</sup>It is hardly the case to say how this setting can be used to represent  $\mathcal{A}$  as a multiplication operator: one equips  $\mathbb{N}$  with the counting measure  $\#$  and introduces the Hilbertian isomorphism  $\mathcal{I} : L^2(\Omega) \rightarrow$



**Theorem 2.73.** *i) For any  $n \in \mathbb{N}$ , there holds  $F_n \in C^\infty(\overline{\Omega})$ ; in addition, for any  $j \in \mathbb{N}$  and for any  $\vartheta \in (0, +\infty)$ , there exists a positive constant  $\Lambda_{j,\vartheta}$  such that*

$$\|F_n\|_{C^j} \leq \Lambda_{j,\vartheta} \omega_n^{j+d/2+\vartheta} \quad (2.276)$$

(where  $\|\cdot\|_{C^j}$  is the norm defined in Eq. (2.12)).

*ii) There holds the Weyl asymptotic relation*

$$\lim_{n \rightarrow +\infty} \frac{\omega_n^2}{n^{2/d}} = C_d, \quad C_d := \frac{4\pi}{|\Omega|^{-2/d}} \Gamma\left(\frac{d}{2}+1\right)^{2/d}. \quad (2.277)$$

*Proof.* i) Let  $n \in \mathbb{N}$ . For any  $r \in \mathbb{R}$  we have  $F_n \in \text{Dom}(\mathcal{A}^{r/2}) \subset \mathcal{H}^r$  and  $\mathcal{A}^{r/2}F_n = \omega_n^r F_n$ , whence  $\|F_n\|_r = \omega_n^r \|F_n\|_{L^2} = \omega_n^r$ . Now let  $j \in \mathbb{N}$ ,  $\vartheta \in (0, +\infty)$  and put  $r = j + d/2 + \vartheta$ ; then  $\mathcal{H}^r \hookrightarrow C^j(\overline{\Omega})$ , so there is a constant  $\Lambda_{j,\vartheta} > 0$  such that  $\|\cdot\|_{C^j} \leq \Lambda_{j,\vartheta} \|\cdot\|_r$  on  $\mathcal{H}^r$ . In particular  $F_n \in C^j(\overline{\Omega})$  and  $\|F_n\|_{C^j} \leq \Lambda_{j,\vartheta} \|F_n\|_r = \Lambda_{j,\vartheta} \omega_n^r$ ; this justifies Eq. (2.276). In these considerations  $j$  is any natural number; from  $F_n \in C^j(\overline{\Omega})$  for all  $j \in \mathbb{N}$  it follows that  $F_n \in C^\infty(\overline{\Omega})$ .

ii) See, e.g., [109], Theorem 5, page 189 and [55], §8.2, pages 99–101 for elementary derivations of Eq. (2.277).  $\square$

Now, let us consider a bounded function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ ; then  $\phi(\mathcal{A}) \in \mathfrak{B}(\mathcal{H})$ . The operators  $\mathcal{A}^\dagger \mathcal{A}$  and  $|\mathcal{A}|$  have eigenvalues  $|\phi(\omega_n^2)|^2$  and  $|\phi(\omega_n^2)|$ , respectively, (with eigenfunctions  $F_n$ ), so that

$$\text{Tr}(\mathcal{A}^\dagger \mathcal{A}) = \sum_{n=1}^{+\infty} |\phi(\omega_n^2)|^2, \quad (2.278)$$

$$\text{Tr}(|\phi(\mathcal{A})|) = \sum_{n=1}^{+\infty} |\phi(\omega_n^2)|. \quad (2.279)$$

Thus,  $\phi(\mathcal{A})$  is of Hilbert-Schmidt class (resp., trace class) if and only if the series (2.278) (resp., then series (2.279)) converges.

In the Hilbert-Schmidt case,  $\phi(\mathcal{A})$  has a kernel of class  $L^2$ ; this admits the expansion

$$\phi(\mathcal{A})(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{+\infty} \phi(\omega_n^2) F_n(\mathbf{x}) \overline{F}_n(\mathbf{y}) \quad (\mathbf{x}, \mathbf{y} \in \Omega), \quad (2.280)$$

---

$L^2(\mathbb{N}, \#)$  sending a function  $f$  into the sequence  $\mathcal{I}f$  of elements  $(\mathcal{I}f)_n = \langle F_n | f \rangle$  ( $n \in \mathbb{N}$ ). Then,  $\mathcal{I} \mathcal{A} \mathcal{I}^{-1}$  is the operator of multiplication by the sequence  $(\omega_n^2)_{n \in \mathbb{N}}$  and, for each measurable function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$ ,  $\mathcal{I} \phi(\mathcal{A}) \mathcal{I}^{-1}$  is the operator of multiplication by the sequence  $(\phi(\omega_n^2))_{n \in \mathbb{N}}$ .

All these statements are rather obvious; the purpose of this footnote is just to connect the case under analysis to the general “multiplication operator formalism” that we have employed to build the scale of Hilbert spaces associated to any positive self-adjoint operator.

converging in  $L^2(\Omega \times \Omega)$  (see subsection 2.3, especially Eq. (2.63)). In the trace class case we can of course define the trace of  $\phi(\mathcal{A})$ , given by

$$\text{Tr } \phi(\mathcal{A}) = \sum_{n=0}^{+\infty} \phi(\omega_n^2). \quad (2.281)$$

Hereafter we infer convergence results for the previous series, assuming  $\phi$  to fulfill a suitable decay condition at infinity, and using the results of Theorem 2.73. Our decay assumptions on  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  involve condition (2.90) (for suitable values of the real exponent  $b$ ), i.e.,

$$\sup_{\lambda \in \sigma(\mathcal{A})} \lambda^b |\phi(\lambda)| < +\infty.$$

Let us recall that kernel  $\phi(\mathcal{A})(\cdot, \cdot)$  is of class  $C^j(\overline{\Omega} \times \overline{\Omega})$  ( $j \in \mathbb{N}$ ) if (2.90) holds for a  $b$  such that  $b > (j + d)/2$  (see Lemma 2.54 and Lemma 2.55).

**Proposition 2.74.** *Assume  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  to fulfill Eq. (2.90) for some real  $b$ ; then the following holds.*

- i) *If  $b > d/4$ , then  $\phi(\mathcal{A})$  is of Hilbert-Schmidt class; so, the eigenfunction expansion (2.280) for the kernel  $\phi(\mathcal{A})(\cdot, \cdot)$  converges in  $L^2(\Omega \times \Omega)$ .*
- ii) *If  $b > j/2 + d$  for some  $j \in \mathbb{N}$ , then the eigenfunction expansion (2.280) for the kernel  $\phi(\mathcal{A})(\cdot, \cdot)$  converges absolutely in  $C^j(\overline{\Omega} \times \overline{\Omega})$ .*
- iii) *If  $b > d/2$ , then  $\phi(\mathcal{A})$  is of trace class.*
- iv) *If  $b > d$ , then*

$$\text{Tr } \phi(\mathcal{A}) = \int_{\Omega} d\mathbf{x} \phi(\mathcal{A})(\mathbf{x}, \mathbf{x}) \quad (2.282)$$

(note that the integrand function in the right-hand side is of class  $C^0(\overline{\Omega})$ ).

*Proof.* First of all, let us note that the assumption (2.90) and the Weyl asymptotic relation (2.277) imply the existence of some positive constants  $c, c'$  such that

$$\begin{aligned} |\phi(\omega_n^2)| &\leq c \omega_n^{-2b} && \text{for all } n \in \mathbb{N}, \\ \omega_n &\geq c' n^{1/d} && \text{for all } n \in \mathbb{N} \setminus \{0\}. \end{aligned} \quad (2.283)$$

Keeping in mind these facts, let us prove statements i)-iv).

i) Let  $b > d/4$ . To prove the thesis, on the grounds of Eq. (2.278) we must show that

$$\sum_{n=0}^{+\infty} |\phi(\omega_n^2)|^2 < +\infty.$$

On the other hand, due to Eq. (2.283), for each  $n \geq 1$  we have

$$|\phi(\omega_n^2)|^2 \leq \text{const. } \omega_n^{-4b} \leq \text{const. } n^{-4b/d}$$

and the series  $\sum_{n=1}^{+\infty} n^{-4b/d}$  is convergent.

ii) Let  $b > j/2 + d$ . To infer the thesis, it suffices prove the absolute convergence in  $C^j(\overline{\Omega} \times \overline{\Omega})$  of the series (2.280), i.e., that

$$\sum_{n=0}^{+\infty} |\phi(\omega_n^2)| \|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} < +\infty ; \quad (2.284)$$

here, in analogy with Eq. (2.12) we have set

$$\|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} := \max_{|\alpha|+|\beta|\leq j, \mathbf{x}, \mathbf{y} \in \overline{\Omega}} |\partial^\alpha F_n(\mathbf{x}) \overline{\partial^\beta F}_n(\mathbf{y})| . \quad (2.285)$$

If Eq. (2.284) is proved, we have convergence in  $C^j(\overline{\Omega} \times \overline{\Omega})$  of the series (2.280); but  $C^j(\overline{\Omega} \times \overline{\Omega}) \hookrightarrow L^2(\Omega \times \Omega)$ , so the sum of the series in  $C^j$  equals its sum in  $L^2$ , that we know to be the kernel of  $\phi(\mathcal{A})$ .

In order to derive Eq. (2.284), let us point out that that definition (2.285) yields automatically  $\|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} \leq \max_{j_1+j_2 \leq j} \|F_n\|_{C^{j_1}} \|F_n\|_{C^{j_2}}$ ; so, for any  $\vartheta \in (0, +\infty)$ , the bound in Eq. (2.276) gives

$$\|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} \leq \max_{j_1+j_2 \leq j} \left( \Lambda_{j_1, \vartheta} \Lambda_{j_2, \vartheta} \omega_n^{j_1+j_2+d+2\vartheta} \right) .$$

Moreover, recalling that  $\omega_n \geq \omega_0 > 0$  (for all  $n \in \mathbb{N}$ ), one has  $\omega_n^{j_1+j_2} = \omega_0^{j_1+j_2} (\omega_n/\omega_0)^{j_1+j_2} \leq \omega_0^{j_1+j_2} (\omega_n/\omega_0)^j = \omega_n^j / \omega_0^{j-j_1-j_2}$ , so that

$$\|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} \leq \left( \max_{j_1+j_2 \leq j} \frac{\Lambda_{j_1, \vartheta} \Lambda_{j_2, \vartheta}}{\omega_0^{j-j_1-j_2}} \right) \omega_n^{j+d+2\vartheta} . \quad (2.286)$$

Eq.s (2.283) and (2.286) imply the following, for each  $n \geq 1$ :

$$|\phi(\omega_n^2)| \|F_n(\cdot) \overline{F}_n(\cdot)\|_{C^j} \leq \text{const.} \omega_n^{-2b-j-d-2\vartheta} \leq \text{const.} n^{-\frac{2b-j-d-2\vartheta}{d}} .$$

Now the thesis follows noting that the series  $\sum_{n=1}^{+\infty} n^{-\frac{2b-j-d-2\vartheta}{d}}$  converges for any  $\vartheta \in (0, b - j/2 - d)$ .

iii) Let  $b > d/2$ . To prove the thesis, on the grounds of Eq. (2.279) we must show that

$$\sum_{n=0}^{+\infty} |\phi(\omega_n^2)| < +\infty ;$$

to this purpose, arguments very similar to the ones employed for item i) can be used.

iv) Let  $b > d$ . By item ii) with  $j = 0$ , the expansion (2.280) of the kernel  $\phi(\mathcal{A})(, )$  converges in  $C^0(\overline{\Omega} \times \overline{\Omega})$ . In particular, along the diagonal we have the expansion

$$\phi(\mathcal{A})(\mathbf{x}, \mathbf{x}) = \sum_{n=0}^{+\infty} \phi(\omega_n^2) |F_n(\mathbf{x})|^2 , \quad (2.287)$$

converging in  $C^0(\overline{\Omega})$ . Of course the map  $C^0(\overline{\Omega}) \ni f \mapsto \int_{\Omega} f$  is a continuous linear form with respect to the topology of  $C^0(\overline{\Omega})$ ; so, we can integrate term by term Eq. (2.287) and infer

$$\int_{\Omega} d\mathbf{x} \phi(\mathcal{A})(\mathbf{x}, \mathbf{x}) = \sum_{n=0}^{+\infty} \phi(\omega_n^2) \int_{\Omega} d\mathbf{x} |F_n(\mathbf{x})|^2 = \sum_{n=0}^{+\infty} \phi(\omega_n^2) = \text{Tr}(\mathcal{A}) .$$

□

**Corollary 2.75.** *i) For all  $s \in \Sigma_{d/4}$ , the operator  $\mathcal{A}^{-s}$  is of Hilbert-Schmidt class; so, its integral kernel  $\mathcal{A}^{-s}(\cdot, \cdot)$  admits the  $L^2$ -convergent eigenfunction expansion*

$$\mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{+\infty} \omega_n^{-2s} F_n(\mathbf{x}) \overline{F}_n(\mathbf{y}) \quad (\mathbf{x}, \mathbf{y} \in \Omega) . \quad (2.288)$$

*ii) For any  $j \in \mathbb{N}$  and for all  $s \in \Sigma_{j/2+d}$ , the eigenfunction expansion (2.288) for  $\mathcal{A}^{-s}(\cdot, \cdot)$  converges absolutely in  $C^j(\overline{\Omega} \times \overline{\Omega})$ .*

*iii) For all  $s \in \Sigma_{d/2}$ ,  $\mathcal{A}^{-s}$  is a trace class operator whose trace is given by the absolutely convergent series*

$$\text{Tr} \mathcal{A}^{-s} = \sum_{n=0}^{+\infty} \omega_n^{-2s} . \quad (2.289)$$

*In addition, the map  $\Sigma_{d/2} \ni s \mapsto \text{Tr} \mathcal{A}^{-s}$  is analytic <sup>(32)</sup>.*

*iv) For all  $s \in \Sigma_d$ , there holds*

$$\text{Tr} \mathcal{A}^{-s} = \int_{\Omega} d\mathbf{x} \mathcal{A}^{-s}(\mathbf{x}, \mathbf{x}) . \quad (2.290)$$

*Proof.* i)-ii) The thesis follows from items i) (resp. ii)) of Proposition 2.74 noting that, for any  $s \in \Sigma_{d/4}$  (resp.  $s \in \Sigma_{j/2+d}$ ), there exists some  $b > d/4$  (resp.  $b > j/2 + d$ ) such that  $\sup_{\lambda \in \sigma(\mathcal{A})} \lambda^{b-\Re s} < +\infty$  (e.g., choose  $b = d/4 + (\Re s - d/4)/2$ , resp.  $b = j/2 + d + (\Re s - j/2 - d)/2$ ).

iii) The series representation (2.289) and its absolute convergence can be inferred by arguments similar to those employed in the proof of items i) and ii), using item iii) of Proposition 2.74. To prove the analyticity of the map  $\Sigma_{d/2} \ni s \mapsto \text{Tr} \mathcal{A}^{-s}$ , it suffices to show the existence of the complex derivative  $\frac{d}{ds} \text{Tr} \mathcal{A}^{-s}$ ; in view of the series expansion (2.289), the last statement follows from Lebesgue dominated convergence theorem if there exists a summable, local dominant for  $\frac{d}{dt} \omega_n^{-2s} = -2\omega_n^{-2s} \ln \omega_n$ . To obtain such a dominant, let us fix  $s \in \Sigma_{d/2}$  and choose a constant  $\sigma \in (d/2, \Re s)$  (note that  $\Re s - \sigma > d/2$ ); then, for any  $s' \in \Sigma_{(\Re s - \sigma, \Re s + \sigma)}$ , it can be proved by elementary methods that  $|\omega_n^{-2s'} \ln \omega_n| \leq c \omega_n^{-2(\Re s - \sigma)}$  for some positive constant  $c$ , (depending on  $\omega_0$  and on the fixed parameters  $s, \sigma$ ). On the other hand, since  $\Re s - \sigma > d/2$ , the Weyl asymptotic relation (2.277) allows to infer that

<sup>32</sup>We also refer to [56, 84, 115, 116] for alternative derivations of this and other related results.

$\sum_{n=0}^{+\infty} \omega_n^{-2(\Re s - \sigma)} < +\infty$  (by arguments similar to those employed to prove the convergence of the series (2.289)). Summing up,  $c \omega_n^{-2(\Re s - \sigma)}$  yields the required local dominant, thus concluding the proof.

iv) The thesis follows by arguments similar to those employed in the proof of items i), ii), using item iv) of Proposition 2.74.  $\square$

**Corollary 2.76.** *The following statements hold for all  $\mathbf{t} \in \Sigma_0$ .*

i) *The operator  $e^{-\mathbf{t}\mathcal{A}}$  is of Hilbert-Schmidt class; so, its integral kernel  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  admits the  $L^2$ -convergent eigenfunction expansion*

$$e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{+\infty} e^{-\mathbf{t}\omega_n^2} F_n(\mathbf{x}) \overline{F}_n(\mathbf{y}) \quad (\mathbf{x}, \mathbf{y} \in \Omega). \quad (2.291)$$

ii) *The eigenfunction expansion (2.291) for  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  converges absolutely in  $C^\infty(\overline{\Omega} \times \overline{\Omega})$ .*

iii)  *$e^{-\mathbf{t}\mathcal{A}}$  is a trace class operator whose trace is given by the absolutely convergent series*

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} = \sum_{n=0}^{+\infty} e^{-\mathbf{t}\omega_n^2}. \quad (2.292)$$

*In addition, the map  $\Sigma_0 \ni \mathbf{t} \mapsto \text{Tr} e^{-\mathbf{t}\mathcal{A}}$  is analytic.*

iv) *There holds*

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} = \int_{\Omega} d\mathbf{x} e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{x}). \quad (2.293)$$

*Results analogous to statements i)-iv) hold, respectively, for the exponential operators  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$ .*

*Proof.* i)-ii) The thesis follows from items i) and ii) of Proposition 2.74 noting that, for any  $\mathbf{t} \in \Sigma_0$  and for all  $b \in \mathbb{R}$  there holds  $\sup_{\lambda \in \sigma(\mathcal{A})} \lambda^b e^{-\Re \mathbf{t} \lambda} < +\infty$ .

iii) Also in this case, arguments similar to those employed in the proof of items i) and ii) allow to obtain the series representation (2.292) and its absolute convergence, using again item iii) of Proposition 2.74. Next, let us prove the existence of the complex derivative  $\frac{d}{d\mathbf{t}} \text{Tr} e^{-\mathbf{t}\mathcal{A}}$ , granting the analyticity of the map  $\Sigma_0 \ni \mathbf{t} \mapsto \text{Tr} e^{-\mathbf{t}\mathcal{A}}$ . Notice that, in view of the series expansion (2.292), this fact follows from Lebesgue dominated convergence theorem if there exists a summable, local dominant for  $\frac{d}{d\mathbf{t}} e^{-\mathbf{t}\omega_n^2} = -\omega_n^2 e^{-\mathbf{t}\omega_n^2}$ . To obtain such a dominant let us fix, for any  $\mathbf{t} \in \Sigma_0$ , a constant  $T \in (0, \Re \mathbf{t})$ ; then, for any  $\mathbf{t}' \in \Sigma_{T_0}$ , there holds  $|\omega_n^2 e^{-\mathbf{t}'\omega_n^2}| \leq \omega_n^2 e^{-T\omega_n^2}$ . Now notice that  $\sum_{n=0}^{+\infty} \omega_n^2 e^{-T\omega_n^2} < +\infty$ , due to the Weyl asymptotic relation (2.277). Summing up,  $\omega_n^2 e^{-T\omega_n^2}$  yields the required dominant, thus yielding the thesis.

iv) Again, the thesis follows by arguments similar to those employed in the proof of items i), ii), using item iv) of Proposition 2.74.  $\square$

For completeness, let us mention that the topic of eigenfunction expansions for integral kernels associated to self-adjoint operators could also be addressed resorting to the theory

of rigged Hilbert spaces, within a much more general framework [78, 106, 17, 18]. As well-known, assuming there to exist a nuclear space  $\mathcal{N} \subset \mathcal{H}$  such that  $\mathcal{N} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{N}'$  is a Gelfand triplet, any self-adjoint operator  $\mathcal{B}$  on  $\mathcal{H}$  admits a complete system of generalized eigenfunctions belonging to  $\mathcal{N}'$  (see, e.g., [78], page 190, theorem 1) which can be used to give an expansion of the integral kernel associated to  $\mathcal{B}$ . Within this framework, much more can be said in the case of a self-adjoint operator  $\mathcal{A}$  given by the closure of an elliptic differential operator (such as the Schrödinger operator to be considered in Section 2.6) defined on any (not necessarily bounded) domain  $\Omega \subset \mathbb{R}^d$ , with minimal assumptions of regularity for its coefficients and for the boundary conditions. In particular, the corresponding generalized eigenfunctions are in fact sufficiently smooth; moreover, they can be used to give an expansion of the integral kernel associated to the operator  $\phi(\mathcal{A})$  for any function  $\phi : \sigma(\mathcal{A}) \rightarrow \mathbb{C}$  decreasing rapidly enough (see [17], page 398, Theorem 2.1 for more details).

### Asymptotic behaviours of the heat and cylinder traces

The results reported in this paragraph constitute the global counterparts of the local analysis described in subsection 2.7, where the topic of asymptotic behaviour of the heat and cylinder kernels was addressed.

More precisely, hereafter we report some results describing the small and large  $\mathbf{t}$  expansions of the heat and cylinder traces  $\text{Tr} e^{-\mathbf{t}\mathcal{A}}$ ,  $\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ .

**Proposition 2.77.** *The map  $\Sigma_0 \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto \text{Tr} e^{-\mathbf{t}\mathcal{A}}$  decays exponentially for  $\Re \mathbf{t} \rightarrow +\infty$ ; more precisely, for any fixed  $T \in (0, +\infty)$  and for all  $\mathbf{t} \in \Sigma_T$ , there holds*

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} \leq C_T e^{-\Re \mathbf{t} \omega_0^2}, \quad C_T := \text{Tr} e^{-T(\mathcal{A} - \omega_0^2 \mathbb{I})} < +\infty \quad (2.294)$$

(recall that  $\omega_0 > 0$  is the minimum eigenvalue of  $\mathcal{A}$ ;  $\mathbb{I}$  is the identity operator on  $\mathcal{H}$ ).

Analogous results hold for the other exponential traces  $\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $\text{Tr}(e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})$ .

*Proof.* Consider again the series expansion (2.292) and recall that  $\omega_n \geq \omega_0$ , for all  $n \in \mathbb{N}$ ; therefore, for all  $T > 0$  and for all  $\mathbf{t} \in \Sigma_T$ , there holds  $|e^{-\mathbf{t}\omega_n^2}| = e^{-\Re \mathbf{t} \omega_0^2} e^{-\Re \mathbf{t} (\omega_n^2 - \omega_0^2)} \leq e^{-\Re \mathbf{t} \omega_0^2} e^{-T(\omega_n^2 - \omega_0^2)}$ . Then, the thesis (2.294) follows noting that the Weyl asymptotic relation (2.277) implies  $\text{Tr} e^{-T(\mathcal{A} - \omega_0^2 \mathbb{I})} = \sum_{n=0}^{+\infty} e^{-T(\omega_n^2 - \omega_0^2)} < +\infty$ , by a slight variation of the arguments used in the proof of Corollary 2.76.  $\square$

Clearly, the previous proposition only deals with the large  $\mathbf{t}$  behaviour of the exponential traces. The small  $\mathbf{t}$  asymptotics of these traces is described instead by the forthcoming Theorems 2.78–2.79; these theorems contain results analogous to those reported in Theorems 2.68–2.69 of subsection 2.7 and, also in this case, we refer to [20, 80, 91] and to [73, 74, 76] for their respective proofs.

**Theorem 2.78.** *Let the assumptions (2.159) and (2.209) be fulfilled; moreover, assume  $V$  to be positive definite. Then there exists a unique sequence of real coefficients  $a_n \in \mathbb{R}$*

( $n \in \mathbb{N}$ ) such that for any  $N \in \mathbb{N}$ , in the limit  $\mathbf{t} \rightarrow 0^+$  ( $\mathbf{t} \in (0, +\infty)$ ), there holds

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} = \frac{1}{\mathbf{t}^{d/2}} \left( \sum_{n=1}^N a_n \mathbf{t}^{n/2} + O(\mathbf{t}^{\frac{N+1}{2}}) \right). \quad (2.295)$$

**Theorem 2.79.** *Let the assumptions (2.159) and (2.209) be fulfilled; moreover, assume  $V$  to be positive definite. Then, there exist a unique pair of sequences  $e_n, f_n \in \mathbb{R}$  ( $n \in \mathbb{N}$ ) such that, for any  $N \in \mathbb{N}$  and for  $\mathbf{t} \rightarrow 0^+$  ( $\mathbf{t} \in (0, +\infty)$ ), there holds*

$$\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}} = \frac{1}{\mathbf{t}^d} \left( \sum_{n=0}^N e_n \mathbf{t}^n + \sum_{\substack{n=d+1 \\ n-d \text{ odd}}}^N f_n \mathbf{t}^n \ln \mathbf{t} + O(\mathbf{t}^{N+1} \ln \mathbf{t}) \right). \quad (2.296)$$

### Integral representations for $\text{Tr} \mathcal{A}^{-s}$ .

The forthcoming Proposition 2.80 allows to express the trace  $\text{Tr} \mathcal{A}^{-s}$  in terms of some integral transforms related to the exponential traces  $\text{Tr} e^{-\mathbf{t}\mathcal{A}}$ ,  $\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $\text{Tr} (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})$ , thus giving a global analogous of Proposition 2.70.

**Proposition 2.80.** *Let the assumptions (2.159) and (2.209) be fulfilled (so that Dirichlet boundary conditions are prescribed on  $\partial\Omega$ ); then, for all  $s \in \Sigma_{d/2}$  there hold*

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \mathbf{t}^{s-1} \text{Tr} e^{-\mathbf{t}\mathcal{A}}, \quad (2.297)$$

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(2s)} \int_0^{+\infty} dt \mathbf{t}^{2s-1} \text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}}, \quad (2.298)$$

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(2s-1)} \int_0^{+\infty} dt \mathbf{t}^{2s-2} \text{Tr} (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}). \quad (2.299)$$

*Proof.* As an example, we show how to derive Eq. (2.297). To this purpose, recall once more the series expansions (2.289)–(2.292) for  $\text{Tr} \mathcal{A}^{-s}$  and  $\text{Tr} e^{-\mathbf{t}\mathcal{A}}$ , respectively; these allow to rephrase Eq. (2.297) as

$$\sum_{n=0}^{+\infty} \omega_n^{-2s} = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \mathbf{t}^{s-1} \sum_{n=0}^{+\infty} e^{-\mathbf{t}\omega_n^2}. \quad (2.300)$$

Therefore, in view of the identity  $z^{-s} = \frac{1}{\Gamma(s)} \int_0^{+\infty} dt \mathbf{t}^{s-1} e^{-tz}$  (see [122], page 139, Eq. 5.9.1), the thesis follows if the integral and the series in Eq. (2.300) can be interchanged. In fact, the mentioned operation can be performed in consequence of the Fubini-Tonelli theorem [134] since

$$\sum_{n=0}^{+\infty} \int_0^{+\infty} dt |\mathbf{t}^{s-1} e^{-\mathbf{t}\omega_n^2}| = \sum_{n=0}^{+\infty} \omega_n^{-2\Re s} < +\infty,$$

where the finiteness of the last expression is granted by item ii) of Corollary 2.75.  $\square$

## 2.8 Mellin transforms and their analytic continuation.

### General definitions and some basic relations.

Let us first fix a few notations to be employed throughout the present section. We indicate with  $\overline{\mathbb{R}}$  the system of extended real numbers, i.e.,

$$\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\} \equiv [-\infty, +\infty] ; \quad (2.301)$$

moreover, for any pair  $r_1, r_2 \in \overline{\mathbb{R}}$  with  $r_1 < r_2$ , we put

$$\Sigma_{(r_1, r_2)} := \{s \in \mathbb{C} \mid r_1 < \Re s < r_2\} . \quad (2.302)$$

If  $r_2 = +\infty$ , in accordance with Eq. (2.133), we use the short-hand notation

$$\Sigma_{r_1} \equiv \Sigma_{(r_1, +\infty)} . \quad (2.303)$$

**Definition 2.81.** Let  $r_1, r_2 \in \overline{\mathbb{R}}$  with  $r_1 < r_2$ . A measurable function  $F : (0, +\infty) \rightarrow \mathbb{C}$  is said to be of *type*  $(r_1, r_2)$  if the map  $(0, +\infty) \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto \mathbf{t}^{s-1} F(\mathbf{t})$  is integrable for all  $s \in \Sigma_{(r_1, r_2)}$ ; we use the notation

$$\mathcal{M}_{(r_1, r_2)} := \{F : (0, +\infty) \rightarrow \mathbb{C} \mid F \text{ is of type } (r_1, r_2)\} \quad (\mathcal{M}_{r_1} \equiv \mathcal{M}_{(r_1, +\infty)}) . \quad (2.304)$$

For  $F \in \mathcal{M}_{(r_1, r_2)}$  and  $s \in \Sigma_{(r_1, r_2)}$ , we put

$$\mathfrak{M}[F](s) := \int_0^{+\infty} dt \, \mathbf{t}^{s-1} F(\mathbf{t}) , \quad (2.305)$$

and refer to the map  $\mathfrak{M}[F] : \Sigma_{(r_1, r_2)} \rightarrow \mathbb{C}$ ,  $s \mapsto \mathfrak{M}[F](s)$  as the *Mellin transform* of  $F$ ; the complex domain  $\Sigma_{(r_1, r_2)}$  will be called the *strip of definition* of  $\mathfrak{M}[F]$ .

*Remark 2.26.* The whole theory of Mellin transforms could be formulated with much more generality; for example, one could only replace the function  $F$  with a distribution-like object acting on some suitable space of test functions. As a matter of fact, many of the results discussed in the present subsection continue to hold also in this generalized framework (for further details on this topic, see, e.g., [157, 30]). Nevertheless, such a broader generality is unnecessary in the present work and will therefore be neglected: we only consider the Mellin transform of ordinary, Lebesgue-integrable functions, since this is the case of interest for the applications to be studied in the following.

**Lemma 2.82.** (Operational relations). *Let  $F : (0, +\infty) \rightarrow \mathbb{C}$ . Then, for all  $r_1, r_2 \in \overline{\mathbb{R}}$  with  $r_1 < r_2$  the following results are fulfilled.*

*i) Let  $a \in (0, +\infty)$  and consider the function*

$$F_a : (0, +\infty) \rightarrow \mathbb{C} , \quad t \mapsto F_a(\mathbf{t}) := F(a\mathbf{t}) . \quad (2.306)$$



Then, there hold

$$F_a \in \mathcal{M}_{(r_2, r_1)} \Leftrightarrow F \in \mathcal{M}_{(r_1, r_2)} ; \quad (2.307)$$

$$\mathfrak{M}[F_a](s) = a^{-s} \mathfrak{M}[F](s) \quad \text{for all } s \in \Sigma_{(r_1, r_2)} . \quad (2.308)$$

ii) Let  $a \in \mathbb{R} \setminus \{0\}$  and consider the function

$$G_a : (0, +\infty) \rightarrow \mathbb{C} , \quad \mathbf{t} \mapsto G_a(\mathbf{t}) := F(\mathbf{t}^a) . \quad (2.309)$$

Then, there hold

$$G_a \in \mathcal{M}_{(ar_2, ar_1)} \Leftrightarrow F \in \mathcal{M}_{(r_1, r_2)} ; \quad (2.310)$$

$$\mathfrak{M}[G_a](s) = \frac{1}{|a|} \mathfrak{M}[F]\left(\frac{s}{a}\right) \quad \text{for all } s \in \Sigma_{(ar_1, ar_2)} . \quad (2.311)$$

iii) Let  $\alpha \in \mathbb{C}$  and consider the function

$$H_\alpha : (0, +\infty) \rightarrow \mathbb{C} , \quad \mathbf{t} \mapsto H_\alpha(\mathbf{t}) = \mathbf{t}^\alpha F(\mathbf{t}) . \quad (2.312)$$

Then, there hold

$$H_\alpha \in \mathcal{M}_{(r_1 - \Re \alpha, r_2 - \Re \alpha)} \Leftrightarrow F \in \mathcal{M}_{(r_1, r_2)} ; \quad (2.313)$$

$$\mathfrak{M}[H_\alpha](s) = \mathfrak{M}[F](s + \alpha) \quad \text{for all } s \in \Sigma_{(r_1 - \Re \alpha, r_2 - \Re \alpha)} . \quad (2.314)$$

*Proof.* All the statements i)-iii) follow from Definition 2.81 by simple changes of the variable of integration, suitably defined in view of the explicit expressions (2.306), (2.309) and (2.312) for the functions  $F_a$ ,  $G_a$  and  $H_\alpha$  in terms of  $F$ .

As an example, let us give a few more details about the derivation of Eq. (2.311). First note that, Eq. (2.309) and the definition (2.305) of Mellin transform give  $\mathfrak{M}[G_a](s) = \int_0^{+\infty} dt \, \mathbf{t}^{s-1} F(\mathbf{t}^a)$ ; making the change of variable  $\mathbf{t} \mapsto \mathbf{t}^{1/a}$  <sup>(33)</sup>, one infers  $\mathfrak{M}[G_a](s) = \frac{1}{|a|} \int_0^{+\infty} dt \, \mathbf{t}^{\frac{s}{a}-1} F(\mathbf{t})$ . Then, Eq. (2.311) follows recalling again the definition (2.305).  $\square$

**Lemma 2.83.** Let  $F \in L_{loc}^1(0, +\infty)$  and assume that, for some  $r_1, r_2 \in \overline{\mathbb{R}}$  with  $r_1 < r_2$ ,

$$F(\mathbf{t}) = \begin{cases} O(\mathbf{t}^{-r_1}) & \text{for } \mathbf{t} \rightarrow 0^+ , \\ O(\mathbf{t}^{-r_2}) & \text{for } \mathbf{t} \rightarrow +\infty . \end{cases} \quad (2.315)$$

Then,  $F \in \mathcal{M}_{(r_1, r_2)}$ .

*Remark 2.27.* In particular, if  $r_1 = -\infty$  or  $r_2 = +\infty$ , the notations  $F(\mathbf{t}) = O(\mathbf{t}^{+\infty})$  for  $\mathbf{t} \rightarrow 0^+$  and  $F(\mathbf{t}) = O(\mathbf{t}^{-\infty})$  for  $\mathbf{t} \rightarrow +\infty$  in Eq. (2.315) mean, respectively,  $F(\mathbf{t}) = O(\mathbf{t}^r)$  and  $F(\mathbf{t}) = O(\mathbf{t}^{-r})$  for each  $r \in (0, +\infty)$ .

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<sup>33</sup>Of course, the restriction on the real parameter  $a$  in both items i) and ii) are necessary in order to guarantee that the change of variables to be employed in the proof (such as  $\mathbf{t} \mapsto \mathbf{t}^{1/a}$ ) are well defined.

*Proof.* First note that, for any  $T_1, T_2 \in (0, +\infty)$ , there holds the following decomposition:

$$\int_0^{+\infty} dt |\mathbf{t}^{s-1} F(\mathbf{t})| = \int_0^{T_1} dt |\mathbf{t}^{s-1} F(\mathbf{t})| + \int_{T_1}^{T_2} dt |\mathbf{t}^{s-1} F(\mathbf{t})| + \int_{T_2}^{+\infty} dt |\mathbf{t}^{s-1} F(\mathbf{t})|. \quad (2.316)$$

By definition,  $F$  is of type  $(r_1, r_2)$  if and only if the integral in the left-hand side of the above equation is finite for all  $s \in \Sigma_{(r_1, r_2)}$ ; this happens if and only if each of the integrals in the right-hand side of Eq. (2.316) are finite, since the integrand functions are all positive. Hereafter we prove the last statement which, according to the previous considerations, gives the thesis.

Of course, the assumption (2.315) means that there exist  $T_1^*, T_2^* \in (0, +\infty)$  and a pair of positive constants  $M_1, M_2$  such that

$$|F(\mathbf{t})| \leq \begin{cases} M_1 \mathbf{t}^{-r_1} & \text{for } 0 < \mathbf{t} < T_1^* \\ M_2 \mathbf{t}^{-r_2} & \text{for } \mathbf{t} > T_2^* \end{cases};$$

this fact allows to infer easily the bounds

$$\begin{aligned} \int_0^{T_1^*} dt |\mathbf{t}^{s-1} F(\mathbf{t})| &\leq M_1 \frac{(T_1^*)^{\Re s - r_1}}{\Re s - r_1} && \text{for all } s \in \mathbb{C} \text{ with } \Re s > r_1, \\ \int_{T_2^*}^{+\infty} dt |\mathbf{t}^{s-1} F(\mathbf{t})| &\leq M_2 \frac{(T_2^*)^{\Re s - r_2}}{r_2 - \Re s} && \text{for all } s \in \mathbb{C} \text{ with } \Re s < r_2. \end{aligned}$$

Next note that, for  $T_1^*, T_2^* \in (0, +\infty)$  as above and for all  $s \in \mathbb{C}$ , there holds

$$\int_{T_1^*}^{T_2^*} dt |\mathbf{t}^{s-1} F(\mathbf{t})| \leq \max((T_1^*)^{\Re s - 1}, (T_2^*)^{\Re s - 1}) \int_{T_1^*}^{T_2^*} dt |F(\mathbf{t})| < +\infty,$$

where the finiteness of the integral on the right-hand side is granted by the assumption  $F \in L_{loc}^1(0, +\infty)$ .

Summing up, we have shown that the three integrals on the right-hand side of Eq. (2.316) are all finite at the same time for  $s \in \mathbb{C}$  with  $r_1 < \Re s < r_2$ , i.e., for  $s \in \Sigma_{(r_1, r_2)}$ ; as anticipated above, this yields the thesis.  $\square$

*Remark 2.28.* The arguments presented in the proof of Lemma 2.83 allow to infer the results discussed hereafter, giving a partial converse of the cited lemma.

On the one hand, the assumption  $F \in L_{loc}^1(0, +\infty)$  is in fact a necessary condition in order to have  $F \in \mathcal{M}_{(r_1, r_2)}$  for some  $r_1, r_2 \in \mathbb{R}$  ( $r_1 < r_2$ ) <sup>(34)</sup>.

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<sup>34</sup>To prove this fact note that, for any  $T_1, T_2 \in (0, +\infty)$  and for all  $s \in \mathbb{C}$ , there holds

$$\int_{T_1}^{T_2} dt |F(\mathbf{t})| \leq \max(T_1^{1-\Re s}, T_2^{1-\Re s}) \int_{T_1}^{T_2} dt |\mathbf{t}^{s-1} F(\mathbf{t})|.$$

On the other hand, it appears that the restrictions  $\Re s > r_1$  and  $\Re s < r_2$  descend, respectively, from the small and large  $\mathbf{t}$  behaviour of  $F$ ; more precisely, the following bounds must hold:

$$\begin{aligned} r_1 &\geq \inf \{r \in \mathbb{R} \mid \mathbf{t}^{r-1} f(\mathbf{t}) \in L^1(0, T) \text{ for some } T > 0\} ; \\ r_2 &\leq \sup \{r \in \mathbb{R} \mid \mathbf{t}^{r-1} f(\mathbf{t}) \in L^1(T, +\infty) \text{ for some } T > 0\} . \end{aligned} \quad (2.317)$$

**Proposition 2.84.** *Let  $r_1, r_2 \in \overline{\mathbb{R}}$  with  $r_1 < r_2$  and let  $F \in \mathcal{M}_{(r_1, r_2)}$ . Then, the Mellin transform  $\mathfrak{M}[F]$  of  $F$  is analytic in the strip  $\Sigma_{(r_1, r_2)}$ ; moreover, for any  $k \in \mathbb{N}$  and for all  $s \in \Sigma_{(r_1, r_2)}$ , there holds*

$$\frac{d^k \mathfrak{M}[F]}{ds^k}(s) = \int_0^{+\infty} dt \mathbf{t}^{s-1} (\ln \mathbf{t})^k F(\mathbf{t}) . \quad (2.318)$$

*Proof.* It suffices to prove that Eq. (2.318) holds for any  $k \in \mathbb{N}$  and for all  $s \in \Sigma_{(r_1, r_2)}$ ; indeed, for  $k = 1$  this fact shows, in particular, that  $\mathfrak{M}[f]$  is holomorphic on the strip  $\Sigma_{(r_1, r_2)}$ , hence analytic therein.

To derive Eq. (2.318), first consider the definition (2.305) of  $\mathfrak{M}[f]$  and note that  $\partial_s^k \mathbf{t}^{s-1} = \mathbf{t}^{s-1} (\ln \mathbf{t})^k$ ; then, it appears that Eq. (2.318) follows from the Lebesgue dominated convergence theorem if, locally for  $s \in \Sigma_{(r_1, r_2)}$ , the map  $(0, +\infty) \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto \mathbf{t}^{s-1} (\ln \mathbf{t})^k F(\mathbf{t})$  admits an integrable dominant function (independent of  $s$ ). To prove the last statement, let us fix  $s_0 \in (r_1, r_2)$  arbitrarily and choose  $\vartheta > 0$  so that  $s_0 \pm 2\vartheta \in (r_1, r_2)$  (such a  $\vartheta$  always exists since  $(r_1, r_2)$  is open); for any  $k \in \mathbb{N}$ , there exists a pair of positive constants  $C_1, C_2$  (depending on  $\vartheta, k$ ) such that <sup>(35)</sup>

$$|(\ln \mathbf{t})^k| \leq \begin{cases} C_1 \mathbf{t}^{-\vartheta} & \text{for } \mathbf{t} \in (0, 1), \\ C_2 \mathbf{t}^{\vartheta} & \text{for } \mathbf{t} \in (1, +\infty). \end{cases}$$

Then, for all  $s \in \Sigma_{(s_0 - \vartheta, s_0 + \vartheta)}$  it follows that

$$|\mathbf{t}^{s-1} (\ln \mathbf{t})^k F(\mathbf{t})| \leq C_1 |\mathbf{t}^{s_0 - 2\vartheta - 1} F(\mathbf{t})| + C_2 |\mathbf{t}^{s_0 + 2\vartheta - 1} F(\mathbf{t})| . \quad (2.319)$$

Since  $F \in \mathcal{M}_{(r_1, r_2)}$  and we have chosen  $\vartheta > 0$  such that  $s_0 \pm 2\vartheta \in (r_1, r_2)$ , the right-hand side of the inequality (2.319) gives a dominant function which is integrable over  $(0, +\infty)$ ; due to the above considerations, this completes the proof.  $\square$

*Remark 2.29.* The previous Proposition 2.84 grants the analyticity of the Mellin transform  $\mathfrak{M}[F]$  of any given function  $F \in \mathcal{M}_{(r_1, r_2)}$  inside the open strip  $\Sigma_{(r_1, r_2)}$ . Then, it is natural to try and extend  $\mathfrak{M}[F]$  to a wider region of the complex plane by means of analytic continuation, a topic we discuss in the remainder of the present section; more precisely, we present three main methods allowing to construct the mentioned analytic continuation of  $\mathfrak{M}[F]$ , under suitable (increasingly stricter) hypotheses for the function  $F$ .

<sup>35</sup>It can be show by elementary methods that the optimal choice for both  $C_1$  and  $C_2$  is

$$C_1 = C_2 = \left( \frac{k}{\vartheta e} \right)^k .$$

### Analytic continuation of Mellin transforms.

**Proposition 2.85.** (First method for analytic continuation: asymptotic expansion). *Let  $F \in L^1_{loc}(0, +\infty)$ . Assume there exist  $N, P \in \mathbb{N}$  and two families of coefficients  $\mathbf{a}_n, \mathbf{f}_{np}$  ( $n \in \{0, \dots, N+1\}$ ,  $p \in \{0, \dots, P\}$ ) with*

$$\mathbf{a}_n \in \mathbb{R}, \quad \mathbf{a}_0 < \mathbf{a}_1 < \dots < \mathbf{a}_N < \mathbf{a}_{N+1} \quad \text{and} \quad \mathbf{f}_{np} \in \mathbb{C}, \quad (2.320)$$

such that there holds the asymptotic expansion

$$F(\mathbf{t}) = \sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \mathbf{t}^{\mathbf{a}_n} (\ln \mathbf{t})^p + O(\mathbf{t}^{\mathbf{a}_{N+1}}) \quad \text{for } \mathbf{t} \rightarrow 0^+; \quad (2.321)$$

moreover, assume there exists  $r \in \overline{\mathbb{R}}$  with  $r > -\mathbf{a}_0$  such that

$$F(\mathbf{t}) = O(\mathbf{t}^{-r}) \quad \text{for } \mathbf{t} \rightarrow +\infty. \quad (2.322)$$

Then  $F \in \mathcal{M}_{(-\mathbf{a}_0, r)}$  and its Mellin transform  $\mathfrak{M}[F]$  can be analytically continued to a function which is meromorphic in the strip  $\Sigma_{(-\mathbf{a}_{N+1}, r)}$ , possibly with pole singularities at  $s \in \{-\mathbf{a}_0, \dots, -\mathbf{a}_N\}$ . Furthermore, the analytic continuation of  $\mathfrak{M}[F]$  (indicated with the same symbol) can be represented as follows, for all  $s \in \Sigma_{(-\mathbf{a}_{N+1}, r)}$ :

$$\begin{aligned} \mathfrak{M}[F](s) &= \sum_{n=0}^N \sum_{p=0}^P \sum_{j=0}^p \left( \frac{(-1)^j p!}{(p-j)!} \right) \frac{\mathbf{f}_{np} T^{s+\mathbf{a}_n} (\ln T)^{p-j}}{(s+\mathbf{a}_n)^j} + \\ &+ \int_0^T dt \mathbf{t}^{s-1} \left( F(\mathbf{t}) - \sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \mathbf{t}^{\mathbf{a}_n} (\ln \mathbf{t})^p \right) + \int_T^{+\infty} dt \mathbf{t}^{s-1} F(\mathbf{t}). \end{aligned} \quad (2.323)$$

*Proof.* First note that  $F(\mathbf{t}) = O(\mathbf{t}^{\mathbf{a}_0})$  for  $\mathbf{t} \rightarrow 0^+$  in consequence of the assumption (2.321); this fact and the other hypotheses on  $F$  made in the present proposition grant, in view of Lemma 2.83, that  $F \in \mathcal{M}_{(-\mathbf{a}_0, r)}$ .

Next, let us pass to the construction of the analytic continuation of the Mellin transform  $\mathfrak{M}[F]$ . To this purpose, recall that the expression  $O(\mathbf{t}^{\mathbf{a}_{N+1}})$  for  $\mathbf{t} \rightarrow 0^+$  by definition means that

$$\exists T, M > 0 \text{ such that } |O(\mathbf{t}^{\mathbf{a}_{N+1}})| \leq M \mathbf{t}^{\mathbf{a}_{N+1}} \text{ for all } 0 < \mathbf{t} < T; \quad (2.324)$$

for any such  $T$  and for all  $s \in \Sigma_{(-\mathbf{a}_0, r)}$ , using the expansion (2.321), the definition (2.305) of  $\mathfrak{M}[F]$  can be rephrased as

$$\begin{aligned} \mathfrak{M}[F](s) &= \\ &\sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \int_0^T dt \mathbf{t}^{s+\mathbf{a}_n-1} (\ln \mathbf{t})^p + \int_0^T dt \mathbf{t}^{s-1} O(\mathbf{t}^{\mathbf{a}_{N+1}}) + \int_T^{+\infty} dt \mathbf{t}^{s-1} F(\mathbf{t}). \end{aligned} \quad (2.325)$$

Hereafter we discuss in detail each of the terms in the right-hand side of Eq. (2.325); the conclusion of this analysis will be the proof of Eq. (2.323), giving the analytic continuation of  $\mathfrak{M}[F]$  as stated in the proposition.

First, let us fix  $n \in \{0, \dots, N\}$ ,  $p \in \{0, \dots, P\}$  and consider the corresponding integral in the first sum on the right-hand side of Eq. (2.325); this integral can be evaluated explicitly, for all  $s \in \Sigma_{-\mathbf{a}_n}$ , giving <sup>(36)</sup>

$$\int_0^T dt \mathbf{t}^{s+\mathbf{a}_n-1} (\ln \mathbf{t})^p = T^{s+\mathbf{a}_n} \sum_{j=0}^p \left( \frac{(-1)^j p!}{(p-j)!} \right) \frac{(\ln T)^{p-j}}{(s+\mathbf{a}_n)^j}. \quad (2.326)$$

Despite the above identity is derived under the assumption  $\Re s > -\mathbf{a}_n$ , it can be interpreted to give the analytic continuation of the integral on the left-hand side to a function which is meromorphic on the whole complex plane and whose only singularity is a pole of order  $p$  at  $s = -\mathbf{a}_n$ .

Concerning the second and the third integral in Eq. (2.325), we state that these integrals are finite and determine analytic functions of  $s$  for all  $s \in \mathbb{C}$  with  $\Re s > -\mathbf{a}_{N+1}$  and  $\Re s < r$ , respectively. In fact, the convergence of  $\int_0^T dt \mathbf{t}^{s-1} O(\mathbf{t}^{\mathbf{a}_{N+1}})$  follows easily using the bound (2.324), while the integral  $\int_T^{+\infty} dt \mathbf{t}^{s-1} F(\mathbf{t})$  can be shown to be finite moving along the same lines as in the proof of Lemma 2.83; the analyticity of these expressions can be proved by arguments similar to the ones presented in the proof of Proposition 2.84. So, as anticipated before, Eq.s (2.325) (2.326) imply the representation (2.323) which gives the analytic continuation of  $\mathfrak{M}[F]$  to a function meromorphic in the strip  $\Sigma_{(-\mathbf{a}_{N+1}, r)}$ , with poles at  $s \in \{-\mathbf{a}_0, \dots, -\mathbf{a}_N\}$ .  $\square$

**Corollary 2.86.** *Let  $k \in \mathbb{N}$  and  $F \in C^{k+1}([0, +\infty))$ ; moreover assume that, for some  $r \in \mathbb{R}$  with  $r > 0$ , there holds*

$$F(\mathbf{t}) = O(\mathbf{t}^{-r}) \quad \text{for } \mathbf{t} \rightarrow +\infty. \quad (2.327)$$

Then  $F \in \mathcal{M}_{(0,r)}$  and its Mellin transform  $\mathfrak{M}[F]$  can be analytically continued to a function meromorphic on the strip  $\Sigma_{(-(k+1), r)}$ , possibly with simple poles at  $s \in \{0, -1, \dots, -k\}$ ; in particular, for  $s \in \Sigma_{(-(k+1), r)}$  there holds

$$\mathfrak{M}[F](s) = \sum_{n=0}^k \frac{F^{(n)}(0)}{n!(s+n)} T^{s+n} + \int_0^T dt \mathbf{t}^{s-1} \left( F(\mathbf{t}) - \sum_{n=0}^k \frac{F^{(n)}(0)}{n!} \mathbf{t}^n \right) + \int_T^{+\infty} dt \mathbf{t}^{s-1} F(\mathbf{t}). \quad (2.328)$$

<sup>36</sup>In order to prove Eq. (2.326), first note that  $\mathbf{t}^{s+\mathbf{a}_n-1} (\ln \mathbf{t})^p = \partial_s^p (\mathbf{t}^{s+\mathbf{a}_n-1})$ ; then, for all  $s \in \mathbb{C}$  with  $\Re s > -\mathbf{a}_n$ , by arguments similar to those presented in the proof of Proposition 2.84 one can resort to the Lebesgue dominated convergence theorem to infer

$$\int_0^T dt \mathbf{t}^{s+\mathbf{a}_n-1} (\ln \mathbf{t})^p = \frac{d^p}{ds^p} \int_0^T dt \mathbf{t}^{s+\mathbf{a}_n-1} = \frac{d^p}{ds^p} \left( \frac{T^{s+\mathbf{a}_n}}{s+\mathbf{a}_n} \right).$$

Eq. (2.326) follows straightforwardly from the last expression above using the general Leibnitz rule.

*Proof.* The assumption  $F \in C^{k+1}([0, +\infty))$  ensures, in particular, that both  $F \in L^1_{loc}(0, +\infty)$  and

$$F(\mathbf{t}) = \sum_{n=0}^{k-1} \frac{F^{(n)}(0)}{n!} \mathbf{t}^n + O(\mathbf{t}^k) \quad \text{for } \mathbf{t} \rightarrow 0^+ ;$$

then, the thesis follows straightforwardly from Proposition 2.85.  $\square$

**Corollary 2.87.** *Let  $F \in L^1_{loc}(0, +\infty)$ . Assume there exist  $N, P \in \mathbb{N}$ , and two families of coefficients  $\mathbf{c}_n, \mathbf{f}_{np}$  ( $n \in \{0, \dots, N\}$ ,  $p \in \{0, \dots, P\}$ ) with*

$$\mathbf{c}_n \in \mathbb{R} , \quad \mathbf{c}_0 < \mathbf{c}_1 < \dots < \mathbf{c}_N < \mathbf{c}_{N+1} \quad \text{and} \quad \mathbf{f}_{np} \in \mathbb{C} , \quad (2.329)$$

*such that there holds the asymptotic expansion*

$$F(\mathbf{t}) = \sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \mathbf{t}^{-\mathbf{c}_n} (\ln \mathbf{t})^p + O(\mathbf{t}^{-\mathbf{c}_{N+1}}) \quad \text{for } \mathbf{t} \rightarrow +\infty ; \quad (2.330)$$

*moreover, assume there exist  $r \in \overline{\mathbb{R}}$  with  $r > -\mathbf{c}_0$  such that*

$$F(\mathbf{t}) = O(\mathbf{t}^r) \quad \text{for } \mathbf{t} \rightarrow 0^+ . \quad (2.331)$$

*Then  $F \in \mathcal{M}_{(-r, \mathbf{c}_0)}$  and its Mellin transform  $\mathfrak{M}[F]$  can be analytically continued to a function which is meromorphic on the strip  $\Sigma_{(-r, \mathbf{c}_{N+1})}$ , possibly with pole singularities at  $s \in \{\mathbf{c}_0, \dots, \mathbf{c}_N\}$ . Furthermore, the analytic continuation of  $\mathfrak{M}[F]$  (indicated with the same symbol) can be represented as follows, for all  $s \in \Sigma_{(-r, \mathbf{c}_{N+1})}$ :*

$$\begin{aligned} \mathfrak{M}[F](s) &= \sum_{n=0}^N \sum_{p=0}^P \sum_{j=0}^p \left( \frac{(-1)^j p!}{(p-j)!} \right) \mathbf{f}_{np} \frac{T^{s-\mathbf{c}_n} (\ln T)^{p-j}}{(s-\mathbf{c}_n)^j} + \\ &+ \int_T^{+\infty} dt \mathbf{t}^{s-1} \left( F(\mathbf{t}) - \sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \mathbf{t}^{\mathbf{c}_n} (\ln \mathbf{t})^p \right) + \int_0^T dt \mathbf{t}^{s-1} F(\mathbf{t}) . \end{aligned} \quad (2.332)$$

*Proof.* Consider the function  $F_{-1} : (0, +\infty) \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto F_{-1}(\mathbf{t}) := F(1/\mathbf{t})$  (see Eq. (2.306), with  $a = -1$ ). Of course,  $F_{-1} \in L^1_{loc}(0, +\infty)$ ; moreover, there hold the following relations:

$$F_{-1}(\mathbf{t}) = \begin{cases} \sum_{n=0}^N \sum_{p=0}^P \mathbf{f}_{np} \mathbf{t}^{\mathbf{c}_n} (-\ln \mathbf{t})^p + O(\mathbf{t}^0) & \text{for } \mathbf{t} \rightarrow 0^+ \\ O(\mathbf{t}^{-r}) & \text{for } \mathbf{t} \rightarrow +\infty \end{cases} .$$

Therefore, due to Proposition 2.85, we have  $F_{-1} \in \mathcal{M}_{(-r, \mathbf{c}_N)}$ ; furthermore, the Mellin transform  $\mathfrak{M}[F_{-1}]$  can be analytically continued to the strip  $\Sigma_{(-r, \mathbf{c}_N)}$  and therein it admits the

following representation, for any  $T_\star \in (0, +\infty)$ :

$$\begin{aligned} \mathfrak{M}[F_{-1}](s) &= \sum_{n=0}^N \sum_{p=0}^P \sum_{j=0}^p \left( \frac{(-1)^{p-j} p!}{(p-j)!} \right) \frac{\mathfrak{f}_{np} T_\star^{s+\mathfrak{c}_n} (\ln T_\star)^{p-j}}{(s+\mathfrak{c}_n)^j} + \\ &+ \int_0^{T_\star} dt \, \mathbf{t}^{s-1} \left( F_{-1}(\mathbf{t}) - \sum_{n=0}^N \sum_{p=0}^P (-1)^p \mathfrak{f}_{np} \mathbf{t}^{+\mathfrak{c}_n} (\ln \mathbf{t})^p \right) + \int_{T_\star}^{+\infty} dt \, \mathbf{t}^{s-1} F_{-1}(\mathbf{t}) . \end{aligned} \quad (2.333)$$

The thesis can be easily inferred using statement i) in Lemma 2.82; in particular, Eq. (2.332) follows from Eq. (2.333) recalling that  $\mathfrak{M}[F](s) = \mathfrak{M}[F_{-1}](-s)$  (see Eq. (2.308), again with  $a = -1$ ), performing the change of variable  $\mathbf{t} \mapsto 1/\mathbf{t}$  in the integrals appearing in Eq. (2.333) and setting  $T := 1/T_\star$ .  $\square$

**Proposition 2.88.** (Second method for analytic continuation: integration by parts). *Let  $F \in C^k([0, +\infty))$  for some  $k \in \mathbb{N}$ ; moreover, assume there exist  $r \in \overline{\mathbb{R}}$  with  $r > 0$  and a family of coefficients  $r_n$  ( $n \in \{0, \dots, k-1\}$ ) with*

$$r_n \geq r + n , \quad (2.334)$$

such that

$$F^{(n)}(\mathbf{t}) = O(\mathbf{t}^{-r_n}) \quad \text{for } \mathbf{t} \rightarrow +\infty . \quad (2.335)$$

Then  $F \in \mathcal{M}_{(0,r)}$  and its Mellin transform  $\mathfrak{M}[F]$  can be analytically continued to a function which is meromorphic on the strip  $\Sigma_{(-k, r_k - k)}$ , possibly with simple poles at  $s \in \{0, -1, \dots, -(k-1)\}$ ; in particular, for  $s \in \Sigma_{(-k, r_k - k)}$  there holds

$$\mathfrak{M}[F](s) = \frac{(-1)^k}{s(s+1)\dots(s+k-1)} \mathfrak{M}[F^{(k)}](s+k) . \quad (2.336)$$

*Proof.* First note that the function  $F$  fulfills all the hypotheses of Corollary 2.86, since  $F \in C^k([0, +\infty))$  and  $F(\mathbf{t}) = O(\mathbf{t}^{-r_0})$  in the limit  $\mathbf{t} \rightarrow +\infty$  for some  $r_0 \geq r > 0$ ; in particular, this suffices to infer that  $F \in \mathcal{M}_{(0,r)}$ .

In order to derive the representation (2.336) for the Mellin transform  $\mathfrak{M}[F]$ , consider the general definition (2.305); integrating by parts  $k$  times, we obtain

$$\mathfrak{M}[F](s) = \quad (2.337)$$

$$\sum_{n=0}^{k-1} \frac{(-1)^n}{s(s+1)\dots(s+n)} \left[ \mathbf{t}^{s+n} F^{(n)}(\mathbf{t}) \right]_0^{+\infty} + \frac{(-1)^k}{s(s+1)\dots(s+k-1)} \int_0^{+\infty} dt \, \mathbf{t}^{s+k-1} F^{(k)}(\mathbf{t}) .$$

Now, fix  $n \in \{0, \dots, k-1\}$  and consider the boundary term  $[\mathbf{t}^{s+n} F^{(n)}(\mathbf{t})]_0^{+\infty}$ . On the one hand, since  $F \in C^k([0, +\infty))$  ( $k \geq n$ ), there holds

$$\lim_{\mathbf{t} \rightarrow 0^+} \left( \mathbf{t}^{s+n} F^{(n)}(\mathbf{t}) \right) = 0 \quad \text{for } s \in \mathbb{C} \text{ with } \Re s > -n ;$$

on the other hand, the assumption (2.335) allows to infer

$$\lim_{\mathbf{t} \rightarrow +\infty} \left( \mathbf{t}^{s+n} F^{(n)}(\mathbf{t}) \right) = 0 \quad \text{for } s \in \mathbb{C} \text{ with } \Re s < r_n - n .$$

The hypothesis (2.334) grants that the above results do indeed hold for all  $s \in \Sigma_{(0,r)}$ ; thus, within this strip Eq. (2.337) reduces to  $\mathfrak{M}[F](s) = \frac{(-1)^k}{s(s+1)\dots(s+k-1)} \int_0^{+\infty} dt \mathbf{t}^{s+k-1} F^{(k)}(\mathbf{t})$ , which is equivalent to Eq. (2.336) by the definition (2.305) of Mellin transform.

To conclude note that, since  $F$  fulfills the hypotheses of Corollary 2.86 (here employed with  $k+1$  replaced by  $k$ ), there holds  $F^{(k)} \in \mathfrak{M}_{(0,r_k)}$ ; therefore, the integral in Eq. (2.336) converges for all  $s \in \Sigma_{(-k,r_k-k)}$ . Since  $\Sigma_{(-k,r_k-k)} \supset \Sigma_{(0,r)}$ , the representation (2.336) gives the analytic continuation of  $\mathfrak{M}[F]$  within this strip to a meromorphic function with possible poles at  $s \in \{0, -1, \dots, -(k-1)\}$ .  $\square$

**Proposition 2.89.** (Third method for analytic continuation: complex integration). *Let  $F : (0, +\infty) \rightarrow \mathbb{C}$  be a function admitting an analytic extension (indicated with the same symbol) to a complex open neighbour  $\mathcal{U} \subset \mathbb{C}$ , such that*

$$[0, +\infty) \subset \mathcal{U} \quad \text{and} \quad \sup_{z \in \mathcal{U}} |\Im z| > 0 ; \quad (2.338)$$

moreover, assume that, for some  $r \in \overline{\mathbb{R}}$  with  $r > 0$ ,

$$F(\mathbf{t}) = O((\Re \mathbf{t})^{-r}) \quad \text{for } \Re \mathbf{t} \rightarrow +\infty . \quad (2.339)$$

Then  $F \in \mathcal{M}_{(0,r)}$  and its Mellin transform  $\mathfrak{M}[F]$  can be analytically continued to a function meromorphic on the infinite left strip  $\Sigma_{(-\infty,r)}$ , possibly with simple poles at  $s \in \mathbb{Z} \cap (-\infty, r)$ ; in particular, for  $s \in \Sigma_{(-\infty,r)} \setminus \{\mathbb{Z} \cap (-\infty, r)\}$  there holds

$$\mathfrak{M}[F](s) = \frac{e^{-i\pi s}}{2i \sin(\pi s)} \int_{\mathfrak{H}} dt \mathbf{t}^{s-1} F(\mathbf{t}) , \quad (2.340)$$

where  $\mathfrak{H} \subset \mathcal{U}$  denotes the Hankel contour, that is a simple path contained in the open neighbour  $\mathcal{U}$  that starts in the upper half-plane near  $+\infty$ , encircles the origin counter-clockwise and returns to  $+\infty$  in the lower half-plane (see Fig. 2.1 below).

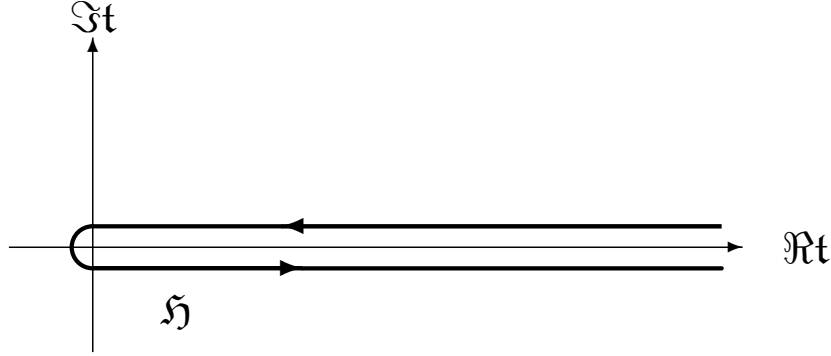
*Proof.* Also in this case the assumptions made for the function  $F$  are sufficient to infer that  $F \in \mathfrak{M}_{(0,r)}$ , by Corollary 2.86.

Next, let us show how to derive the representation (2.340) for the Mellin transform  $\mathfrak{M}[F]$ ; to this purpose, fix  $s \in \Sigma_{(0,r)}$  and consider the integral

$$\mathfrak{N}[F](s) := \int_{\mathfrak{H}} dt \mathbf{t}^{s-1} F(\mathbf{t}) \quad (2.341)$$

(note that the assumption  $\Re s < r$  and the hypotheses made for  $F$  ensure that the above integral is well-defined). To proceed note that, for any  $\delta$  with  $0 < \delta < \sup_{z \in \mathcal{U}} |\Im z|$ , the



Figure 2.1: The Hankel contour  $\mathfrak{H}$ .

Hankel contour  $\mathfrak{H}$  is homotopic to the path  $\mathfrak{H}_\delta$  described as follows:

$$\begin{aligned} \mathfrak{H}_\delta &= \mathfrak{H}_\delta^+ \cup \mathfrak{H}_\delta^0 \cup \mathfrak{H}_\delta^- , \quad \text{with} \\ \mathfrak{H}_\delta^\pm &:= \{ \mathbf{t} \in \mathbb{C} \mid \mathbf{t} = \tau \pm i\delta, \tau \in [0, +\infty) \} , \\ \mathfrak{H}_\delta^0 &:= \{ \mathbf{t} \in \mathbb{C} \mid \mathbf{t} = \delta e^{i\theta}, \theta \in (\pi/2, 3\pi/2) \} . \end{aligned}$$

Due to this fact and to the analyticity of  $F$ , the path  $\mathfrak{H}$  in Eq. (2.341) can be replaced with  $\mathfrak{H}_\delta$ ; thus,

$$\begin{aligned} \mathfrak{N}[F](s) &= \mathfrak{N}_\delta^+[F](s) + \mathfrak{N}_\delta^0[F](s) + \mathfrak{N}_\delta^-[F](s) , \\ \mathfrak{N}_\delta^\pm[F](s) &:= \mp \int_0^{+\infty} d\tau (\tau \pm i\delta)^{s-1} F(\tau \pm i\delta) , \\ \mathfrak{N}_\delta^0[F](s) &:= i \int_{\pi/2}^{3\pi/2} d\theta (\delta e^{i\theta})^s F(\delta e^{i\theta}) . \end{aligned} \tag{2.342}$$

Consider the limit  $\delta \rightarrow 0^+$ . Notice that, in this limit,  $(\tau + i\delta)^{s-1} \rightarrow \tau^{s-1}$  while  $(\tau - i\delta)^{s-1} \rightarrow e^{2i\pi(s-1)} \tau^{s-1} = e^{2i\pi s} \tau^{s-1}$ ; moreover,  $F(\tau \pm i\delta) \rightarrow F(\tau)$ . Due to these results, by Lebesgue dominated convergence theorem it follows that  $\lim_{\delta \rightarrow 0^+} \mathfrak{N}_\delta^+[F](s) = - \int_0^{+\infty} d\tau \tau^{s-1} F(\tau)$  and  $\lim_{\delta \rightarrow 0^+} \mathfrak{N}_\delta^-[F](s) = e^{2i\pi s} \int_0^{+\infty} d\tau \tau^{s-1} F(\tau)$ . Concerning the integral  $\mathfrak{N}_\delta^0[F](s)$ , note that the analyticity of  $F$  implies the existence of a positive constant  $C$  such that  $|F(\delta e^{i\theta})| \leq C$  for all  $\theta \in (0, 2\pi)$ ; thus, for  $\Re s > 0$ , one has

$$|\mathfrak{N}_\delta^0[F](s)| \leq C \delta^{\Re s} \int_{\pi/2}^{3\pi/2} d\theta e^{-(\Im s)\theta} \rightarrow 0 \quad \text{for } \delta \rightarrow 0^+ . \tag{2.343}$$

Summing up, in the limit  $\delta \rightarrow 0^+$  Eq. (2.342) gives

$$\mathfrak{N}[F](s) = (e^{2i\pi s} - 1) \int_0^{+\infty} d\tau \tau^{s-1} F(\tau) . \tag{2.344}$$

Noting that  $e^{2i\pi s} - 1 = 2ie^{i\pi s} \sin(\pi s)$  and recalling the definitions (2.305) (2.341) of  $\mathfrak{M}[F]$ ,  $\mathfrak{N}[F]$ , Eq. (2.344) allow us to obtain the representation (2.340) of the Mellin transform  $\mathfrak{M}[F]$  for all  $s \in \Sigma_{(0,r)} \setminus \{\mathbb{Z} \cap (0, r)\}$ .

To conclude, note that the hypothesis  $\Re s > 0$  was employed only to justify the intermediate result (2.343); nevertheless, to grant the finiteness of the integral  $\mathfrak{M}[F]$  of Eq. (2.341) it suffices to require  $\Re s < r$ . Therefore, the representation (2.340) makes sense for all  $s \in \Sigma_{(-\infty, r)}$  and can be interpreted as the analytic continuation of  $\mathfrak{M}[F]$  to this strip, yielding the thesis.  $\square$

*Remark 2.30.* i) Let  $F : (0, +\infty) \rightarrow \mathbb{C}$  be an analytic function fulfilling all the hypotheses of Proposition 2.89; for any  $q \in \mathbb{Z}$ , consider the analytic extension of the function introduced in Eq. (2.312):

$$H_q : \mathcal{U} \rightarrow \mathbb{C}, \quad \mathbf{t} \mapsto H_q(\mathbf{t}) := \mathbf{t}^q F(\mathbf{t}). \quad (2.345)$$

Proposition 2.89 and the statement iii) of Lemma 2.82 allow to infer that  $H_q$  can be analytically continued to a function which is meromorphic on the infinite left strip  $\Sigma_{(-\infty, r-q)}$ ; due to the results in Eq.s (2.314) (2.340), this analytic continuation can be represented as

$$\mathfrak{M}[H_q](s) = \frac{e^{-i\pi s}}{2i \sin(\pi s)} \int_{\mathfrak{H}} d\mathbf{t} \mathbf{t}^{s-1} H_q(\mathbf{t}), \quad (2.346)$$

where it was also used the fact that

$$e^{-i\pi q} / \sin(\pi(s+q)) = 1 / \sin(\pi s) \quad \text{for } q \in \mathbb{Z}. \quad (2.347)$$

ii) Consider the very well-known *reflection relation* (see, e.g., [122], page 138, Eq. 5.5.3)

$$\Gamma(s) \Gamma(1-s) = \frac{\pi}{\sin(\pi s)} \quad \text{for } s \in \mathbb{C} \setminus \mathbb{Z}. \quad (2.348)$$

Using this identity, Eq. (2.340) can be reformulated as follows, for all  $s \in \mathbb{C} \setminus \mathbb{Z}$ :

$$\frac{1}{\Gamma(s)} \mathfrak{M}[F](s) = \frac{e^{-i\pi s} \Gamma(1-s)}{2\pi i} \int_{\mathfrak{H}} d\mathbf{t} \mathbf{t}^{s-1} F(\mathbf{t}), \quad (2.349)$$

In some cases of interest for the applications to be considered in the following, Eq. (2.349) yields a very effective method for computing explicitly the analytic continuation of the Mellin transform of certain functions; in fact, for suitable  $s \in \mathbb{Z}$ , the integral in the right-hand side of Eq. (2.349) can be easily computed via the residue theorem, since  $F$  is assumed to be analytic in the region enclosed by the Hankel contour  $\mathfrak{H}$ .

### Analytic continuation of the Dirichlet kernels.

Let us consider the framework of Sections 2.6 and 2.7; so, assume again  $\Omega \subset \mathbb{R}^d$  to be an arbitrary domain and let  $\mathcal{A}$  be the admissible operator obtained restricting the differential operator  $A = -\Delta + V$  ( $V \in C^\infty(\Omega)$ ) to an admissible domain  $\text{Dom}(\mathcal{A}) \subset L^2(\Omega)$ .

Consider the heat, cylinder and modified cylinder kernels associated to  $\mathcal{A}$ ; recall that the features possessed by these kernels have been discussed extensively in subsection 2.7. The results obtained therein allow, in particular, to derive the following lemma.

**Lemma 2.90.** *Let  $j \in \mathbb{N}$  and let  $\alpha, \beta$  be any pair of multi-indices such that  $|\alpha| + |\beta| \leq j$ . For any fixed  $\mathbf{x}, \mathbf{y} \in \Omega$ , consider the maps  $(0, +\infty) \rightarrow \mathbb{C}$ ,  $\mathbf{t} \mapsto \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$ ,  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y})$ ,  $\partial_1^\alpha \partial_2^\beta (e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\mathbf{x}, \mathbf{y})$ ; each one of these maps admits a Mellin transform. More precisely, there holds*

$$\begin{aligned} \partial_1^\alpha \partial_2^\beta e^{-\bullet\mathcal{A}}(\mathbf{x}, \mathbf{y}) &\in \mathcal{M}_{(j+d)/2}, \\ \partial_1^\alpha \partial_2^\beta e^{-\bullet\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y}) &\in \mathcal{M}_{j+d}, \\ \partial_1^\alpha \partial_2^\beta (e^{-\bullet\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\mathbf{x}, \mathbf{y}) &\in \mathcal{M}_{j+d-1}. \end{aligned} \quad (2.350)$$

Moreover, for all  $s \in \Sigma_{(j+d)/2}$ , the derivative  $\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})$  of the Dirichlet kernel can be expressed as follows in terms of the Mellin transforms of the above maps:

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(s)} \mathfrak{M}[\partial_1^\alpha \partial_2^\beta e^{-\bullet\mathcal{A}}(\mathbf{x}, \mathbf{y})](s), \quad (2.351)$$

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(2s)} \mathfrak{M}[\partial_1^\alpha \partial_2^\beta e^{-\bullet\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y})](2s), \quad (2.352)$$

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Gamma(2s-1)} \mathfrak{M}[\partial_1^\alpha \partial_2^\beta (e^{-\bullet\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}})(\mathbf{x}, \mathbf{y})](2s-1). \quad (2.353)$$

*Remark 2.31.* The identities in Eq.s (2.351-2.353) must be meant to hold pointwisely, for all fixed  $\mathbf{x}, \mathbf{y} \in \Omega$  (and for all  $s \in \Sigma_{(j+d)/2}$ ).

*Proof.* Recall the small and large  $\mathbf{t}$  bounds derived in point ii) of Proposition 2.65 for the exponential kernels; see, in particular, Eq.s (2.249), (2.254) and (2.255). Then, the first part of the thesis (namely, Eq. (2.350)) follows easily from Lemma 2.83.

On the other hand, the identities in Eq.s (2.351-2.353) are simply a restatement of Eq.s (2.266-2.268) (see Proposition 2.70) in the language of Mellin transforms.  $\square$

Let us anticipate that, for the physical applications to be considered in the subsequent Chapters 3 and 4, it is of utmost interest the evaluation along the diagonal ( $\mathbf{y} = \mathbf{x}$ ) of the Dirichlet kernel and of its derivatives, as well as the computation of their analytic continuations with respect to the complex parameter defining their order.

Having in mind these developments, hereafter we proceed to construct the required analytic continuations, making suitable hypotheses for the small  $\mathbf{t}$  asymptotic behaviour of the corresponding derivatives of the heat and cylinder kernels (to be evaluated along the diagonal, as well). The main results are contained in the forthcoming Theorems 2.91, 2.92 and 2.93; in the related Remarks 2.32, 2.33 and 2.34 we will comment on the hypotheses mentioned above for the exponential kernels, pointing out that they are typically fulfilled in most cases of interest.

Before proceeding, let us recall once more that, for any  $\mathbf{x} \in \Omega$  and for any pair of multi-indexes  $\alpha, \beta$ , the maps  $(0, +\infty) \ni \mathbf{t} \mapsto \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$ ,  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\sqrt{\mathcal{A}}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  are analytic and decay exponentially for  $\mathbf{t} \rightarrow +\infty$  (see Proposition 2.65). On the other hand, all the hypotheses made in Theorems 2.91, 2.92 and 2.93 contain only assumptions about the asymptotics of the above maps in the limit  $\mathbf{t} \rightarrow 0^+$ .

**Theorem 2.91.** *Let  $\alpha, \beta$  be any pair of multi-indexes and consider the derivative  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$  of the heat kernel, for  $\mathbf{t} \in (0, +\infty)$  and  $\mathbf{x}, \mathbf{y} \in \Omega$ . Assume there exist  $N \in \mathbb{N}$  and a family of coefficients  $b_n : \Omega \rightarrow \mathbb{R}$  ( $n \in \{0, \dots, N\}$ ) such that along the diagonal  $\mathbf{y} = \mathbf{x}$ , there holds the following asymptotic expansion for  $\mathbf{t} \rightarrow 0^+$  :*

$$\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{1}{\mathbf{t}^{(|\alpha|+|\beta|+d)/2}} \left( \sum_{n=1}^N b_n(\mathbf{x}) \mathbf{t}^n + O(\mathbf{t}^{N+1}) \right). \quad (2.354)$$

Then, the map  $\Sigma_{(|\alpha|+|\beta|+d)/2} \rightarrow \mathbb{C}$ ,  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{x})$  (for all  $\mathbf{x} \in \Omega$ ) can be analytically continued to a function which is meromorphic in the strip  $\Sigma_{(|\alpha|+|\beta|+d)/2-N}$  and possesses only possible simple pole singularities at  $s = \frac{|\alpha|+|\beta|+d}{2} - n$ , for  $n \in \{0, \dots, N\}$ . More precisely, the analytic continuation is given by

$$\begin{aligned} \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= \frac{1}{\Gamma(s)} \left[ \sum_{n=0}^N \frac{b_n(\mathbf{x}) T^{s-d/2+n}}{s - \frac{|\alpha|+|\beta|+d}{2} + n} + \right. \\ &+ \left. \int_0^T dt \mathbf{t}^{s-1} \left( \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} - \frac{1}{\mathbf{t}^{(|\alpha|+|\beta|+d)/2}} \sum_{n=0}^N b_n(\mathbf{x}) \mathbf{t}^n \right) + \int_T^{+\infty} dt \mathbf{t}^{s-1} \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \right]. \end{aligned} \quad (2.355)$$

*Proof.* First of all, recall that the results of Proposition 2.65 allow to infer the following estimate, for any fixed  $\mathbf{x} \in \Omega$ :

$$\left| \partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \right| \leq C_{\alpha,\beta}(\mathbf{x}) e^{-\varepsilon \mathbf{t}} \quad \text{for } \mathbf{t} > T_{\alpha,\beta}(\mathbf{x}),$$

where the positive constants  $C_{\alpha,\beta}(\mathbf{x}), T_{\alpha,\beta}(\mathbf{x})$  can be determined explicitly according to Eq. (2.249) and  $\varepsilon > 0$  is such that  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ . Then, due to Proposition 2.85, the map  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}$  can be analytically continued to the (right-infinite) strip  $\Sigma_{((|\alpha|+|\beta|+d)/2-N, +\infty)} \equiv \Sigma_{(|\alpha|+|\beta|+d)/2-N}$ . Moreover, the analytic continuation can be determined explicitly starting with Eq. (2.351); it suffices to keep in mind the asymptotic expansion (2.354) and to resort to the general relation (2.323), here employed with  $P = 0$  and  $\mathbf{a}_n = n - (|\alpha| + |\beta| + d)/2$ , ( $n = 0, \dots, N$ ). This suffices to infer the thesis.  $\square$

*Remark 2.32.* i) As anticipated previously, the hypotheses made in the above theorem are well-known to be fulfilled in many cases of interest. For example, expansions of the form (2.354) for the diagonal heat kernel derivatives can be easily derived for arbitrary  $N \in \mathbb{N}$  under the assumptions (2.159) for the domain  $\Omega$  and for the potential  $V$ , starting from the expression in Eq. (2.262); in this case the coefficients  $b_n$  in Eq. (2.354) can all be determined in terms of the HDSM-coefficients  $a_n$  and of their derivatives. Analogous results for the heat kernel also hold in case the domain is a (possibly unbounded) subset  $R^d$  delimited by flat boundaries (namely, parallel or perpendicular planes), on which suitable boundary conditions are prescribed (<sup>37</sup>). Let us also mention that, when the domain  $\Omega$

<sup>37</sup>This statement can be checked by direct computations, starting with the heat kernel  $K_0(\mathbf{t}; \mathbf{x}, \mathbf{y}) := \frac{1}{(4\pi\mathbf{t})^{d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\mathbf{t}}}$  (see Eq. (2.263)) and using the method of images.

is the whole space  $\mathbb{R}^d$  and the potential  $V$  is either a mass term ( $V = m^2$ , for some  $m \in \mathbb{R}$ ) or an harmonic-type background ( $V(\mathbf{x}) = \lambda^4|\mathbf{x}|^2$ , for some  $\lambda \in \mathbb{R}$ ), the well-known explicit expressions for the corresponding heat kernels are easily seen to possess asymptotic expansions of the type (2.354).

ii) Whenever the hypotheses of Theorem 2.91 are fulfilled, it can be proved by Riesz means methods (see, e.g., [60, 73, 76]) that the derivative  $\partial_1^\alpha \partial_2^\beta e^{-t\sqrt{A}}(\mathbf{x}, \mathbf{y})$  of the cylinder kernel evaluated along the diagonal admits a corresponding asymptotic expansion, for  $\mathbf{t} \rightarrow 0^+$ , given by (compare with (2.265))

$$\frac{\partial_1^\alpha \partial_2^\beta e^{-t\sqrt{A}}(\mathbf{x}, \mathbf{y})}{\mathbf{t}^{d+|\alpha|+|\beta|}} \Big|_{\mathbf{y}=\mathbf{x}} = \frac{1}{\mathbf{t}^{d+|\alpha|+|\beta|}} \left( \sum_{n=0}^N g_n(\mathbf{x}) \mathbf{t}^n + \sum_{\substack{n=d+|\alpha|+|\beta|+1 \\ n-(d+|\alpha|+|\beta|) \text{ odd}}}^N h_n(\mathbf{x}) \mathbf{t}^n \ln \mathbf{t} + O(\mathbf{t}^{N+1} \ln \mathbf{t}) \right), \tag{2.356}$$

for some  $N \in \mathbb{N}$  and for two families of coefficients  $g_n, h_n : \Omega \rightarrow \mathbb{R}$  ( $n \in \{0, \dots, N\}$ ) <sup>(38)</sup>. Then, a simple variation of the above Theorem 2.91 can be derived starting from the asymptotic expansion (2.356); since this alternative formulation will never be used in the applications to be considered in the following, it will not be reported in the present work.

In most of the cases mentioned in item i) of Remark 2.32 much more can be said about the small  $\mathbf{t}$  behaviour of either the heat or cylinder kernel and of their derivatives. Having in mind these considerations, we state the following Theorems 2.92, 2.93; therein, under slightly stronger assumptions, we present other methods which allow to construct the analytic continuations of the maps  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$ , typically in a more efficient way from a computational point of view.

**Theorem 2.92.** *Let  $\alpha, \beta$  be any pair of multi-indexes. Assume there exist  $N \in \mathbb{N}$  and a function  $H^{(\alpha, \beta)} : [0, +\infty) \times \Omega \rightarrow \mathbb{R}$ ,  $(\mathbf{t}, \mathbf{x}) \mapsto H^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  such that, for any fixed  $\mathbf{x} \in \Omega$ :*

- i) the map  $\mathbf{t} \mapsto H^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  is of class  $C^N$ ;*
- ii) for  $\mathbf{t} \in (0, +\infty)$ , the derivative  $\partial_1^\alpha \partial_2^\beta e^{-tA}(\mathbf{x}, \mathbf{y})$  of the heat kernel evaluated along the diagonal is given by*

$$\partial_1^\alpha \partial_2^\beta e^{-tA}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{1}{\mathbf{t}^{(|\alpha|+|\beta|+d)/2}} H^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x}) . \tag{2.357}$$

*Then, for any fixed  $\mathbf{x} \in \Omega$ , the map  $\Sigma_{(d+|\alpha|+|\beta|)/2} \rightarrow \mathbb{C}$ ,  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  can be analytically continued to a function which is meromorphic in the strip  $\Sigma_{(d+|\alpha|+|\beta|)/2-N}$  and possesses only possible simple pole singularities at  $s = \frac{|\alpha|+|\beta|+d}{2} - n$ , for  $n \in \{0, \dots, N\}$ . More precisely, the analytic continuation is given by*

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<sup>38</sup>As pointed out by Fulling in the already cited works [60, 73, 76], some but not all of the coefficients  $g_n, h_n$  can be determined in terms of the heat kernel coefficients  $b_n$ .

$$\begin{aligned} \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= \tag{2.358} \\ \frac{(-1)^N}{\Gamma(s)(s - \frac{|\alpha+|\beta|+d}{2}) \dots (s - \frac{|\alpha+|\beta|+d}{2} - 1 + N)} \int_0^{+\infty} dt \, t^{s - \frac{|\alpha+|\beta|+d}{2} - 1 + N} \partial_{\mathbf{t}}^N H^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x}) . \end{aligned}$$

*Proof.* The thesis can be derived following the same arguments presented in the proof of Theorem 2.91, using Proposition 2.88 (and the corresponding Eq. (2.336)) in place of Proposition 2.85.  $\square$

*Remark 2.33.* The hypotheses made in the above theorem are known to hold when  $\Omega$  is bounded with smooth boundary and  $V = 0$  <sup>(39)</sup>, or when  $\Omega = \mathbb{R}^d$  and the potential is either  $V = m^2$  ( $m \in \mathbb{R}$ ) or  $V(\mathbf{x}) = \lambda^4 |\mathbf{x}|^2$  ( $\lambda \in \mathbb{R}$ ).

**Theorem 2.93.** *Let  $\alpha, \beta$  be any pair of multi-indices. Assume there to exist a function  $J^{(\alpha, \beta)} : (0, +\infty) \times \Omega \rightarrow \mathbb{R}$ ,  $(\mathbf{t}, \mathbf{x}) \mapsto J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  such that, for any fixed  $\mathbf{x} \in \Omega$ :*

- i) the map  $\mathbf{t} \mapsto J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  admits an analytic extension to a complex open neighbour  $\mathcal{U} \subset \mathbb{C}$  of the positive real semi-axis  $[0, +\infty)$ ;*
- ii) for  $\mathbf{t} \in (0, +\infty)$ , the derivative  $\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\sqrt{A}}(\mathbf{x}, \mathbf{y})$  of the cylinder kernel evaluated along the diagonal is given by*

$$\partial_1^\alpha \partial_2^\beta e^{-\mathbf{t}\sqrt{A}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{1}{\mathbf{t}^{|\alpha+|\beta|+d}} J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x}) . \tag{2.359}$$

*Then, the map  $\Sigma_{(|\alpha+|\beta|+d)/2} \rightarrow \mathbb{C}$ ,  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}$  can be analytically continued to a function, which is meromorphic on the whole complex plane and possesses only possible simple pole singularities at  $s = k/2$ , for  $k \in \{1, \dots, |\alpha| + |\beta| + d\}$ . More precisely, the analytic continuation is given by*

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{e^{-2i\pi s} \Gamma(1-2s)}{2\pi i} \int_{\mathfrak{S}} dt \, t^{2s-|\alpha+|\beta|-d-1} J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x}) ; \tag{2.360}$$

*in particular, for  $s = -k/2$ ,  $k \in \mathbb{N}$ , there holds*

$$\partial_1^\alpha \partial_2^\beta \mathcal{A}^{k/2}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = (-1)^k \Gamma(k+1) \operatorname{Res} \left( \mathbf{t}^{-(k+|\alpha+|\beta|+d+1)} J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x}) ; \mathbf{t} = 0 \right) . \tag{2.361}$$

*Proof.* Also in this case the thesis can be derived following the same arguments presented in the proof of Theorem 2.91; this time, in place of Proposition 2.85, one must resort to Proposition 2.89 and to the related Remark 2.30 (see, in particular, item i) therein which must be employed here with  $q = |\alpha| + |\beta| + d$  and  $F(\mathbf{t}) = J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$ . Finally, Eq. (2.361) follows easily by the residue theorem, recalling that the map  $\mathbf{t} \mapsto J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  is analytic for all  $\Re \mathbf{t} > 0$ .  $\square$

<sup>39</sup>In fact, in this case all the HDMS coefficients of any order vanish except for  $a_0(\mathbf{x}, \mathbf{x}) = 1$ .

*Remark 2.34.* i) The hypotheses made in Theorem 2.93 can be easily checked by direct computation in many cases of interest. For example, they are fulfilled when the potential is null ( $V = 0$ ) and the domain is a subset of  $\mathbb{R}^d$  delimited by flat boundaries consisting, namely, of parallel and/or perpendicular planes on which either Dirichlet or Neumann conditions are prescribed (see [65] and the forthcoming Section 4.3 of Chapter 4).

ii) Consider the analytic continuation of  $\partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  determined according to Eq. (2.360). It appears that the singular behaviour at the points  $s = k/2$ ,  $k \in \{1, \dots, |\alpha| + |\beta| + d\}$  descends from the pole singularity of the Gamma function evaluated at non-positive integers. Due to the same considerations, one could expect any of the points  $s = k/2$ , with  $k \in \mathbb{N}$  unrestricted, to be singular; however, it is known a priori that the map  $s \mapsto \partial_1^\alpha \partial_2^\beta \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  is analytic for  $s \in \Sigma_{(|\alpha|+|\beta|+d)/2}$ , so that no singularity exists therein (nor can it arise by analytic continuation). Let us stress that there is no contradiction; in fact, for  $s = k/2$  with  $k \in \mathbb{N}$  and  $k > |\alpha| + |\beta| + d$ , the integral along the Hankel contour in Eq. (2.360) can be easily seen to vanish via the residue theorem so that there appears an indeterminate form of the type  $\infty \cdot 0$ , which has to be evaluated by alternative methods.

Before moving on, let us point out that the results derived in the above Theorems 2.91, 2.92 and 2.93 continue to hold also for boundary points  $\mathbf{x} \in \partial\Omega$  whenever stronger regularity assumptions (such as those in Eq. (2.159)) are fulfilled by the domain  $\Omega$  and by the potential  $V$ , and suitable boundary conditions are prescribed on  $\partial\Omega$ .

### Analytic continuation of the trace $\text{Tr } \mathcal{A}^{-s}$ .

Assume the stricter regularity hypotheses (2.159) and (2.209) to be fulfilled (so that  $\Omega$  is bounded with boundary of class  $C^\infty$ ,  $A = -\Delta + V$  with  $V \in C^\infty(\bar{\Omega})$ , and Dirichlet boundary conditions are prescribed on  $\partial\Omega$ ).

Let us recall that, under the above assumptions, the heat and cylinder traces  $\text{Tr } e^{-\mathbf{t}A}$ ,  $\text{Tr } e^{-\mathbf{t}\sqrt{A}}$  exist and are analytic for  $\mathbf{t} \in \Sigma_0$ ; moreover, these traces decay exponentially for  $\Re \mathbf{t} \rightarrow +\infty$  (see Proposition 2.77). These facts can be employed, along with suitable hypotheses about the small  $\mathbf{t}$  behaviour of the mentioned traces, to construct the analytic continuation of the complex trace  $\text{Tr } \mathcal{A}^{-s}$  (recall that this is granted to exist and to be analytic for  $s \in \Sigma_{d/2}$ ; see Corollary 2.75).

The forthcoming Theorems 2.94, 2.95 and 2.96 essentially contain global analogues of Theorems 2.91, 2.92 and 2.93, discussed in the previous subsection.

**Theorem 2.94.** *Consider the heat trace  $\text{Tr } e^{-\mathbf{t}A}$ , for  $\mathbf{t} \in (0, +\infty)$ . Assume there exist  $N \in \mathbb{N}$  and a family of coefficients  $b_n \in \mathbb{R}$  ( $n \in \{0, \dots, N\}$ ) such that, for  $\mathbf{t} \rightarrow 0^+$ , this trace possesses an asymptotic expansion of the form*

$$\text{Tr } e^{-\mathbf{t}A} = \frac{1}{\mathbf{t}^{d/2}} \left( \sum_{n=1}^N b_n \mathbf{t}^{n/2} + O(\mathbf{t}^{(N+1)/2}) \right). \tag{2.362}$$

Then  $\text{Tr} e^{-\bullet \mathcal{A}} \in \mathcal{M}_{d/2}$ , and there holds

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(s)} \mathfrak{M}[\text{Tr} e^{-\bullet \mathcal{A}}](s) . \quad (2.363)$$

Moreover, the map  $\Sigma_{d/2} \rightarrow \mathbb{C}$ ,  $s \mapsto \text{Tr} \mathcal{A}^{-s}$  can be analytically continued to a function which is meromorphic on the strip  $\Sigma_{(d-N)/2}$  and possesses only possible simple pole singularities at  $s = (d-n)/2$ , for  $n \in \{0, \dots, N\}$ ; more precisely, the analytic continuation is given by

$$\begin{aligned} \text{Tr} \mathcal{A}^{-s} = & \quad (2.364) \\ \frac{1}{\Gamma(s)} & \left[ \sum_{n=0}^N \frac{b_n T^{s-d/2+n}}{s - \frac{d}{2} + \frac{n}{2}} + \int_0^T dt \, \mathbf{t}^{s-1} \left( \text{Tr} e^{-\mathbf{t} \mathcal{A}} - \frac{1}{\mathbf{t}^{d/2}} \sum_{n=0}^N b_n \mathbf{t}^{n/2} \right) + \int_T^{+\infty} dt \, \mathbf{t}^{s-1} \text{Tr} e^{-\mathbf{t} \mathcal{A}} \right] . \end{aligned}$$

*Proof.* Recall again that the heat trace  $\text{Tr} e^{-\mathbf{t} \mathcal{A}}$  is analytic for  $\mathbf{t} \in \Sigma_0$  and vanishes exponentially for  $\Re \mathbf{t} \rightarrow +\infty$  (see Proposition 2.77); these facts and the asymptotic expansion (2.362) suffice to infer that  $\text{Tr} e^{-\bullet \mathcal{A}} \in \mathcal{M}_{d/2}$ , due to Lemma 2.83. Eq. (2.363) is just a restatement of the integral relation (2.297).

Also in this case, the explicit expression (2.364) for the analytic continuation of  $\text{Tr} \mathcal{A}^{-s}$  can be derived resorting to the general relation (2.323), here employed with  $P = 0$  and  $\mathbf{a}_n = (n - |\alpha| + |\beta| + d)/2$ , ( $n = 0, \dots, N$ ).  $\square$

**Theorem 2.95.** Consider the heat trace  $\text{Tr} e^{-\mathbf{t} \mathcal{A}}$ , for  $\mathbf{t} \in (0, +\infty)$ . Assume there exist  $N \in \mathbb{N}$  and a function  $H \in C^N([0, +\infty); \mathbb{R})$  such that

$$\text{Tr} e^{-\mathbf{t} \mathcal{A}} = \frac{1}{\mathbf{t}^{d/2}} H(\mathbf{t}) . \quad (2.365)$$

Then  $\text{Tr} e^{-\bullet \mathcal{A}} \in \mathcal{M}_{d/2}$ , and there holds Eq. (2.363), i.e.,

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(s)} \mathfrak{M}[\text{Tr} e^{-\bullet \mathcal{A}}](s) .$$

Moreover, the map  $\Sigma_{d/2} \rightarrow \mathbb{C}$ ,  $s \mapsto \text{Tr} \mathcal{A}^{-s}$  can be analytically continued to a function which is meromorphic on the strip  $\Sigma_{(d-N)/2}$  and possesses only possible simple pole singularities at  $s = (d-n)/2$ , for  $n \in \{0, \dots, N\}$ ; more precisely, the analytic continuation is given by

$$\text{Tr} \mathcal{A}^{-s} = \frac{(-1)^N}{\Gamma(s)(s - \frac{d}{2}) \dots (s - \frac{d-N}{2} - 1)} \int_0^{+\infty} dt \, \mathbf{t}^{s - \frac{d-N}{2} - 1} \partial_{\mathbf{t}}^N H(\mathbf{t}) . \quad (2.366)$$

*Proof.* The thesis can be derived following the same arguments presented in the proof of Theorem 2.94, using Proposition 2.88 (and the corresponding Eq. (2.336)) in place of Proposition 2.85.  $\square$



**Theorem 2.96.** Consider the cylinder trace  $\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ , for  $\mathbf{t} \in (0, +\infty)$ . Assume there exists a function  $J : (0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto J(\mathbf{t})$  admitting an analytic extension to a complex neighbour  $\mathcal{U} \subset \mathbb{C}$  of the positive real semi-axis  $[0, +\infty)$ , such that

$$\text{Tr} e^{-\mathbf{t}\sqrt{\mathcal{A}}} = \frac{1}{\mathbf{t}^d} J(\mathbf{t}) . \quad (2.367)$$

Then  $\text{Tr} e^{-\bullet\sqrt{\mathcal{A}}} \in \mathcal{M}_d$ , and there holds Eq. (2.363), i.e.,

$$\text{Tr} \mathcal{A}^{-s} = \frac{1}{\Gamma(2s)} \mathfrak{M}[\text{Tr} e^{-\bullet\sqrt{\mathcal{A}}}] (2s) .$$

Moreover, the map  $\Sigma_d \rightarrow \mathbb{C}$ ,  $s \mapsto \text{Tr} \mathcal{A}^{-s}$  can be analytically continued to a function, which is meromorphic on the whole complex plane and possesses only possible simple pole singularities at  $s = k/2$ , for  $k \in \{1, \dots, d\}$ . The analytic continuation is given by

$$\text{Tr} \mathcal{A}^{-s} = \frac{e^{-2i\pi s} \Gamma(1-2s)}{2\pi i} \int_{\mathfrak{S}} dt \mathbf{t}^{2s-d-1} J(\mathbf{t}) ; \quad (2.368)$$

in particular, for  $s = -k/2$ ,  $k \in \mathbb{N}$ , there holds

$$\text{Tr} \mathcal{A}^{k/2} = (-1)^k \Gamma(k+1) \text{Res} \left( \mathbf{t}^{-(k+d+1)} J(\mathbf{t}) ; \mathbf{t} = 0 \right) . \quad (2.369)$$

*Proof.* Also in this case the thesis can be derived following the same arguments presented in the proof of Theorem 2.94; this time, in place of Proposition 2.85, one must resort to Proposition 2.89 and to the related Remark 2.30 (see, in particular, item i) therein which must be employed here with  $q = d$  and  $F(\mathbf{t}) = J(\mathbf{t})$ . Finally, Eq. (2.361) follows easily by the residue theorem, recalling that  $J$  is analytic.  $\square$

*Remark 2.35.* Of course, the results derived in the above theorems continue to hold whenever the heat and cylinder traces are well-posed, decay exponentially at infinity and possess small  $\mathbf{t}$  asymptotic behaviours such as those described in Eq.s (2.362), (2.365) and (2.367). In this sense, the assumptions (2.159) are sufficient but not necessary; for example, it can be checked by explicit computations that the heat trace is well-defined, analytic and exponentially vanishing at infinity if  $\Omega = \mathbb{R}^d$  and  $\mathcal{A} = -\Delta + V$ , with  $V(\mathbf{x}) = \lambda^4 |\mathbf{x}|^2$  ( $\lambda \in \mathbb{R}$ ) (see Section 4.1).



## Chapter 3

# Quantum field theory on spatial domains with boundaries

In the present chapter we review the theory of canonical quantization for a Hermitian scalar field living on a suitable spatial domain  $\Omega$  (which is assigned once and for all and has arbitrary dimension); possible conditions prescribed on the boundary of the domain and the interaction with a classical background potential are also taken into account. The implementation of local zeta regularization (ZR) within this framework is discussed in detail. The physical setting is the one which was described in Chapter 1 of the present manuscript, of which we retain the same notations and conventions; however, the language adopted here is more rigorous and precise from a mathematical point of view.

In Section 3.1 we review some well-known Fock space techniques, referring in particular to the Segal approach to quantization (see, e.g., [43, 58, 129, 130]). We give an abstract formulation of these topics, using the framework developed in Chapter 2 in terms of scales of Hilbert spaces associated to the real powers of a given strictly positive, self-adjoint operator (acting on the single particle space). In Section 3.2, this abstract framework is specialized to the case where the single particle Hilbert space consists of square-integrable functions on a fixed spatial domain  $\Omega \subset \mathbb{R}^d$  and the positive, self-adjoint operator is a Schrödinger-type differential operator of the form  $\mathcal{A} = -\Delta + V$ , with  $V$  a smooth potential on  $\Omega$ . Next, we use the complex powers  $\mathcal{A}^{-s}$  ( $s \in \mathbb{C}$ ) to define a zeta-regularized Wightman field; this is employed, in turn, to construct a zeta-regularized version of the propagator and of some related observables (in particular, of the stress-energy VEV), thus making connection with the theory of the Casimir effect. In the end, we describe the zeta approach to renormalization in the most general formulation proposed in [64]; it is shown that this approach is granted to give finite values for the renormalized observables in many cases of interest.

Before proceeding, let us recall that we consider only a purely classical description of the above mentioned spatial domain  $\Omega$ , of its boundary  $\partial\Omega$  and of the background potential  $V$ ; in particular, no back-reaction effect produced by the interaction with the quantum field is ever taken into account.

### 3.1 Canonical quantization of an abstract Hermitian scalar field.

In this section we review the theory of canonical quantization for an Hermitian scalar field. We develop an abstract formulation of this subject, making only minimal assumptions on the objects to be employed in the subsequent constructions. To this purpose, and in order to fix the notations and some conventions, we first recall some basic definitions and some well-known results, rephrasing them in the language developed in Chapter 2 of this work. For further details on the topics discussed hereafter (and, in particular, for the proofs of some statements), we refer mainly to the books of Reed and Simon [129] and of Moretti [119].

#### The bosonic Fock space.

Let  $(\mathcal{H}, \langle \cdot | \cdot \rangle)$  be an abstract, separable Hilbert space and let  $n \in \{1, 2, 3, \dots\}$  be any given positive integer.

Consider the  $n$ -th tensor power  $\mathcal{H}^{\otimes n} = \mathcal{H} \otimes \dots \otimes \mathcal{H}$  ( $n$  times); this is the Hilbert space obtained by completing the algebraic tensor product  $\otimes_{\text{alg}}^n \mathcal{H}$  of the underlying vector spaces with respect to the Hermitian inner product  $(\cdot | \cdot)_n : \otimes_{\text{alg}}^n \mathcal{H} \times \otimes_{\text{alg}}^n \mathcal{H} \rightarrow \mathbb{C}$ , defined as the unique sesquilinear extension <sup>(1)</sup> of the map which, for any pair of factorized elements  $f^{(n)} = f_1 \otimes \dots \otimes f_n$ ,  $g^{(n)} = g_1 \otimes \dots \otimes g_n \in \otimes_{\text{alg}}^n \mathcal{H}$  ( $f_i, g_i \in \mathcal{H}$  for all  $i = 1, \dots, n$ ), gives

$$(f^{(n)} | g^{(n)})_n = \prod_{i=1}^n \langle f_i | g_i \rangle . \quad (3.1)$$

In order to avoid confusion, we will indicate with  $o$  the null element of  $\mathcal{H}$  and with  $o^{(n)}$  the null vector of  $\mathcal{H}^{\otimes n}$ .

Next, consider the group of permutations of  $n$  elements, which we indicate with  $\mathbb{P}_n$ . For any  $\pi \in \mathbb{P}_n$ , let  $U_\pi \in \mathfrak{B}(\mathcal{H}^{\otimes n})$  denote the unitary operator which, for any  $f_1, \dots, f_n \in \mathcal{H}$ , gives

$$U_\pi(f_1 \otimes \dots \otimes f_n) = f_{\pi^{-1}(1)} \otimes \dots \otimes f_{\pi^{-1}(n)} ; \quad (3.2)$$

it can be easily checked that the map  $U : \mathbb{P}_n \rightarrow \mathfrak{B}(\mathcal{H}^{\otimes n})$ ,  $\pi \mapsto U_\pi$  yields a faithful unitary representation of  $\mathbb{P}_n$  (see, e.g., Proposition 13.41 on page 661 of [119]).

The  $n$ -th totally symmetric tensor power  $\mathcal{H}^{\vee n}$  is, by definition, the closed linear subspace of  $\mathcal{H}^{\otimes n}$  formed by the elements which are  $U_\pi$ -invariant for all  $\pi \in \mathbb{P}_n$ . Of course,  $\mathcal{H}^{\vee n}$  is itself a Hilbert space with the inner product  $(\cdot | \cdot)_n$  inherited from  $\mathcal{H}^{\otimes n}$  and its null element is  $o^{(n)}$ .

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<sup>1</sup>This extension is defined by antilinearity in the left argument and by linearity in the right one, respectively; for the proof of its uniqueness, see, e.g., [129], page 49, Proposition 1 or [119], page 451, Proposition 10.23.

For any  $f_1, \dots, f_n \in \mathcal{H}$ , let us define the *symmetrized tensor product*

$$f_1 \vee \dots \vee f_n := \frac{1}{n!} \sum_{\pi \in \mathcal{P}_n} f_{\pi(1)} \otimes \dots \otimes f_{\pi(n)} ; \quad (3.3)$$

as well-known,  $\mathcal{H}^{\vee n}$  coincides with the closed subspace of  $\mathcal{H}^{\otimes n}$  generated by products of the form (3.3) (which explains the notation  $\vee^n$ ).

Let us point out that, following the usual convention, we set  $\mathcal{H}^{\otimes 0} := \mathbb{C}$  (with null vector  $o^{(0)} := 0 \in \mathbb{C}$ ); consequently, we also have  $\mathcal{H}^{\vee 0} = \mathbb{C}$ .

*Remark 3.1.* The factor  $1/n!$  on the right-hand side of Eq. (3.3) is just an arbitrary normalization choice; the subsequent items i) and ii) point out some facts descending from this choice.

i) Let  $f \in \mathcal{H}$  and consider the totally symmetric element  $f \vee \dots \vee f \in \mathcal{H}^{\vee n}$ . It follows straightforwardly from the definition (3.3) (here employed with  $f_i = f$  for all  $i = 1, \dots, n$ ) that

$$f \vee \dots \vee f = f \otimes \dots \otimes f ; \quad (3.4)$$

in particular, one has  $o \vee \dots \vee o = o^{(n)}$ .

ii) Let  $f^{(n)} = f_1 \vee \dots \vee f_n$ ,  $g^{(n)} = g_1 \vee \dots \vee g_n \in \mathcal{H}^{\vee n}$  ( $f_i, g_i \in \mathcal{H}$  for all  $i = 1, \dots, n$ ) be any pair of totally symmetric elements. Then, using Eq.s (3.1) (3.3), it can be easily inferred that the inner product  $(f^{(n)}|g^{(n)})_n$  can be expressed as follows:

$$(f^{(n)}|g^{(n)})_n = \frac{1}{n!} \sum_{\pi \in \mathcal{P}_n} \prod_{i=1}^n \langle f_i | g_{\pi(i)} \rangle = \frac{1}{n!} \sum_{\pi \in \mathcal{P}_n} \prod_{i=1}^n \langle f_{\pi(i)} | g_i \rangle . \quad (3.5)$$

In particular, if  $f^{(n)} = f \vee \dots \vee f$  for some  $f \in \mathcal{H}$ , one has

$$(f^{(n)}|f^{(n)})_n = \langle f | f \rangle^n . \quad (3.6)$$

Now, consider the infinite collection of all totally symmetric Hilbert tensor powers of  $\mathcal{H}$ :

$$\mathcal{H}^{\vee n} \quad (n \in \{0, 1, 2, \dots\}) . \quad (3.7)$$

**Definition 3.1.** The *symmetric Fock space* over  $\mathcal{H}$  is

$$\mathfrak{F}^{\vee}(\mathcal{H}) := \bigoplus_{n=0}^{+\infty} \mathcal{H}^{\vee n} , \quad (3.8)$$

where  $\bigoplus$  indicates the Hilbert direct sum. The corresponding inner product is denoted with  $( | )$ .

*Remark 3.2.* According to the theory of Hilbert direct sums <sup>(2)</sup>,  $(\mathfrak{F}^{\vee}(\mathcal{H}), ( | ))$  is (up to isomorphisms) the unique Hilbert space possessing the forthcoming features i) and ii).

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<sup>2</sup>For a precise definition of Hilbert tensor product and Hilbert direct sum in the case of infinitely many countable or uncountable spaces (to be intended properly in the sense of nets), see, e.g., [27, 119].

- i) For any  $n \in \{0, 1, 2, \dots\}$ ,  $\mathcal{H}^{\vee n}$  is a closed subspace of  $\mathfrak{F}^{\vee}(\mathcal{H})$  and the corresponding inner product  $(\cdot | \cdot)_n$  coincides with the restriction of  $(\cdot | \cdot)$  to  $\mathcal{H}^{\vee n}$ .
- ii) The summands  $\mathcal{H}^{\vee n}$  ( $n \in \{0, 1, 2, \dots\}$ ) are mutually orthogonal with respect to  $(\cdot | \cdot)$  and the closed subspace they generate coincides with the whole Fock space  $\mathfrak{F}^{\vee}(\mathcal{H})$ .

It should be noted that any element  $\mathbf{f} \in \mathfrak{F}^{\vee}(\mathcal{H})$  has a unique representation

$$\mathbf{f} = \sum_{n=0}^{+\infty} f^{(n)} \quad (f^{(n)} \in \mathcal{H}^{\vee n}) ; \quad (3.9)$$

for any  $n \in \{0, 1, 2, \dots\}$ ,  $f^{(n)}$  is called the  $n$ -th *component* of  $\mathbf{f}$ .

Let us point out that, for any  $\mathbf{f}$  as above and for any  $\mathbf{g} = \sum_n g^{(n)} \in \mathfrak{F}^{\vee}(\mathcal{H})$ , there holds

$$(\mathbf{f} | \mathbf{g}) = \sum_{n=0}^{+\infty} (f^{(n)} | g^{(n)})_n . \quad (3.10)$$

We put

$$\mathbf{o} := \text{the null vector of } \mathfrak{F}^{\vee}(\mathcal{H}) ; \quad (3.11)$$

on the other hand, we will refer to the normalized vector

$$\mathbf{v} := 1 \in \mathbb{C} \equiv \mathcal{H}^{\vee 0} \subset \mathfrak{F}^{\vee}(\mathcal{H}) \quad (3.12)$$

(<sup>3</sup>). Moreover, we indicate with  $\hat{\mathbb{O}}_{\mathfrak{F}}$  and  $\hat{\mathbb{I}}_{\mathfrak{F}}$  the null and the identity operators on  $\mathfrak{F}^{\vee}(\mathcal{H})$ , respectively.

In the sequel we will be often interested in the space

$$\mathfrak{D}^{\vee}(\mathcal{H}) := \{ \mathbf{f} = \sum_n f^{(n)} \in \mathfrak{F}^{\vee}(\mathcal{H}) \mid f^{(n)} = 0 \text{ for almost all } n \in \{0, 1, 2, \dots\} \} ; \quad (3.13)$$

the above expression means that there exists  $N_{\mathbf{f}} \in \mathbb{N}$  (depending on  $\mathbf{f}$ ) such that  $f^{(n)} = 0$  for all  $n \geq N_{\mathbf{f}}$ . Of course,  $\mathfrak{D}^{\vee}(\mathcal{H})$  is a dense linear subspace of the Fock space  $\mathfrak{F}^{\vee}(\mathcal{H})$ ; whenever we will need a topology on  $\mathfrak{D}^{\vee}(\mathcal{H})$ , we will use the (non-complete) topology induced by the restriction of the inner product  $(\cdot | \cdot)$ .

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<sup>3</sup> Let us mention that  $\mathfrak{F}^{\vee}(\mathcal{H})$  could be defined as the set of sequences of the form

$$\mathbf{f} \equiv (f^{(n)}) = (f^{(0)}, f^{(1)}, f^{(2)}, \dots) ,$$

with  $f^{(n)} \in \mathcal{H}^{\vee n}$  for each  $n \in \{0, 1, 2, \dots\}$ , such that  $\sum_n (f^{(n)} | f^{(n)})_n < +\infty$ . This is a Hilbert space with the inner product  $(\cdot | \cdot)$ , defined according to Eq. (3.10). An element  $f^{(n)} \in \mathcal{H}^{\vee n}$  can be identified with the sequence  $(o^{(0)}, \dots, o^{(n-1)}, f^{(n)}, o^{(n+1)}, \dots) \in \mathfrak{F}^{\vee}(\mathcal{H})$ , where  $o^{(n)}$  is the null element of  $\mathcal{H}^{\vee n}$  ( $n \in \{0, 1, 2, \dots\}$ ). In this sense  $\mathcal{H}^{\vee n}$  is a linear subspace of  $\mathfrak{F}^{\vee}(\mathcal{H})$ , for each  $n \in \{0, 1, 2, \dots\}$ , and Eq. (3.9) holds for any  $\mathbf{f}$  as above; moreover, using the language of the present footnote, Eq.s (3.11) and (3.12) can be rephrased, respectively, as

$$\mathbf{o} := (o^{(0)}, o^{(1)}, o^{(2)}, \dots) , \quad \mathbf{v} := (1, o^{(1)}, o^{(2)}, \dots) .$$

Needless to say, both  $\mathbf{o}$  and  $\mathbf{v}$  (see Eq.s (3.11) (3.12)) do, in fact, belong to  $\mathfrak{D}^\vee(\mathcal{H})$ .

The space of all linear (unbounded) operators on  $\mathfrak{D}^\vee(\mathcal{H})$  is  $\mathcal{L}(\mathfrak{D}^\vee(\mathcal{H}))$ . In particular, we indicate with  $\hat{\mathbb{O}}_{\mathfrak{D}}$  and  $\hat{\mathbb{I}}_{\mathfrak{D}}$  ( $\in \mathcal{L}(\mathfrak{D}^\vee(\mathcal{H}))$ ) the restrictions to  $\mathfrak{D}^\vee(\mathcal{H})$  of the null and the identity operators on  $\mathfrak{F}^\vee(\mathcal{H})$  (i.e., of  $\hat{\mathbb{O}}_{\mathfrak{F}}$  and  $\hat{\mathbb{I}}_{\mathfrak{F}}$ ), respectively; so, for any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$ , there hold

$$\hat{\mathbb{O}}_{\mathfrak{D}} \mathbf{f} = \mathbf{o} , \quad \hat{\mathbb{I}}_{\mathfrak{D}} \mathbf{f} = \mathbf{f} . \quad (3.14)$$

One can also consider the *particle number operator*; this is the essentially self-adjoint operator  $\hat{\mathcal{N}} : \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{F}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  which is defined by components setting, for any  $\mathbf{f} = \sum_n f^{(n)}$ ,

$$\hat{\mathcal{N}} \mathbf{f} := \sum_n n f^{(n)} . \quad (3.15)$$

In the following, we adopt systematically the standard terminology indicated hereafter.

**Definition 3.2.** For any  $n \in \{1, 2, 3, \dots\}$ ,  $\mathcal{H}^{\vee n}$  is called the *n-particle Hilbert space* ( $\mathcal{H}$  is the *single particle space*) and its elements are the *totally symmetric states* of  $n$  particles.  $\mathcal{H}^{\vee 0}$  is the *Fock vacuum*; this is generated by the normalized vector  $\mathbf{v} \in \mathfrak{F}^\vee(\mathcal{H})$  (see Eq. (3.12)) which is called the *vacuum state*.  $\mathfrak{D}^\vee(\mathcal{H})$  is the *finite-particle subspace* and  $\mathfrak{F}^\vee(\mathcal{H})$  is the *bosonic Fock space* on  $\mathcal{H}$ .

*Remark 3.3.* In this work we will only consider a *scalar* field theory; therefore, since no confusion shall arise, the adjectives “totally symmetric” and “bosonic” will often be omitted and implicitly understood.

Finally, let us point out that in the physical applications that we are going to discuss in the following, we shall mainly be interested with expressions of the form described hereafter.

**Definition 3.3.** Let  $\hat{\mathcal{O}} : \text{Dom}(\hat{\mathcal{O}}) \subset \mathfrak{F}^\vee(\mathcal{H}) \rightarrow \mathfrak{F}^\vee(\mathcal{H})$  be any operator with domain containing (at least) the vacuum state  $\mathbf{v}$  ( $\mathbf{v} \in \text{Dom}(\hat{\mathcal{O}})$ ). The *vacuum expectation value* (in brief, *VEV*) of  $\hat{\mathcal{O}}$  is the complex number  $(\mathbf{v} | \hat{\mathcal{O}} \mathbf{v}) \in \mathbb{C}$ .

## Creation and annihilation operators.

Let again  $(\mathcal{H}, \langle | \rangle)$  be any abstract Hilbert space and consider the Fock space  $\mathfrak{F}^\vee(\mathcal{H})$ , in the formulation given in the previous subsection; hereafter, using the language described therein, we introduce the creation and annihilation operators on  $\mathfrak{F}^\vee(\mathcal{H})$  and analyze their main features.

**Definition 3.4.** For any given  $h \in \mathcal{H}$ , the (*h-smearred*) *creation* and *annihilation operators* are, respectively, the  $\mathbb{R}$ -linear maps

$$\hat{a}^+(h), \hat{a}^-(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H}) \quad (3.16)$$

defined “by components” as follows <sup>(4)</sup>. For any  $n \in \{1, 2, 3, \dots\}$ ,  $\hat{a}^+(h)$  and  $\hat{a}^-(h)$  are the unique linear maps sending  $\mathcal{H}^{\vee n}$  respectively into  $\mathcal{H}^{\vee(n+1)}$  and  $\mathcal{H}^{\vee(n-1)}$  which, for any element  $f^{(n)} \in \mathcal{H}^{\vee n}$  of the form  $f^{(n)} = f_1 \vee \dots \vee f_n$  ( $f_i \in \mathcal{H}$  for  $i = 1, \dots, n$ ), give

$$\hat{a}^+(h)(f_1 \vee \dots \vee f_n) = \sqrt{n+1} \ h \vee f_1 \vee \dots \vee f_n , \quad (3.17)$$

$$\hat{a}^-(h)(f_1 \vee \dots \vee f_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \langle h | f_i \rangle f_1 \vee \dots \vee \cancel{f_i} \vee \dots \vee f_n ; \quad (3.18)$$

here the notation  $f_1 \vee \dots \vee \cancel{f_i} \vee \dots \vee f_n$  indicates the symmetrized tensor product of the  $n-1$  elements obtained eliminating  $f_i$  from the collection  $\{f_1, \dots, f_n\}$ . In particular, for  $n=1$  and  $f^{(1)} \equiv f_1$ , Eq. (3.18) must be meant to hold in the sense that

$$\hat{a}^-(h)f^{(1)} = \langle h | f_1 \rangle \mathbf{v} . \quad (3.19)$$

Moreover, we put by convention

$$\hat{a}^-(h) \mathbf{v} := \mathbf{o} , \quad \hat{a}^+(h) \mathbf{v} := h \in \mathcal{H} \equiv \mathcal{H}^{\vee 1} , \quad (3.20)$$

with  $\mathbf{o}$  and  $\mathbf{v}$  indicating as usual the null vector and the vacuum state, respectively.

As well-known [130], for any  $h \in \mathcal{H}$ , both  $\hat{a}^+(h)$  and  $\hat{a}^-(h)$  are closable unbounded linear operators on  $\mathfrak{F}^{\vee}(\mathcal{H})$ , defined on the dense domain  $\mathfrak{D}^{\vee}(\mathcal{H})$ ; unless otherwise stated, from here on the symbols  $\hat{a}^+(h)$  and  $\hat{a}^-(h)$  will be used to indicate the closures of the operators defined in Eq.s (3.17) and (3.18), respectively.

Let us also point out a fact made evident by the definitions (3.17) (3.18): namely, that the maps  $h \mapsto \hat{a}^+(h)$  and  $h \mapsto \hat{a}^-(h)$  are  $\mathbb{C}$ -linear and  $\mathbb{C}$ -antilinear, respectively.

**Proposition 3.5.** *For any  $h \in \mathcal{H}$ , the creation and annihilation operators  $\hat{a}^+(h), \hat{a}^-(h)$  are the adjoints of each other; in particular, for all  $\mathbf{f}, \mathbf{g} \in \mathfrak{D}^{\vee}(\mathcal{H})$ , there holds*

$$(\hat{a}^+(h) \mathbf{f} | \mathbf{g}) = (\mathbf{f} | \hat{a}^-(h) \mathbf{g}) . \quad (3.21)$$

*Proof.* Due to the definition of the operators  $\hat{a}^+(h), \hat{a}^-(h)$ , it suffices to show that, for any  $n \in \mathbb{N}$  the maps  $\hat{a}^+(h) : \mathcal{H}^{\vee n} \rightarrow \mathcal{H}^{\vee(n+1)}$  and  $\hat{a}^-(h) : \mathcal{H}^{\vee(n+1)} \rightarrow \mathcal{H}^{\vee n}$  are (Banach) adjoints of each other; since  $\mathcal{H}^{\vee n}$  and  $\mathcal{H}^{\vee(n+1)}$  are respectively spanned by elements of the form  $f^{(n)} = f_1 \vee \dots \vee f_n$  and  $g^{(n+1)} = g_1 \vee \dots \vee g_{n+1} \in \mathcal{H}^{\vee(n+1)}$ , this amounts to prove that for any such pair  $f^{(n)}, g^{(n+1)}$ , there holds

$$(\hat{a}^+(h) f^{(n)} | g^{(n+1)})_{n+1} = (f^{(n)} | \hat{a}^-(h) g^{(n+1)})_n$$

where  $( | )_n$  and  $( | )_{n+1}$  indicate the inner products defined according to Eq. (3.1). On the other hand, the above identity can be easily checked keeping in mind Eq.s (3.17) (3.18) for  $\hat{a}^+(h), \hat{a}^-(h)$  and recalling the identities in Eq. (3.5) for the inner product  $( | )_n$  (and the corresponding ones for  $( | )_{n+1}$ ).  $\square$

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<sup>4</sup>Recall the considerations below Eq. (3.3) on page 113. In particular, let us recall that the finite particle subspace  $\mathfrak{D}^{\vee}(\mathcal{H})$  (as well as the Fock space  $\mathfrak{F}^{\vee}(\mathcal{H})$ ) is spanned by elements of the form  $f_1 \vee \dots \vee f_n$  ( $f_i \in \mathcal{H}$ , for  $i = 1, \dots, n, n \in \{0, 1, 2, \dots\}$ ).



To go on let us notice that, for any  $n \in \{1, 2, 3, \dots\}$  and for any family  $h_i \in \mathcal{H}$  ( $i = 1, \dots, n$ ), the multiple product  $\hat{a}^+(h_1) \dots \hat{a}^+(h_n)$  and the analogous expressions obtained replacing some of the  $\hat{a}^+$  with  $\hat{a}^-$  are all well-defined operators on the finite particle subspace  $\mathfrak{D}^\vee(\mathcal{H})$ . In particular, there holds the subsequent proposition, where we introduce the notation

$$[X, Y] := XY - YX , \quad (3.22)$$

to be respected thoroughout the remainder of this manuscript.

**Proposition 3.6.** *There hold the results enumerated hereafter.*

i) For any  $n \in \{1, 2, 3, \dots\}$ , the set  $\{\hat{a}^+(h_1) \dots \hat{a}^+(h_n) \mathbf{v} \mid h_i \in \mathcal{H}, i = 1, \dots, n, n \in \mathbb{N}\}$  spans  $\mathfrak{D}^\vee(\mathcal{H})$ , (i.e., it is total in  $\mathfrak{F}^\vee(\mathcal{H})$ ).

ii) For any  $h, k \in \mathcal{H}$ , there hold the canonical commutation relations (CCR)

$$\begin{aligned} [\hat{a}^+(h), \hat{a}^+(k)] &= \hat{\mathbf{O}}_{\mathfrak{D}} , \\ [\hat{a}^-(h), \hat{a}^-(k)] &= \hat{\mathbf{O}}_{\mathfrak{D}} , \\ [\hat{a}^-(h), \hat{a}^+(k)] &= \langle h|k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} . \end{aligned} \quad (3.23)$$

iii) For any  $h, k \in \mathcal{H}$ , the VEVs of monomials of degree two of the creation and annihilation operators are given by <sup>(5)</sup>

$$\begin{aligned} (\mathbf{v} | \hat{a}^+(h) \hat{a}^+(k) \mathbf{v}) &= (\mathbf{v} | \hat{a}^+(h) \hat{a}^-(k) \mathbf{v}) = (\mathbf{v} | \hat{a}^-(h) \hat{a}^-(k) \mathbf{v}) = 0 , \\ (\mathbf{v} | \hat{a}^-(h) \hat{a}^+(k) \mathbf{v}) &= \langle h|k \rangle . \end{aligned} \quad (3.24)$$

*Remark 3.4.* Statement i) can be expressed in other terms saying that the vacuum state  $\mathbf{v}$  is *cyclic* for the algebra generated by the identity operator  $\hat{\mathbb{I}}_{\mathfrak{D}}$  and by the set of all creation and annihilation operators  $\hat{a}^+(h), \hat{a}^-(h)$  ( $h \in \mathcal{H}$ ).

*Proof.* i) Recalling the definition (3.17) of  $\hat{a}^+(h)$  ( $h \in \mathcal{H}$ ), it can be trivially proved by induction on  $n \in \{1, 2, 3, \dots\}$  that

$$\hat{a}^+(h_1) \dots \hat{a}^+(h_n) \mathbf{v} = \sqrt{(n+1)!} h_1 \vee \dots \vee h_n ; \quad (3.25)$$

in view of the definition of  $\mathfrak{D}^\vee(\mathcal{H})$ , the above identity allows to infer the thesis.

ii) The thesis follows if one can prove the component-wise versions of the relations in Eq. (3.23). To this purpose, first notice that, due to the relations in Eq. (3.20), there hold  $[\hat{a}^+(h), \hat{a}^+(k)] \mathbf{v} = \sqrt{2} (h \vee k - k \vee h) = \mathbf{o}$ ,  $[\hat{a}^-(h), \hat{a}^-(k)] \mathbf{v} = \mathbf{o}$  and  $[\hat{a}^-(h), \hat{a}^+(k)] \mathbf{v} = \hat{a}^-(h) k = \langle h|k \rangle$ . Next, let us show that, for any  $n \in \{1, 2, 3, \dots\}$  and for any factorized element  $f^{(n)} = f_1 \vee \dots \vee f_n \in \mathcal{H}^{\vee n}$ , there holds

$$[\hat{a}^+(h), \hat{a}^+(k)] f^{(n)} = 0^{(n)} , \quad (3.26)$$

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<sup>5</sup>Of course, with some computational effort, this result could be generalized by Wick's theorem [142, 146] to a monomial of any order in the creation and annihilation operators; we do not report the general result here for the pursue of brevity, since we will only need the relations in Eq. (3.24) for the developments to be discussed in the following.

$$[\hat{a}^-(h), \hat{a}^-(k)] f^{(n)} = 0^{(n)} , \quad (3.27)$$

$$[\hat{a}^-(h), \hat{a}^+(k)] f^{(n)} = \langle h|k \rangle f^{(n)} . \quad (3.28)$$

Eq. (3.26) follows trivially from the definition of symmetrized tensor product (see Eq. (3.3)) noting that  $\hat{a}^+(h) \hat{a}^+(k) f^{(n)} = \sqrt{(n+1)(n+2)} h \vee k \vee f_1 \vee \dots \vee f_n$ . Once Eq. (3.26) has been established, one can easily infer Eq. (3.27) recalling that  $\hat{a}^-(h)$  is the adjoint of  $\hat{a}^+(h)$  for all  $h \in \mathcal{H}$  (see Proposition 3.5). Finally, keeping in mind the definitions (3.17) (3.18) of the creation and annihilation operators, one obtains

$$\begin{aligned} \hat{a}^-(h) \hat{a}^+(k) f^{(n)} &= \hat{a}^-(h) (\sqrt{n+1} k \vee f_1 \vee \dots \vee f_n) = \\ &= \frac{1}{n+1} \left( \langle h|k \rangle f_1 \vee \dots \vee f_n + \sum_{i=1}^n \langle h|f_i \rangle k \vee f_1 \vee \dots \vee \cancel{f_i} \vee \dots \vee f_n \right) , \\ \hat{a}^+(k) \hat{a}^-(h) f^{(n)} &= \frac{1}{n} \sum_{i=1}^n \langle h|f_i \rangle \hat{a}^+(k) (f_1 \vee \dots \vee \cancel{f_i} \vee \dots \vee f_n) = \\ &= \frac{1}{n} \sum_{i=1}^n \langle h|f_i \rangle k \vee f_1 \vee \dots \vee \cancel{f_i} \vee \dots \vee f_n ; \end{aligned}$$

the thesis (3.28) follows by taking the difference of the above expressions.

iii) First notice that, due to Proposition 3.5, there holds

$$(\mathbf{v} | \hat{a}^+(h) \hat{a}^+(k) \mathbf{v}) = (\hat{a}^-(k) \hat{a}^-(h) \mathbf{v} | \mathbf{v}) ;$$

then, all the expressions in the first line of Eq. (3.24) are easily seen to vanish because of the convention (3.20). On the other hand, due to (the already proved) item ii) of the present theorem, there holds  $\hat{a}^-(h) \hat{a}^+(k) = [\hat{a}^-(h), \hat{a}^+(k)] + \hat{a}^+(k) \hat{a}^-(h)$ ; then, the identity in the second line of Eq. (3.24) follows using again item ii) of the present theorem and recalling once more the convention (3.20).  $\square$

For completeness, let us also give the following result.

**Lemma 3.7.** *Let  $h \in \mathcal{H}$  and consider the creation and annihilation operators  $\hat{a}^+(h), \hat{a}^-(h)$ , along with the particle number operator  $\hat{\mathcal{N}}$  <sup>(6)</sup>. Then, there hold*

$$\begin{aligned} [\hat{\mathcal{N}}, \hat{a}^+(h)] &= \hat{a}^+(h) , \\ [\hat{\mathcal{N}}, \hat{a}^-(h)] &= -\hat{a}^-(h) . \end{aligned} \quad (3.29)$$

*Proof.* Also in this case the thesis follows by proving component-wise versions of the relations in Eq. (3.29). First notice that, due to Eq. (3.20),  $[\hat{\mathcal{N}}, \hat{a}^+(h)] \mathbf{v} = \hat{\mathcal{N}} h = h = \hat{a}^+(h) \mathbf{v}$  and  $[\hat{\mathcal{N}}, \hat{a}^-(h)] \mathbf{v} = \mathbf{o} = \hat{a}^-(h) \mathbf{v}$ . Then, it suffices to show that, for all  $n \in \{1, 2, 3, \dots\}$  and for all  $f^{(n)} \in \mathcal{H}^{\vee n}$  of the form  $f^{(n)} = f_1 \vee \dots \vee f_n$ , one has  $[\hat{\mathcal{N}}, \hat{a}^+(h)] f^{(n)} = \hat{a}^+(h) f^{(n)}$  and  $[\hat{\mathcal{N}}, \hat{a}^-(h)] f^{(n)} = -\hat{a}^-(h) f^{(n)}$ . In fact, the latter identities can be inferred by straightforward computations, recalling the definitions (3.15) and (3.17) (3.18) of  $\hat{\mathcal{N}}$  and  $\hat{a}^+(h), \hat{a}^-(h)$ ; this yields the thesis.  $\square$

<sup>6</sup>Recall that all these operators are defined on the common dense domain  $\mathfrak{D}^{\vee}(\mathcal{H})$ .

### Segal quantization.

Let again  $\mathfrak{F}^\vee(\mathcal{H})$  denote the Fock space constructed on any given, abstract Hilbert space  $\mathcal{H}$ , with inner product  $\langle \cdot | \cdot \rangle$ . In accordance with Segal's approach to field quantization (see, e.g., [43, 58, 130]), we give the following definition.

**Definition 3.8.** For any  $h \in \mathcal{H}$ , the ( $h$ -smeared) Segal field and conjugate momentum are the (unbounded) operators  $\hat{\Phi}_S(h), \hat{\Pi}_S(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  given, respectively, by

$$\hat{\Phi}_S(h) := \frac{1}{\sqrt{2}} \left( \hat{a}^-(h) + \hat{a}^+(h) \right), \quad (3.30)$$

$$\hat{\Pi}_S(h) := \frac{1}{i\sqrt{2}} \left( \hat{a}^-(h) - \hat{a}^+(h) \right). \quad (3.31)$$

*Remark 3.5.* It can be readily checked that, for any  $h \in \mathcal{H}$ , there holds

$$\hat{\Pi}_S(h) = \hat{\Phi}_S(ih); \quad (3.32)$$

so, the Segal momentum is not strictly necessary within the framework considered in this subsection. For this reason, most of the forthcoming results will be formulated only in terms of the Segal field  $\hat{\Phi}_S(h)$ . Nevertheless, let us anticipate that the Segal momentum  $\hat{\Pi}_S(h)$  turns out to be useful in order to motivate the definition of Wightman conjugate momentum, as well as in certain related considerations, to be discussed in the following subsection 3.1.

Recall that the maps  $h \mapsto \hat{a}^+(h), h \mapsto \hat{a}^-(h)$  are, respectively,  $\mathbb{C}$ -linear and  $\mathbb{C}$ -antilinear (see the comments below Definition 3.4); in consequence of this, the map  $h \mapsto \hat{\Phi}_S(h)$  (usually referred to as *Segal quantization*) is neither  $\mathbb{C}$ -linear nor  $\mathbb{C}$ -antilinear, but only  $\mathbb{R}$ -linear.

It is well-known [43, 130] that, for any  $h \in \mathcal{H}$ ,  $\hat{\Phi}_S(h)$  extends to an essentially self-adjoint (closed) operator of  $\mathfrak{F}^\vee(\mathcal{H})$  with domain of self-adjointness  $\mathfrak{D}^\vee(\mathcal{H})$ . Moreover, for any  $n \in \{1, 2, 3, \dots\}$  and for any family  $h_i \in \mathcal{H}^1, i = 1, \dots, n$ , the finite product  $\hat{\Phi}_S(h_1) \dots \hat{\Phi}_S(h_n)$  is well-defined on the finite particle subspace  $\mathfrak{D}^\vee(\mathcal{H})$ .

**Proposition 3.9.** *There hold the following results.*

i) For any  $n \in \{1, 2, 3, \dots\}$ , the set  $\{\hat{\Phi}_S(h_1) \dots \hat{\Phi}_S(h_n) \mathbf{v} \mid h_i \in \mathcal{H}, \text{ for } i = 1, \dots, n, n \in \{1, 2, 3, \dots\}\}$  spans  $\mathfrak{D}^\vee(\mathcal{H})$ .

ii) For any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$ , the map  $\mathcal{H} \rightarrow \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{F}^\vee(\mathcal{H}), h \mapsto \hat{\Phi}_S(h)\mathbf{f}$  is continuous.

iii) For any  $h, k \in \mathcal{H}$ , there holds the commutation relation

$$[\hat{\Phi}_S(h), \hat{\Phi}_S(k)] = i\Im\langle h|k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} \quad (3.33)$$

(here  $\Im\langle h|k \rangle$  indicates the imaginary part of the inner product  $\langle h|k \rangle \in \mathbb{C}$ ).

iv) For any  $h, k \in \mathcal{H}$ , the VEV of the second-order monomial  $\hat{\Phi}_S(h)\hat{\Phi}_S(k)$  is

$$\langle \mathbf{v} \mid \hat{\Phi}_S(h) \hat{\Phi}_S(k) \mathbf{v} \rangle = \frac{1}{2} \langle h|k \rangle. \quad (3.34)$$

*Remark 3.6.* In consequence of statement i), the vacuum state  $\mathbf{v}$  is cyclic for the algebra generated by the identity operator  $\hat{\mathbb{I}}_{\mathfrak{D}}$  and by the set of Segal field operators  $\hat{\Phi}_S(h)$  ( $h \in \mathcal{H}$ ).

*Proof.* i) Recalling the definition (3.20) and the identity (3.25), also in this case the thesis can be proved by induction on  $n \in \{1, 2, 3, \dots\}$ , with some computational effort.

ii) This is a well-known fact; see, e.g., the proof of item (d) of Theorem X.41 in [130].

iii) First notice that, in view of the definition (3.30) of the Segal field, one easily infers

$$[\hat{\Phi}_S(h), \hat{\Phi}_S(k)] = \frac{1}{2} \left( [\hat{a}^-(h), \hat{a}^-(k)] + [\hat{a}^-(h), \hat{a}^+(k)] + [\hat{a}^+(h), \hat{a}^-(k)] + [\hat{a}^+(h), \hat{a}^+(k)] \right);$$

due to the CCR (3.23), the above identity implies  $[\hat{\Phi}_S(h), \hat{\Phi}_S(k)] = (\langle h|k \rangle - \langle k|h \rangle)/2 \hat{\mathbb{I}}_{\mathfrak{D}}$ , which yields Eq. (3.33).

iv) Recalling again the definition (3.30) of  $\hat{\Phi}_S(h)$  ( $h \in \mathcal{H}$ ), one has

$$\begin{aligned} & (\mathbf{v} | \hat{\Phi}_S(h) \hat{\Phi}_S(k) \mathbf{v}) = \\ & \frac{1}{2} \left( (\mathbf{v} | \hat{a}^-(h) \hat{a}^-(k) \mathbf{v}) + (\mathbf{v} | \hat{a}^-(h) \hat{a}^+(k) \mathbf{v}) + (\mathbf{v} | \hat{a}^+(h) \hat{a}^-(k) \mathbf{v}) + (\mathbf{v} | \hat{a}^+(h) \hat{a}^+(k) \mathbf{v}) \right); \end{aligned}$$

now, Eq. (3.34) follows straightforwardly using the CCR (3.23). □

Now, let us recall some well-known facts about second quantization; these facts will be employed in the following to introduce a notion of time evolution for the physical theory of a scalar field, to be described later on. We refer to [43, 130] for the proof of the forthcoming Proposition 3.11 (as well as for more general formulations, which can be derived under much weaker assumptions).

**Definition 3.10.** Consider the single particle Hilbert space  $\mathcal{H}$  and let  $\mathcal{U}$  be any unitary operator on it; the *second quantization* of  $\mathcal{U}$  is the unitary operator  $\Gamma(\mathcal{U}) : \mathfrak{F}^\vee(\mathcal{H}) \rightarrow \mathfrak{F}^\vee(\mathcal{H})$  defined so that, for all  $n \in \{1, 2, 3, \dots\}$ , there holds

$$\Gamma(\mathcal{U}) \upharpoonright \mathcal{H}^{\vee n} = \underbrace{\mathcal{U} \otimes \dots \otimes \mathcal{U}}_{n \text{ times}}. \quad (3.35)$$

*Remark 3.7.* Note that  $\Gamma(\mathcal{U}) \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{D}^\vee(\mathcal{H})$ .

**Proposition 3.11.** Let  $\mathcal{U}$  be any unitary operator on  $\mathcal{H}$ ; for any  $h \in \mathcal{H}$  and for all  $\mathbf{f} \in \mathfrak{D}^\vee$ , the Segal field  $\hat{\Phi}_S(h)$  fulfills

$$\Gamma(\mathcal{U}) \hat{\Phi}_S(h) \Gamma(\mathcal{U})^{-1} \mathbf{f} = \hat{\Phi}_S(\mathcal{U}h) \mathbf{f}. \quad (3.36)$$

*Proof.* First of all notice that, for any  $n \in \{1, 2, 3, \dots\}$  and for any  $f^{(n)} \in \mathcal{H}^{\vee n}$  of the form  $f^{(n)} = f_1 \vee \dots \vee f_n$  ( $f_i \in \mathcal{H}$ ,  $i = 1, \dots, n$ ), there holds

$$\begin{aligned} & \Gamma(\mathcal{U}) \hat{a}^+(h) \Gamma(\mathcal{U})^{-1} f^{(n)} = \Gamma(\mathcal{U}) \hat{a}^+(h) (\mathcal{U}^{-1} f_1 \vee \dots \vee \mathcal{U}^{-1} f_n) = \\ & = \sqrt{n+1} \Gamma(\mathcal{U}) (h \vee \mathcal{U}^{-1} f_1 \vee \dots \vee \mathcal{U}^{-1} f_n) = \sqrt{n+1} (\mathcal{U}h) \vee f_1 \vee \dots \vee f_n = \hat{a}^+(\mathcal{U}h) f^{(n)}; \end{aligned}$$

by the usual linearity and density arguments, the above chain of equalities allows to infer that  $\Gamma(\mathcal{U}) \hat{a}^+(h) \Gamma(\mathcal{U})^{-1} = \hat{a}^+(\mathcal{U}h)$  on  $\mathfrak{D}^\vee$ . On the other hand, keeping in mind Proposition 3.5 and taking the adjoint, one readily infers  $\Gamma(\mathcal{U}) \hat{a}^-(h) \Gamma(\mathcal{U})^{-1} = \hat{a}^-(\mathcal{U}h)$  on  $\mathfrak{D}^\vee$ . Then the thesis follows recalling the definition (3.30) of  $\hat{\Phi}_S(H)$ .  $\square$

### The Wightman field at time zero.

Let  $(\mathcal{H}, \langle \cdot | \cdot \rangle)$  be any abstract Hilbert space endowed with a conjugation  $\mathcal{J} : \mathcal{H} \rightarrow \mathcal{H}$  (see subsection 2.5); moreover, let  $\mathcal{A}$  be some strictly positive, self-adjoint operator on  $\mathcal{H}$  (with spectrum  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ , for some  $\varepsilon > 0$ ). We assume  $\mathcal{A}$  to be  $\mathcal{J}$ -real.

On the one hand, following the general construction developed in Chapter 2 (see, in particular, Proposition 2.4 of Section 2.5), one can consider the scale of Hilbert spaces  $\mathcal{H}^r \equiv (\mathcal{H}^r, \langle \cdot | \cdot \rangle_r)$  ( $r \in [-\infty, +\infty]$ ) associated to the real powers  $\mathcal{A}^{r/2}$ . On the other hand, the conjugation over  $\mathcal{H}$  admits a continuous extension  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$ , (see Proposition 2.25). So, we can introduce the linear subspaces

$$\mathcal{H}_\pm^{-\infty} := \{f \in \mathcal{H}^{-\infty} \mid \mathcal{J}f = \pm f\}, \quad (3.37)$$

fulfilling

$$\mathcal{H}^{-\infty} = \mathcal{H}_+^{-\infty} \oplus \mathcal{H}_-^{-\infty}, \quad \mathcal{H}_-^{-\infty} = i\mathcal{H}_+^{-\infty}. \quad (3.38)$$

The projectors of  $\mathcal{H}^{-\infty}$  onto  $\mathcal{H}_\pm^{-\infty}$  are

$$\mathcal{P}_\pm := \frac{\mathbb{I} \pm \mathcal{J}}{2} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}_\pm^{-\infty} \quad (3.39)$$

and, for each  $h \in \mathcal{H}^{-\infty}$ , one has

$$h = \mathcal{P}_+ h + \mathcal{P}_- h, \quad \mathcal{P}_- h = i\mathcal{P}_+(-i h). \quad (3.40)$$

Again from Proposition 2.25, we know that  $\mathcal{J}\mathcal{H}^r = \mathcal{H}^r$  for each  $r \in [-\infty, +\infty]$ . Of course, we can define the subspaces  $\mathcal{H}_\pm^r := \{f \in \mathcal{H}^r \mid \mathcal{J}f = \pm f\}$  and write an analogue of Eq. (3.38) with  $-\infty$  replaced by  $r$ ; the projections of  $\mathcal{H}^r$  onto  $\mathcal{H}_\pm^r$  are the maps  $\mathcal{P}_\pm \upharpoonright \mathcal{H}^r$ .

In view of the forthcoming physical applications, we choose  $\mathcal{H} \equiv \mathcal{H}^0$  as the fundamental, single particle Hilbert space and consider the bosonic Fock space  $\mathfrak{F}^\vee(\mathcal{H})$  on it. Nonetheless, we will often employ the spaces  $\mathcal{H}^{\pm 1/2}$ , as well as spaces of other orders; in particular, let us recall that  $\mathcal{H}^{1/2} \xrightarrow{\text{dense}} \mathcal{H} \xrightarrow{\text{dense}} \mathcal{H}^{-1/2}$  (see item ii) of Proposition 2.5 in Chapter 2).

Next, consider the Segal field  $\hat{\Phi}_S(h)$  along with the conjugate momentum  $\hat{\Pi}_S(h)$  ( $h \in \mathcal{H}$ ); hereafter we will use them to define the so-called Wightman field and its conjugate momentum, which are more closely related to the Wightman axioms for field quantization (and, in particular, are  $\mathbb{C}$ -linear in the “test function”  $h$ , as required by the Wightman axioms). These fields will be the subject of the forthcoming Definition 3.13, which is preceded by the following proposition.

**Proposition 3.12.** *Consider the  $\mathbb{R}$ -linear maps*

$$\hat{\varphi} : \mathcal{H}_+^{-1/2} \rightarrow \mathfrak{L}(\mathfrak{D}^\vee(\mathcal{H})) , \quad h \mapsto \hat{\varphi}(h) := \hat{\Phi}_S(\mathcal{A}^{-1/4}h) , \quad (3.41)$$

$$\hat{\pi} : \mathcal{H}_+^{1/2} \rightarrow \mathfrak{L}(\mathfrak{D}^\vee(\mathcal{H})) , \quad h \mapsto \hat{\pi}(h) := \hat{\Pi}_S(\mathcal{A}^{1/4}h) . \quad (3.42)$$

*These possess unique  $\mathbb{C}$ -linear extensions*

$$\hat{\varphi} : \mathcal{H}^{-1/2} \rightarrow \mathfrak{L}(\mathfrak{D}^\vee(\mathcal{H})) , \quad \hat{\pi} : \mathcal{H}^{1/2} \rightarrow \mathfrak{L}(\mathfrak{D}^\vee(\mathcal{H})) , \quad (3.43)$$

*given by*

$$\hat{\varphi}(h) = \hat{\Phi}_S(\mathcal{P}_+(\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(\mathcal{P}_+(-i\mathcal{A}^{-1/4}h)) \quad \text{for } h \in \mathcal{H}^{-1/2} , \quad (3.44)$$

$$\hat{\pi}(h) = \hat{\Pi}_S(\mathcal{P}_+(\mathcal{A}^{1/4}h)) + i\hat{\Pi}_S(\mathcal{P}_+(-i\mathcal{A}^{1/4}h)) \quad \text{for } h \in \mathcal{H}^{1/2} . \quad (3.45)$$

*Remark 3.8.* i) The assumptions  $h \in \mathcal{H}^{-1/2}$  and  $h \in \mathcal{H}^{1/2}$  in Eq.s (3.44) and (3.45), respectively, are both necessary and sufficient in order for the expressions in the cited equations to make sense. In fact, due to Corollary 2.13 (see, in particular, Eq. (2.95)), one has  $\mathcal{A}^{-1/4}h \in \mathcal{H}^0 \equiv \mathcal{H}$  and  $\mathcal{A}^{1/4}h \in \mathcal{H}^0 \equiv \mathcal{H}$  if and only if  $h \in \mathcal{H}^{-1/2}$  and  $h \in \mathcal{H}^{1/2}$ , respectively; this grants the well-posedness of the Segal fields and of the conjugate momentums appearing in Eq. (3.44) (3.45).

ii) Of course, the maps  $\mathcal{H}^{-1/2} \ni h \mapsto \hat{\varphi}(h)$  and  $\mathcal{H}^{1/2} \ni h \mapsto \hat{\pi}(h)$  are both  $\mathbb{C}$ -linear.

iii) Keeping in mind the identity  $\mathcal{P}_+h = i\mathcal{P}_-(-ih)$  (see Eq. (3.40)) and recalling that  $\hat{\Pi}_S(\mathcal{A}^{1/4}h) = \hat{\Phi}_S(i\mathcal{A}^{1/4}h)$  (see Eq. (3.32)), Eq. (3.45) can be easily re-expressed in terms of the Segal field as

$$\hat{\pi}(h) = i\left(\hat{\Phi}_S(\mathcal{P}_-(\mathcal{A}^{1/4}h)) + i\hat{\Phi}_S(\mathcal{P}_-(-i\mathcal{A}^{1/4}h))\right) \quad \text{for } h \in \mathcal{H}^{1/2} . \quad (3.46)$$

*Proof.* . We are going to show how to derive Eq. (3.44) under the only assumption that  $\mathcal{H}^{-1/2} \ni h \mapsto \hat{\varphi}(h)$  is a  $\mathbb{C}$ -linear extension of the map  $\mathcal{H}_+^{-1/2} \ni h \mapsto \hat{\Phi}_S(\mathcal{A}^{-1/4}h)$ ; of course, this automatically grants that the map under analysis exists and is uniquely determined. The analogous statement for  $h \mapsto \hat{\pi}(h)$  can be proved similarly, in view of the identity  $\hat{\Pi}_S(\mathcal{A}^{1/4}h) = \hat{\Phi}_S(i\mathcal{A}^{1/4}h)$  ( $h \in \mathcal{H}^{1/2}$ ).

So, let us first recall that  $h = \mathcal{P}_+h + i\mathcal{P}_+(-ih)$  for all  $h \in \mathcal{H}^{-1/2}$  (see Eq. (3.40)); of course  $\mathcal{P}_+h, \mathcal{P}_+(-ih) \in \mathcal{H}_+^{-1/2}$ . Next, let  $\hat{\varphi} : \mathcal{H}^{-1/2} \rightarrow \mathfrak{L}(\mathfrak{D}^\vee(\mathcal{H}))$  be any  $\mathbb{C}$ -linear map; in view of the previous considerations, for any  $h \in \mathcal{H}^{-1/2}$ , by complex-linearity it follows that  $\hat{\varphi}(h) = \hat{\varphi}(\mathcal{P}_+h) + i\hat{\varphi}(\mathcal{P}_+(-ih))$ . Moreover, requiring  $\hat{\varphi}$  to fulfill  $\hat{\varphi}(h_+) = \hat{\Phi}_S(\mathcal{A}^{-1/4}h_+)$  for all  $h_+ \in \mathcal{H}_+^{-1/2}$ , one has  $\hat{\varphi}(\mathcal{P}_+h) + i\hat{\varphi}(\mathcal{P}_+(-ih)) = \hat{\Phi}_S(\mathcal{A}^{-1/4}(\mathcal{P}_+h)) + i\hat{\Phi}_S(\mathcal{A}^{-1/4}(\mathcal{P}_+(-ih)))$ . Since  $\mathcal{P}_+$  commutes with any real function of  $\mathcal{A}$  (see Corollary 2.26), Eq. (3.44) follows easily. In conclusion, the arbitrariness of  $h \in \mathcal{H}^{-1/2}$  yields the thesis.  $\square$

**Definition 3.13.** The ( $h$ -smeared) *Wightman field* and the related *conjugate momentum at time zero*, respectively, the (unbounded) operators  $\hat{\varphi}(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  (for  $h \in \mathcal{H}^{-1/2}$ ) and  $\hat{\pi}(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  (for  $h \in \mathcal{H}^{1/2}$ ) introduced in Proposition 3.12.

*Remark 3.9.* The nomenclature at “time zero” might seem unclear at this stage; its meaning will become apparent in the next subsection, when a notion of *time evolution* for the field theory discussed here will be described.

**Lemma 3.14.** *For any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$ , the maps  $\mathcal{H}^{-1/2} \rightarrow \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{F}^\vee(\mathcal{H})$ ,  $h \mapsto \hat{\varphi}(h)\mathbf{f}$  and  $\mathcal{H}^{1/2} \rightarrow \mathfrak{D}^\vee(\mathcal{H})$ ,  $h \mapsto \hat{\pi}(h)\mathbf{f}$  are continuous.*

*Proof.* First consider the representations (3.44) and (3.45) of the Wightman field and of the conjugate momentum, respectively. Next, recall that the maps  $\mathcal{A}^{\pm 1/4} : \mathcal{H}^{\pm 1/2} \rightarrow \mathcal{H}$  are Hilbertian isomorphisms (see Corollary 2.13); whence, in particular, they are continuous. On the other hand, in view of the continuity of the extension  $\mathcal{J} : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  of the conjugation operator (see Proposition 2.25), the restriction of the projector  $\mathcal{P}_+ : \mathcal{H}^r \rightarrow \mathcal{H}^r$  is also continuous for all  $r \in \mathbb{R}$ . Then, the thesis follows from the continuity of the map  $\mathcal{H} \ni h \mapsto \hat{\Phi}_S(h)\mathbf{f}$  (see item ii) of Proposition 3.9).  $\square$

Now, let us give an auxiliary result which allows to make contact with the standard literature on the Wightman field [130]; this result also allows to derive easier proofs of the subsequent statements.

**Lemma 3.15.** *The Wightman field and conjugate momentum operators at time zero possess, respectively, the following representations in terms of the creation and annihilation operators  $\hat{a}^+(\cdot)$ ,  $\hat{a}^-(\cdot)$ :*

$$\hat{\varphi}(h) = \frac{1}{\sqrt{2}} \left( \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}h)) + \hat{a}^+(\mathcal{A}^{-1/4}h) \right) \quad (h \in \mathcal{H}^{-1/2}), \quad (3.47)$$

$$\hat{\pi}(h) = \frac{1}{i\sqrt{2}} \left( \hat{a}^-(\mathcal{J}(\mathcal{A}^{1/4}h)) - \hat{a}^+(\mathcal{A}^{1/4}h) \right) \quad (h \in \mathcal{H}^{1/2}). \quad (3.48)$$

*Proof.* As an example, we show how to derive Eq. (3.47); the analogous relation (3.48) can be derived by similar means. First of all, consider the identity (3.44) for the Wightman field  $\hat{\varphi}(h)$  ( $h \in \mathcal{H}^{-1/2}$ ); expressing the Segal field  $\hat{\Phi}_S$  appearing therein in terms of the creation and annihilation operators  $\hat{a}^\pm(\cdot)$  according to Eq. (3.30), it can be readily inferred that

$$\hat{\varphi}(h) = \frac{1}{\sqrt{2}} \left( \hat{a}^-(\mathcal{P}_+(\mathcal{A}^{-1/4}h)) + \hat{a}^+(\mathcal{P}_+(\mathcal{A}^{-1/4}h)) + i\hat{a}^-(-i\mathcal{P}_-(\mathcal{A}^{-1/4}h)) + i\hat{a}^+(-i\mathcal{P}_-(\mathcal{A}^{-1/4}h)) \right).$$

Then, recalling that the maps  $h \mapsto \hat{a}^+(h)$  and  $h \mapsto \hat{a}^-(h)$  are, respectively,  $\mathbb{C}$ -linear and  $\mathbb{C}$ -antilinear, it follows that

$$\hat{\varphi}(h) = \frac{1}{\sqrt{2}} \left( \hat{a}^-((\mathcal{P}_+ - \mathcal{P}_-)\mathcal{A}^{-1/4}h) + \hat{a}^+((\mathcal{P}_+ + \mathcal{P}_-)\mathcal{A}^{-1/4}h) \right);$$

the above identity proves the thesis (3.47) since, in view of the definitions of  $\mathcal{P}_\pm$  in Eq. (3.39),  $\mathcal{P}_+ - \mathcal{P}_- = \mathcal{J}$  and  $\mathcal{P}_+ + \mathcal{P}_- = \mathbb{I}$  (with  $\mathbb{I}$  indicating the identity operator on  $\mathcal{H}$ ).  $\square$

**Proposition 3.16.** *There hold the following commutation relations:*

$$\begin{aligned} [\hat{\varphi}(h), \hat{\varphi}(k)] &= \hat{\mathcal{O}}_{\mathfrak{D}} && \text{for } h, k \in \mathcal{H}^{-1/2}, \\ [\hat{\varphi}(h), \hat{\pi}(k)] &= i \langle \mathcal{J}h|k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} && \text{for } h \in \mathcal{H}^{-1/2}, k \in \mathcal{H}^{1/2}, \\ [\hat{\pi}(h), \hat{\pi}(k)] &= \hat{\mathcal{O}}_{\mathfrak{D}} && \text{for } h, k \in \mathcal{H}^{1/2} \end{aligned} \quad (3.49)$$

where  $\langle | \rangle$  indicates the extension (2.103) to  $\mathcal{H}^{-1/2} \times \mathcal{H}^{1/2}$  of the inner product on  $\mathcal{H}$ .

*Remark 3.10.* Let  $k \in \mathcal{H}^{1/2}$  be any given element; then, if  $h$  belongs to of the subspace  $\mathcal{H}_+^{-1/2} \subset \mathcal{H}^{-1/2}$  (which is invariant under the action of  $\mathcal{J}$ ), the second relation in Eq. (3.49) reduces to

$$[\hat{\varphi}(h), \hat{\pi}(k)] = i \langle h|k \rangle \hat{\mathbb{I}}_{\mathfrak{D}}. \quad (3.50)$$

*Proof.* Let us compute, for example, the only non-vanishing commutator in Eq. (3.49), i.e.,  $[\hat{\varphi}(h), \hat{\pi}(k)]$ . Keeping in mind the expressions derived in Lemma 3.15 (giving the Wightman field and the conjugate momentum in terms of creation and annihilation operators) and recalling the CCR (3.23), one easily infers that

$$[\hat{\varphi}(h), \hat{\pi}(k)] = -\frac{1}{2i} \left( \langle \mathcal{J}(\mathcal{A}^{-1/4}h)|\mathcal{A}^{1/4}k \rangle + \langle \mathcal{J}(\mathcal{A}^{1/4}k)|\mathcal{A}^{-1/4}h \rangle \right) \hat{\mathbb{I}}_{\mathfrak{D}}$$

where  $\langle | \rangle$  indicates the (non-extended) inner product on  $\mathcal{H}$ . Since this map is sesquilinear, the basic properties (2.64) of the conjugation  $\mathcal{J}$  yield

$$\langle \mathcal{J}(\mathcal{A}^{1/4}k)|\mathcal{A}^{-1/4}h \rangle = \overline{\langle \mathcal{A}^{1/4}k|\mathcal{J}(\mathcal{A}^{-1/4}h) \rangle} = \langle \mathcal{J}(\mathcal{A}^{-1/4}h)|\mathcal{A}^{1/4}k \rangle.$$

Next, notice that  $\mathcal{J}\mathcal{A}^{-1/4} = \mathcal{A}^{-1/4}\mathcal{J}$ , due to Corollary 2.26; moreover, interpreting the expression  $\langle | \rangle$  as the extension (2.103) to  $\mathcal{H}^{-1/2} \times \mathcal{H}^{1/2}$  of the inner product on  $\mathcal{H}$  and keeping in mind the results of Corollary 2.24 on the Banach adjoints of powers of  $\mathcal{A}$ , it follows that  $\langle \mathcal{A}^{-1/4}\mathcal{J}h|\mathcal{A}^{1/4}k \rangle = \langle \mathcal{J}h|k \rangle$ . Summing up, the above mentioned facts prove the thesis.  $\square$

**Lemma 3.17.** *The VEVs of the second order monomials in the Wightman field  $\hat{\varphi}(h)$  and in the conjugate momentum  $\hat{\pi}(h)$  are the following:*

$$\begin{aligned} (\mathbf{v}|\hat{\varphi}(h)\hat{\varphi}(k)\mathbf{v}) &= \frac{1}{2} \langle \mathcal{J}(\mathcal{A}^{-1/4}h)|\mathcal{A}^{-1/4}k \rangle && \text{for } h, k \in \mathcal{H}^{-1/2}, \\ (\mathbf{v}|\hat{\varphi}(h)\hat{\pi}(k)\mathbf{v}) &= -(\mathbf{v}|\hat{\pi}(h)\hat{\varphi}(k)\mathbf{v}) = \frac{i}{2} \langle \mathcal{J}h|k \rangle && \text{for } h \in \mathcal{H}^{-1/2}, k \in \mathcal{H}^{1/2}, \\ (\mathbf{v}|\hat{\pi}(h)\hat{\pi}(k)\mathbf{v}) &= \frac{1}{2} \langle \mathcal{J}(\mathcal{A}^{1/4}h)|\mathcal{A}^{1/4}k \rangle && \text{for } h, k \in \mathcal{H}^{1/2} \end{aligned} \quad (3.51)$$

where  $\langle | \rangle$  indicates the usual inner product on  $\mathcal{H}$ .



*Proof.* As an example, let us evaluate the VEV  $(\mathbf{v} | \hat{\varphi}(h) \hat{\varphi}(k) \mathbf{v})$ . Recalling once more Eq.s (3.47) and (3.48) for the Wightman field and the conjugate momentum, respectively, one easily obtains

$$\begin{aligned} (\mathbf{v} | \hat{\varphi}(h) \hat{\varphi}(k) \mathbf{v}) = & \\ \frac{1}{2} \left( (\mathbf{v} | \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}h)) \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}k)) \mathbf{v}) + (\mathbf{v} | \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}h)) \hat{a}^+(\mathcal{A}^{-1/4}k) \mathbf{v}) + \right. & \\ \left. + (\mathbf{v} | \hat{a}^+(\mathcal{A}^{-1/4}h) \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}k)) \mathbf{v}) + (\mathbf{v} | \hat{a}^+(\mathcal{A}^{-1/4}h) \hat{a}^+(\mathcal{A}^{-1/4}k) \mathbf{v}) \right). & \end{aligned}$$

Due to item iii) of Proposition 3.6 (see, in particular, Eq. (3.24)), all the VEVs on the right-hand side vanish except for  $(\mathbf{v} | \hat{a}^-(\mathcal{J}(\mathcal{A}^{-1/4}h)) \hat{a}^+(\mathcal{A}^{-1/4}k) \mathbf{v}) = \langle \mathcal{J}(\mathcal{A}^{-1/4}h) | \mathcal{A}^{-1/4}k \rangle$  which gives the thesis.

Let us also point out that, in order to derive the explicit expression in Eq. (3.51) for  $(\mathbf{v} | \hat{\varphi}(h) \hat{\pi}(k) \mathbf{v})$ ,  $(\mathbf{v} | \hat{\pi}(h) \hat{\varphi}(k) \mathbf{v})$ , one should also recall that  $\mathcal{J}\sqrt{\mathcal{A}} = \sqrt{\mathcal{A}}\mathcal{J}$  (see Corollary 2.26).  $\square$

### Time evolution for the Wightman field.

Let  $\mathcal{A}$  denote again a strictly positive, self-adjoint operator on some given Hilbert space  $\mathcal{H}$ , which we assume to be endowed with a conjugation  $\mathcal{J}$  (such that  $\mathcal{A}$  is  $\mathcal{J}$ -real).

In order to introduce a notion of “time evolution” for the Wightman field, let us first assume that the space  $\mathcal{H}$  is used to describe a physical theory where the role of the *single particle Hamiltonian* is played by the square root of the admissible operator  $\mathcal{A}$ , i.e.,

$$\sqrt{\mathcal{A}} : \text{Dom}(\mathcal{A}^{1/2}) \equiv \mathcal{H}^1 \subset \mathcal{H} \rightarrow \mathcal{H}. \quad (3.52)$$

Due to the abstract formulation we are considering, this assumption might appear a bit obscure and short of any real justification. Nevertheless, the motivations lying behind it will soon become clear: in fact, we will show in the forthcoming Corollary 3.23 that in consequence of this choice the time evolution of the Wightman field fulfills, as expected, the Klein-Gordon evolution equation (in a suitable strong sense).

Due to Stone’s theorem [119], the time evolution of the non-interacting single-particle theory is implemented on  $\mathcal{H}$  in the Schrödinger picture by the strongly continuous one-parameter unitary group

$$\mathcal{U}_t := e^{-it\sqrt{\mathcal{A}}} : \mathcal{H} \rightarrow \mathcal{H}, \quad (3.53)$$

where the (otherwise arbitrary) parameter  $t \in \mathbb{R}$  plays the role of *time*.

*Remark 3.11.* The time parameter  $t$  shall not be confused with the other variable  $\mathbf{t} \in \mathbb{R}$  used in Chapter 2 to define the exponential operators  $e^{-\mathbf{t}\mathcal{A}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ ,  $e^{-\mathbf{t}\sqrt{\mathcal{A}}}/\sqrt{\mathcal{A}}$  and the related heat, cylinder and modified cylinder kernels (<sup>7</sup>).

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<sup>7</sup>Nonetheless, let us point out that, with the Wick rotation  $t = -it$ , one has  $\mathcal{U}_{-it} = e^{-\mathbf{t}\sqrt{\mathcal{A}}}$ , i.e.,  $\mathcal{U}_{-it}$  coincides with the cylinder operator.

Before moving on, let us point out a couple of facts on the family of operators  $\mathcal{U}_t$  ( $t \in \mathbb{R}$ ) and on the related operators  $\cos(\sqrt{\mathcal{A}}t) := (\mathcal{U}_t + \mathcal{U}_{-t})/2$ ,  $\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}} := (\mathcal{U}_t - \mathcal{U}_{-t})/2i\sqrt{\mathcal{A}} : \mathcal{H} \rightarrow \mathcal{H}$ , which will be employed in the forthcoming developments. Due to Proposition 2.12 in Chapter 2, all the operators mentioned above (for any  $t \in \mathbb{R}$ ) possess unique, continuous linear extensions to  $\mathcal{H}^{-\infty}$ , indicated with the same symbols:

$$\mathcal{U}_t, \cos(\sqrt{\mathcal{A}}t), (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}}) : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}. \quad (3.54)$$

In particular, due to item ii) of Proposition 2.12, for any  $r \in \mathbb{R}$  and for any  $f \in \mathcal{H}^r$  there hold

$$\begin{aligned} \|\mathcal{U}_t f\|_r &= \|f\|_r, \\ \|\cos(\sqrt{\mathcal{A}}t)f\|_r &\leq \|f\|_r, \quad \|(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})f\|_r \leq \|f\|_{r-1}; \end{aligned} \quad (3.55)$$

moreover, item iii) of the same proposition (here employed with  $b = 0$ ) allows to infer that  $\mathcal{U}_t$  is an Hilbertian automorphism of  $\mathcal{H}^r$ , for any  $t \in \mathbb{R}$  and for any  $r \in \mathbb{R}$ .

Next, following the standard *second quantization* approach (see, Definition 3.10), we introduce the one-parameter unitary group given by

$$\Gamma(\mathcal{U}_t) : \mathfrak{F}^\vee(\mathcal{H}) \rightarrow \mathfrak{F}^\vee(\mathcal{H}) \quad (t \in \mathbb{R}); \quad (3.56)$$

then, from Definition 3.10, it follows straightforwardly that

$$\Gamma(\mathcal{U}_t)^{-1} = \Gamma(\mathcal{U}_t^{-1}) \quad (3.57)$$

(<sup>8</sup>). In the spirit of Heisenberg picture for time evolution, we give the following definition.

**Definition 3.18.** The *Wightman field* and *conjugate momentum at time  $t \in \mathbb{R}$*  are the (unbounded) operators  $\hat{\varphi}_t(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  and  $\hat{\pi}_t(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  defined, respectively, as

$$\hat{\varphi}_t(h) := \Gamma(\mathcal{U}_t)^{-1} \hat{\varphi}(h) \Gamma(\mathcal{U}_t) \quad \text{for } h \in \mathcal{H}^{-1/2}, \quad (3.58)$$

$$\hat{\pi}_t(h) := \Gamma(\mathcal{U}_t)^{-1} \hat{\pi}(h) \Gamma(\mathcal{U}_t) \quad \text{for } h \in \mathcal{H}^{1/2}. \quad (3.59)$$

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<sup>8</sup>For completeness, let us also mention that, setting

$$\mathfrak{D}_1 := \left\{ f \sum_n f^{(n)} \in \mathfrak{D}^\vee(\mathcal{H}) \mid f^{(n)} \in (\text{Dom}(\sqrt{\mathcal{A}}))^{\vee n} \equiv (\mathcal{H}^1)^{\vee n}, \text{ for all } n \in \mathbb{N} \right\},$$

one could also consider the *free Hamiltonian* for the Hermitian scalar field; this is the densely defined operator  $d\Gamma(\sqrt{\mathcal{A}}) : \mathfrak{D}_1 \subset \mathfrak{F}^\vee(\mathcal{H}) \rightarrow \mathfrak{F}^\vee(\mathcal{H})$  which, for all  $n \in \mathbb{N}$ , fulfills

$$d\Gamma(\sqrt{\mathcal{A}}) \upharpoonright (\mathfrak{D}_1 \cap \mathcal{H}^{\vee n}) = \sum_{i=1}^n (\sqrt{\mathcal{A}})^{\delta_{i,1}} \otimes \dots \otimes (\sqrt{\mathcal{A}})^{\delta_{i,n}}$$

where  $\delta$  indicates the Kronecker delta ( $\delta_{ij} = 1$  if  $i = j$ ,  $\delta_{ij} = 0$  if  $i \neq j$ ) and, by convention, we put  $(\sqrt{\mathcal{A}})^0 := \mathbb{I}_{\mathcal{H}^{-1/2}}$  (i.e., the identity operator on  $\mathcal{H}^{-1/2}$ ). As well-known [130],  $d\Gamma(\sqrt{\mathcal{A}})$  is essentially self-adjoint on  $\mathfrak{D}_1$  and there holds

$$\Gamma(\mathcal{U}_t) = e^{-it d\Gamma(\sqrt{\mathcal{A}})}.$$

*Remark 3.12.* Of course, for  $t = 0$  there holds  $\mathcal{U}_0 = \mathbb{I}$  (the identity operator on  $\mathcal{H}$ ); on the other hand, it follows straightforwardly from Definition 3.10 that  $\Gamma(\mathbb{I}) = \hat{\mathbb{I}}_{\mathfrak{F}}$  (the identity on the Fock space). Therefore, there holds

$$\hat{\varphi}_0(h) = \hat{\varphi}(h) \quad (h \in \mathcal{H}^{-1/2}), \quad \hat{\pi}_0(h) = \hat{\pi}(h) \quad (h \in \mathcal{H}^{1/2}); \quad (3.60)$$

this justifies the nomenclature ‘‘at time zero’’ adopted in Definition 3.13 for the Wightman field  $\hat{\varphi}(h)$  and for the conjugate momentum  $\hat{\pi}(h)$ .

**Proposition 3.19.** *The Wightman field  $\hat{\varphi}_t(h)$  and conjugate momentum  $\hat{\pi}_t(h)$  at any time  $t \in \mathbb{R}$  can be expressed as follows in terms of their time zero analogues  $\hat{\varphi}(h), \hat{\pi}(h)$ :*

$$\hat{\varphi}_t(h) = \hat{\varphi}\left(\cos(\sqrt{\mathcal{A}}t)h\right) + \hat{\pi}\left((\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h\right) \quad (h \in \mathcal{H}^{-1/2}), \quad (3.61)$$

$$\hat{\pi}_t(h) = \hat{\pi}\left(\cos(\sqrt{\mathcal{A}}t)h\right) - \hat{\varphi}\left(\mathcal{A}(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h\right) \quad (h \in \mathcal{H}^{1/2}). \quad (3.62)$$

*Remark 3.13.* In analogy with the considerations of Remark 3.8 (see, in particular, item i) therein), it appears that the expressions (3.61) and (3.62) do in fact make sense for the respective choices of  $h$  indicated therein. In fact,  $\cos(\sqrt{\mathcal{A}}t)h \in \mathcal{H}^{-1/2}$  and  $(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h \in \mathcal{H}^{1/2}$  for all  $h \in \mathcal{H}^{-1/2}$ , while  $\cos(\sqrt{\mathcal{A}}t)h \in \mathcal{H}^{1/2}$  and  $\mathcal{A}(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h \in \mathcal{H}^{-1/2}$  for all  $h \in \mathcal{H}^{1/2}$ ; therefore, all the Wightman fields and conjugate momentums at time zero appearing in the cited equations are well-defined.

*Proof.* We only show, as an example, how to derive Eq. (3.61). To this purpose, first recall the identity (3.44), expressing the Wightman field in terms of the Segal field, and the definition (3.58), describing the time evolution of the Wightman field. Then, in view of Proposition 3.11 and of Eq. (3.57), it can be easily inferred that

$$\hat{\varphi}_t(h) = \hat{\Phi}_S(\mathcal{U}_t^{-1}\mathcal{P}_+(\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(\mathcal{U}_t^{-1}\mathcal{P}_+(-i\mathcal{A}^{-1/4}h)).$$

Next, notice that  $\mathcal{U}_t^{-1} = e^{it\sqrt{\mathcal{A}}} = \cos(\sqrt{\mathcal{A}}t) + i\sin(\sqrt{\mathcal{A}}t)$ , for all  $t \in \mathbb{R}$ ; moreover, both the operators  $\cos(\sqrt{\mathcal{A}}t)$  and  $\sin(\sqrt{\mathcal{A}}t)$  are  $\mathcal{J}$ -real due to Proposition 2.25, so that  $\cos(\sqrt{\mathcal{A}}t)\mathcal{J} = \mathcal{J}\cos(\sqrt{\mathcal{A}}t)$  and  $\sin(\sqrt{\mathcal{A}}t)\mathcal{J} = \mathcal{J}\sin(\sqrt{\mathcal{A}}t)$ . Therefore, by the  $\mathbb{R}$ -linearity of the Segal field  $\hat{\Phi}_S$  (recalling that  $\mathcal{P}_{\pm}(if) = i\mathcal{P}_{\mp}f$ ; see Eq. (3.40)), one has

$$\begin{aligned} \hat{\varphi}_t(h) = & \hat{\Phi}_S(\mathcal{P}_+(\cos(\sqrt{\mathcal{A}}t)\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(\mathcal{P}_+(-i\cos(\sqrt{\mathcal{A}}t)\mathcal{A}^{-1/4}h)) + \\ & + \hat{\Phi}_S(i\mathcal{P}_+(\sin(\sqrt{\mathcal{A}}t)\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(i\mathcal{P}_+(-i\sin(\sqrt{\mathcal{A}}t)\mathcal{A}^{-1/4}h)); \end{aligned}$$

then, the thesis follows using, again, the identities (3.44) (3.45) for the Wightman field and the conjugate momentum at time zero (notice that  $\hat{\Phi}_S(i\mathcal{P}_+(\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(i\mathcal{P}_+(-i\mathcal{A}^{-1/4}h)) = \hat{\pi}(\mathcal{A}^{-1/2}h)$ , for all  $h \in \mathcal{H}^{-1} \supset \mathcal{H}^{-1/2}$ ).  $\square$

For completeness, let us also report the following result, giving the commutation relations for the Wightman field and the conjugate momentum at unequal times.

**Proposition 3.20.** *For any  $t, t' \in \mathbb{R}$ , there hold the commutation relations at unequal times ( $t \neq t'$ )*

$$\begin{aligned} [\hat{\varphi}_t(h), \hat{\varphi}_{t'}(k)] &= -i \langle \mathcal{J}h | (\sin(\sqrt{\mathcal{A}}(t-t'))/\sqrt{\mathcal{A}}) k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} && \text{for } h, k \in \mathcal{H}^{-1/2}, \\ [\hat{\varphi}_t(h), \hat{\pi}_{t'}(k)] &= +i \langle \mathcal{J}h | \cos(\sqrt{\mathcal{A}}(t-t')) k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} && \text{for } h \in \mathcal{H}^{-1/2}, k \in \mathcal{H}^{1/2}, \\ [\hat{\pi}_t(h), \hat{\pi}_{t'}(k)] &= -i \langle \mathcal{J}h | (\sin(\sqrt{\mathcal{A}}(t-t'))/\sqrt{\mathcal{A}}) k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} && \text{for } h, k \in \mathcal{H}^{1/2} \end{aligned} \quad (3.63)$$

*Proof.* We only compute, as an example, the commutator  $[\hat{\varphi}_t(h), \hat{\varphi}_{t'}(k)]$ . To this purpose, recall the expression (3.61) for the time evolution of the Wightman field, along with the commutation relations at time zero (3.49); these facts allow to infer by elementary computations that

$$\begin{aligned} &[\hat{\varphi}_t(h), \hat{\varphi}_{t'}(k)] = \\ &i \langle \mathcal{J}(\cos(\sqrt{\mathcal{A}}t)h) | (\sin(\sqrt{\mathcal{A}}t')/\sqrt{\mathcal{A}}) k \rangle - i \langle \mathcal{J}(\cos(\sqrt{\mathcal{A}}t')k) | (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}}) h \rangle \hat{\mathbb{I}}_{\mathfrak{D}} . \end{aligned}$$

Next notice that,  $\langle \mathcal{J}(\cos(\sqrt{\mathcal{A}}t')k) | (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}}) h \rangle = \langle \mathcal{J}(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h | \cos(\sqrt{\mathcal{A}}t')k \rangle$  (use the properties of the conjugation  $\mathcal{J}$ , keeping in mind the sesquilinearity of the inner product  $\langle | \rangle$ ). Moreover, recall that  $\cos(\sqrt{\mathcal{A}}t)$  and  $\sin(\sqrt{\mathcal{A}}t')/\sqrt{\mathcal{A}}$  both commute with  $\mathcal{J}$  in consequence of Proposition 2.25; so, due to the results of Corollary 2.24 on Banach adjoints, it follows that

$$[\hat{\varphi}_t(h), \hat{\varphi}_{t'}(k)] = i \langle \mathcal{J}h | \left( (\cos(\sqrt{\mathcal{A}}t) \sin(\sqrt{\mathcal{A}}t') - \cos(\sqrt{\mathcal{A}}t') \sin(\sqrt{\mathcal{A}}t)) / \sqrt{\mathcal{A}} \right) k \rangle \hat{\mathbb{I}}_{\mathfrak{D}} .$$

Then, the thesis follows by elementary functional calculus <sup>(9)</sup>. □

**Proposition 3.21.** *Let  $\mathbf{f} \in \mathfrak{D}^{\vee}(\mathcal{H})$  and  $n \in \mathbb{N}$ . Then, the maps  $\mathbb{R} \mapsto \mathfrak{D}^{\vee}(\mathcal{H}) \subset \mathfrak{F}^{\vee}(\mathcal{H})$ ,  $t \mapsto \hat{\varphi}_t(h) \mathbf{f}$  and  $\mathbb{R} \mapsto \mathfrak{D}^{\vee}(\mathcal{H}) \subset \mathfrak{F}^{\vee}(\mathcal{H})$ ,  $t \mapsto \hat{\pi}_t(h) \mathbf{f}$  are well-posed and of class  $C^n$  for all  $h \in \mathcal{H}^{-1/2+n}$  and all  $h \in \mathcal{H}^{1/2+n}$ , respectively. In particular, for any  $h \in \mathcal{H}^{3/2}$ , the map  $t \mapsto \hat{\varphi}_t(h) \mathbf{f}$  is of class  $C^2$  and its first and second derivative are, respectively, given by*

$$\frac{d}{dt} (\hat{\varphi}_t(h) \mathbf{f}) = \hat{\pi}_t(h) \mathbf{f}, \quad \frac{d^2}{dt^2} (\hat{\varphi}_t(h) \mathbf{f}) = -\hat{\varphi}_t(\mathcal{A}h) \mathbf{f}. \quad (3.64)$$

*Proof.* As an example, we only discuss the differentiability of the map  $t \mapsto \hat{\varphi}_t(h) \mathbf{f}$ . First of all, recall that the Wightman field at any time  $t \in \mathbb{R}$  can be expressed as  $\hat{\varphi}_t(h) = \hat{\varphi}(\cos(\sqrt{\mathcal{A}}t)h) + \hat{\pi}((\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h)$  (see Eq. (3.61)). On the other hand, Proposition 2.30 grants that both the maps  $\mathbb{R} \rightarrow \mathcal{H}^{-1/2}$ ,  $t \mapsto \cos(\sqrt{\mathcal{A}}t)h$  and  $\mathbb{R} \rightarrow \mathcal{H}^{1/2}$ ,  $t \mapsto (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h$  are of class  $C^n$ , for any  $h \in \mathcal{H}^{-1/2+n}$ . Moreover, due to Lemma 3.14, both the  $\mathbb{C}$ -linear maps  $\mathcal{H}^{-1/2} \ni h \mapsto \hat{\varphi}(h) \mathbf{f}$  and  $\mathcal{H}^{1/2} \ni h \mapsto \hat{\pi}(h) \mathbf{f}$  are continuous,

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<sup>9</sup>One should recall the trigonometric identity  $\cos a \sin b - \cos a \sin b = -\sin(a - b)$ , for any  $a, b \in \mathbb{R}$ .

whence analytic, for any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$ . Summing up, the map  $t \mapsto \hat{\varphi}_t(h) \mathbf{f}$  is the composition of functions which are either smooth or of class  $C^n$ , which proves the first part of the thesis.

Finally note that, by linearity and continuity, there hold

$$\begin{aligned} \frac{d^n}{dt^n} (\hat{\varphi}(\cos(\sqrt{\mathcal{A}}t) h) \mathbf{f}) &= \hat{\varphi} \left( \frac{d^n}{dt^n} \cos(\sqrt{\mathcal{A}}t) h \right) \mathbf{f} , \\ \frac{d^n}{dt^n} (\hat{\pi}(\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}}) h) \mathbf{f} &= \hat{\varphi} \left( \frac{d^n}{dt^n} (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}}) h \right) \mathbf{f} ; \end{aligned}$$

then, the identities in Eq. (3.64) can be easily derived computing (via functional calculus) the derivatives  $\frac{d^n}{dt^n} \cos(\sqrt{\mathcal{A}}t)$ ,  $\frac{d^n}{dt^n} (\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})$  and keeping in mind the identities in Eq.s (3.61) and (3.62).  $\square$

*Remark 3.14.* Starting from the identities in Eq. (3.64) and working by recursion, one can derive explicit expressions also for the higher order derivatives of both the maps  $t \mapsto \hat{\varphi}_t(h) \mathbf{f}$ ,  $\hat{\pi}_t(h) \mathbf{f}$  (making suitable assumptions for  $h$ , in order to grant their existence). We will not report these expressions here because for the following developments we shall only need at most second order “time derivatives” of the Wightman field.

In view of the results established in the above Proposition 3.21, we give the forthcoming definition.

**Definition 3.22.** For any  $n \in \mathbb{N}$  and for all  $h \in \mathcal{H}^{-1/2+n}$ , the ( $h$ -smeared)  $n$ -th derivative of the Wightman field at time  $t$  is the unbounded operator  $\partial_t^n \hat{\varphi}_t(h) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  which, for all  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$ , fulfills

$$\partial_t^n \hat{\varphi}_t(h) \mathbf{f} = \frac{d^n}{dt^n} (\hat{\varphi}_t(h) \mathbf{f}) . \quad (3.65)$$

**Corollary 3.23.** For any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$  and for any  $h \in \mathcal{H}^{3/2}$ , the time-evolved Wightman field fulfills the strong form of the abstract Klein-Gordon evolution equation

$$\begin{cases} \left( \partial_{tt} \hat{\varphi}_t(h) + \hat{\varphi}_t(\mathcal{A}h) \right) \mathbf{f} = \mathbf{o} , \\ \hat{\varphi}_t(h) \mathbf{f} \Big|_{t=0} = \hat{\varphi}(h) \mathbf{f} , \\ \partial_t \hat{\varphi}_t(h) \mathbf{f} \Big|_{t=0} = \hat{\pi}(h) \mathbf{f} \end{cases} \quad (3.66)$$

where  $\mathbf{o} \in \mathfrak{D}^\vee(\mathcal{H})$  is the null element of the Fock space  $\mathfrak{F}^\vee(\mathcal{H})$ .

*Proof.* The thesis follows straightforwardly from the results derived in Proposition 3.21, keeping in mind the considerations of Remark 3.12 and of item i) of Remark 3.14.  $\square$

*Remark 3.15.* i) It appears that Eq. (3.66) can be interpreted as the second quantized version of the classical Klein-Gordon equation, that is the evolution equation

$$\begin{cases} (\partial_{tt} + \mathcal{A})\varphi_t = 0 , \\ \varphi_t|_{t=0} = \varphi , \\ \partial_t\varphi_t|_{t=0} = \pi \end{cases} \quad (3.67)$$

where  $\mathcal{A}$  is some suitable, second order elliptic differential operator (e.g., of Schrödinger type),  $t \mapsto \varphi_t$  is a function-valued map and  $\varphi, \pi$  are prescribed initial data. In view of this correspondence, it appears that the parameter  $t$  can in fact be interpreted as the time also in the abstract Klein-Gordon equation.

ii) Consider the ordinary differential equation corresponding to Eq. (3.67)

$$\begin{cases} (\partial_{tt} + \lambda)\varphi(t) = 0 , \\ \varphi(t)|_{t=0} = \varphi_0 , \\ \partial_t\varphi(t)|_{t=0} = \pi_0 \end{cases} \quad (3.68)$$

where  $\omega > 0$  and  $\varphi_0, \pi_0 \in \mathbb{R}$  are assigned and  $t \mapsto \varphi(t)$  is an at least twice-differentiable function; by elementary arguments it follows that the solution of Eq. (3.68) is given by

$$\varphi(t) = \varphi_0 \cos(\sqrt{\omega}t) + \pi_0 \sin(\sqrt{\omega}t)/\sqrt{\omega} . \quad (3.69)$$

In view of this fact, working backwards, one could have started with an ansatz and define the Wightman field  $\hat{\varphi}_t(h)$  at time  $t \in \mathbb{R}$  ( $h \in \mathcal{H}^1$ ) according to Eq. (3.61) (which in our approach is instead a consequence derived by more primitive definitions).

Using the above results and those reported in Lemma 3.17, one can evaluate the VEVs of the monomials of any order in the Wightman field (as well as the VEVs involving the conjugate momentum and their time derivatives). As well-known, due to Wick's theorem [142, 146], this operation reduces to the computation of the VEV of the field squared. Let us first give the following corollary descending straightforwardly from Proposition 3.21.

**Corollary 3.24.** *Let  $\mathbf{v} \in \mathfrak{D}^\vee(\mathcal{H})$  be the vacuum state and let  $n \in \mathbb{N}$ .*

*i) For any pair  $h \in \mathcal{H}^{-1/2+n}$ ,  $k \in \mathcal{H}^{-1/2}$  and for any fixed  $t' \in \mathbb{R}$ , the map  $\mathbb{R} \rightarrow \mathbb{C}$ ,  $t \mapsto (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v})$  is of class  $C^n$ ; for any  $j \leq n$ , there holds*

$$\frac{d^j}{dt^j} (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = (\mathbf{v} | \partial_t^j \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) . \quad (3.70)$$

*ii) For any pair  $h \in \mathcal{H}^{-1/2}$ ,  $k \in \mathcal{H}^{-1/2+n}$  and for any fixed  $t \in \mathbb{R}$ , the map  $\mathbb{R} \rightarrow \mathbb{C}$ ,  $t' \mapsto (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v})$  is of class  $C^n$ ; for any  $j \leq n$ , there holds*

$$\frac{d^j}{dt'^j} (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = (\mathbf{v} | \hat{\varphi}_t(h) \partial_{t'}^j \hat{\varphi}_{t'}(k) \mathbf{v}) . \quad (3.71)$$

*Remark 3.16.* i) Of course, it follows that if both  $h \in \mathcal{H}^{-1/2+n}$  and  $k \in \mathcal{H}^{-1/2+n}$  for some  $n \in \mathbb{N}$ , then the map  $\mathbb{R}^2 \rightarrow \mathbb{C}$ ,  $(t, t') \mapsto (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v})$  is of class  $C^n$  jointly in the two variables. Moreover, for any  $j, j' \leq n$ , there holds

$$\partial_t^j \partial_{t'}^{j'} (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = (\mathbf{v} | \partial_t^j \hat{\varphi}_t(h) \partial_{t'}^{j'} \hat{\varphi}_{t'}(k) \mathbf{v}) . \quad (3.72)$$

ii) From the forthcoming proof, it appears that all the above statements can be easily generalized to any expectation value of the form  $(\mathbf{f} | \partial_t^j \hat{\varphi}_t(h) \partial_{t'}^{j'} \hat{\varphi}_{t'}(k) \mathbf{g})$ , for any given  $\mathbf{f}, \mathbf{g} \in \mathfrak{D}^\vee(\mathcal{H})$ .

*Proof.* As an example, we show how to prove statement i). First notice that, for any  $\mathbf{v} \in \mathfrak{D}^\vee(\mathcal{H})$ ,  $k \in \mathcal{H}^{-1/2}$  and for any fixed  $t' \in \mathbb{R}$ , one has  $\hat{\varphi}_{t'}(k) \mathbf{v} \in \mathfrak{D}^\vee(\mathcal{H})$ . On the other hand, due to Proposition 3.21, the map  $t \mapsto \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}$  is of class  $C^n$  for any  $h \in \mathcal{H}^{-1/2+n}$ . Then, the thesis follows easily from the linearity and continuity (whence, analyticity) of the inner product  $( | )$  on  $\mathfrak{F}^\vee(\mathcal{H})$ .  $\square$

**Proposition 3.25.** *Let  $h, k \in \mathcal{H}^{-1/2}$  and let  $t, t' \in \mathbb{R}$ ; then the VEV of the Wightman field squared  $(\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v})$  can be expressed as follows:*

$$(\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = \frac{1}{2} \langle \mathcal{J}h | (e^{-i(t-t')\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}}) k \rangle , \quad (3.73)$$

where  $\langle | \rangle$  indicates the extension to  $\mathcal{H}^{-1/2} \times \mathcal{H}^{1/2}$  of the inner product on  $\mathcal{H}$  <sup>(10)</sup>.

*Proof.* First notice that, using the expression (3.61) for the Wightman field  $\hat{\varphi}_t(h)$  at time  $t \in \mathbb{R}$ , one has

$$\begin{aligned} & (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = \\ & (\mathbf{v} | \left[ \hat{\varphi}(\cos(\sqrt{\mathcal{A}}t)h) \hat{\varphi}(\cos(\sqrt{\mathcal{A}}t')k) + \hat{\pi}((\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h) \hat{\pi}((\sin(\sqrt{\mathcal{A}}t')/\sqrt{\mathcal{A}})k) + \right. \\ & \quad \left. + \hat{\varphi}(\cos(\sqrt{\mathcal{A}}t)h) \hat{\pi}((\sin(\sqrt{\mathcal{A}}t')/\sqrt{\mathcal{A}})k) + \hat{\pi}((\sin(\sqrt{\mathcal{A}}t)/\sqrt{\mathcal{A}})h) \hat{\varphi}(\cos(\sqrt{\mathcal{A}}t')k) \right] \mathbf{v}) . \end{aligned}$$

To proceed, let us evaluate each of the terms at time zero in the right-hand side of the above equality, using the results derived in Lemma 3.17. Next, recall that the conjugation  $\mathcal{J}$  commutes with  $\cos(\sqrt{\mathcal{A}}t)$ ,  $\sin(\sqrt{\mathcal{A}}t)$  and with any real power of  $\mathcal{A}$  (see Corollary 2.26); interpreting the inner products  $\langle | \rangle$  so obtained in terms of the extension (2.103) and using Corollary 2.24 for the (Banach) adjoints of  $\cos(\sqrt{\mathcal{A}}t)$ ,  $\sin(\sqrt{\mathcal{A}}t)$ ,  $\mathcal{A}^r$  ( $r \in \mathbb{R}$ ), it can be inferred that

$$\begin{aligned} & (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v}) = \\ & \frac{1}{2} \langle \mathcal{J}h | \mathcal{A}^{-1/2} \left[ (\cos(\sqrt{\mathcal{A}}t) \cos(\sqrt{\mathcal{A}}t') + \sin(\sqrt{\mathcal{A}}t) \sin(\sqrt{\mathcal{A}}t')) + \right. \\ & \quad \left. + i (\cos(\sqrt{\mathcal{A}}t) \sin(\sqrt{\mathcal{A}}t') - \sin(\sqrt{\mathcal{A}}t) \cos(\sqrt{\mathcal{A}}t')) \right] k \rangle . \end{aligned}$$

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<sup>10</sup>In fact, for any  $k \in \mathcal{H}^{-1/2}$ , there holds  $(e^{-i(t-t')\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}})k \in \mathcal{H}^{1/2}$  (see Lemma 2.27).

Then, the thesis follows again by elementary functional calculus <sup>(11)</sup>.  $\square$

For the subsequent developments, only the evaluation of the VEVs at equal time is required; these are reported in the forthcoming corollary.

**Corollary 3.26.** *For any pair  $h, k \in \mathcal{H}^{3/2}$ , the VEVs of the second order monomials in the Wightman field (and the related time derivatives of degree two at most), evaluated at equal times are the following:*

$$\begin{aligned} (\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_t(k) \mathbf{v}) &= \frac{1}{2} \langle \mathcal{J}h | \mathcal{A}^{-1/2} k \rangle, \\ (\mathbf{v} | \hat{\varphi}_t(h) \partial_t \hat{\varphi}_t(k) \mathbf{v}) &= - (\mathbf{v} | \partial_t \hat{\varphi}_t(h) \hat{\varphi}_t(k) \mathbf{v}) = \frac{i}{2} \langle \mathcal{J}h | k \rangle, \end{aligned} \quad (3.74)$$

$(\mathbf{v} | \partial_t \hat{\varphi}_t(h) \partial_t \hat{\varphi}_t(k) \mathbf{v}) = - (\mathbf{v} | \partial_{tt} \hat{\varphi}_t(h) \hat{\varphi}_t(k) \mathbf{v}) = - (\mathbf{v} | \hat{\varphi}_t(h) \partial_{tt} \hat{\varphi}_t(k) \mathbf{v}) = \frac{1}{2} \langle \mathcal{J}h | \mathcal{A}^{1/2} k \rangle$ ; again,  $\langle | \rangle$  indicates, in general, the extension to  $\mathcal{H}^{(2)}$  of the inner product on  $\mathcal{H}$  <sup>(12)</sup>.

*Proof.* First recall the identity (3.72), which allows to express the VEVs in the left-hand sides of Eq. (3.74) in terms of the derivatives of  $(\mathbf{v} | \hat{\varphi}_t(h) \hat{\varphi}_{t'}(k) \mathbf{v})$  evaluated at equal times ( $t' = t$ ); then, the thesis follows easily using the explicit expression (3.73).  $\square$

*Remark 3.17.* All the expressions on the left-hand sides of the identities in Eq. (3.74) do, in principle, depend on the time parameter  $t \in \mathbb{R}$ , which however does not appear in the corresponding right-hand sides. This fact shows that the VEV of the Wick polynomials evaluated at equal times are actually time independent; as a matter of fact, this was to be expected due to the staticity features of the configuration under analysis. We will return on this topic in the following (see Proposition 3.37).

## 3.2 Scalar quantum field on a spatial domain.

Hereafter we employ the abstract framework developed in the previous section to analyze the case of an Hermitian scalar field living on a suitable open subset of  $(d+1)$ -dimensional Minkowski spacetime  $\mathcal{M}_{d+1}$  (with  $d \in \{1, 2, 3, \dots\}$  arbitrary). Let us recall that this setting was already considered in Chapter 1, where the main ideas were presented using a language somehow less precise than the mathematically rigorous one developed in Chapter 2 and in Section 3.1 of the present chapter.

We refer to the same framework described in Chapter 1; in particular, let us recall that we employ natural units (so that  $c = 1$  and  $\hbar = 1$ ) and that we identify Minkowski spacetime with  $\mathbb{R}^{d+1}$  using the set of global inertial coordinates

$$x = (x^\mu)_{\mu=0,1,\dots,d} \equiv (x^0, \mathbf{x}) \equiv (t, \mathbf{x}) : \mathcal{M}_{d+1} \rightarrow \mathbb{R}^{d+1},$$

<sup>11</sup>Just notice that  $(\cos a \cos b + \sin a \sin b) + i(\cos a \sin b - \sin a \cos b) = e^{-i(a-b)}$ , for all  $a, b \in \mathbb{R}$ .

<sup>12</sup>In fact, under the assumptions made for  $h, k$ , the expressions in the right-hand sides of Eq. (3.74) can also be interpreted, a posteriori, in terms of the non-extended inner product on  $\mathcal{H}$ .



in terms of which the Minkowski metric  $\eta$  has coefficients  $(\eta_{\mu\nu}) = \text{diag}(-1, 1, \dots, 1)$  (see Eq.s (1.1-1.3)). We make reference to the theory of a scalar field living on a fixed spatial domain  $\Omega \subset \mathbb{R}^d$ , which we assume to be open and connected but otherwise arbitrary (possibly, unbounded); time evolution is described on the open subset of Minkowski spacetime given by  $\mathbb{R} \times \Omega \subset \mathbb{R}^{d+1} \simeq \mathcal{M}_{d+1}$ . Prescribed boundary conditions on  $\partial\Omega$  for the field are properly taken into account, as well as the interaction with an assigned scalar potential  $V \in C^\infty(\Omega)$ .

We first reconsider the canonical quantization of the classical theory; this is obtained specializing the general formulation of Section 3.1 to the explicit model under analysis. Next, we implement ZR within the present setting to define a regularized version of the Wightman field evaluated at a spacetime point  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$ , depending on a complex parameter  $u$  introduced on purpose. This regularized field is used to construct natural quantized counterparts of the classical observables, such as the stress-energy tensor, the total energy and the pressure on the boundary. The VEVs of this regularized observables are computed explicitly using the integral kernels analyzed in Chapter 2 of this manuscript. Finally, the renormalized VEVs are defined in terms of the analytic continuation of the corresponding regularized expressions at  $u = 0$ , which is the value corresponding formally to the non-regularized field operator.

Let us recall once more that the spatial domain  $\Omega$ , its boundary  $\partial\Omega$  and the potential  $V$  are assigned classical objects which do not evolve in time; moreover no back-reaction exerted on them by the quantum field is ever considered in the analysis to be described in the following.

### Canonical quantization (revisited).

To make contact with the standard literature [58, 130], let us specialize the abstract approach to canonical quantization described in Section 3.1 for the particular case we are considering in this section.

First of all, we define the single particle Hilbert space to be

$$\mathcal{H} = L^2(\Omega, d\mathbf{x}) \equiv L^2(\Omega) \quad (3.75)$$

(with inner product  $\langle f|g\rangle_{L^2} := \int_{\Omega} d\mathbf{x} \bar{f}(\mathbf{x}) g(\mathbf{x})$ ), i.e., as the space of square-integrable functions on  $\Omega$  with respect to the standard Lebesgue measure  $d\mathbf{x}$ .

The corresponding bosonic Fock space  $\mathfrak{F}^\vee(\mathcal{H}) = \mathfrak{F}^\vee(L^2(\Omega))$  is the direct sum of the totally symmetric tensor powers  $\mathcal{H}^{\vee n} = (L^2(\Omega))^{\vee n}$  ( $n \in \mathbb{N}$ ); as well known, each of these tensor powers coincides with the space of square-integrable functions on the  $n$ -fold cartesian product  $\Omega \times \dots \times \Omega$  which are invariant under permutation of the coordinates. So,

$$\mathfrak{F}^\vee(\mathcal{H}) = \bigoplus_{n=0}^{+\infty} \mathcal{H}^{\vee n} \quad (3.76)$$

with  $\mathcal{H}^{\vee 0} := \mathbb{C}$  and  $\mathcal{H}^{\vee n} = L^2_{\vee}(\times_{i=1}^n \Omega, \otimes_{i=1}^n d\mathbf{x}) \equiv L^2_{\vee}(\times_{i=1}^n \Omega)$  for  $n \in \{1, 2, 3, \dots\}$ , where

$$L^2_{\vee}(\times_{i=1}^n \Omega) := \{f^{(n)} \in L^2(\times_{i=1}^n \Omega, \otimes_{i=1}^n d\mathbf{x}) \mid f^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = f^{(n)}(\mathbf{x}_{\pi(1)}, \dots, \mathbf{x}_{\pi(n)}), \forall \pi \in \mathbb{P}_n\} \quad (3.77)$$

(here  $\mathbf{x}_i \in \Omega$  for  $i = 1, \dots, n$  and  $\mathbb{P}_n$  is the permutation group of  $n$  elements).

For any  $h \in L^2(\Omega)$ , the creation and annihilation operators  $\hat{a}^-(h), \hat{a}^+(h)$  defined in Eq.s (3.17) (3.18) are easily seen to map any finite-particle element  $\mathbf{f} = (f^{(n)}) \in \mathfrak{D}^\vee(\mathcal{H})$  (with  $f^{(n)} \in L^2_\vee(\times_{i=1}^n \Omega)$ ) into  $\hat{a}^\pm(h) \mathbf{f} = ((\hat{a}^\pm(h) \mathbf{f})^{(n)}) \in \mathfrak{D}^\vee(\mathcal{H})$ , where

$$(\hat{a}^-(h) \mathbf{f})^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \sqrt{n+1} \int_\Omega d\mathbf{y} \bar{h}(\mathbf{y}) f^{(n+1)}(\mathbf{y}, \mathbf{x}_1, \dots, \mathbf{x}_n), \quad (3.78)$$

$$(\hat{a}^+(h) \mathbf{f})^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^n h(\mathbf{x}_i) f^{(n-1)}(\mathbf{x}_1, \dots, \hat{\mathbf{x}}_i, \dots, \mathbf{x}_n). \quad (3.79)$$

The Segal field and conjugate momentum are defined again according to Eq.s (3.30) (3.31) and, of course, all the results of subsection 3.1 continue to hold.

In order to proceed, let us consider the strictly positive, self-adjoint Schrödinger-type differential operator  $\mathcal{A} = (-\Delta + V) \upharpoonright \mathcal{D}_\mathcal{A} : \mathcal{D}_\mathcal{A} \subset L^2(\Omega) \rightarrow L^2(\Omega)$ , defined on a dense admissible domain  $\mathcal{D}_\mathcal{A} \subset L^2(\Omega)$ . Since  $\mathcal{A}$  fulfills the general hypotheses of Section 2.5, we can consider the scale of Hilbert spaces  $\mathcal{H}^r$  ( $r \in [-\infty, +\infty]$ ) related to it. Of course, complex conjugation on  $L^2(\Omega)$  commutes with  $\mathcal{A}$  (i.e.,  $\overline{\mathcal{A}f} = \mathcal{A}\bar{f}$ , for all  $f \in \mathcal{D}_\mathcal{A}$ ), so that it can be uniquely extended to a continuous antilinear involution on  $\mathcal{H}^{-\infty}$  according to Proposition 2.25. Moreover, the projectors  $\mathcal{P}_\pm$  related to complex conjugation (see Eq. (2.68)) map any function  $f \in L^2(\Omega)$  into its real and imaginary parts; more precisely, there holds  $\mathcal{P}_+f = \Re f$  and  $\mathcal{P}_-f = i\Im f$ . In view of this, when considering the extensions  $\mathcal{P}_\pm : \mathcal{H}^{-\infty} \rightarrow \mathcal{H}^{-\infty}$  of these operators defined according to Eq. (2.127), with a slight abuse of notation we will write, for any  $f \in \mathcal{H}^{-\infty}$ ,

$$\mathcal{P}_+f = \Re f, \quad \mathcal{P}_-f = i\Im f. \quad (3.80)$$

The Wightman field and the conjugate momentum at time zero can be expressed according to Eq.s (3.44) (3.45), which with the present assumptions read

$$\hat{\varphi}(h) = \hat{\Phi}_S(\Re(\mathcal{A}^{-1/4}h)) + i\hat{\Phi}_S(\Im(\mathcal{A}^{-1/4}h)) \quad \text{for } h \in \mathcal{H}^{-1/2}, \quad (3.81)$$

$$\hat{\pi}(h) = \hat{\Pi}_S(\Re(\mathcal{A}^{1/4}h)) + i\hat{\Pi}_S(\Im(\mathcal{A}^{1/4}h)) \quad \text{for } h \in \mathcal{H}^{1/2}. \quad (3.82)$$

Time evolution is implemented again via second quantization; this allows to define the time evolved Wightman field  $\hat{\varphi}_t(h)$  ( $t \in \mathbb{R}$ ), for any  $h \in \mathcal{H}^{-1/2}$ , as well as its time derivatives  $\partial_t^n \hat{\varphi}_t(h)$ , for any  $h \in \mathcal{H}^{-1/2+n}$  ( $n \in \mathbb{N}$ ). Moreover, there holds the strong version (3.66) of the Klein-Gordon equation.

*Remark 3.18.* The approach to second quantization described above generalizes the corresponding formulation that we considered in Section 1.2 of Chapter 1. Let us spend a few more words about this fact; to this purpose, let us first recall that in Section 1.2 (see, in particular, Eq.s (1.13-1.15)) we gave an expansion of the field operator in terms of the creation and annihilation operators  $\hat{a}_k, \hat{a}_k^\dagger$  associated to a complete orthonormal set of eigenfunctions  $(F_k)_{k \in \mathcal{K}}$  of  $\mathcal{A}$ , with corresponding eigenvalues  $(\omega_k^2)_{k \in \mathcal{K}}$  (where  $\omega_k \geq \varepsilon$ , for

some  $\varepsilon > 0$ , and  $\mathcal{K}$  is an unspecified set of labels). In the present framework, assuming the mentioned *proper* eigenfunctions  $F_k \in \mathcal{H}$  ( $k \in \mathcal{K}$ ) to exist, it appears that the associated operators  $\hat{a}_k, \hat{a}_k^\dagger$  are strictly related to the maps  $\hat{a}^-(\cdot), \hat{a}^+(\cdot) : \mathcal{H} \rightarrow \mathcal{L}(\mathcal{D}^\vee(\mathcal{H}))$ ; more precisely, for any  $k \in \mathcal{K}$ , this connection is established setting

$$\hat{a}_k := \hat{a}^-(\overline{F}_k) . \quad (3.83)$$

Then, since  $\hat{a}_k^\dagger$  is the adjoint of  $\hat{a}_k$ , due to Proposition 3.5 the above definition also yields

$$\hat{a}_k^\dagger = (\hat{a}^-(\overline{F}_k))^\dagger = \hat{a}^+(\overline{F}_k) . \quad (3.84)$$

In view of the above correspondences, the identities in Eq.s (1.14) and (1.15) are an obvious reformulation of Eq.s (3.23) and (3.20), respectively <sup>(13)</sup>. To conclude, let us point out that the field expansion (1.13) evaluated at time zero can be derived starting from the expression (3.47) for the Wightman field in terms of the operators  $\hat{a}^-, \hat{a}^+$  <sup>(14)</sup>.

### The zeta-regularized Wightman field.

The analysis to be presented in the following will be mainly focused on the Wightman field operator. Analogous results could be easily derived also for the conjugate momentum operator; however, for brevity, we shall not report them within this manuscript since they are not strictly necessary for the applications that will be discussed in the following.

In the mathematical formulation described so far, only a suitably smeared version of the Wightman field (at time  $t \in \mathbb{R}$ ) can be properly defined, i.e.,  $\hat{\varphi}_t(h)$  for  $h \in \mathcal{H}^{-1/2}$ . Nevertheless, in many physical applications, it is of interest to *evaluate the field at a point*  $\mathbf{x} \in \Omega$ ; this operation could be formally accounted for by considering the Wightman field evaluated on the Dirac delta element  $\delta_{\mathbf{x}} \in \mathcal{H}^{-r}$  ( $r > d/2$ ), setting

$$\text{“ } \hat{\varphi}(x) \equiv \hat{\varphi}_t(\mathbf{x}) := \hat{\varphi}_t(\delta_{\mathbf{x}}) \text{ ”} \quad (x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega) . \quad (3.85)$$

<sup>13</sup>Recalling that  $\langle F_k | F_h \rangle_{L^2} = \delta(k, h)$ , where  $\delta(k, h)$  is the Dirac delta on the label space  $\mathcal{K}$ .

<sup>14</sup>Let us account briefly for this statement. To this purpose, for any given  $h \in \mathcal{H}$  consider the representation (3.47) for the Wightman field at time zero  $\hat{\varphi}(h)$  in terms of the operators  $\hat{a}^-(\mathcal{A}^{-1/4}h)$  and  $\hat{a}^+(\mathcal{A}^{-1/4}h)$ . Using the eigenfunction expansions  $h = \int_{\mathcal{K}} dk \langle F_k | h \rangle_{L^2} F_k$  and  $h = \int_{\mathcal{K}} dk \langle \overline{F}_k | h \rangle_{L^2} \overline{F}_k$  and recalling that the maps  $\hat{a}^-$  and  $\hat{a}^+$  are respectively  $\mathbb{C}$ -antilinear and  $\mathbb{C}$ -linear, by linearity we formally obtain

$$\hat{\varphi}(h) = \frac{1}{\sqrt{2}} \int_{\mathcal{K}} dk \left( \langle F_k | h \rangle_{L^2} \hat{a}^-(\overline{\mathcal{A}^{-1/4}F_k}) + \langle \overline{F}_k | h \rangle_{L^2} \hat{a}^+(\mathcal{A}^{-1/4}\overline{F}_k) \right) .$$

Next, notice that  $\mathcal{A}^{-1/4}F_k = \omega_k^{-1/2}F_k$  and  $\mathcal{A}^{-1/4}\overline{F}_k = \omega_k^{-1/2}\overline{F}_k$ , so that

$$\hat{\varphi}(h) = \int_{\mathcal{K}} \frac{dk}{\sqrt{2\omega_k}} \left( \langle F_k | h \rangle_{L^2} \hat{a}^-(\overline{F}_k) + \langle \overline{F}_k | h \rangle_{L^2} \hat{a}^+(\overline{F}_k) \right) = \int_{\mathcal{K}} \frac{dk}{\sqrt{2\omega_k}} \left( \langle F_k | h \rangle_{L^2} \hat{a}_k + \langle \overline{F}_k | h \rangle_{L^2} \hat{a}_k^\dagger \right) ,$$

where the second identity follows from the relations in Eq.s (3.83) (3.84). The last expression written above can be formally interpreted as the smearing of the field (1.13) with the function  $h \in L^2(\Omega)$ .

On the other hand, since  $\delta_{\mathbf{x}}$  does not belong to the proper test-function space  $\mathcal{H}^{-1/2}$  (for any  $d \in \{1, 2, 3, \dots\}$ ), it appears that no rigorous meaning can be directly attributed to expressions like  $\hat{\varphi}_t(\delta_{\mathbf{x}})$  (appearing in Eq. (3.85)) within the framework developed in Section 3.1.

A natural approach to give an admissible definition of point-wise evaluation for the Wightman field operator is to introduce a family of suitably regularized Dirac delta elements, depending on a parameter; at the end the regularizing parameter has to be removed via a limiting procedure, to be properly interpreted. In the spirit of ZR, we give the forthcoming definition.

**Definition 3.27.** Let  $\kappa > 0$  be any fixed, real parameter and put (see Eq. (1.17))

$$\mathcal{A}_\kappa := \mathcal{A}/\kappa^2 . \quad (3.86)$$

For any fixed  $\mathbf{x} \in \Omega$  and for any  $u \in \mathbb{C}$ , the *zeta-regularized Dirac delta* at  $\mathbf{x}$  is

$$\delta_{\mathbf{x}}^u := \mathcal{A}_\kappa^{-u/4} \delta_{\mathbf{x}} . \quad (3.87)$$

*Remark 3.19.* i) Following the considerations of Section 1.3, we will refer to  $\kappa$  as *mass parameter*; this is introduced in the definition of the zeta-regularized Dirac delta for dimensional reasons, in order to make the rescaled operator  $\mathcal{A}_\kappa$  adimensional<sup>(15)</sup>. Of course,  $\delta_{\mathbf{x}}^u$  also depends on  $\kappa$ ; however, we assume  $\kappa$  to be assigned once and for all and, in pursue of notational simplicity, we choose to not indicate explicitly the dependence on this parameter when writing the regularized Dirac delta  $\delta_{\mathbf{x}}^u$ .

ii) Other regularized versions of the Dirac delta could, of course, be considered in alternative to (3.87). For example, having in mind an exponential type regularization, one could put (for  $\mathbf{t} \in \Sigma_0$ )

$$\delta_{\mathbf{x}}^{\mathbf{t}} := e^{-\mathbf{t}\mathcal{A}_\kappa} \delta_{\mathbf{x}} \quad \text{or} \quad \delta_{\mathbf{x}}^{\mathbf{t}} := e^{-\mathbf{t}\sqrt{\mathcal{A}_\kappa}} \delta_{\mathbf{x}} . \quad (3.88)$$

These alternative definitions will not be considered within this work. We plan to discuss them and their relation to ZR elsewhere.

**Lemma 3.28.** *i) For any fixed  $j \in \mathbb{N}$ ,  $r \in \mathbb{R}$  and for any  $u \in \Sigma_{2j+d-2r}$ , the map  $\delta^u : \Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto \delta_{\mathbf{x}}^u$  is of class  $C^j$ ; moreover, for any multi-index  $\alpha$  of order  $\leq j$ , the  $\alpha$ -th derivative of this map is given by*

$$(\partial^\alpha \delta^u)_{\mathbf{x}} = \mathcal{A}_\kappa^{-u/4} (\partial^\alpha \delta)_{\mathbf{x}} \in \mathcal{H}^{-r} \quad \text{for } u \in \Sigma_{2|\alpha|+d-2r} . \quad (3.89)$$

*ii) Let  $\bar{\phantom{x}}$  indicate the extension of the complex conjugation on  $\mathcal{H} = L^2(\Omega)$  to  $\mathcal{H}^{-\infty}$ ; then, for all  $u \in \mathbb{C}$  and for all  $\mathbf{x} \in \Omega$ , there holds*

$$\overline{\delta_{\mathbf{x}}^u} = \delta_{\mathbf{x}}^{\bar{u}} . \quad (3.90)$$

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<sup>15</sup>In fact, by standard dimensional analysis, the Schrödinger-type operator  $\mathcal{A} := -\Delta + V$  can be attributed the dimension of a momentum squared; due to the convention  $c = \hbar = 1$  observed in the present manuscript, this means that, dimensionally speaking,  $\mathcal{A}$  is a mass squared.

*Proof.* i) By definition (see Eq. (3.87)), the map  $\mathbf{x} \mapsto \delta_{\mathbf{x}}^u$  is given by the composition of the maps  $\mathbf{x} \mapsto \delta_{\mathbf{x}}$  and  $h \mapsto \kappa^{u/2} \mathcal{A}^{-u/4} h$ . Next, recall that the map  $\Omega \rightarrow \mathcal{H}^{-r'}$ ,  $\mathbf{x} \mapsto \delta_{\mathbf{x}}$  is of class  $C^j$  for all  $r' > j + d/2$  (see Proposition 2.48). On the other hand, due to Corollary 2.13, the map  $\mathcal{A}^{-u/4} : \mathcal{H}^{-(r+\Re u/2)} \rightarrow \mathcal{H}^{-r}$  is an Hilbertian isomorphism; so, in particular, it is a linear and continuous (whence analytic) map. The above facts, employed with  $r' = r + \Re u/2$ , suffice to infer the thesis.

ii) In order to avoid confusion, let us temporarily indicate with  $\mathcal{J}$  the extension to  $\mathcal{H}^{-\infty}$  of the complex conjugation. Then, notice that  $\overline{\delta_{\mathbf{x}}^u} = \mathcal{J}(\kappa^{u/2} \mathcal{A}^{-u/4} \delta_{\mathbf{x}}) = \kappa^{\bar{u}/2} \mathcal{J} \mathcal{A}^{-u/4} \mathcal{J}^{-1} \mathcal{J} \delta_{\mathbf{x}}$ . Due to Corollary 2.26, there holds  $\mathcal{J} \mathcal{A}^{-u/4} \mathcal{J}^{-1} = \mathcal{A}^{-\bar{u}/4}$ ; on the other hand, Lemma 2.52 allows to infer that  $\mathcal{J} \delta_{\mathbf{x}} = \delta_{\mathbf{x}}$ . Summing up, one has  $\overline{\delta_{\mathbf{x}}^u} = \kappa^{\bar{u}/2} \mathcal{A}^{-\bar{u}/4} \delta_{\mathbf{x}} = \mathcal{A}_{\kappa}^{-\bar{u}/4} \delta_{\mathbf{x}} = \delta_{\mathbf{x}}^{\bar{u}}$ , which proves Eq. (3.90).  $\square$

*Remark 3.20.* Recall the definition (2.237) of the Dirichlet kernel  $\mathcal{A}^{-u/4}(\cdot, \cdot)$ . Then, for all  $\mathbf{x} \in \Omega$ , it appears that the above relations (3.87)–(3.89) can be rephrased as follows:

$$\begin{aligned} \delta_{\mathbf{x}}^u &= \kappa^{u/2} \mathcal{A}^{-u/4}(\cdot, \mathbf{x}) && \text{for } u \in \Sigma_{2d} ; \\ (\partial^\alpha \delta^u)_{\mathbf{x}} &= \kappa^{u/2} \partial_2^\alpha \mathcal{A}^{-u/4}(\cdot, \mathbf{x}) && \text{for } u \in \Sigma_{2(|\alpha|+d)} . \end{aligned} \quad (3.91)$$

The above relations show that, for  $\Re u$  large enough,  $\delta_{\mathbf{x}}^u$  ( $\mathbf{x} \in \Omega$ ) coincides with the  $\kappa$ -rescaled Dirichlet kernel of  $\mathcal{A}$ , with one of the second argument fixed; so, for any fixed  $\mathbf{x} \in \Omega$ ,  $\delta_{\mathbf{x}}^u$  is in fact an ordinary (continuous and differentiable) function.

In view of Lemma 3.28, the forthcoming definition is well-posed.

**Definition 3.29.** The *zeta-regularized Wightman field* at  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$  (i.e., at time  $t \in \mathbb{R}$  and space position  $\mathbf{x} \in \Omega$ ) is

$$\hat{\varphi}^u(x) \equiv \hat{\varphi}^u(t, \mathbf{x}) := \hat{\varphi}_t(\delta_{\mathbf{x}}^u) \quad \text{for } u \in \Sigma_{d-1} . \quad (3.92)$$

*Remark 3.21.* Due to Lemma 3.28,  $\delta_{\mathbf{x}}^u \in \mathcal{H}^{-1/2}$  whenever  $\Re u > d - 1$ ; this suffices to infer that the right-hand side of Eq. (3.92) makes sense according to Definition 3.13, so that  $\hat{\varphi}^u(x)$  defined above is well posed.

**Proposition 3.30.** Let  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$  be any finite particle state; then, for any  $n \in \mathbb{N}$  and for all  $u \in \Sigma_{2n+d-1}$ , the map  $\mathbb{R} \times \Omega \rightarrow \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{F}^\vee(\mathcal{H})$ ,  $x \mapsto \hat{\varphi}^u(x) \mathbf{f}$  is of class  $C^n$ . Moreover, for any (spatial) multi-index  $\alpha$  and any  $j \in \mathbb{N}$  with  $j + |\alpha| \leq n$ , there holds

$$\partial_t^j \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}) = \partial_t^j \hat{\varphi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f} \quad \text{for } u \in \Sigma_{2(j+|\alpha|)+d-1} ; \quad (3.93)$$

in addition the order of the derivatives can be interchanged arbitrarily.

*Proof.* First of all, recall the definition (3.92) of the zeta-regularized Wightman field  $\hat{\varphi}^u(x)$ . In order to prove the thesis, we show hereafter in several steps that all the partial derivatives (with respect to  $t$  and  $\mathbf{x}$ ) of order  $\leq n$  exist and are continuous on  $\mathbb{R} \times \Omega$ .

*Step 1 - Existence and continuity of the time derivatives (of any order  $j \in \mathbb{N}$  with  $j \leq n$ ).* This statement follows easily from Proposition 3.21, simply noting that  $\delta_{\mathbf{x}}^u \in \mathcal{H}^{-1/2+j}$  for all  $u \in \Sigma_{d-1+2j}$  (see Lemma 3.28).

*Step 2 - Existence and continuity of the spatial derivatives (of any order  $j \in \mathbb{N}$  with  $j \leq n$ ); proof of Eq. (3.93) for  $j = 0$ .* First recall that, due to Lemma 3.14 and to Proposition 3.19, the map  $\mathcal{H}^{-1/2} \rightarrow \mathfrak{D}^\vee(\mathcal{H}) \subset \mathfrak{F}^\vee(\mathcal{H})$ ,  $h \mapsto \hat{\varphi}_t(h) \mathbf{f}$  is linear and continuous, whence analytic; on the other hand, the map  $\Omega \rightarrow \mathcal{H}^{-r}$ ,  $\mathbf{x} \mapsto \delta_{\mathbf{x}}^u$  is of class  $C^j$  for all  $u \in \Sigma_{d+2j-2r}$  (see Lemma 3.28). Since  $\mathbf{x} \mapsto \hat{\varphi}_t(\delta_{\mathbf{x}}^u) \mathbf{f}$  is given by the composition of the previous two maps (set  $r = 1/2$ ), the regularity results discussed above for the latter suffice to infer the first part of the thesis. Eq. (3.93) with  $j = 0$  follows easily by continuity arguments, recalling that  $(\partial^\alpha \delta^u)_{\mathbf{x}}$  is the  $\alpha$ -th derivative of the map  $\mathbf{x} \mapsto \delta_{\mathbf{x}}^u$  (see Lemma 3.28).

*Step 3 - Existence and continuity of the mixed derivatives of the form  $\partial_t^j \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f})$  (for  $j \in \mathbb{N}$  and  $\alpha$  a multi-index with  $j+|\alpha| \leq n$ ).* Notice that, due to the previously proved identity (3.93) with  $j = 0$ , there holds  $\partial_t^j \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}) = \partial_t^j (\hat{\varphi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f})$ . Then, one can proceed as in Step 1 of the present proof to show that the map  $(t, \mathbf{x}) \mapsto \partial_t^j (\hat{\varphi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f})$  is well-posed and continuous; indeed, it suffices to notice that the map  $\Omega \rightarrow \mathcal{H}^{-1/2+j}$ ,  $\mathbf{x} \mapsto (\partial^\alpha \delta^u)_{\mathbf{x}}$  is continuous for all  $u \in \Sigma_{d-1+2(j+|\alpha|)}$  (see Lemma 3.28). This suffices to infer the thesis.

*Step 4 - Commutativity of the partial derivatives  $\partial_t^j$  and  $\partial_{\mathbf{x}}^\alpha$ .* As an example, consider the expression  $\partial_t \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f})$ , for  $|\alpha| \leq n - 1$  and recall that, using Eq. (3.93) with  $j = 1$ , this can be re-written as  $\partial_t (\hat{\varphi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f})$ . Next, notice that, due to Lemma 3.21 (see, in particular, the second identity in Eq. (3.64)), there holds  $\partial_t (\hat{\varphi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f}) = \hat{\pi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f}$ . Moreover, by arguments similar to those of Step 2 it can be proved that, for all multi-indexes  $\beta$  with  $\beta \leq \alpha$  <sup>(16)</sup>,  $\hat{\pi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f} = \partial_{\mathbf{x}}^{\alpha-\beta} (\hat{\pi}_t((\partial^\beta \delta^u)_{\mathbf{x}}) \mathbf{f})$ ; recalling again Eq. (3.64), this yields  $\hat{\pi}_t((\partial^\alpha \delta^u)_{\mathbf{x}}) \mathbf{f} = \partial_{\mathbf{x}}^{\alpha-\beta} \partial_t \partial_{\mathbf{x}}^\beta (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f})$ . Summing up, the above facts show that  $\partial_t \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}) = \partial_{\mathbf{x}}^{\alpha-\beta} \partial_t \partial_{\mathbf{x}}^\beta (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f})$ , for all  $\beta \leq \alpha$ . Finally, one can proceed by induction to prove that analogous identities hold with higher order time derivatives; this, along with Step 3, yields Eq. (3.93).  $\square$

In view of the previous proposition, the following definition is well posed.

**Definition 3.31.** Let  $\alpha$  be any multi-index and let  $j \in \mathbb{N}$ ; for any  $u \in \Sigma_{d-1+2(j+|\alpha|)}$  the  $j$ -th time,  $\alpha$ -th spatial derivative of the zeta-regularized Wightman field at time  $t \in \mathbb{R}$  and space position  $\mathbf{x} \in \Omega$  is the unique operator  $\partial_t^j \partial_{\mathbf{x}}^\alpha \hat{\varphi}^u(t, \mathbf{x}) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  (coinciding with similar expressions obtained by exchanging the differentiation order) which fulfills

$$(\partial_t^j \partial_{\mathbf{x}}^\alpha \hat{\varphi}^u(t, \mathbf{x})) \mathbf{f} = \partial_t^j \partial_{\mathbf{x}}^\alpha (\hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}) \quad \text{for all } \mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H}) . \quad (3.94)$$

**Corollary 3.32.** For any  $\mathbf{f} \in \mathfrak{D}^\vee(\mathcal{H})$  and for all  $u \in \Sigma_{d+3}$ , the zeta-regularized Wightman field fulfills the following version of the Klein-Gordon equation:

$$\begin{cases} (\partial_{tt} - \Delta_{\mathbf{x}} + V(\mathbf{x})) \hat{\varphi}^u(t, \mathbf{x}) \mathbf{f} = \mathbf{o} , \\ \hat{\varphi}^u(t, \mathbf{x}) \mathbf{f} \Big|_{t=0} = \hat{\varphi}(\delta_{\mathbf{x}}^u) \mathbf{f} , \\ (\partial_t \hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}) \Big|_{t=0} = \hat{\pi}(\delta_{\mathbf{x}}^u) \mathbf{f} \end{cases} \quad (3.95)$$

<sup>16</sup>With the notation  $\beta \leq \alpha$ , we mean that  $\beta_i \leq \alpha_i$  for all  $i \in \{1, \dots, d\}$ .

where  $\mathbf{o} \in \mathfrak{D}^\vee(\mathcal{H})$  is the null element of the Fock space  $\mathfrak{F}^\vee(\mathcal{H})$ .

*Proof.* First of all, let us notice that  $\delta_{\mathbf{x}}^u \in \text{Dom}(\mathcal{A}) \subset \mathcal{H}$  for all  $u \in \Sigma_d \supset \Sigma_{d+3}$  (see Lemma 3.28, here employed with  $r = 0$ ), so that  $\mathcal{A} \delta_{\mathbf{x}}^u = (-\Delta_{\mathbf{x}} + V(\mathbf{x})) \delta_{\mathbf{x}}^u$  <sup>(17)</sup>. This fact and Proposition 3.30 (see, in particular, Eq. (3.93)) imply, by linearity and continuity, that  $\hat{\varphi}_t(\mathcal{A} \delta_{\mathbf{x}}^u) \mathbf{f} = (-\Delta_{\mathbf{x}} + V(\mathbf{x})) \hat{\varphi}^u(t, \mathbf{x}) \mathbf{f}$  (one should also recall the definition (3.92) of the zeta-regularized Wightman field  $\hat{\varphi}^u(t, \mathbf{x})$ ). Then the thesis follows straightforwardly from Corollary 3.23 (see, in particular, Eq. (3.66)), to be employed here with  $h = \delta_{\mathbf{x}}^u$  (for  $u \in \Sigma_{d-1}$ ).  $\square$

Before proceeding, let us also point out that, once the zeta-regularized Wightman field has been defined according to Eq. (3.92), one can consider the corresponding regularized VEV of the field squared at any two (possibly coinciding) spacetime points, i.e., the *zeta-regularized propagator*. Concerning this quantity, the subsequent results can be proved.

**Corollary 3.33.** *Let  $\mathbf{v} \in \mathfrak{D}^\vee(\mathcal{H})$  be the vacuum state and let  $n \in \mathbb{N}$ . Then, for any  $u \in \Sigma_{d-1+2n}$ , the map  $(\mathbb{R} \times \Omega)^2 \rightarrow \mathbb{C}$ ,  $(x, y) \mapsto (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v})$  is of class  $C^n$ . Moreover, for any  $j, j' \in \mathbb{N}$  and any pair of multi-indices  $\alpha, \alpha'$  with  $j + |\alpha|, j' + |\alpha'| \leq n$ , there holds*

$$\partial_{x^0}^j \partial_{y^0}^{j'} \partial_{\mathbf{x}}^\alpha \partial_{\mathbf{y}}^{\alpha'} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = (\mathbf{v} | (\partial_{x^0}^j \partial_{\mathbf{x}}^\alpha \hat{\varphi}^u(x)) (\partial_{y^0}^{j'} \partial_{\mathbf{y}}^{\alpha'} \hat{\varphi}^u(y)) \mathbf{v}) . \quad (3.96)$$

*Proof.* Due to the results Proposition 3.30, the thesis can be easily proved moving along the same lines as in the proof of Corollary 3.24.  $\square$

**Lemma 3.34.** *For any two spacetime points  $x = (x^0, \mathbf{x}), y = (y^0, \mathbf{y}) \in \mathbb{R} \times \Omega$  and any  $u \in \Sigma_{d-1}$ , consider the VEV  $(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v})$ ; this can be expressed as follows*

$$(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \frac{\kappa^u}{2} \langle \delta_{\mathbf{x}} | (e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} / \mathcal{A}^{\frac{u+1}{2}}) \delta_{\mathbf{y}} \rangle , \quad (3.97)$$

where  $\langle | \rangle$  indicates the extension to  $\mathcal{H}^{(2)}$  of the inner product on  $\mathcal{H}$ .

*Remark 3.22.* Of course, the identity in Eq. (3.97) could be re-expressed as follows, using the language of integral kernels:

$$(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \frac{\kappa^u}{2} (e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} \mathcal{A}^{-\frac{u+1}{2}})(\mathbf{x}, \mathbf{y}) . \quad (3.98)$$

Nonethelss, in view of the following applications, it is advisable to keep in mind the mentioned identity in the version given in the above Lemma.

<sup>17</sup>Indeed, for any  $f \in \mathcal{H}^r$  with  $r > 2 + d/2$ , there holds

$$\langle \mathcal{A} \delta_{\mathbf{x}}^u | f \rangle = \langle \delta_{\mathbf{x}} | \mathcal{A} \mathcal{A}^{-\bar{u}/4} f \rangle = (-\Delta + V)(\mathcal{A}^{-\bar{u}/4} f)(\mathbf{x}) = (-\Delta_{\mathbf{x}} + V(\mathbf{x})) \langle \delta_{\mathbf{x}}^u | f \rangle ,$$

where, in the last passage, we have used the fact that

$$(\mathcal{A}^{-\bar{u}/4} f)(\mathbf{x}) = \langle \delta_{\mathbf{x}} | \mathcal{A}^{-\bar{u}/4} f \rangle = \langle \mathcal{A}^{-u/4} \delta_{\mathbf{x}} | f \rangle = \langle \delta_{\mathbf{x}}^u | f \rangle .$$

Then, the identity  $\mathcal{A} \delta_{\mathbf{x}}^u = (-\Delta_{\mathbf{x}} + V(\mathbf{x})) \delta_{\mathbf{x}}^u$  follows by linearity and continuity.

*Proof.* First notice that the definition (3.92) and the identity (3.73) of Proposition 3.25 allow to infer  $(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \frac{1}{2} \langle \bar{\delta}_{\mathbf{x}}^u | (e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}}) \delta_{\mathbf{y}}^u \rangle$ ; on the other hand, the definition (3.87) (along with the identity (3.90)) yields

$$\langle \bar{\delta}_{\mathbf{x}}^u | (e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}}) \delta_{\mathbf{y}}^u \rangle = \kappa^u \langle \mathcal{A}^{-\bar{u}/4} \delta_{\mathbf{x}} | (e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}}) \mathcal{A}^{-u/4} \delta_{\mathbf{y}} \rangle . \quad (3.99)$$

To proceed, notice that for any  $u \in \Sigma_{d-1}$  there exists  $r, r' \in \mathbb{R}$  such that  $\Re u > d - 2r$ ,  $\Re u > d - 2r' - 2$  and  $-r' > r$ ; then, due to Lemma 3.28, one has  $\mathcal{A}^{-\bar{u}/4} \delta_{\mathbf{x}} \in \mathcal{H}^{-r}$  and  $(e^{-i(x^0-y^0)\sqrt{\mathcal{A}}} / \sqrt{\mathcal{A}}) \mathcal{A}^{-u/4} \delta_{\mathbf{y}} \in \mathcal{H}^{-r'} \hookrightarrow \mathcal{H}^r$ . Therefore, the pairing  $\langle | \rangle$  in the right-hand side of Eq. (3.99) can be interpreted as the extension to  $\mathcal{H}^{-r} \times \mathcal{H}^r$  of the inner product on  $L^2(\Omega)$  (defined according to Proposition 2.16). Then, the thesis follows recalling that the Banach adjoint of  $\mathcal{A}^{-\bar{u}/2}$  is  $\mathcal{A}^{-u/2}$  (see Corollary 2.24).  $\square$

*Remark 3.23.* In the following we will mainly consider second order derivatives of the zeta-regularized Wightman field. In order to adopt a more standard and concise nomenclature, we will use for such quantities the short-hand notation

$$\partial_{\mu\nu} \hat{\varphi}^u(x) \quad \text{for } u \in \Sigma_{d+3} \text{ and } \mu, \nu \in \{0, 1, \dots, d\} , \quad (3.100)$$

where we have introduced the following conventions, for  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$  and  $i, j \in \{1, \dots, d\}$ :

$$\begin{aligned} \partial_{00} \hat{\varphi}^u(x) &:= \partial_t^2 \hat{\varphi}^u(t, \mathbf{x}) , \\ \partial_{i0} \hat{\varphi}^u(x) &\equiv \partial_{0i} \hat{\varphi}^u(t, \mathbf{x}) := \partial_t \partial_{x^i} \hat{\varphi}^u(t, \mathbf{x}) , \\ \partial_{ij} \hat{\varphi}^u(x) &\equiv \partial_{ji} \hat{\varphi}^u(t, \mathbf{x}) := \partial_{x^i x^j} \hat{\varphi}^u(t, \mathbf{x}) . \end{aligned} \quad (3.101)$$

### The zeta-regularized stress-energy tensor and its VEV.

We now consider one of the main observables of interest for the applications, i.e., the stress-energy tensor. By analogy with the classical expression (1.7), we consider the following definition for the corresponding quantum version; here, in order to deal with the non-commutativity of the operators involved, we choose to replace the pointwise products with the symmetrized Jordan's product

$$A \circ B := \frac{1}{2} (AB + BA) , \quad (3.102)$$

for all linear operators  $A, B : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$ .

**Definition 3.35.** For any  $u \in \Sigma_{d+3}$ , the *zeta-regularized stress-energy tensor* at  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$  (i.e., at time  $t \in \mathbb{R}$  and evaluated at the space position  $\mathbf{x} \in \Omega$ ) is the operator  $\hat{T}_{\mu\nu}^u(x) : \mathfrak{D}^\vee(\mathcal{H}) \rightarrow \mathfrak{D}^\vee(\mathcal{H})$  given by

$$\begin{aligned} \hat{T}_{\mu\nu}^u(x) &:= \\ &(1 - 2\xi) \partial_\mu \hat{\varphi}^u(x) \circ \partial_\nu \hat{\varphi}^u(x) \\ &- \left( \frac{1}{2} - 2\xi \right) \eta_{\mu\nu} \left( \partial^\lambda \hat{\varphi}^u(x) \partial_\lambda \hat{\varphi}^u(x) + V(\mathbf{x}) (\hat{\varphi}^u(x))^2 \right) - 2\xi \hat{\varphi}^u(x) \circ \partial_{\mu\nu} \hat{\varphi}^u(x) , \end{aligned} \quad (3.103)$$



where  $\xi \in \mathbb{R}$  is an assigned parameter.

The *zeta-regularized stress-energy VEV* at  $x$  is  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(x) \mathbf{v})$ , where  $\mathbf{v} \in \mathfrak{D}^\vee(\mathcal{H})$  indicates as usual the vacuum state of the Fock space  $\mathfrak{F}^\vee(\mathcal{H})$ .

*Remark 3.24.* i) This is a proposed regularization of

$$\begin{aligned} \hat{T}_{\mu\nu}(x) &:= (1 - 2\xi) \partial_\mu \hat{\varphi}(x) \circ \partial_\nu \hat{\varphi}(x) \\ &- \left( \frac{1}{2} - 2\xi \right) \eta_{\mu\nu} \left( \partial^\lambda \hat{\varphi}(x) \partial_\lambda \hat{\varphi}(x) + V(\mathbf{x})(\hat{\varphi}(x))^2 \right) - 2\xi \hat{\varphi}(x) \circ \partial_{\mu\nu} \hat{\varphi}(x) , \end{aligned} \quad (3.104)$$

which is ill-defined. See, e.g., [64] for some basic information on this object (and, in particular, on the role of the parameter  $\xi$ ).

ii) Let us stress that, due to Proposition 3.30 and to the related Definition 3.31 of the zeta-regularized Wightman field (see also the notations introduced in Eq. (3.101)), all the expressions on the right-hand side of Eq. (3.103) are in fact well-defined under the assumption  $u \in \Sigma_{d+3}$ , since there appear only derivatives of the zeta-regularized Wightman field of second order at most.

iii) The choice we made to replace the point-wise products in the classical expression with the symmetrized Jordan's product (3.102) of the corresponding operators, grants automatically the symmetry of the zeta-regularized stress-energy tensor  $\hat{T}_{\mu\nu}^u(x)$  under exchange of the indexes  $\mu, \nu \in \{0, \dots, d\}$ , i.e., that

$$\hat{T}_{\mu\nu}^u(x) = \hat{T}_{\nu\mu}^u(x) . \quad (3.105)$$

The zeta-regularized stress-energy VEV can be expressed in terms of the zeta-regularized propagator  $(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v})$  and of its space-time derivatives, evaluated along the diagonal  $y = x$ . More precisely, there holds the following result.

**Lemma 3.36.** *For any  $u \in \Sigma_{d+3}$  and for any  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$ , the regularized VEV of the stress-energy tensor can be expressed as*

$$\begin{aligned} (\mathbf{v} | \hat{T}_{\mu\nu}^u(x) \mathbf{v}) &= \\ &\left( \frac{1}{2} - \xi \right) (\partial_{x^\mu y^\nu} + \partial_{x^\nu y^\mu}) - \left( \frac{1}{2} - 2\xi \right) \eta_{\mu\nu} \left( \partial^{x^\lambda} \partial_{y^\lambda} + V(\mathbf{x}) \right) - \xi (\partial_{x^\mu x^\nu} + \partial_{y^\mu y^\nu}) \Big|_{y=x} \\ &(\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) . \end{aligned} \quad (3.106)$$

*Proof.* The thesis can be easily proved keeping in mind the definition (3.103) for the zeta-regularized stress-energy tensor operator and using the results of Corollary 3.33.  $\square$

Due to the above lemma, the zeta-regularized stress-energy VEV can be explicitly computed in terms of the Dirichlet kernel and of its derivatives evaluated along the diagonal. More precisely, there holds the forthcoming proposition.

**Proposition 3.37.** *For any  $u \in \Sigma_{d+3}$ , the components of the zeta-regularized stress-energy VEV at  $x = (t, \mathbf{x}) \in \mathbb{R} \times \Omega$  admit the following representations (for  $i, j \in \{1, \dots, d\}$ ):*

$$(\mathbf{v} | \hat{T}_{00}^u(t, \mathbf{x}) \mathbf{v}) = \kappa^u \left[ \left( \frac{1}{4} + \xi \right) \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) + \left( \frac{1}{4} - \xi \right) (\partial^{x^\ell} \partial_{y^\ell} + V(\mathbf{x})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}}, \quad (3.107)$$

$$(\mathbf{v} | \hat{T}_{0i}^u(t, \mathbf{x}) \mathbf{v}) = (\mathbf{v} | \hat{T}_{i0}^u(t, \mathbf{x}) \mathbf{v}) = 0, \quad (3.108)$$

$$\begin{aligned} (\mathbf{v} | \hat{T}_{ij}^u(t, \mathbf{x}) \mathbf{v}) &= (\mathbf{v} | \hat{T}_{ji}^u(t, \mathbf{x}) \mathbf{v}) = \\ \kappa^u &\left[ \left( \frac{1}{4} - \xi \right) \delta_{ij} \left( \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) - (\partial^{x^\ell} \partial_{y^\ell} + V(\mathbf{x})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right) + \right. \\ &\left. + \left( \left( \frac{1}{2} - \xi \right) \partial_{x^i} \partial_{y^j} - \xi \partial_{x^i x^j} \right) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}}. \end{aligned} \quad (3.109)$$

Here the notation  $[ ]_{\mathbf{y}=\mathbf{x}}$  is used to indicate that the expressions within the square brackets must be evaluated along the diagonal  $\mathbf{y} = \mathbf{x}$ .

*Proof.* First consider the expression (3.106) for the zeta-regularized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(x) \mathbf{v})$  ( $\mu, \nu \in \{0, \dots, d\}$ ) in terms of the propagator; then, Eq.s (3.107-3.109) follow by simple algebraic computations if one can prove the forthcoming identities for the VEVs of the second order monomials of the zeta-regularized field, for  $i, j \in \{1, \dots, d\}$ :

$$\begin{aligned} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(x) \mathbf{v}) &= \frac{\kappa^u}{2} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}, \\ \partial_{x^0 y^0} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) &= -\partial_{x^0 x^0} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = -\partial_{y^0 y^0} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \\ &= \frac{\kappa^u}{2} \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}, \\ \partial_{x^i y^0} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(y) \hat{\varphi}^u(x) \mathbf{v}) &= -\partial_{x^0 y^i} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \\ \partial_{y^0 y^i} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) &= -\partial_{x^0 x^i} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(x) \mathbf{v}) = \frac{i \kappa^u}{2} \partial_{x^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}, \\ \partial_{x^i y^j} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) &= \frac{\kappa^u}{2} \partial_{x^i y^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}, \\ \partial_{x^i x^j} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) &= \partial_{y^i y^j} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \frac{\kappa^u}{2} \partial_{x^i x^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}. \end{aligned}$$

All the above identities can be derived by elementary manipulations, recalling the explicit expression (3.97) given in Lemma 3.34 for the zeta-regularized propagator. As an example, we show how to compute the VEV  $\partial_{x^0 y^i} \Big|_{\mathbf{y}=\mathbf{x}} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v})$  (the other identities can be

obtained in a similar fashion). To this purpose first notice that, using the cited lemma, one has

$$\partial_{x^0 y^i} \Big|_{y=x} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = \frac{\kappa^u}{2} \partial_{x^0} \partial_{y^i} \langle \delta_{\mathbf{x}} | (e^{-i(x^0 - y^0)\sqrt{\mathcal{A}}} / \mathcal{A}^{\frac{u+1}{2}}) \delta_{\mathbf{y}} \rangle \Big|_{y=x} ;$$

this allows to infer that  $\partial_{x^0 y^i} \Big|_{y=x} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = -\frac{i\kappa^u}{2} \langle \delta_{\mathbf{x}} | \mathcal{A}^{-\frac{u}{2}} (\partial_i \delta)_{\mathbf{y}} \rangle \Big|_{y=x}$ , which in terms of integral kernels (see Eq. (2.221)) gives

$$\partial_{x^0 y^i} \Big|_{y=x} (\mathbf{v} | \hat{\varphi}^u(x) \hat{\varphi}^u(y) \mathbf{v}) = -\frac{i\kappa^u}{2} \partial_{y^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} .$$

In conclusion, the thesis follows noting that  $\partial_{y^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \partial_{x^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}$ , due to item i) of Proposition 2.64 <sup>(18)</sup>.  $\square$

*Remark 3.25.* Let us stress that, in principle, the zeta-regularized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(x) \mathbf{v}) \equiv (\mathbf{v} | \hat{T}_{\mu\nu}^u(t, \mathbf{x}) \mathbf{v})$  does depend on both the time ( $t \in \mathbb{R}$ ) and spatial ( $\mathbf{x} \in \Omega$ ) coordinates; nevertheless, the expressions obtained in the right-hand sides of Eq.s (3.107-3.109) for the components of the mentioned VEV show that the latter is, in fact, independent of the time variable  $t$ . This property was to be expected as a natural consequence of the staticity features of the setting under analysis.

In view of the considerations discussed in the above remark, in pursue of brevity, we adopt the following (slightly abusive) convention.

**Notation 3.38.** For all  $(t, \mathbf{x}) \in \mathbb{R} \times \Omega$ ,  $\mu, \nu \in \{0, \dots, d\}$  and for any  $u \in \Sigma_{d+3}$ , we put

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) \equiv (\mathbf{v} | \hat{T}_{\mu\nu}^u(t, \mathbf{x}) \mathbf{v}) . \quad (3.110)$$

*Remark 3.26.* The hypothesis  $u \in \Sigma_{d+3}$  made in Proposition 3.37 is necessary to grant the existence of the stress-energy tensor operator  $\hat{T}_{\mu\nu}^u(\mathbf{x})$  appearing in the left-hand sides of Eq.s (3.107-3.109). However, keeping in mind the results of Proposition 2.64, it appears that the expressions on the right-hand sides of the cited equations continue to make sense under the weaker assumption  $u \in \Sigma_{d+1}$ ; as a matter of fact, this is also the minimum requirement necessary to ensure the continuity of the map  $\mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$ , thus granting the well-posedness of the point-wise evaluation of the stress-energy VEV.

The considerations of Remark 3.26 can be interpreted in the sense of analytic continuation, meaning that the right-hand sides of Eq.s (3.107-3.109) give the analytic continuation to  $\Sigma_{d+1}$ . More precisely, there hold the results reported in the subsequent Corollary.

<sup>18</sup>In fact, Eq. (2.240) yields, in particular,

$$\partial_{y^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) = \partial_{y^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{y}, \mathbf{x}) ;$$

on the other hand, when evaluation along the diagonal  $\mathbf{y} = \mathbf{x}$  is being considered, one can relabel the variables in the right-hand side of the the above identity ( $\mathbf{x} \leftrightarrow \mathbf{y}$ ), thus obtaining  $\partial_{y^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \partial_{x^i} \mathcal{A}^{-\frac{u}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}$ .

**Corollary 3.39.** *There hold the following statements.*

i) *For any  $j \in \mathbb{N}$  and  $u \in \Sigma_{d+1+j}$ , the map  $\Omega \rightarrow \mathbb{C}$ ,  $\mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  is of class  $C^j$  (whence, in particular, continuous for  $u \in \Sigma_{d+1}$ ).*

ii) *For any fixed  $\mathbf{x} \in \Omega$  and for any multi-index  $\alpha$  of order  $\leq j$ , the map  $\Sigma_{d+1+j} \rightarrow \mathbb{C}$ ,  $u \mapsto \partial_{\mathbf{x}}^{\alpha}(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  is analytic.*

*Proof.* First of all, recall the expressions (3.107-3.109) derived in Proposition 3.37 for the components of the zeta-regularized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  in terms of the Dirichlet kernel and of its derivatives (evaluated along the diagonal  $\mathbf{y} = \mathbf{x}$ ). Then, both statements i) and ii) can be easily inferred from the results of Proposition 2.64, granting the differentiability of the Dirichlet kernel (also along the diagonal) with respect to the spatial variables and its analyticity with respect to the complex index; one should recall, as well, that  $V$  was assumed to be smooth.  $\square$

*Remark 3.27.* When the domain and the potential fulfill the stronger regularity assumptions (2.159) and suitable conditions are prescribed on the boundary (see the comments at the end of subsection 2.6), the results of Corollary 3.39 can be extended up to the boundary. More precisely, item i) of the above Corollary holds with  $\Omega$  replaced by  $\bar{\Omega} = \Omega \cup \partial\Omega$ , while item ii) holds for any  $\mathbf{x} \in \bar{\Omega}$ .

Next, let us state two results which will turn out to be crucial for the developments to be discussed in the following (in particular, to define a renormalized version of the stress-energy VEV).

**Theorem 3.40.** *Assume the domain  $\Omega$ , its boundary  $\partial\Omega$  and the potential  $V$  to be such that, for any pair of multi-indexes  $\alpha, \beta$  with  $|\alpha| + |\beta| \leq 2$ , for any  $\mathbf{x} \in \Omega$  and for some  $N \in \mathbb{N}$ , the diagonal heat kernel derivative  $\partial_1^{\alpha} \partial_2^{\beta} e^{-tA}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  has the form (2.354) (or even (2.357); see pages 104 and 105, respectively). Then, for any  $\mu, \nu \in \{0, \dots, d\}$  and for fixed  $\mathbf{x} \in \Omega$ , the map  $\Sigma_{d+1} \rightarrow \mathbb{C}$ ,  $u \mapsto (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  can be analytically continued to a function, which is meromorphic on the strip  $\Sigma_{d+1-2N}$  and possesses only possible simple pole singularities at  $u = d + 1 - 2n$ , for  $n \in \{0, \dots, N\}$ . In particular, if  $N > (d + 1)/2$  the mentioned analytic continuation extends to a neighbour of  $u = 0$ ; moreover, whenever the spatial dimension  $d$  is even,  $u = 0$  is a regular point for the mentioned analytic continuation.*

*Proof.* Consider once more the representations (3.107-3.109) for the components of the zeta-regularized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$ ; in particular, notice that these representations involve the functions  $\mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})$ ,  $\partial_{w^i z^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})$  (with  $w, z \in \{x, y\}$  and  $i, j \in \{1, \dots, d\}$ ), evaluated along the diagonal  $\mathbf{y} = \mathbf{x}$ . Then the thesis follows easily from Theorem 2.91, whose hypotheses are assumed to be fulfilled in the present theorem.  $\square$

**Theorem 3.41.** *Assume the domain  $\Omega$ , its boundary  $\partial\Omega$  and the potential  $V$  to be such that, for any pair of multi-indexes  $\alpha, \beta$  with  $|\alpha| + |\beta| \leq 2$  and for any  $\mathbf{x} \in \Omega$ , the diagonal cylinder kernel derivative  $\partial_1^{\alpha} \partial_2^{\beta} e^{-t\sqrt{A}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  has the form (2.359) for some function such that the map  $[0, +\infty) \ni \mathbf{t} \mapsto J^{(\alpha, \beta)}(\mathbf{t}; \mathbf{x})$  admits an analytic extension to a complex*

open neighbour  $\mathcal{U} \subset \mathbb{C}$  of  $[0, +\infty)$  (see page 106). Then, for any  $\mu, \nu \in \{0, \dots, d\}$  and for fixed  $\mathbf{x} \in \Omega$ , the map  $\Sigma_{d+1} \rightarrow \mathbb{C}$ ,  $u \mapsto (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  can be analytically continued to a function, which is meromorphic on the whole complex plane and possesses only possible simple pole singularities at  $u = k$ , for  $k \in \{0, \dots, d+1\}$ .

*Proof.* The thesis can be derived as in the proof of in Theorem 3.40, using Theorem 2.92 in place of Theorem 2.91.  $\square$

### The zeta-regularized vacuum energy and pressure.

Following the analysis presented in Section 4 of our previous work [64], we are now going to consider other physical observables (aside from the stress-energy tensor), which are of direct interest for studying the Casimir effect. In particular, keeping in mind the results derived in the previous subsection for the VEV of the zeta-regularized stress-energy tensor (recalling, especially, that it is time independent), we can define zeta-regularized versions for both the vacuum energy and the vacuum pressure on the boundary  $\partial\Omega$  of the spatial domain  $\Omega$ . More precisely, proceeding again by analogy with the classical field theory described in subsection 1.1, we give the following definitions, which are well-posed under the specified assumptions.

**Definition 3.42.** Assume the zeta-regularized VEV of the energy density  $(\mathbf{v} | \hat{T}_{00}^u \mathbf{v})$  to fulfill the following hypothesis:

$$\begin{aligned} & \exists r_1, r_2 \in \mathbb{R} \text{ with } r_1 < r_2 \text{ s.t. } \forall u \in \Sigma_{(r_1, r_2)} \\ & \text{the map } \Omega \rightarrow \mathbb{C}, \mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v}) \text{ belongs to } L^1(\Omega), \end{aligned} \quad (3.111)$$

(recall that  $\Sigma_{(r_1, r_2)}$  indicates the strip  $\{u \in \mathbb{C} \mid r_1 < \Re u < r_2\}$ ). Then, for all  $u \in \Sigma_{(r_1, r_2)}$  the *zeta-regularized vacuum total energy* is (compare with Eq. (1.8))

$$\mathcal{E}^u := \int_{\Omega} d\mathbf{x} (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v}). \quad (3.112)$$

*Remark 3.28.* i) In the next paragraph we will show that the assumption (3.111) holds in the case where  $\Omega$  is a bounded domain with smooth boundary  $\partial\Omega$ ,  $V \in C^\infty(\bar{\Omega})$  and Dirichlet boundary conditions are prescribed.

ii) Recall that the map  $\Omega \ni \mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})$  is granted to be continuous for all  $u \in \Sigma_{d+1}$ , due to Corollary 3.39 (see, in particular, item i) therein); therefore, the assumption (3.111) can be checked by studying the behaviour of  $(\mathbf{v} | \hat{T}_{00}^u \mathbf{v})$  near the boundary  $\partial\Omega$  and, when  $\Omega$  is unbounded, at spatial infinity.

When the boundary  $\partial\Omega$  is non-empty and sufficiently regular, one can also consider the pressure exerted on it by the field confined within the spatial domain  $\Omega$ .

**Definition 3.43.** Let  $\partial\Omega$  be piecewise differentiable; consider the subset

$$\partial\Omega' := \{\mathbf{x} \in \partial\Omega \mid \exists \mathbf{n}(\mathbf{x}) \equiv (n^i(\mathbf{x})) = \text{unit outer normal at } \mathbf{x}\} \quad (3.113)$$

and assume the zeta-regularized VEV of the spatial components of the stress-energy tensor  $(\mathbf{v} | \hat{T}_{ij}^u \mathbf{v})$  ( $i, j \in \{1, \dots, d\}$ ) to fulfill the following hypothesis:

$$\begin{aligned} & \exists r_1, r_2 \in \mathbb{R} \text{ with } r_1 < r_2 \text{ s.t. } \forall u \in \Sigma_{(r_1, r_2)}, i \in \{1, \dots, d\} \\ & \text{the map } \partial\Omega' \rightarrow \mathbb{C}, \mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{ij}^u(\mathbf{x}) \mathbf{v}) n^j(\mathbf{x}) \text{ is locally bounded.} \end{aligned} \quad (3.114)$$

Then, for all  $u \in \Sigma_{(r_1, r_2)}$ , the *zeta-regularized vacuum pressure* at  $\mathbf{x} \in \partial\Omega'$  is the vector  $\mathbf{p}^u(\mathbf{x}) \equiv (p_i^u(\mathbf{x}))$  whose components are defined as (compare with Eq. (1.9))

$$p_i^u(\mathbf{x}) := (\mathbf{v} | \hat{T}_{ij}^u(\mathbf{x}) \mathbf{v}) n^j(\mathbf{x}) \quad (i \in \{1, \dots, d\}). \quad (3.115)$$

### The case of a bounded domain.

Let us now restrict the attention to a particular type of settings; more precisely, we consider configurations fulfilling the assumptions (2.159) and (2.209):

$$\begin{aligned} & \Omega \subset \mathbb{R}^d \text{ is bounded with compact boundary } \partial\Omega \text{ of class } C^\infty, \\ & V \in C^\infty(\bar{\Omega}), \text{ Dirichlet boundary conditions are prescribed on } \partial\Omega. \end{aligned} \quad (3.116)$$

In these cases, it can be shown that the regularized vacuum energy  $\mathcal{E}^u$  and pressure  $\mathbf{p}^u$  introduced above are well-defined; as a matter of fact, much more can be said about these observables. Hereafter we report some results which we already derived in our previous work [64]; therein we employed systematically eigenfunction expansion techniques, while the arguments presented here rely on more general considerations.

Before proceeding, let us point out that some of the forthcoming results continue hold also under assumptions more general than those in Eq. (3.116).

**Proposition 3.44.** *Assume the hypotheses (3.116) to be fulfilled; then, the map  $\Sigma_{d+1} \rightarrow \mathbb{C}, u \mapsto \mathcal{E}^u$  is (well-defined and) analytic.*

*Proof.* First of all, consider the representation (3.107) which allows to express the VEV  $(\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})$  in terms of the diagonal kernels  $\mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}, \partial^{x^\ell} \partial_{y^\ell} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$ . Recall that, due to Proposition 2.64, these kernels are all continuous functions of  $\mathbf{x}$  on  $\bar{\Omega} = \Omega \cup \partial\Omega$ ; this suffices to infer that the map  $\Omega \ni \mathbf{x} \mapsto (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})$  is integrable, so that  $\mathcal{E}^u$  is well-defined according to Eq. (3.112).

Let us now pass to show the analyticity of the map  $\Sigma_{d+1} \ni u \mapsto \mathcal{E}^u$ . To this purpose, it suffices to show that there exists the complex derivative  $\frac{d}{du} \mathcal{E}^u$ , for all  $u \in \Sigma_{d+1}$ ; this fact follows, in turn, from Lebesgue's dominated convergence theorem if we can prove that, for any fixed  $u_0 > d + 1$ , there exist  $\delta > 0$  and a function  $\mathcal{T} \in L^1(\Omega)$  such that  $|\partial_u (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})| \leq \mathcal{T}(\mathbf{x})$  for all  $u \in \Sigma_{(u_0-\delta, u_0+\delta)} \cap \Sigma_{d+1}$  and for all  $\mathbf{x} \in \Omega$ .

So, let us proceed to prove the last statement above. Keeping in mind the representation (3.107) and recalling item v) of Proposition 2.64, it can be easily inferred that the complex derivative  $\partial_u (\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})$  is given by a sum of integral kernels of the form

$$\langle \delta_{\mathbf{x}} | (\partial_u \mathcal{A}^{-\frac{u+1}{2}}) \delta_{\mathbf{x}} \rangle = -\frac{1}{2} \langle \delta_{\mathbf{x}} | (\mathcal{A}^{-\frac{u+1}{2}} \ln \mathcal{A}) \delta_{\mathbf{x}} \rangle,$$

$$\langle \partial_i \delta_{\mathbf{x}} | (\partial_u \mathcal{A}^{-\frac{u+1}{2}}) \partial_i \delta_{\mathbf{x}} \rangle = -\frac{1}{2} \langle \partial_i \delta_{\mathbf{x}} | (\mathcal{A}^{-\frac{u+1}{2}} \ln \mathcal{A}) \partial_i \delta_{\mathbf{x}} \rangle \quad (i \in \{1, \dots, d\}) .$$

To proceed, notice that all the above mentioned kernels are of the form  $\langle f | (\mathcal{A}^{-\frac{u\pm 1}{2}} \ln \mathcal{A}) f \rangle$ , for  $f = \delta_{\mathbf{x}}$  or  $\partial_i \delta_{\mathbf{x}}$ ; on the other hand, it can be easily proved by functional analytic methods that, for any  $\delta \in (0, (u_0 - d - 1)/2)$  and for all  $u \in \Sigma_{(u_0 - \delta, u_0 + \delta)} (\subset \Sigma_{d+1})$ , there exists a positive constant  $c_{u_0, \delta}$  such that  $|\langle f | (\mathcal{A}^{-\frac{u\pm 1}{2}} \ln \mathcal{A}) f \rangle| \leq 2 c_{u_0, \delta} \langle f | \mathcal{A}^{-\frac{u_0\pm 1}{2} + \delta} f \rangle$  <sup>(19)</sup>. In consequence of this, there holds

$$|\langle \delta_{\mathbf{x}} | (\partial_u \mathcal{A}^{-\frac{u\pm 1}{2}}) \delta_{\mathbf{x}} \rangle| \leq c_{u_0, \delta, \varepsilon} \mathcal{A}^{-\frac{u_0\pm 1}{2} + \delta}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} ,$$

$$|\langle \partial_i \delta_{\mathbf{x}} | (\partial_u \mathcal{A}^{-\frac{u\pm 1}{2}}) \partial_i \delta_{\mathbf{x}} \rangle| \leq c_{u_0, \delta, \varepsilon} \partial_{x^i y^i} \mathcal{A}^{-\frac{u_0\pm 1}{2} + \delta}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \quad (i \in \{1, \dots, d\}) ,$$

which allows to infer

$$|\partial_u(\mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v})| \leq c_{u_0, \delta, \varepsilon} \kappa^{\Re u} \left[ \left( \frac{1}{4} + |\xi| \right) \mathcal{A}^{-\frac{u_0-1}{2} + \delta}(\mathbf{x}, \mathbf{y}) + \left( \frac{1}{4} + |\xi| \right) (\partial^{x^\ell} \partial_{y^\ell} + |V(\mathbf{x})|) \mathcal{A}^{-\frac{u_0+1}{2} + \delta}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}} .$$

To conclude notice that, since  $u_0 \pm 1 + 2\delta \in \Sigma_{d+1\pm 1}$ , due to Proposition 2.64 (keeping in mind that the potential  $V$  is assumed to be smooth on  $\overline{\Omega}$ ), the expression on the right-hand side of the last inequality is in fact a continuous function of  $\mathbf{x}$  on  $\overline{\Omega}$ . Therefore, the mentioned right-hand side yields the sought-for summable dominant; this proves the thesis.  $\square$

**Proposition 3.45.** *Assume the hypotheses (3.116) to be fulfilled; then, the regularized vacuum energy  $\mathcal{E}^u$  can be expressed as the sum*

$$\mathcal{E}^u = E^u + B^u , \quad (3.117)$$

where we introduced the zeta regularized bulk and boundary vacuum energies which are, respectively,

$$E^u := \frac{\kappa^u}{2} \int_{\Omega} d\mathbf{x} \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{x}) , \quad (3.118)$$

<sup>19</sup>To prove this fact consider the realization (2.54-2.56) of  $\mathcal{H}$  and  $\mathcal{A}$ , which were often employed in Chapter 2 of the present work; this allows to infer

$$|\langle f | (\mathcal{A}^{-\frac{u\pm 1}{2}} \ln \mathcal{A}) f \rangle| = 2 \int_K d\mu w^{-(\Re u \pm 1)} |\ln w| |f|^2 .$$

On the other hand, for all  $\Re u \in (u_0 - \delta, u_0 + \delta)$ , by elementary calculus one has (for  $w \in [\varepsilon, +\infty)$ )

$$w^{-(\Re u \pm 1)} |\ln w| \leq c_{u_0, \delta} w^{-(u_0 \pm 1) + \delta} \quad \text{with } c_{u_0, \delta} := \max\{\varepsilon^{-\delta} |\ln \varepsilon|, \varepsilon^{-3\delta} |\ln \varepsilon|, e^{-\delta}, e^{-3\delta}\} .$$

Then, the thesis follows noting that  $\int_K d\mu w^{-(u_0 \pm 1) + 2\delta} |f|^2 = \langle f | \mathcal{A}^{-\frac{u_0 \pm 1}{2} + \delta} f \rangle$ .

$$B^u := \kappa^u \left( \frac{1}{4} - \xi \right) \int_{\partial\Omega} da(\mathbf{x}) n^i(\mathbf{x}) \partial_{y^i} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}}. \quad (3.119)$$

*Remark 3.29.* In particular notice that, in view of Eq. (3.118), the regularized bulk energy can be equivalently expressed as

$$E^u := \frac{\kappa^u}{2} \text{Tr} \mathcal{A}^{-\frac{u-1}{2}}. \quad (3.120)$$

Indeed, under the assumptions (3.116),  $\mathcal{A}$  has purely discrete spectrum and explicit estimates are available for the eigenvalues; moreover, due to Corollary 2.75,  $\mathcal{A}^{-\frac{u-1}{2}}$  is of trace class and  $\text{Tr} \mathcal{A}^{-\frac{u-1}{2}}$  is an analytic function of  $u$  for  $u \in \Sigma_{d+1}$ .

Recalling that  $\mathcal{E}^u$  is analytic in the very same strip  $\Sigma_{d+1}$  due to Proposition 3.44, this suffices to infer that also  $B^u$  is analytic therein. Moreover, due to the results of item vi) of Proposition 2.64 (see also Proposition 2.72 and the related Remark 2.25), one readily infers that the regularized boundary energy  $B^u$  defined according to Eq. (3.119) vanishes identically whenever either Dirichlet or Neumann conditions are prescribed on the boundary of the domain  $\Omega$ .

*Proof.* Recalling the definition (3.112) and considering again the expression (3.107) for the regularized VEV  $\langle \mathbf{v} | \hat{T}_{00}^u(\mathbf{x}) \mathbf{v} \rangle$ , one has

$$\mathcal{E}^u = \kappa^u \int_{\Omega} d\mathbf{x} \left[ \left( \frac{1}{4} + \xi \right) \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) + \left( \frac{1}{4} - \xi \right) (\partial^{x^\ell} \partial_{y^\ell} + V(\mathbf{x})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}}.$$

Now, notice that  $[\partial^{x^\ell} \partial_{y^\ell} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})]_{\mathbf{y}=\mathbf{x}} = \partial^{x^\ell} ([\partial_{y^\ell} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})]_{\mathbf{y}=\mathbf{x}}) - [\Delta_{\mathbf{y}} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})]_{\mathbf{y}=\mathbf{x}}$  (by the Leibnitz rule); therefore, by the divergence theorem it follows that

$$\begin{aligned} & \int_{\Omega} d\mathbf{x} \left[ (\partial^{x^\ell} \partial_{y^\ell} + V(\mathbf{x})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}} = \\ & \int_{\partial\Omega} da(\mathbf{x}) n^\ell(\mathbf{x}) \left[ \partial_{y^\ell} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}} + \int_{\Omega} d\mathbf{x} \left[ (-\Delta_{\mathbf{y}} + V(\mathbf{y})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}}. \end{aligned}$$

In view of this, the thesis follows by simple algebraic computations if we can show that  $(-\Delta_{\mathbf{y}} + V(\mathbf{y})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) = \mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y})$ . Indeed, to prove this fact it suffices to notice that  $(-\Delta_{\mathbf{y}} + V(\mathbf{y})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) = \langle \delta_{\mathbf{x}} | \mathcal{A}^{-\frac{u+1}{2}}(-\Delta_{\mathbf{y}} + V(\mathbf{y})) \delta_{\mathbf{y}} \rangle$  by continuity (see Eq. (2.221)), and to recall that  $\Delta_{\mathbf{y}} \delta_{\mathbf{y}} = \Delta \delta_{\mathbf{y}}$  (compare with Eq. (2.196)), so that  $(-\Delta_{\mathbf{y}} + V(\mathbf{y})) \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) = \langle \delta_{\mathbf{x}} | \mathcal{A}^{-\frac{u+1}{2}} \mathcal{A} \delta_{\mathbf{y}} \rangle$ , which yields the thesis.  $\square$

**Proposition 3.46.** *Assume the hypotheses (3.116) to be fulfilled; then, for any boundary point  $\mathbf{x} \in \partial\Omega$ , the map  $\Sigma_{d+1} \rightarrow \mathbb{C}$ ,  $u \mapsto \mathbf{p}^u(\mathbf{x})$  is (well-defined and) analytic.*

*Proof.* Consider the expression (3.109) giving  $\langle \mathbf{v} | \hat{T}_{ij}^u \mathbf{v} \rangle$  in terms of the Dirichlet kernel and of its derivatives evaluated along the diagonal. By a simple generalization of item i) of Proposition 2.64 it follows that  $\mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$ ,  $\partial_{zw} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  are continuous functions of  $\mathbf{x}$  up to the boundary; moreover, for any fixed  $\mathbf{x} \in \partial\Omega$  the mentioned kernels are analytic functions of  $u$ , for  $u \in \Sigma_{d+1}$ , and the unit outer normal  $\mathbf{n}(\mathbf{x})$  exists. This suffices to infer the thesis.  $\square$



Finally, let us state two results which will turn out to be crucial for the developments to be discussed in the following (in particular, to define a renormalized version of the bulk energy).

**Theorem 3.47.** *Assume the heat trace to fulfill the assumptions of Theorem 2.94 (see, in particular, Eq. (2.362)) for some  $N \in \mathbb{N}$ . Then, the map  $\Sigma_{d+1} \rightarrow \mathbb{C}$ ,  $u \mapsto E^u$  can be analytically continued to a function which is meromorphic on the strip  $\Sigma_{d+1-2N}$  and possesses only possible simple pole singularities at  $u = d + 1 - n$ , for  $n \in \{0, \dots, 2N\}$ . In particular, if  $N > (d + 1)/2$  the mentioned analytic continuation extends to a neighbour of  $u = 0$ .*

*Proof.* Consider the representation (3.120) for the zeta-regularized bulk energy  $E^u$ , in terms of the trace  $\text{Tr} \mathcal{A}^{-\frac{u-1}{2}}$ . Then the thesis follows easily from Theorem 2.94.  $\square$

**Theorem 3.48.** *Assume the cylinder trace to fulfill the assumptions of Theorem 2.96 (see, in particular, Eq. (2.367)). Then, the map  $\Sigma_{d+1} \rightarrow \mathbb{C}$ ,  $u \mapsto E^u$  can be analytically continued to a function which is meromorphic on the whole complex plane and possesses only possible simple pole singularities at  $u = k$ , for  $k \in \{0, \dots, d + 1\}$ .*

*Proof.* Consider once more the representation (3.120) for the zeta-regularized bulk energy  $E^u$ , in terms of the trace  $\text{Tr} \mathcal{A}^{-\frac{u-1}{2}}$ . Then the thesis follows by arguments similar to those employed in the proof of Theorem 3.40, using Theorem 2.96 in place of Theorem 2.94.  $\square$

## Renormalized observables.

Let us consider the zeta-regularized versions of the stress-energy VEV ( $\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}$ ) ( $\mu, \nu \in \{0, \dots, d\}$ ,  $\mathbf{x} \in \Omega$ ), of the vacuum bulk and boundary energies  $E^u$ ,  $B^u$ , and of the vacuum pressure  $\mathbf{p}^u(\mathbf{x})$  ( $\mathbf{x} \in \partial\Omega$ ) introduced in the previous subsection. In view of the results derived therein for these observables (see, in particular, Corollary 3.39 and Propositions 3.44, 3.46), it appears that the mentioned observables are typically analytic functions of  $u$ , for  $\Re u$  sufficiently large (i.e., for  $u \in \Sigma_{d+1}$ ); moreover, they can be analytically continued to wider regions of the complex plane, possibly including a neighbour of the origin, where they are meromorphic and possess only simple pole singularities.

Therefore, in general, we can proceed to define the renormalized versions of the above mentioned zeta-regularized observables following the general (“extended”) approach presented in [64]. To this purpose, let us indicate with  $F(u)$  any one of ( $\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}$ ),  $E^u$ ,  $B^u$ ,  $\mathbf{p}^u(\mathbf{x})$  and state the following definition.

**Definition 3.49.** (*Zeta approach to renormalization*). Assume there exist  $r_1, r_2 \in \mathbb{R}$  with  $r_1 < r_2$  such that the map  $\Sigma_{(r_1, r_2)} \rightarrow \mathbb{C}$ ,  $u \mapsto F(u)$  is analytic; moreover, assume this map to possess an analytic continuation to a function (indicated again with  $F$ ) which is meromorphic on the larger strip  $\Sigma_{(r_-, r_+)} \supset \Sigma_{(r_1, r_2)}$  including the origin ( $0 \in \Sigma_{(r_-, r_+)}$ ). Then, the *renormalized value of  $F$*  is

$$F_{ren} := RP \Big|_{u=0} F(u) , \quad (3.121)$$

where  $RP|_{u=0}$  indicates the evaluation in  $u = 0$  of the regular part of the Laurent expansion centered at the same point.

*Remark 3.30.* i) In order to avoid misunderstandings, let us mention that, for any meromorphic function  $F$  with a pole of order  $N$  ( $N \in \mathbb{N}$ ) at  $u = 0$ , the Laurent expansion centered at the same point ( $u = 0$ ) is

$$F(u) = \sum_{k=-N}^{+\infty} F_k u^k ; \quad (3.122)$$

its regular part is given by  $(RP F)(u) := \sum_{k=0}^{+\infty} F_k u^k$ , so that

$$RP|_{u=0} F(u) = F_0 .$$

ii) Let us stress that the prescription (3.121) is a quite straightforward generalization of the approach considered, e.g., in [22, 56], where  $F$  was assumed to possess a simple pole in  $u = 0$  (i.e., it was assumed that  $N = 1$ ). On the other hand it is apparent that, whenever  $F$  is analytic at  $u = 0$ , the prescription (3.121) reduces to

$$F_{ren} := F(0) , \quad (3.123)$$

which was referred to as “restricted” zeta approach in our previous work [64].

For future reference, let us specify the definition (3.121) for the cases of main interest in the applications.

**Definition 3.50.** Assume the regularized expressions  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$  ( $\mathbf{x} \in \Omega$ ),  $E^u$ ,  $B^u$  and  $\mathbf{p}^u(\mathbf{x})$  ( $\mathbf{x} \in \partial\Omega$ ) to fulfill the assumptions considered in Definition 3.49. Then, we consider the corresponding renormalized versions reported hereafter.

i) For any  $\mathbf{x} \in \Omega$  and  $\mu, \nu \in \{0, \dots, d\}$ , the *renormalized stress-energy VEV* is

$$(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren} := RP|_{u=0} (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) . \quad (3.124)$$

ii) The *renormalized bulk and boundary energies* are, respectively,

$$E^{ren} := RP|_{u=0} E^u , \quad B^{ren} := RP|_{u=0} B^u . \quad (3.125)$$

iii) The *renormalized pressure*, at any point  $\mathbf{x} \in \partial\Omega$  where the outer normal  $\mathbf{n}(\mathbf{x})$  is well defined, is

$$\mathbf{p}^{ren}(\mathbf{x}) := RP|_{u=0} \mathbf{p}^u(\mathbf{x}) . \quad (3.126)$$

*Remark 3.31.* Let us stress that, in particular, whenever the diagonal heat or cylinder kernel derivatives fulfill the hypotheses of Theorem 2.91 (with  $N > (d+1)/2$ ) or of Theorem 2.93, respectively, then Eq. (3.124) is granted to give a finite value for  $(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren}$  in consequence of Theorems 3.40 and 3.41, respectively. On the other hand, Theorems 3.47 and 3.48 show that the renormalized bulk energy  $E^{ren}$  is also finite under suitable hypothesis.

### Conformal and non-conformal parts of the stress-energy tensor.

In the literature [21, 119, 153] it is customary to write the stress-energy tensor (here to be intended as the zeta-regularized operator  $\hat{T}_{\mu\nu}^u$ , its VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  or the renormalized version  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$ ) as the sum of a conformal and a non-conformal part. In order to define these quantities, let us consider for  $\xi$  the critical value

$$\xi_d := \frac{d-1}{4d} . \quad (3.127)$$

*Remark 3.32.* As well-known, when coupling of the scalar field to gravity is taken into account and no external potential is present (for  $V = 0$ ), the theory is invariant under conformal transformations of the spacetime line element if  $\xi$  has the critical value (3.127) (see, e.g., [153], page 447).

In the sequel we adopt systematically the notations

$$\diamond \equiv \text{conformal} , \quad \blacksquare \equiv \text{non-conformal} ; \quad (3.128)$$

in particular, in accordance with them, we give the following definition.

**Definition 3.51.** Consider the renormalized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$ ; its *conformal* and *non-conformal parts* are, respectively,

$$(\mathbf{v} | \hat{T}_{\mu\nu}^{(\diamond)} \mathbf{v})_{ren} := (\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren} \Big|_{\xi=\xi_d} , \quad (3.129)$$

$$(\mathbf{v} | \hat{T}_{\mu\nu}^{(\blacksquare)} \mathbf{v})_{ren} := \frac{1}{\xi - \xi_d} \left( (\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren} - (\mathbf{v} | \hat{T}_{\mu\nu}^{(\diamond)} \mathbf{v})_{ren} \right) . \quad (3.130)$$

*Remark 3.33.* i) Of course, in view of the above definitions, there holds

$$(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren} = (\mathbf{v} | \hat{T}_{\mu\nu}^{(\diamond)} \mathbf{v})_{ren} + (\xi - \xi_d) (\mathbf{v} | \hat{T}_{\mu\nu}^{(\blacksquare)} \mathbf{v})_{ren} . \quad (3.131)$$

ii) In the applications to be considered in the forthcoming Chapter 4, when presenting our final results for the renormalized stress-energy VEV, we will either write them in the form (3.131) or give separately the conformal and non-conformal parts (3.129) (3.130).

### Anomalies.

As we pointed out in our previous work [64], Eq.s (3.125) and (3.126) are not the only reasonable ways to define renormalized versions of the bulk/boundary energies and of the boundary pressure, respectively. For example, starting with the renormalized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$ , one could consider the quite natural alternative definitions described hereafter.

On the one hand, one could define the *renormalized total energy* as

$$\mathcal{E}^{ren} := \int_{\Omega} d\mathbf{x} (\mathbf{v} | \hat{T}_{00}(\mathbf{x}) \mathbf{v})_{ren} \quad (3.132)$$

(in few words: in the approach (3.112)-(3.125), one integrates over the domain  $\Omega$  the regularized energy density and next renormalizes; in the approach (3.132), one first renormalizes the energy density and then integrates it over  $\Omega$ ).

On the other hand, the *renormalized pressure*  $\mathbf{p}^{ren}(\mathbf{x}) \equiv (p_i^{ren}(\mathbf{x}))$  at any boundary point  $\mathbf{x} \in \partial\Omega'$  (see Eq. (3.113)) with outer unit normal  $\mathbf{n}(\mathbf{x})$  could be defined as

$$p_i^{ren}(\mathbf{x}) := \left( \lim_{\mathbf{x}' \in \Omega, \mathbf{x}' \rightarrow \mathbf{x}} (\mathbf{v} | \hat{T}_{ij}(\mathbf{x}') \mathbf{v})_{ren} \right) n^j(\mathbf{x}) \quad (3.133)$$

(in few words: in the approach (3.115)-(3.126), one stays at a point on the boundary, and performs therein the renormalization; in the approach (3.133), one renormalizes at points inside  $\Omega$ , and then moves towards the boundary <sup>(20)</sup>).

Let us recall a fact that we already stressed in [64]: namely, that *the possibilities (3.132) and (3.133) are not granted a priori to be equivalent, respectively, to the definitions (3.125) and (3.126) considered in the previous subsection.* For example, it may happen that the integral in the right-hand side of Eq. (3.132) is divergent, while the prescription (3.125) always gives a finite result by construction (assuming  $\mathcal{E}^u$  can be analytically continued in a neighbour of  $u = 0$ ). Similarly, the renormalized VEV  $(\mathbf{v} | \hat{T}_{ij}(\mathbf{x}') \mathbf{v})_{ren}$  ( $\mathbf{x}' \in \Omega$ ) might have no finite limit for  $\mathbf{x}' \rightarrow \mathbf{x} \in \partial\Omega$ , thus making ill-defined the prescription (3.133) for the renormalized pressure.

As a matter of fact, in our previous series of works [64, 65, 66, 67] we showed with some explicit examples that, in general, the prescriptions (3.132) and (3.133) give infinite results for  $\mathcal{E}^{ren}$  and  $\mathbf{p}^{ren}$  due to the singular behaviours of the renormalized stress-energy VEV near the boundary. In consequence of this, there arise unavoidable ambiguities, or *anomalies*, when talking about these renormalized observables. On the other hand, let us stress that the above mentioned boundary singularities of the renormalized stress-energy VEV are not a specific consequence of the ZR approach which we are considering in the present manuscript; indeed, they also appear if one uses a point-splitting approach, as indicated by the very systematic analysis of Deutsch and Candelas [49].

For the moment, these anomalies must be accepted as a problematic aspect which is common to all the main regularization schemes; what we can do is just to record them when they appear, and hope that in the future they can be better understood. Most probably, their origin should be looked for in some excessive idealization of the physical model. For example, one could try to describe in a more realistic manner the boundaries of the spatial domain; these are “hard” and “deterministic” in the present formulation, but could perhaps be replaced with “soft” or “stochastic” boundaries, following an idea which was first proposed by Ford and Svaiter [70].

To conclude, let us also report a supposition we made in [64]. Therein, motivated by some explicit results derived in our series of papers [64, 65, 66, 67], we advanced the following

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<sup>20</sup>Notice that both the mentioned approaches require the existence of the normal  $\mathbf{n}(\mathbf{x})$ ; therefore, they both lose meaning on the eventual edges and corner points of  $\partial\Omega$ .

conjecture about the pressure anomaly discussed before:

“at points  $\mathbf{x} \in \partial\Omega$  where the normal is well defined and the approach (3.133) gives a finite pressure, the result obtained according to the latter prescription (3.134) agrees with the renormalized pressure defined by Eq. (3.126).”



# Chapter 4

## Some explicitly solvable models

In this conclusive chapter we describe some applications of the abstract framework developed previously in this manuscript; in particular, we analyze some models which can be treated exactly, i.e., without resorting to any perturbative method.

First of all, we briefly report some results obtained in our series of papers [64, 65, 66, 67]: more precisely, we consider the case of a scalar field interacting with a background harmonic potential and that of a field confined within a rectangular box. Next, in Section 4.3 we consider the configuration involving two parallel planes; this model was analyzed in [65] for Dirichlet, Neumann and periodic boundary conditions (we make reference to some of the results obtained for these configurations). In the present work we describe some novel results obtained for a particular subcase which, to the best of our knowledge, was never treated previously by means of zeta techniques: we assume Robin boundary conditions are prescribed on each one of the planes and we compute all the components of the renormalized stress-energy VEV. Our main motivation in the analysis of this configuration is to study the changes arising in the passage from Dirichlet to Neumann boundary conditions in a case which can be solved explicitly; in particular, we are interested in the analysis of the boundary behaviour of the renormalized stress-energy VEV which, as mentioned in subsection 3.2 and exemplified in the forthcoming Sections 4.1 and 4.2, can cause the appearance of anomalies within the physical framework under analysis.

Before moving on, let us stress the following facts.

*Remark 4.1.* In all the settings to be studied in the present chapter, for simplicity, we restrict attention to the case of a massless field; nevertheless, most of the results to be reported in the sequel could be generalized to the case of a massive field, with some additional computational effort. Furthermore, the computational methods we are going to present can be employed for an arbitrary spatial dimension  $d \in \{1, 2, 3, \dots\}$ . As examples, at the end of each section we report the explicit results which can be obtained performing the numerical computations required by the previously mentioned general methods for some specific choice of  $d$ ; we typically fix  $d = 3$  in these computations, for clear physical interest (except for Section 4.2, where we choose  $d = 2$  for simplicity of exposition).

## 4.1 The case with a background harmonic potential.

The configuration under investigation in the present section is that of a scalar quantum field interacting with a background harmonic potential, in arbitrary spatial dimension  $d \in \{1, 2, 3, \dots\}$ . Hereafter, we report some of the results which were derived in our previous work [66], to which we refer for a more detailed analysis; following the cited work, for simplicity, we restrict the attention to the case where the field is *massless* and the background potential is *isotropic*. Nevertheless, our approach could be extended with some computational effort to anisotropic harmonic potentials and to the case of a massive scalar field, as well.

The main result of our analysis is the computation of the renormalized stress-energy VEV, obtained by applying the general framework described in Chapters 2 and 3 (see also [64]) to the present configuration; we also consider the total energy, referring to both bulk and boundary contributions. For all the mentioned observables we derive, by analytic methods, fully explicit integral representations; ultimately, these representation must be computed numerically. However, they can also be used to derive asymptotic expansions (complete with remainder estimates) for the stress-energy VEV components when the radius goes to zero or to infinity.

In subsection 4.1, we report the results obtained using the framework mentioned above and performing the required explicit computations for  $d = 3$ , with the aid of `Mathematica`; in particular, we restrict the attention to the renormalized energy density  $(\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$  and to the renormalized bulk energy  $E^{ren}$ .

Before proceeding, let us mention that the idea to replace sharp boundaries with suitable background potentials is well-known in the literature on the Casimir effect. Typically (see, e.g., [15, 23, 81, 105, 120]), delta-like potentials are introduced in order to mimic boundary conditions in a “physically more realistic” framework; the ultimate purpose is to obtain less singular behaviours of the renormalized quantities, avoiding, e.g., boundary divergences such as the ones mentioned in subsection 3.2 (see also [64, 65]). The case of a scalar field interacting with an external harmonic potential has been formerly considered by Actor and Bender [2, 5], who have determined the renormalized VEV of the total (bulk) energy via global zeta regularization (using ad hoc results on the analytic continuations for the special functions involved in this specific case)<sup>(1)</sup>; as far as we know, the stress-energy tensor has not been previously computed for the present configuration.

### Introducing the problem.

As anticipated previously, we consider the case of a massless scalar field on  $\mathbb{R}^d$  in presence of a classical isotropic harmonic potential. More precisely, we assume

$$\Omega := \mathbb{R}^d, \quad V(\mathbf{x}) := \lambda^4 |\mathbf{x}|^2, \quad (4.1)$$

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<sup>1</sup>In [66] we point out that our results for the renormalized bulk energy agree with the ones of Actor and Bender [5] for  $d \in \{1, 2, 3\}$ .



where  $\lambda > 0$  and  $|\mathbf{x}| := \sqrt{(x^1)^2 + \dots + (x^d)^2}$ ; the constant  $\lambda$  is, dimensionally, a mass (or an inverse length) like the parameter  $\kappa$  employed to define the zeta-regularized Wightman field (see Eq. (3.92) and the related comments). In this case, we put

$$\mathcal{A} := -\Delta + V ; \quad (4.2)$$

this is an *admissible operator* in the sense of definition 2.37 (see page 55). In fact, as well known,  $\mathcal{A}$  is strictly positive and self-adjoint on the single particle Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^d)$ , with admissible domain  $\mathcal{D}_{\mathcal{A}} := \{f \in L^2(\mathbb{R}^d) \mid (-\Delta + V)f \in L^2(\mathbb{R}^d)\}$ . Moreover,  $\mathcal{A}$  has purely discrete spectrum, given by

$$\sigma(\mathcal{A}) = \left\{ \lambda^2 \left( 2(n_1 + \dots + n_d) + d \right) \mid n_i \in \mathbb{N}, i = 1, \dots, d \right\} \quad (4.3)$$

(<sup>2</sup>). In view of the above considerations, we can employ the functional analytic framework developed in Chapter 2 to analyze the present setting; in particular, we can consider the Dirichlet and heat kernels associated to the admissible operator  $\mathcal{A}$ , as well as the related traces.

### The heat kernel and the heat trace.

Notice that the configuration described in Eq. (4.1) is of product type. Therefore, the heat kernel  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  (for  $\mathbf{t} \in \Sigma_0$ ) related to the admissible operator  $\mathcal{A} = -\Delta + V$  (with  $V(\mathbf{x}) = \lambda^4 |\mathbf{x}|^2$ , for  $\mathbf{x} \in \mathbb{R}^d$ ) can be easily determined, starting from the one-dimensional *Mehler kernel* [108] (see also [20, 33, 46, 82]); for any  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ , the final result is [66]

$$e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \left( \frac{\lambda}{\sqrt{2\pi \sinh(2\lambda^2 \mathbf{t})}} \right)^d \exp \left[ -\lambda^2 \left( \frac{|\mathbf{x}|^2 + |\mathbf{y}|^2}{2 \tanh(2\lambda^2 \mathbf{t})} - \frac{\mathbf{x} \cdot \mathbf{y}}{\sinh(2\lambda^2 \mathbf{t})} \right) \right] \quad (4.4)$$

(where  $\mathbf{x} \cdot \mathbf{y} := \sum_{i=1}^d x^i y^i$ ). Moreover, by a slight variation of Proposition 2.74 and of the related Corollary 2.76, it appears that the exponential operator  $e^{-\mathbf{t}\mathcal{A}}$  is of trace class for all  $\mathbf{t} \in \Sigma_0$ ; so, the heat trace  $\text{Tr} e^{-\mathbf{t}\mathcal{A}}$  exists and is finite. It can be proved by simple computations (<sup>3</sup>) that

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} = \left( \frac{1}{2 \sinh(k^2 \mathbf{t})} \right)^d . \quad (4.5)$$

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<sup>2</sup>Note that the parameter  $\varepsilon > 0$ , which is generally chosen so as to fulfill  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ , can be fixed explicitly in the case under analysis, setting  $\varepsilon := \lambda^2 d$ .

<sup>3</sup>Eq. (4.5) can be easily derived as follows, recalling that the spectrum of  $\mathcal{A}$  is given by (4.3):

$$\text{Tr} e^{-\mathbf{t}\mathcal{A}} = \sum_{n_1, \dots, n_d \in \mathbb{N}} e^{-\mathbf{t}\lambda^2(2(n_1 + \dots + n_d) + d)} = e^{-\mathbf{t}\lambda^2 d} \left( \sum_{n=0}^{+\infty} e^{-\mathbf{t}\lambda^2 n} \right)^d = \frac{e^{-\mathbf{t}\lambda^2 d}}{(1 - e^{-\mathbf{t}\lambda^2})^d} = \left( \frac{1}{2 \sinh(k^2 \mathbf{t})} \right)^d .$$

For an alternative derivation, using the explicit expression (4.4) of the heat kernel, see [66], page 8, footnote 4.

**Rescaled spherical coordinates.**

Next, notice that the configuration (4.1) is patently spherically symmetric; therefore, it is natural to pass to a set of curvilinear coordinates which best fit the symmetries of the problem. To this purpose, we introduce the spherical “ $\lambda$ -rescaled” coordinates

$$\mathbf{x} \mapsto \mathbf{q}(\mathbf{x}) \equiv (r(\mathbf{x}), \theta_1(\mathbf{x}), \dots, \theta_{d-2}(\mathbf{x}), \theta_{d-1}(\mathbf{x})) \in (0, +\infty) \times (0, \pi) \times \dots \times (0, \pi) \times (0, 2\pi) \quad (4.6)$$

whose inverse map  $\mathbf{q} \mapsto \mathbf{x}(\mathbf{q})$  is described by the equations

$$\begin{aligned} \lambda x^1 &= r \cos(\theta_1) , \\ \lambda x^2 &= r \sin(\theta_1) \cos(\theta_2) , \\ &\vdots \\ \lambda x^{d-1} &= r \sin(\theta_1) \dots \sin(\theta_{d-2}) \cos(\theta_{d-1}) , \\ \lambda x^d &= r \sin(\theta_1) \dots \sin(\theta_{d-1}) . \end{aligned} \quad (4.7)$$

Let us stress that, for any spatial dimension  $d$ , there holds

$$r = \lambda |\mathbf{x}| ; \quad (4.8)$$

thus, the coordinate  $r$  is an adimensional radius.

In order to avoid cumbersome notations, given a function  $\mathbb{R}^d \rightarrow Y$ ,  $\mathbf{x} \mapsto f(\mathbf{x})$  (with  $Y$  any set), we indicate the composition  $\mathbf{q} \mapsto f(\mathbf{x}(\mathbf{q}))$  as  $\mathbf{q} \mapsto f(\mathbf{q})$ ; we will use similar conventions for functions on  $\mathbb{R}^d \times \mathbb{R}^d$ .

Of course, the curvilinear coordinates  $\mathbf{q}$  induce a set of spacetime coordinates  $q \equiv (q^\mu) \equiv (t, \mathbf{q})$ . The spatial and space-time line elements are, respectively,

$$\begin{aligned} dl^2 &= a_{ij}(\mathbf{q}) dq^i dq^j ; & ds^2 &= -dt^2 + dl^2 = g_{\mu\nu}(q) dq^\mu dq^\nu , \\ g_{00} &:= -1 , & g_{i0} = g_{0i} &:= 0 , & g_{ij}(q) &:= a_{ij}(\mathbf{q}) \quad \text{for } i, j \in \{r, \theta_1, \dots, \theta_{d-1}\} , \end{aligned} \quad (4.9)$$

where  $a_{ij}$  indicates the flat metric on  $\mathbb{R}^d$  expressed in the curvilinear coordinates  $\mathbf{q}$ . Most results of the previous Chapters 1-3 are readily rephrased in the present framework; in particular, the analogue of Eq. (3.103) in the coordinate system  $(q^\mu)$  is

$$\hat{T}_{\mu\nu}^u := (1 - 2\xi) \partial_\mu \hat{\varphi}^u \circ \partial_\nu \hat{\varphi}^u - \left( \frac{1}{2} - 2\xi \right) \eta_{\mu\nu} (\partial^\rho \hat{\varphi}^u \partial_\rho \hat{\varphi}^u + V(\hat{\varphi}^u)^2) - 2\xi \hat{\varphi}^u \circ \nabla_{\mu\nu} \hat{\varphi}^u , \quad (4.10)$$

where  $\nabla_\mu$  denotes the covariant derivative induced by the metric (4.9). Notice that, indicating with  $\gamma_{ij}^k$  the Christoffel symbols for the spatial metric  $(a_{ij}(\mathbf{q}))$  and with  $D_i$  the corresponding covariant derivative, for any scalar function  $f$  there hold  $(i, j \in \{r, \theta_1, \dots, \theta_{d-1}\})$

$$\begin{aligned} \nabla_\mu f &= \partial_\mu f , & \nabla_{ij} f &= D_{ij} f = \partial_{ij} f - \gamma_{ij}^k \partial_k f , \\ \nabla_{0i} f &= \partial_0(\partial_i f) = \partial_i(\partial_0 f) = \nabla_{i0} f , & \nabla_{00} f &= \partial_{00} f . \end{aligned} \quad (4.11)$$

Before proceeding, let us also point out that, in view of the explicit expressions (4.4) and (4.5) for the heat kernel and trace, respectively, it is natural to introduce the rescaled parameter

$$\tau := \lambda^2 \mathbf{t} \in (0, +\infty) . \quad (4.12)$$

In the sequel, for any pair

$$\mathbf{q} = (r, \theta_1, \dots, \theta_{d-1}) \equiv (r, \boldsymbol{\theta}) , \quad \mathbf{p} = (r', \theta'_1, \dots, \theta'_{d-1}) \equiv (r', \boldsymbol{\theta}') , \quad (4.13)$$

we write  $\mathcal{A}^{-s}(\mathbf{q}, \mathbf{p})$  and  $e^{-\tau\mathcal{A}}(\mathbf{q}, \mathbf{p})$ , respectively, for the Dirichlet and heat kernels at two points  $\mathbf{x}, \mathbf{y}$  of (rescaled) spherical coordinates  $\mathbf{q}, \mathbf{p}$ , and with  $\tau$  related to  $\mathbf{t}$  by Eq. (4.12). In particular, Eq. (4.4) implies

$$e^{-\tau\mathcal{A}}(\mathbf{q}, \mathbf{p}) = \left( \frac{\lambda}{\sqrt{2\pi \sinh(2\tau)}} \right)^d \exp \left[ - \left( \frac{r^2 + r'^2}{2 \tanh(2\tau)} - \frac{r r' S(\boldsymbol{\theta}) S(\boldsymbol{\theta}')}{\sinh(2\tau)} \right) \right] \quad (4.14)$$

where  $S(\boldsymbol{\theta})$  and  $S(\boldsymbol{\theta}')$  are the products of cosines and sines of the angular coordinates  $(\theta_1, \dots, \theta_{d-1})$  and  $(\theta'_1, \dots, \theta'_{d-1})$  of Eq. (4.13), corresponding to the scalar product  $\mathbf{x} \cdot \mathbf{y}$ .

### The zeta-regularized stress-energy VEV.

Hereafter we are going to derive integral representations for the regularized stress-energy VEV components, using the ‘‘rescaled’’ heat kernel  $e^{-\tau\mathcal{A}}(\mathbf{q}, \mathbf{p})$  (of Eq. (4.14)). To this purpose, let us first point out that the Mellin relation (2.266) can be rephrased in the present setting as

$$\mathcal{A}^{-s}(\mathbf{q}, \mathbf{p}) = \frac{\lambda^{-2s}}{\Gamma(s)} \int_0^{+\infty} d\tau \tau^{s-1} e^{-\tau\mathcal{A}}(\mathbf{q}, \mathbf{p}) , \quad (4.15)$$

along with analogous relations for its (covariant) derivatives.

Next notice that, starting from Eq. (4.10), expressions analogous to those in Eq.s (3.107-3.109) can be derived for  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  in terms of the Dirichlet kernel and of its derivatives in curvilinear coordinates. Using these expressions for the zeta-regularized stress-energy VEV along with Eq. (4.15) and the corresponding ones for the derivatives of  $\mathcal{A}^{-s}(\cdot, \cdot)$ , it follows that

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v}) = \frac{\lambda^{d+1}}{\Gamma(\frac{u+1}{2})} \left( \frac{\kappa}{\lambda} \right)^u \int_0^{+\infty} d\tau \tau^{\frac{u-d-3}{2}} \mathbf{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}) \quad (\mu, \nu \in \{0, r, \theta_1, \dots, \theta_{d-1}\}) \quad (4.16)$$

where the coefficients  $\mathbf{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$  are as follows (for  $i, j, h, \ell \in \{r, \theta_1, \dots, \theta_{d-1}\}$ ; here  $D$  is the spatial covariant derivative of Eq. (4.11)):

$$\mathbf{H}_{00}^{(u)}(\tau; \mathbf{q}) := \left( \frac{\tau}{\lambda^2} \right)^{d/2} \left[ \left( \frac{1}{4} + \xi \right) \left( \frac{u-1}{2} \right) + \left( \frac{1}{4} - \xi \right) \tau \left( a^{h\ell}(\mathbf{q}) D_{q^h p^\ell} + r^2 \right) \right] \Big|_{\mathbf{p}=\mathbf{q}} e^{-\tau\mathcal{A}}(\mathbf{q}, \mathbf{p}) , \quad (4.17)$$

$$\mathbf{H}_{0i}^{(u)}(\tau; \mathbf{q}) = \mathbf{H}_{i0}^{(u)}(\tau; \mathbf{q}) := 0 , \quad (4.18)$$

$$\begin{aligned}
\mathbb{H}_{ij}^{(u)}(\tau; \mathbf{q}) &= \mathbb{H}_{ji}^{(u)}(\tau; \mathbf{q}) := \\
\left(\frac{\tau}{\lambda^2}\right)^{d/2} &\left[ \left(\frac{1}{4} - \xi\right) a_{ij}(\mathbf{q}) \left(\frac{u-1}{2} - \tau \left(a^{h\ell}(\mathbf{q}) D_{q^h p^\ell} + r^2\right)\right) + \right. \\
&\left. + \left(\frac{\tau}{\lambda^2}\right) \left(\left(\frac{1}{2} - \xi\right) D_{q^i p^j} - \xi D_{q^i q^j}\right) \right] \Bigg|_{\mathbf{p}=\mathbf{q}} e^{-\tau \mathcal{A}}(\mathbf{q}, \mathbf{p}) .
\end{aligned} \tag{4.19}$$

Here and in the remainder of this section, we are implicitly understanding the dependence on the parameter  $\xi$  for simplicity of notation: so,  $\mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$  stands for  $\mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}; \xi)$ . Using the explicit expression (4.14) for the heat kernel in rescaled spherical coordinates, one can infer the following notable properties i)-v) of the coefficients  $\mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$ ; these properties could be proved for arbitrary  $d$  (in [66] we checked them by explicit computations in the cases  $d \in \{1, 2, 3\}$ ).

- i) For any fixed  $\tau, \mathbf{q}$  and any  $\mu, \nu \in \{0, r, \theta_1, \dots, \theta_{d-1}\}$ , the map  $u \mapsto \mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$  is affine.
- ii) For any fixed  $\mathbf{q}, u \in \mathbb{C}$  and any  $\mu, \nu \in \{0, r, \theta_1, \dots, \theta_{d-1}\}$ , the map  $\tau \mapsto \mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$  is smooth (i.e., of class  $C^\infty$ ) on  $[0, +\infty)$  and exponentially vanishing for  $\tau \rightarrow +\infty$ .
- iii) The final expressions for the coefficients  $\mathbb{H}_{\mu\nu}^{(u)}$  do not depend on the parameter  $\lambda$ , even though it appears in the right-hand sides of Eq.s (4.17-4.19).
- iv) There holds

$$\begin{aligned}
\mathbb{H}_{\mu\nu}^{(u)} &= 0 \quad \text{for } \mu \neq \nu , \\
\mathbb{H}_{\theta_{d-1}\theta_{d-1}}^{(u)} &= \sin^2(\theta_{d-2}) \mathbb{H}_{\theta_{d-2}\theta_{d-2}}^{(u)} = \dots = \sin^2(\theta_{d-2}) \dots \sin^2(\theta_1) \mathbb{H}_{\theta_1\theta_1}^{(u)} .
\end{aligned} \tag{4.20}$$

- v) For  $\mu = \nu \in \{0, r, \theta_1\}$ , there hold

$$\mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}) = e^{-r^2 \tanh \tau} \mathcal{M}_{\mu\nu}^{(u)}(\tau; r) \tag{4.21}$$

where  $\mathcal{M}_{\mu\nu}^{(u)}(\tau; r)$  is a polynomial in  $r, u$  of degree 1 in both these variables, with coefficients depending smoothly on  $\tau$ .

Before moving on, let us make a few remarks concerning the integral representation (4.16) for the regularized stress-energy VEV. First notice that, in consequence of item iii) above, this VEV only depends on the parameter  $\lambda$  through the multiplicative coefficient  $\lambda^{d+1}(\kappa/\lambda)^u$  in front of the integral in the cited equation. On the other hand, Eq. (4.20) of point iv) indicates that the VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  is diagonal and that the only independent components are those with  $\mu = \nu \in \{0, r, \theta_1\}$ ; finally, these components only depend on the radial coordinate  $r$  (and not on the angular ones  $\{\theta_1, \dots, \theta_{d-1}\}$ ), in accordance with the spherical symmetry of the configuration under analysis.

### Analytic continuation.

Let us move on to determine the analytic continuation of the regularized stress-energy VEV. To this purpose, consider the integral representation (4.16) of  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  along with the general framework of subsection 2.8, where several methods are proposed to construct

the analytic continuation of Mellin transforms. In particular, Proposition 2.88 can be employed in the case under analysis, setting  $F = \mathbb{H}_{\mu\nu}^{(u)}(\cdot; \mathbf{x})$  and  $s = (u - d - 1)/2$ ; this allows to infer (compare with Eq. (2.336)), for any  $N \in \mathbb{N}$ ,

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v}) = \frac{\lambda^{d+1}}{\Gamma(\frac{u+1}{2})} \frac{(-1)^N}{(\frac{u-d-1}{2}) \dots (\frac{u-d-1}{2} + N - 1)} \left(\frac{\kappa}{\lambda}\right)^u \int_0^{+\infty} d\tau \tau^{\frac{u-d-3}{2} + N} \partial_\tau^N \mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}). \quad (4.22)$$

Due to the features of the coefficients  $\mathbb{H}_{\mu\nu}^{(u)}$  pointed out in the previous subsection, the integral in the above expression converges for  $u \in \Sigma_{d+1-2N}$ , so that Eq. (4.22) yields the required analytic continuation of  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  to the very same region; this region includes the value  $u = 0$ , required for the zeta approach to renormalization (see Eq. (3.124)), whenever

$$N > \frac{d+1}{2}. \quad (4.23)$$

Under this assumption, following Eq. (3.124), in general we define

$$(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{q}) \mathbf{v})_{ren} := RP \Big|_{u=0} (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v}). \quad (4.24)$$

For  $N$  as in Eq. (4.23), consider the expression in the second line of Eq. (4.22); for any even spatial dimension  $d$  this expression is regular in  $u = 0$ , so that we can simply evaluate  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v})$  at this point to obtain the renormalized stress-energy VEV. On the other hand, for odd  $d$  we must in fact discard a singular contribution in the Laurent expansion at  $u = 0$ , since the function under analysis has a simple pole in  $u = 0$ . Because of this pole singularity, the procedure of evaluating the regular part of Eq. (4.22) in  $u = 0$  in the case of odd  $d$  implies the appearance of a logarithmic term in  $\tau$  in the integrand<sup>(4)</sup>.

Simple but rather lengthy computations give the following results, for  $d$  either odd or even and  $\mu, \nu \in \{0, r, \theta_1\}$ :

$$\begin{aligned} (\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{q}) \mathbf{v})_{ren} &= \lambda^{d+1} \left( T_{\mu\nu}^{(0)}(r) + M_{\kappa,\lambda} T_{\mu\nu}^{(1)}(r) \right), \quad \text{where} \\ T_{\mu\nu}^{(0)}(r) &:= \int_0^{+\infty} d\tau \tau^{N-\frac{d+3}{2}} e^{-r^2 \tanh \tau} \left[ \mathcal{P}_{\mu\nu}^{(0)}(\tau; r) + \ln \tau \mathcal{P}_{\mu\nu}^{(1)}(\tau; r) \right], \\ T_{\mu\nu}^{(1)}(r) &:= \int_0^{+\infty} d\tau \tau^{N-\frac{d+3}{2}} e^{-r^2 \tanh \tau} \mathcal{P}_{\mu\nu}^{(1)}(\tau; r), \quad M_{\kappa,\lambda} := \gamma_{EM} + 2 \ln \left( \frac{2\kappa}{\lambda} \right) \end{aligned} \quad (4.25)$$

<sup>4</sup>In fact

$$\tau^{u/2} = e^{\frac{u}{2} \ln \tau} = 1 + \frac{u}{2} \ln \tau + O(u^2) \quad \text{for } u \rightarrow 0.$$

The logarithmic term proportional to  $u$  is not relevant in the case of even  $d$ , where analytic continuation exists up to  $u = 0$  and it is simply obtained setting  $u = 0$  in (4.22). On the contrary, for odd  $d$  we must take the regular part at  $u = 0$  of the expression (4.22) and the above term  $\frac{u}{2} \ln \tau$  contributes to it, since it is multiplied by a term proportional to  $1/u$  that comes from the  $u \rightarrow 0$  expansion of the factor  $1/(\frac{u-d-3}{2}+1) \dots (\frac{u-d-3}{2}+N)$  in (4.22).

( $\gamma_{EM} \simeq 0.577$  is the Euler-Mascheroni constant). In the above definitions  $\mathcal{P}_{\mu\nu}^{(0)}(\tau; r)$  and  $\mathcal{P}_{\mu\nu}^{(1)}(\tau; r)$  are suitable functions determined by  $\mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q})$ ; these functions are in fact polynomials in  $r^2$  of order  $N + 1$ , with coefficients which are smooth functions of  $\tau$  on  $[0, +\infty)$ . Let us stress that

$$\mathcal{P}_{\mu\nu}^{(1)}(\tau; r) = 0 \quad \text{and} \quad T_{\mu\nu}^{(1)}(r) = 0 \quad \text{for } d \text{ even ,} \quad (4.26)$$

a fact corresponding to the previous comments on the logarithmic terms.

Next note that, in consequence of the remarks at the end of subsection 4.1, the renormalized VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$  only depends on the parameter  $\lambda$  through the coefficients  $\lambda^{d+1}$  and  $M_{\kappa, \lambda}$  in the first equation of (4.25). In particular, the functions  $T_{\mu\nu}^{(a)}(r)$  ( $a \in \{0, 1\}$ ) introduced therein do not depend on  $\lambda$  and we can evaluate them computing the integrals in Eq. (4.25) numerically, for any fixed  $r \in (0, +\infty)$ . In fact, the same integrals can also be used to derive explicit expressions (complete with remainder estimates) for the asymptotic expansions of  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$  in the limits  $r \rightarrow 0^+$  and  $r \rightarrow +\infty$ . We refer to [66] for more details on this topic; in the present manuscript we only report the final results which can be obtained for  $d = 3$  (see the conclusive paragraph of the present section).

To conclude, following Definition 3.51 <sup>(5)</sup>, we introduce the conformal and non-conformal parts of the functions  $r \mapsto T_{\mu\nu}^{(0)}(r), T_{\mu\nu}^{(1)}(r)$ , setting

$$T_{\mu\nu}^{(a, \diamond)} := T_{\mu\nu}^{(a)} \Big|_{\xi=\xi_d}, \quad T_{\mu\nu}^{(a, \blacksquare)} := \frac{1}{\xi - \xi_d} \left( T_{\mu\nu}^{(a)} - T_{\mu\nu}^{(a, \diamond)} \right) \quad (a \in \{0, 1\}) \quad (4.27)$$

where  $\xi_d$  is defined by Eq. (3.127). In the final paragraph we present the functions  $\mathcal{P}_{00}^{(a)}$  ( $a \in \{0, 1\}$ ) and the graphs (obtained via numerical integration) for the functions in Eq. (4.27) corresponding to the energy density ( $\mu = \nu = 0$ ), for  $d = 3$ .

### The total energy.

First note that, by a simple variation of Proposition 3.45, the total energy can be expressed as the sum of a bulk and a boundary contribution as in Eq.s (3.117-3.119); in the following we are going to discuss these two contributions separately.

Let us first consider the *regularized bulk energy*; according to Eq. (3.120), this can be expressed as

$$E^u = \frac{\kappa^u}{2} \text{Tr } \mathcal{A}^{-\frac{u-1}{2}} .$$

The trace appearing in the above equation is connected through Eq. (2.297) to the heat trace which, according to Eq. (4.5), has the form

$$\text{Tr } e^{-\mathbf{t}\mathcal{A}} = \frac{1}{\mathbf{t}^d} H(\mathbf{t}) \quad \text{with} \quad H(\mathbf{t}) := \left( \frac{\mathbf{t}}{2 \sinh(k^2 \mathbf{t})} \right)^d ; \quad (4.28)$$

<sup>5</sup>In particular, recall that the following convention is employed:

$\diamond \equiv$  conformal ,  $\blacksquare \equiv$  non-conformal .

it is patent that the map  $\mathbf{t} \mapsto H(\mathbf{t})$  is smooth on  $[0, +\infty)$  and exponentially vanishing for  $\mathbf{t} \rightarrow +\infty$ . Then, using Theorem 2.95, we obtain for the regularized bulk energy

$$E^u = \frac{(-1)^N \kappa^u}{2 \Gamma(\frac{u-1}{2})(\frac{u-1}{2}-d)\dots(\frac{u-1}{2}-d+N-1)} \int_0^{+\infty} dt \mathbf{t}^{\frac{u-3}{2}-d+N} \frac{d^N}{dt^N} H(\mathbf{t}) . \quad (4.29)$$

The above relation holds for any  $N \in \{1, 2, 3, \dots\}$  and the integral appearing therein converges for any complex  $u \in \Sigma_{2(d-N)+1}$ ; thus, for any integer  $N > d + 1/2$ , Eq. (4.29) gives the analytic continuation of  $E^u$  in a neighborhood of  $u = 0$ . Since here no singularity appears, we can obtain the renormalized bulk energy simply by setting  $u = 0$  in Eq. (4.29); making again the change of integration variable  $\tau := k^2 \mathbf{t}$  (see Eq. (4.12)), we infer

$$E^{ren} = -\frac{k}{2^{d+2-N} \sqrt{\pi}} \left( \prod_{i=0}^{N-1} \frac{1}{2(d-i)+1} \right) \int_0^{+\infty} d\tau \tau^{N-d-\frac{3}{2}} \frac{d^N}{d\tau^N} \mathbf{H}(\tau) \quad (4.30)$$

for any  $N > d + \frac{1}{2}$ , with  $\mathbf{H}(\tau) := \left( \frac{\tau}{\sinh \tau} \right)^d$ .

Now, let us move on to discuss the *boundary energy*  $\mathcal{B}^u$ . This can be defined, according to Eq. (3.119); however, since the spatial domain is  $\mathbb{R}^d$ , the integral over the boundary appearing therein must be properly interpreted as the limit of integrals over the boundary of suitable, bounded subdomains. By quite lengthy computations (see [66]), this procedure allows to infer that  $\mathcal{B}^u = 0$  for all  $u \in \Sigma_{d-3}$ . Therefore, the zeta approach implies that the renormalized boundary energy vanishes identically:

$$B^{ren} := B^u \Big|_{u=0} = 0 . \quad (4.31)$$

*A remark.* Before proceeding, let us point out a fact that we anticipated in subsection 3.2: the renormalized total energy  $\mathcal{E}^{ren}$  (which, due to Eq. (4.31), in the present setting is equal to  $E^{ren}$ ) does not coincide with the integral  $\int_{\mathbb{R}^d} (\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$ . This fact is patently exemplified by the results to be reported in the subsequent paragraph, dealing with a scalar field in presence of an isotropic harmonic potential in spatial dimension  $d = 3$ . Indeed, on the one hand, the forthcoming Eq. (4.46) states that the renormalized total energy  $\mathcal{E}^{ren} = E^{ren}$  is finite; on the other hand, Eq. (4.45) (along with Eq. (4.40)) shows that  $(\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$  diverges in a non-integrable way for  $|\mathbf{x}| (= r/k) \rightarrow +\infty$ . Let us stress that the “energy anomaly”  $\mathcal{E}^{ren} \neq \int (\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$  is not a consequence of some ultraviolet issue specific to the present setting: in fact, it also appears in configurations involving bounded spatial domains (such as the one discussed in the subsequent Section 4.2).

### The previous results in spatial dimension $d = 3$ .

Hereafter we are going to report the results which can be obtained using the general approach presented in the previous paragraphs for the case of spatial dimension  $d = 3$ . We describe this setting using the spherical coordinates  $\mathbf{q} = (r, \theta_1, \theta_2) \in (0, +\infty) \times (0, \pi) \times$

$[0, 2\pi)$ , which are related to the Cartesian coordinates  $\mathbf{x} \equiv (x_1, x_2, x_3) \in \mathbb{R}^3$  via (see Eq. (4.7))

$$\lambda x^1 = r \cos \theta_1, \quad \lambda x^2 = r \sin \theta_1 \cos \theta_2, \quad \lambda x^3 = r \sin \theta_1 \sin \theta_2; \quad (4.32)$$

the corresponding spatial line element is

$$d\ell^2 = \lambda^{-2}(dr^2 + r^2(d\theta_1^2 + \sin^2\theta_1 d\theta_2^2)). \quad (4.33)$$

After lengthy computations, the zeta-regularized stress-energy VEV can be expressed as (compare with Eq. (4.16) and recall that dependence on  $\xi$  is understood implicitly)

$$\langle \mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v} \rangle = \frac{\lambda^4}{\Gamma(\frac{u+1}{2})} \left(\frac{\kappa}{\lambda}\right)^u \int_0^{+\infty} d\tau \tau^{-3+\frac{u}{2}} \mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}) \quad (\mu, \nu \in \{0, r, \theta_1, \theta_2\}), \quad (4.34)$$

where  $\mathbb{H}_{\mu\nu}^{(u)}$  is diagonal and we only have to consider the independent components

$$\begin{aligned} & \mathbb{H}_{00}^{(u)}(\tau; \mathbf{q}) := \\ & A_3(\tau, r) \left[ -(1-u)(1+4\xi) + (1-4\xi) \left( \frac{2\tau}{\sinh 2\tau} \right) \left( 3 + r^2 \frac{\sinh 3\tau - \sinh \tau}{\cosh \tau} \right) \right], \end{aligned} \quad (4.35)$$

$$\begin{aligned} & \mathbb{H}_{rr}^{(u)}(\tau; \mathbf{q}) := \\ & A_3(\tau, r) \left[ 8\xi \frac{\tau}{\tanh \tau} - (1-4\xi) \left( 1-u + \left( \frac{2\tau}{\sinh 2\tau} \right) \left( 1+2r^2 \tanh \tau \right) \right) \right], \end{aligned} \quad (4.36)$$

$$\begin{aligned} & \mathbb{H}_{\theta_1\theta_1}^{(u)}(\tau; \mathbf{q}) := \\ & \left( \frac{r}{\lambda} \right)^2 A_3(\tau, r) \left[ 8\xi \frac{\tau}{\tanh \tau} - (1-4\xi) \left( 1-u + \left( \frac{2\tau}{\sinh 2\tau} \right) \left( 1 + \frac{r^2}{\cosh^2 2\tau} \right) \right) \right] \end{aligned} \quad (4.37)$$

(for the remaining diagonal component, i.e.  $\mathbb{H}_{\theta_2\theta_2}^{(u)}(\tau; \mathbf{q})$ , see Eq. (4.20)). In the above, for simplicity of notation we have put

$$A_3(\tau, r) := \frac{1}{64 \pi^{3/2}} e^{-r^2 \tanh \tau} \left( \frac{2\tau}{\sinh 2\tau} \right)^{3/2}. \quad (4.38)$$

The above expressions for the components of the tensor  $\mathbb{H}_{\mu\nu}^{(u)}$  are easily seen to possess the features anticipated in Eq.s (4.20) (4.21) and in the related comments. Thus, according to the general framework developed in subsection 4.1, we can obtain the analytic continuation of  $\langle \mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v} \rangle$  given in Eq. (4.34) integrating by parts  $N$  times the integral appearing therein, for any  $N > 2$  (see Eq. (4.23)). For definiteness, we fix  $N = 3$  so that Eq. (4.22) reads

$$\langle \mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{q}) \mathbf{v} \rangle = - \frac{\lambda^4}{\Gamma(\frac{u+1}{2})} \frac{1}{(\frac{u}{2}-2)(\frac{u}{2}-1)\frac{u}{2}} \left(\frac{\kappa}{\lambda}\right)^u \int_0^{+\infty} d\tau \tau^{\frac{u}{2}} \partial_\tau^3 \mathbb{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}). \quad (4.39)$$



As in all cases with odd spatial dimension, the analytic continuation of the regularized stress-energy VEV given in Eq. (4.39) has a simple pole in  $u = 0$  (recall the comments made in subsection 4.1). In consequence of this, we have to adopt the extended version of the zeta approach to define the renormalized VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$ , taking the regular part in  $u = 0$  of Eq. (4.39) (see Eq. (4.24)); with some effort, we obtain

$$\begin{aligned} (\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{q}) \mathbf{v})_{ren} &= \lambda^4 \left( T_{\mu\nu}^{(0)}(r) + M_{\kappa,\lambda} T_{\mu\nu}^{(1)}(r) \right), \\ T_{\mu\nu}^{(0)}(r) &:= \int_0^{+\infty} d\tau e^{-r^2 \tanh \tau} \left[ \mathcal{P}_{\mu\nu}^{(0)}(\tau; r) + \ln \tau \mathcal{P}_{\mu\nu}^{(1)}(\tau; r) \right], \\ T_{\mu\nu}^{(1)}(r) &:= \int_0^{+\infty} d\tau e^{-r^2 \tanh \tau} \mathcal{P}_{\mu\nu}^{(1)}(\tau; r), \quad M_{\kappa,\lambda} := \gamma_{EM} + 2 \ln \left( \frac{2\mu}{\lambda} \right), \end{aligned} \quad (4.40)$$

where

$$\begin{aligned} \mathcal{P}_{\mu\nu}^{(0)}(\tau; r) &:= -\frac{1}{4\sqrt{\pi}} e^{r^2 \tanh \tau} \left[ 3 \partial_\tau^3 \mathbf{H}_{\mu\nu}^{(0)}(\tau; \mathbf{q}) + 4 \partial_u \Big|_{u=0} \partial_\tau^3 \mathbf{H}_{\mu\nu}^{(u)}(\tau; \mathbf{q}) \right], \\ \mathcal{P}_{\mu\nu}^{(1)}(\tau; r) &:= -\frac{1}{2\sqrt{\pi}} e^{r^2 \tanh \tau} \partial_\tau^3 \mathbf{H}_{\mu\nu}^{(0)}(\tau; \mathbf{q}). \end{aligned} \quad (4.41)$$

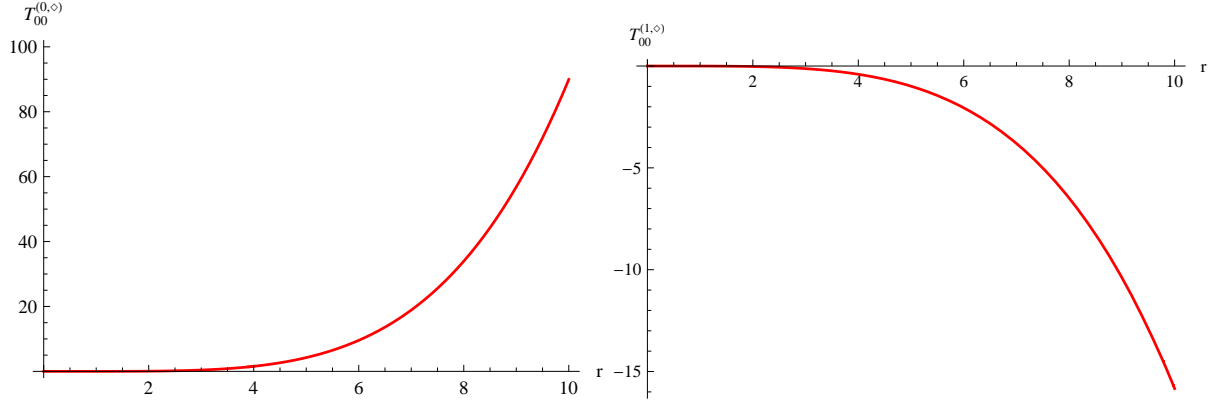
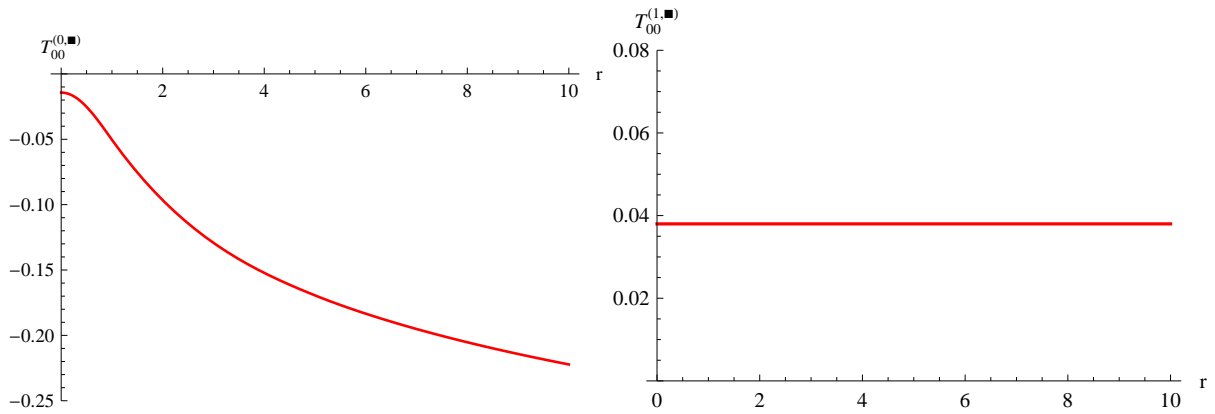
It is readily found that  $\mathcal{P}_{\mu\nu}^{(0)}$ ,  $\mathcal{P}_{\mu\nu}^{(1)}$  are polynomials of fourth order in  $r^2$ . Now, we evaluate numerically the integrals in Eq. (4.40) and distinguish between the conformal and non-conformal parts  $\diamond$ ,  $\blacksquare$  of each component; once more we refer to Eq. (4.27), recalling that for  $d = 3$  we have (see Eq. (3.131))

$$\xi_3 = \frac{1}{6}. \quad (4.42)$$

The forthcoming Figs 4.1 and 4.2 show, as examples, the graphs of the functions determining the renormalized energy density  $(\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$ , i.e.,

$$r \mapsto T_{00}^{(0,\diamond)}(r), T_{00}^{(1,\diamond)}(r), T_{00}^{(0,\blacksquare)}(r), T_{00}^{(1,\blacksquare)}(r). \quad (4.43)$$

We refer to [66] for the graphs of the other components.

Figure 4.1: Graphs of  $T_{00}^{(0, \diamond)}$  and  $T_{00}^{(1, \diamond)}$  ( $d = 3$ ).Figure 4.2: Graphs of  $T_{00}^{(0, \blacksquare)}$  and  $T_{00}^{(1, \blacksquare)}$  ( $d = 3$ ).

In the following we report the asymptotic expansions of the functions in Eq. (4.43) in the limit of small and large values of the radial coordinate  $r$ ; these expansions can be obtained starting from the integral representations (4.40) (see [66] for more details).

On the one hand, for  $r = \lambda|\mathbf{x}| \rightarrow 0^+$  there hold

$$\begin{aligned}
 T_{00}^{(0, \diamond)}(r) &= -0.0047 - 0.0024 r^2 + 0.0028 r^4 + 0.0006 r^6 - 0.0001 r^8 + O(r^{10}) , \\
 T_{00}^{(1, \diamond)}(r) &= -0.0016 r^4 + O(r^{10}) , \\
 T_{00}^{(0, \blacksquare)}(r) &= -0.0143 - 0.0468 r^2 + 0.0134 r^4 - 0.0033 r^6 + 0.0007 r^8 + O(r^{10}) , \\
 T_{00}^{(1, \blacksquare)}(r) &= 0.0380 + O(r^{10}) .
 \end{aligned} \tag{4.44}$$

Let us stress that, using the methods described in [66], all the coefficients in the above expansions could be determined explicitly, complete with quantitative remainder estimates. However the expressions involved are quite cumbersome; for this reason, we have reported here only the first four digits of their numerical evaluation.

On the other hand, in the limit  $r = \lambda|\mathbf{x}| \rightarrow +\infty$ , the following asymptotics can be inferred:

$$\begin{aligned}
T_{00}^{(0,\diamond)}(r) &= \frac{r^4}{64\pi^2} \left( \ln r^2 + \gamma_{EM} + \frac{1}{2} \right) - \frac{5}{96\pi^2} - \frac{23}{2880\pi^2 r^4} + O(r^{-8} \ln r^2) , \\
T_{00}^{(1,\diamond)}(r) &= -\frac{r^4}{64\pi^2} + O(r^{-8} \ln r^2) , \\
T_{00}^{(0,\blacksquare)}(r) &= -\frac{3}{8\pi^2} \left( \ln r^2 + \gamma_{EM} + \frac{2}{3} \right) + \frac{1}{12\pi^2 r^4} + O(r^{-8} \ln r^2) , \\
T_{00}^{(1,\blacksquare)}(r) &= \frac{3}{8\pi^2} + O(r^{-8} \ln r^2) .
\end{aligned} \tag{4.45}$$

In passing, let us point out that the asymptotic expansions in Eq.s (4.44), (4.45) and the corresponding graph in Figure 4.2 suggest that the function  $T_{00}^{(1,\blacksquare)}$  is, in fact, constant (notice that  $3/8\pi^2 \simeq 0.0380\dots$ ).

Finally, Eq. (4.30) with  $N = 4$  and numerical evaluation of the corresponding integral allow us to derive the renormalized bulk energy

$$E^{ren} = -(0.0078607119 \pm 10^{-10}) \lambda . \tag{4.46}$$

This result agrees with the one obtained by Actor and Bender in [5], using a different approach also related to analytic continuation techniques <sup>(6)</sup>.

Since the renormalized boundary energy  $B^{ren}$  vanishes identically in the present configuration (see Eq. (4.31)), the above result for the bulk energy  $E^{ren}$  suffices to infer that the total energy  $\mathcal{E}^{ren} = E^{ren} + B^{ren}$  is finite. On the other hand, it appears from the asymptotic expansions in Eq. (4.45) that the renormalized boundary energy  $(\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$  diverges in a non-integrable manner in the limit  $r \rightarrow +\infty$ ; therefore, the integral  $\int_{\mathbb{R}^d} (\mathbf{v} | \hat{T}_{00} \mathbf{v})_{ren}$  is infinite (or, rather, it does not exist). In view of this, the alternative definition (3.132) for the total energy  $\mathcal{E}^{ren}$  does not yield a finite result in the present case. This is one of the anomalies which we pointed out in the remark at the end of subsection 4.1 (see subsection 3.2 for a general discussion).

## 4.2 The case of a rectangular box.

In the present section we consider a massless field confined within a  $d$ -dimensional rectangular domain  $\Omega = (0, a_1) \times \dots \times (0, a_d)$  ( $d \in \{1, 2, 3, \dots\}$ , arbitrary), with Dirichlet boundary conditions. Our approach could also be generalized, with some computational effort, to include the case of a massive field and to deal with Neumann or periodic boundary conditions; we choose to avoid these generalizations here for the sake of simplicity.

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<sup>6</sup>To check this, one must compare the numerical value reported in the above Eq. (4.46) with the one reported in Eq. (4.4) of [5]. Let us stress that conventions different from ours are used therein. In fact, using our language, the bulk energy is formally defined in [5] as  $E := \sum_n \omega_n$ , while our general prescription (3.120) is formally equivalent to  $E = \frac{1}{2} \sum_n \omega_n$ ; moreover the parameter  $\alpha$  of [5] and our parameter  $\lambda$  are related by  $\alpha = \sqrt{2} \lambda$ . Summing up, the ‘‘total energy’’ derived in [5] has to be multiplied by 1/2 in order to obtain our  $E^{ren}$ .

We follow the analysis presented in our previous work [67]. Our starting point is the heat kernel  $e^{-\mathbf{t}A}(\cdot, \cdot)$ , for which we consider two different series representations describing, respectively, the behavior for small and large  $\mathbf{t}$ ; these are used to produce series expansions giving the analytic continuations of the Dirichlet kernel  $\mathcal{A}^{-s}(\cdot, \cdot)$  and of its derivatives, which converge with exponential speed (we also give fully quantitative remainder estimates). These analytic continuations determine the renormalized VEVs of several observables, namely: the stress-energy tensor, the pressure on boundary points, the total energy and the total force acting on any side of the box. Our results hold for an arbitrary spatial dimension  $d$ ; in the conclusive paragraph of the present section we specialize them to the subcase  $d = 2$ , producing several graphs for the renormalized VEV of the energy density and for the other observables mentioned previously.

Many of the results reported in this Section (such as those in [67]) have been derived with the aid of `Mathematica` for both symbolic and numerical computations.

The Casimir effect for a rectangular box configuration has been discussed in a lot of works; here we only mention some of them. Concerning total energy and boundary forces, the foremost computations were performed by Lukosz [99, 100], by means of exponential regularization and Abel-Plana formula; the same techniques were used by Mamaev and Trunov [102, 103] (also see [104, 105]). Alternative derivations based on global ZR were later given by Ruggerio, Vilanni and Zimmerman [135, 136], Ambjørn and Wolfram [11, 12] and by Li, Cheng et al. [95]; equivalent results were obtained using generalized cut-off techniques by Edery [52, 53] and by Estrada, Fulling et al. [61, 77]. Finally, let us mention the monographies of Elizalde et al. [56, 57] and Bordag et al. [25]; these can be taken as standard references for the study of global aspects. Our series representations for the total energy and for the boundary forces are different, but equivalent to the ones of [25].

On the other hand, local aspects for a scalar field in a rectangular box were first analyzed by Actor in two seminal papers [3, 4]; therein  $d = 3$ , the framework is Euclidean and the author renormalizes, mostly by analytic continuation, the effective Lagrangian density and the VEV  $\langle \mathbf{v} | \hat{\varphi}^2(x) | \mathbf{v} \rangle$ . It is hardly the case to point out that these observables do not determine the renormalized stress-energy VEV; the latter was instead considered in a work of Svaiter et al. [132], again by means of analytic continuation techniques. However, in [132] some additional “empty space” divergences are removed by hand, with the motivation that they are also present when there is no boundary; moreover, [132] considers only a 3-dimensional, infinite rectangular waveguide ( $\Omega = (0, a_1) \times (0, a_2) \times \mathbb{R}$ ), rather than a box of arbitrary dimension. Let us also stress that the methods employed in [132] yield a representation of the renormalized stress-energy VEV via series converging with polynomial speed, which is slower than the exponential convergence of our series expansions. An alternative evaluation of the stress-energy VEV was proposed by Estrada, Fulling et al. in [61, 77], where the case of a 2-dimensional rectangular box is analyzed using exponential cut-off techniques; nevertheless, the position of principle in the cited works is that the theory with a cutoff is a more realistic description of the physical system under investigation, and renormalization is only hinted at for the energy density.

### Introducing the problem.

We consider the model of a massless scalar field confined within a  $d$ -dimensional box, with no external potential; more precisely, we assume

$$\Omega = \times_{i=1}^d (0, a_i) \quad \text{with } a_i > 0 \text{ for } i \in \{1, \dots, d\}, \quad V = 0. \quad (4.47)$$

The boundary  $\partial\Omega$  of the spatial domain is composed by the sides

$$\begin{aligned} \pi_{p,\alpha} := \{ \mathbf{x} \in \mathbb{R}^d \mid x^p = \alpha a_p, x^i \in [0, a_i] \text{ for } i \neq p, i \in \{1, \dots, d\} \} \\ \text{for } p \in \{1, \dots, d\}, \alpha \in \{0, 1\}; \end{aligned} \quad (4.48)$$

for the sake of simplicity, we restrict attention to the case where the field fulfills Dirichlet boundary conditions on each one of these sides. Under the above assumptions, we put

$$\mathcal{A} := -\Delta; \quad (4.49)$$

this is strictly positive and self-adjoint on  $\mathcal{H} = L^2(\Omega)$ , with domain  $\mathcal{D}_{\mathcal{A}} := \{f \in H_0^1(\Omega) \mid \Delta f \in L^2(\Omega)\}$  <sup>(7)</sup>. Also in this case,  $\mathcal{A}$  is an *admissible operator* in the sense of definition 2.37 and it has purely discrete spectrum, given by

$$\sigma(\mathcal{A}) = \left\{ \omega_{\mathbf{m}}^2 := \sum_{i=1}^d \frac{m_i^2 \pi^2}{a_i^2} \mid \mathbf{m} \equiv (m_i)_{i=1, \dots, d}, m_i \in \{1, 2, 3, \dots\} \right\} \quad (4.50)$$

<sup>(8)</sup>; a complete orthonormal set of eigenfunctions of  $\mathcal{A}$  in  $L^2(\Omega)$  corresponding to the eigenvalues  $(\omega_{\mathbf{m}}^2)$  in Eq. (4.50) is

$$F_{\mathbf{m}}(\mathbf{x}) := \prod_{i=1}^d \sqrt{\frac{2}{a_i}} \sin\left(\frac{m_i \pi}{a_i} x^i\right) \quad (\mathbf{x} \in \Omega). \quad (4.51)$$

Again, we can use the general framework of Chapter 2; in particular, we can consider the Dirichlet and heat kernels associated to  $\mathcal{A}$ , along with the related traces.

### The heat kernel.

Similarly to the model with a harmonic potential considered in the previous Section 4.1, in the present setting we are dealing with a product domain configuration. In particular, the heat kernel associated to  $\mathcal{A} = -\Delta$  factorizes; more precisely, we have

$$e^{-t\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^d e^{-t\mathcal{A}_i(x^i, y^i)}, \quad (4.52)$$

<sup>7</sup> Let us point out that, since the boundary  $\partial\Omega$  is Lipschitz, one can still define a notion of trace as in Eq. (2.160) and prove that  $H_0^1(\Omega) = \{f \in H^1(\Omega) \mid f \upharpoonright \partial\Omega = 0\}$  (see [7]). Moreover, it can be proven that  $\mathcal{D}_{\mathcal{A}} = \{f \in H^2(\Omega) \mid f \upharpoonright \partial\Omega = 0\}$ . If  $\Omega$  were smooth, one could infer this fact from Theorem 2.34; in this case  $\partial\Omega$  is not smooth, but the same conclusion can be inferred using the eigenfunction expansion of  $\mathcal{A}$ .

<sup>8</sup>In this case the parameter  $\varepsilon > 0$  fulfilling  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ , can be chosen to be  $\varepsilon := \sum_{i=1}^d (\pi/a_i)^2$ .

where, for  $i \in \{1, \dots, d\}$ , we have put  $\mathcal{A}_i := -\partial_{x^i x^i}$  (with the induced Dirichlet boundary conditions in  $x^i = 0$  and  $x^i = a_i$ ) and  $e^{-\mathbf{t}\mathcal{A}_i}(\cdot, \cdot)$  indicates the corresponding heat kernel. Each of the one-dimensional kernels can be determined by elementary methods; in particular, we showed in [67] that two different representations can be derived for  $e^{-\mathbf{t}\mathcal{A}_i}(\cdot, \cdot)$ , starting from the set of eigenfunctions and eigenvalues in Eq.s (4.50)–(4.51) and using the Poisson summation formula. Of course, these representations determine, according to (4.52), two alternative expressions for the total heat kernel  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$ , which we proceed to report hereafter. It appears that these alternative expressions are suited to describe the behaviour of this kernel for small and large  $\mathbf{t}$ , respectively.

*Large  $\mathbf{t}$  representation of the heat kernel.* This is

$$e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \frac{2^d}{a_1 \dots a_d} \sum_{\mathbf{m} \in \mathbb{N}_\star^d} e^{-\omega_{\mathbf{m}}^2 \mathbf{t}} \mathcal{C}_{\mathbf{m}}(\mathbf{x}, \mathbf{y}), \quad (4.53)$$

where  $\omega_{\mathbf{m}}$  is as in Eq. (4.50) and, for the sake of brevity, we have put

$$\mathbb{N}_\star := \{1, 2, 3, \dots\}, \quad \mathcal{C}_{\mathbf{m}}(\mathbf{x}, \mathbf{y}) := \prod_{i=1}^d \sin\left(\frac{m_i \pi}{a_i} y^i\right) \sin\left(\frac{m_i \pi}{a_i} x^i\right). \quad (4.54)$$

*Small  $\mathbf{t}$  representation of the heat kernel.* This is

$$e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}) = \frac{1}{(4\pi\mathbf{t})^{d/2}} \sum_{\mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1, 2\}^d} \delta_{\mathbf{l}} e^{-\frac{1}{\mathbf{t}} b_{\mathbf{h}\mathbf{l}}(\mathbf{x}, \mathbf{y})}, \quad (4.55)$$

where, for simplicity of notation, we have put

$$\mathbf{h} := (h_i)_{i=1, \dots, d}, \quad \mathbf{l} := (l_i)_{i=1, \dots, d}, \quad \delta_{\mathbf{l}} := \prod_{i=1}^d \delta_{l_i}, \quad \delta_{l_i} := \begin{cases} 1 & \text{for } l_i = 1 \\ -1 & \text{for } l_i = 2 \end{cases}, \quad (4.56)$$

$$b_{\mathbf{h}\mathbf{l}}(\mathbf{x}, \mathbf{y}) := \sum_{i=1}^d a_i^2 (h_i - \mathcal{D}_{l_i}(x^i, y^i))^2, \quad \mathcal{D}_{l_i}(x^i, y^i) := \begin{cases} \frac{x^i - y^i}{2a_i} & \text{for } l_i = 1 \\ \frac{x^i + y^i}{2a_i} & \text{for } l_i = 2 \end{cases}.$$

Before moving on, let us emphasize a number of facts on the expansions (4.53)–(4.55); we will resort to them in the following subsections, when performing the analytic continuation of the Dirichlet kernel and of its derivatives.

i) The expansions in Eq.s (4.53) and (4.55) describe, respectively, the large and small  $\mathbf{t}$  behaviour of  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$  in the following sense. The series over  $\mathbf{m} \in \mathbb{N}_\star^d$  in Eq. (4.53) and the one over  $\mathbf{h} \in \mathbb{Z}^d$  in Eq. (4.55) are mainly determined by the terms corresponding to small values of  $m_i$  and  $|h_i|$  ( $i \in \{1, \dots, d\}$ ), in the limits  $\mathbf{t} \rightarrow +\infty$  and  $\mathbf{t} \rightarrow 0^+$  respectively.

ii) Notice that

$$\omega_{\mathbf{n}}^2 > 0 \quad \text{for all } \mathbf{n} \in \mathbb{N}^d. \quad (4.57)$$

iii) There holds

$$b_{\mathbf{h}\mathbf{l}}(\mathbf{x}, \mathbf{y}) \geq 0 \quad \text{for all } \mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1, 2\}^d, \mathbf{x}, \mathbf{y} \in \Omega. \quad (4.58)$$

In particular, since  $\mathcal{D}_{l_i}(x^i, y^i) \in [-1/2, 1/2]$  for  $l_i = 1$  and  $\mathcal{D}_{l_i}(x^i, y^i) \in [0, 1]$  for  $l_i = 2$  (see the definition of  $\mathcal{D}_{l_i}$  in Eq. (4.56)), it follows that

$$b_{\mathbf{h}\mathbf{l}}(\mathbf{x}, \mathbf{y}) = 0 \Leftrightarrow \text{for each } i \in \{1, \dots, d\}, \text{ one has } \begin{cases} h_i = 0, l_i = 1, y^i = x^i \in [0, a_i] \\ \text{or } h_i = 0, l_i = 2, y^i = x^i = 0; \\ \text{or } h_i = 1, l_i = 2, y^i = x^i = a_i \end{cases} \quad (4.59)$$

let us stress that this implies, in particular,  $b_{\mathbf{h}\mathbf{l}}(\mathbf{x}, \mathbf{y}) \neq 0$  for  $\mathbf{x} \neq \mathbf{y}$ .

### The Dirichlet kernel.

The analytic continuation of  $\mathcal{A}^{-s}(\cdot, \cdot)$  can be constructed in the style of Minakshisundaram [111], starting from the integral representation (2.266) in terms of the heat kernel  $e^{-\mathbf{t}\mathcal{A}}(\cdot, \cdot)$ ; to this purpose, let us fix arbitrarily

$$T \in (0, +\infty) \quad (4.60)$$

and re-express the cited integral representation, for  $\mathbf{x}, \mathbf{y} \in \Omega$ , as

$$\mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = \mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y}) + \mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y}), \quad \text{where} \quad (4.61)$$

$$\mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y}) := \frac{1}{\Gamma(s)} \int_T^{+\infty} dt \mathbf{t}^{s-1} e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y}), \quad \mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y}) := \frac{1}{\Gamma(s)} \int_0^T dt \mathbf{t}^{s-1} e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$$

(notice that  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$  and  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$  depend on  $T$ , but their sum  $\mathcal{A}^{-s}(\cdot, \cdot)$  does not!). To construct the analytic continuation of  $\mathcal{A}^{-s}(\cdot, \cdot)$ , we substitute in the definitions of  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$  and  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$ , respectively, the large and small  $\mathbf{t}$  expansions (4.53) (4.55) for the heat kernel  $e^{-\mathbf{t}\mathcal{A}}(\mathbf{x}, \mathbf{y})$  <sup>9</sup>. We obtain the results reported hereafter.

*Series expansion for  $\mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y})$ .* Using the representation (4.53) for the heat kernel, one can derive [67] the following, for  $\mathbf{x}, \mathbf{y} \in \Omega$ :

$$\mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{2^d}{a_1 \dots a_d \Gamma(s)} \sum_{\mathbf{m} \in \mathbb{N}^d} \omega_{\mathbf{m}}^{-2s} \Gamma(s, \omega_{\mathbf{m}}^2 T) \mathcal{C}_{\mathbf{m}}(\mathbf{x}, \mathbf{y}), \quad (4.62)$$

where, for any  $s \in \mathbb{C}$  and  $z \in (0, +\infty)$ ,  $\Gamma(s, z)$  is the upper incomplete gamma function (see [122], page 174, Eq. 8.2.2). The above expression can also be used to evaluate derivatives

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<sup>9</sup>In these manipulations (and in some related computations) we often take for granted that certain series can be integrated or differentiated term by term. In all cases under analysis, rigorous justifications could be given using the Lebesgue dominated convergence theorem or the Fubini-Tonelli theorem, but we will not go into the details.

of any order of the function  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$ . Moreover, the series in the right-hand sides of Eq. (4.62), along with analogous ones for the derivatives of  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$ , converges for all  $s \in \mathbb{C}$  even for  $\mathbf{y} = \mathbf{x}$  (see the subsequent paragraph); so, Eq. (4.62) yields automatically the analytic continuation of the map  $s \mapsto \mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y})$  to the whole complex plane.

*Series expansion for  $\mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y})$ .* The expression (4.55) for the heat kernel can be used to infer, for  $\mathbf{x}, \mathbf{y} \in \Omega$ ,

$$\mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y}) = \frac{T^{s-\frac{d}{2}}}{(4\pi)^{d/2}\Gamma(s)} \sum_{\mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1,2\}^d} \delta_{\mathbf{l}} \mathcal{P}_{s-\frac{d}{2}} \left( \frac{b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y})}{T} \right). \quad (4.63)$$

Here, for  $\beta \geq 0$  and  $s \in \mathbb{C}$  (recall that  $b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y}) \geq 0$  for all  $\mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1,2\}^d$ ; see Eq. (4.58)), we have introduced the function

$$\mathcal{P}_s(\beta) := \int_0^1 d\tau \tau^{s-1} e^{-\frac{\beta}{\tau}}; \quad (4.64)$$

this map fulfills

$$\mathcal{P}_s(\beta) = \begin{cases} s^{-1} & \text{for } \beta = 0, \Re s > 0 \\ \beta^s \Gamma(-s, \beta) & \text{for } \beta > 0 \end{cases}, \quad (4.65)$$

$$\partial_\beta^\ell \mathcal{P}_s(\beta) = (-1)^\ell \mathcal{P}_{s-\ell}(\beta) \quad \text{for } \ell \in \mathbb{N}$$

(again,  $\Gamma(\cdot, \cdot)$  denotes the upper incomplete gamma function). Let us point out that, due to the results reported in Eq. (4.59), we have

$$b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y}) = 0 \text{ only for } \mathbf{y} = \mathbf{x} \text{ and for a finite number of terms in the series of Eq. (4.63).} \quad (4.66)$$

The above mentioned terms of Eq. (4.63) deserve special attention, and must be evaluated using the first identity in Eq. (4.65); it follows that

$$\begin{aligned} \mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y}) &= \frac{T^{s-\frac{d}{2}}}{(4\pi)^{d/2}\Gamma(s) \left(s - \frac{d}{2}\right)} \sum_{\substack{\mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1,2\}^d \\ \text{s.t. } b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y})=0}} \delta_{\mathbf{l}} + \\ &+ \frac{1}{(4\pi)^{d/2}\Gamma(s)} \sum_{\substack{\mathbf{h} \in \mathbb{Z}^d, \mathbf{l} \in \{1,2\}^d \\ \text{s.t. } b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y})>0}} \delta_{\mathbf{l}} \left( b_{\mathbf{hl}}^{s-\frac{d}{2}} \Gamma\left(\frac{d}{2}-s, \frac{b_{\mathbf{hl}}}{T}\right) \right) (\mathbf{x}, \mathbf{y}). \end{aligned} \quad (4.67)$$

Let us repeat that the first sum in the above expression contains finitely many terms. Notice that the term in the first line of Eq. (4.67) is related to the first equality in Eq. (4.65) which, in principle, would require  $\Re s > d/2$ ; however, this term makes sense for all complex  $s$  except  $s = d/2$ , where a simple pole appears. On the other hand, the series in the second line of Eq.s (4.67) can be proved to converge for any complex  $s$  (see, again,



the forthcoming paragraph). In view of these remarks, Eq. (4.67) gives automatically the analytic continuation of  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$  to a meromorphic function of  $s$  on the whole complex plane, with a simple pole singularity only for

$$\mathbf{y} = \mathbf{x} \quad \text{and} \quad s = d/2 . \quad (4.68)$$

A similar analysis can be made for the derivatives of  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$ , for which series representations analogous to that in Eq. (4.65) can be derived. For brevity, we do not report here the detailed discussion of these quantities, for which we refer to [67]. Let us only mention that, for any two spatial variables  $z, w$  and for any  $\mathbf{x}, \mathbf{y} \in \Omega$ , the map  $s \mapsto \partial_{zw} \mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y})$  can be analytically continued to a function meromorphic on the whole complex plane, with a simple pole singularity only for

$$\mathbf{y} = \mathbf{x} \quad \text{and} \quad s = d/2 + 1 . \quad (4.69)$$

Let us stress that the above facts allow to infer, in particular, that the analytic continuations of  $\mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  and  $\partial_{zw} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\mathbf{x}}$  (required for the evaluation of the regularized stress-energy VEV and pressure) are both regular at  $u = 0$ .

**Convergence and remainder estimates for the series in Eq.s (4.62) and (4.63).**

This subject is discussed in more detail in [67] (see, in particular, subsection 3.4 and the related Appendix A therein); here we only report the main results. To this purpose, some notations are required; first of all we put

$$\begin{aligned} a &:= \min_{i \in \{1, \dots, d\}} \{a_i\} , & A &:= \max_{i \in \{1, \dots, d\}} \{a_i\} , \\ |\mathbf{z}| &:= \left( \sum_{i=1}^d z_i^2 \right)^{1/2} & \text{for } \mathbf{z} = \mathbf{m} \in \mathbb{N}^d \text{ or } \mathbf{z} = \mathbf{h} \in \mathbb{Z}^d . \end{aligned} \quad (4.70)$$

Besides, for  $N \in (2\sqrt{d}, +\infty)$ ,  $\alpha \in (0, 1)$ ,  $\beta \in (0, +\infty)$ ,  $\sigma, \rho \in \mathbb{R}$ , we set

$$\begin{aligned} H_N^{(d)}(\alpha, \beta; \sigma, \rho) &:= \\ &\frac{\pi^{d/2}}{(1-\alpha)^\sigma (\alpha\beta)^{\frac{d+\rho}{2}} \Gamma(\frac{d}{2})} \left( \frac{N-\sqrt{d}}{N-2\sqrt{d}} \right)^{d-1} \Gamma(\sigma, (1-\alpha)\beta N^2) \Gamma\left(\frac{d+\rho}{2}; \alpha\beta(N-2\sqrt{d})^2\right) ; \end{aligned} \quad (4.71)$$

it can be shown that there holds the asymptotic expansion, for  $N \rightarrow +\infty$ ,

$$H_N^{(d)}(\alpha, \beta; \sigma, \rho) = \frac{\pi^{d/2} \beta^{\sigma-2} e^{-4\alpha\beta d}}{\alpha(1-\alpha) \Gamma(\frac{d}{2})} e^{-\beta N(N-4\alpha\beta\sqrt{d})} N^{2\sigma+\rho+d-4} (1 + O(N^{-1})) . \quad (4.72)$$

Finally, we put

$$C_{a,A}^{(d)}(\sigma, N) := \max \left[ \left( a \left( 1 - \frac{\sqrt{d}}{N} \right) \right)^{2\sigma} , \left( A \left( 1 + \frac{\sqrt{d}}{N} \right) \right)^{2\sigma} \right] . \quad (4.73)$$

Having introduced the above notations, let us proceed to give the previously mentioned remainder estimates for the series expansions of  $\mathcal{A}_{(>)}^{-s}$  and  $\mathcal{A}_{(<)}^{-s}$ . In all cases the remainder is controlled by the function  $H_N^{(d)}$ ; due to the exponential decay of this function for large  $N$  described in Eq. (4.72), good approximations of all the series under investigation can be obtained by just summing the first few terms.

*Estimates for the series (4.62).* Let  $s \in \mathbb{C}$ ; keeping in mind Eq. (4.62), for any  $N \in (0, +\infty)$  let us write

$$\begin{aligned} \mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y}) &= \mathcal{A}_{(>),N}^{-s}(\mathbf{x}, \mathbf{y}) + R_{(>),N}^{-s}(\mathbf{x}, \mathbf{y}) , \\ \mathcal{A}_{(>),N}^{-s}(\mathbf{x}, \mathbf{y}) &:= \frac{2^d}{a_1 \dots a_d \Gamma(s)} \sum_{\mathbf{m} \in \mathbb{N}_*^d, |\mathbf{m}| \leq N} \omega_{\mathbf{m}}^{-2s} \Gamma(s, \omega_{\mathbf{m}}^2 T) \mathcal{C}_{\mathbf{m}}(\mathbf{x}, \mathbf{y}) , \\ R_{(>),N}^{-s}(\mathbf{x}, \mathbf{y}) &:= \frac{2^d}{a_1 \dots a_d \Gamma(s)} \sum_{\mathbf{m} \in \mathbb{N}_*^d, |\mathbf{m}| > N} \omega_{\mathbf{m}}^{-2s} \Gamma(s, \omega_{\mathbf{m}}^2 T) \mathcal{C}_{\mathbf{m}}(\mathbf{x}, \mathbf{y}) . \end{aligned} \quad (4.74)$$

For the remainder function  $R_{(>),N}^{-s}(\mathbf{x}, \mathbf{y})$  we have the following uniform estimate

$$\begin{aligned} \left| R_{(>),N}^{-s}(\mathbf{x}, \mathbf{y}) \right| &\leq \frac{\max(a^{2\Re s}, A^{2\Re s})}{a_1 \dots a_d \pi^{2\Re s} |\Gamma(s)|} H_N^{(d)} \left( \alpha, \frac{\pi^2 T}{A^2}; \Re s, -2\Re s \right) \\ &\text{for either } \Re s \geq 0, N > 2\sqrt{d} \quad \text{or } \Re s < 0, N > 2\sqrt{d} + \frac{A}{\pi} \sqrt{\frac{|\Re s|}{\alpha T}} . \end{aligned} \quad (4.75)$$

In the above,  $\alpha$  is a parameter that can be freely chosen in  $(0, 1)$ ; of course, the best choice is the one minimizing the right-hand side of Eq. (4.75), which depends on the other parameters (e.g.,  $N, T$ ) involved in these considerations.

*Estimates for the series (4.63).* Let  $s \in \mathbb{C}$ , and exclude the case (4.68); keeping in mind Eq. (4.63), for any  $N \in (0, +\infty)$  we put

$$\begin{aligned} \mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y}) &= \mathcal{A}_{(<),N}^{-s}(\mathbf{x}, \mathbf{y}) + R_{(<),N}^{-s}(\mathbf{x}, \mathbf{y}) , \\ \mathcal{A}_{(<),N}^{-s}(\mathbf{x}, \mathbf{y}) &:= \frac{T^{s-\frac{d}{2}}}{(4\pi)^{d/2} \Gamma(s)} \sum_{\mathbf{h} \in \mathbb{Z}^d, |\mathbf{h}| \leq N, \mathbf{l} \in \{1,2\}^d} \delta_{\mathbf{l}} \mathcal{P}_{s-\frac{d}{2}} \left( \frac{b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y})}{T} \right) , \\ R_{(<),N}^{-s}(\mathbf{x}, \mathbf{y}) &:= \frac{T^{s-\frac{d}{2}}}{(4\pi)^{d/2} \Gamma(s)} \sum_{\mathbf{h} \in \mathbb{Z}^d, |\mathbf{h}| > N, \mathbf{l} \in \{1,2\}^d} \delta_{\mathbf{l}} \mathcal{P}_{s-\frac{d}{2}} \left( \frac{b_{\mathbf{hl}}(\mathbf{x}, \mathbf{y})}{T} \right) . \end{aligned} \quad (4.76)$$

For the remainder function  $R_{(<),N}^{-s}$ , we have the following uniform estimate:

$$\begin{aligned} \left| R_{(<),N}^{-s}(\mathbf{x}, \mathbf{y}) \right| &\leq \frac{C_{a,A}^{(d)}(\Re s - \frac{d}{2}, N)}{\pi^{d/2} |\Gamma(s)|} H_N^{(d)} \left( \alpha, \frac{a^2(1-\frac{\sqrt{d}}{N})^2}{T}; \frac{d}{2} - \Re s, 2\Re s - d \right) \\ &\text{for either } \Re s \leq \frac{d}{2}, N > 2\sqrt{d} \quad \text{or } \Re s > \frac{d}{2}, N > 3\sqrt{d} + \frac{1}{a} \sqrt{\frac{(\Re s - \frac{d}{2})T}{\alpha}} . \end{aligned} \quad (4.77)$$

Again, the parameter  $\alpha$  can be freely taken in  $(0, 1)$  and it is convenient to choose for it the value minimizing the right-hand sides of Eq. (4.77), keeping into account the choices made for the other parameters (in particular, for  $N$ ).

### The stress-energy tensor.

Consider the representations deduced in the previous paragraph for the analytic continuations of the Dirichlet kernel (and of its derivatives). Resorting to Eq.s (3.107-3.109), one can obtain series expansions for each component of the zeta-regularized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$ . More precisely, for any  $\mathbf{x} \in \Omega$ , we have

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) = T_{\mu\nu}^{u,(>)}(\mathbf{x}) + T_{\mu\nu}^{u,(<)}(\mathbf{x}) , \quad (4.78)$$

where, for  $\bullet$  equal to  $>$  or  $<$ ,  $T_{\mu\nu}^{u,(\bullet)}(\mathbf{x})$  has the expression corresponding to Eq.s (3.107-3.109), with  $\mathcal{A}^{-s}(\cdot, \cdot)$  replaced by  $\mathcal{A}_{(\bullet)}^{-s}(\cdot, \cdot)$ ; thus, for  $i, j \in \{1, \dots, d\}$ , we have

$$T_{00}^{u,(\bullet)}(\mathbf{x}) = \kappa^u \left[ \left( \frac{1}{4} + \xi \right) \mathcal{A}_{(\bullet)}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) + \left( \frac{1}{4} - \xi \right) \partial^{x^\ell} \partial_{y^\ell} \mathcal{A}_{(\bullet)}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}} , \quad (4.79)$$

$$T_{0j}^{u,(\bullet)}(\mathbf{x}) = T_{j0}^{u,(\bullet)}(\mathbf{x}) = 0 , \quad (4.80)$$

$$\begin{aligned} T_{ij}^{u,(\bullet)}(\mathbf{x}) = T_{ji}^{u,(\bullet)}(\mathbf{x}) = \kappa^u & \left[ \left( \frac{1}{4} - \xi \right) \partial_{ij} \left( \mathcal{A}_{(\bullet)}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) - \partial^{x^\ell} \partial_{y^\ell} \mathcal{A}_{(\bullet)}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right) + \right. \\ & \left. + \left( \left( \frac{1}{2} - \xi \right) \partial_{x^i y^j} - \xi \partial_{x^i x^j} \right) \mathcal{A}_{(\bullet)}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}} . \end{aligned} \quad (4.81)$$

In view of the results discussed in the previous paragraphs for the functions  $\mathcal{A}_{(>)}^{-s}(\mathbf{x}, \mathbf{y})$  and  $\mathcal{A}_{(<)}^{-s}(\mathbf{x}, \mathbf{y})$ , it appears that  $u = 0$  is a regular point for each component of  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})$ ; so, the general zeta approach to renormalization (3.121) reduces, in this case, to

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})_{ren} := (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) \Big|_{u=0} . \quad (4.82)$$

In the following, when considering the case in spatial dimension  $d = 2$ , we will use approximate expressions for all the components of  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})_{ren}$  obtained replacing each Dirichlet function  $\mathcal{A}_{(\bullet)}^{-s}(\cdot, \cdot)$  in Eq.s (4.79-4.81) with the truncations  $\mathcal{A}_{(\bullet),N}^{-s}(\cdot, \cdot)$  of a fixed (sufficiently large) order  $N$ , given by Eq.s (4.74) (4.76). Let us recall that we have explicit remainder bounds for these truncations (see Eq.s (4.75) (4.77)); these allow us to infer error estimates for the approximate expressions of  $(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v})_{ren}$  described above.

### The pressure on the boundary.

Let  $\mathbf{x}$  be any point interior to one of the sides  $\pi_{p,\alpha}$ ; we exclude  $\mathbf{x}$  to be on an edge of the box (i.e., on the intersection of two or more sides), where the outer normal is ill-defined. As an example, let us assume  $\mathbf{x}$  to be an inner point of the side  $\pi_{1,0}$ , so that the unit outer

normal at  $\mathbf{x}$  is  $\mathbf{n}(\mathbf{x}) = (-1, 0, \dots, 0)$ . The zeta-regularized pressure at  $\mathbf{x}$  can be defined according to the general prescription (3.115), which in the present case reduces to

$$p_i^u(\mathbf{x}) := (\mathbf{v} | \hat{T}_{ij}^u(\mathbf{x}) \mathbf{v}) n^j(\mathbf{x}) = -(\mathbf{v} | \hat{T}_{i1}^u(\mathbf{x}) \mathbf{v}) ; \quad (4.83)$$

since Dirichlet boundary conditions are prescribed, recalling the general expression (3.109) for  $(\mathbf{v} | \hat{T}_{ij}^u(\mathbf{x}) \mathbf{v})$  and using the decomposition (4.61) for the Dirichlet kernel, the above relation yields <sup>(10)</sup>

$$\begin{aligned} p_i^u(\mathbf{x}) &= -\delta_{i1} \frac{\kappa^u}{4} \partial_{x^1 y^1} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \\ &= -\delta_{i1} \frac{\kappa^u}{4} \left[ \partial_{x^1 y^1} \mathcal{A}_{(>)}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} + \partial_{x^1 y^1} \mathcal{A}_{(<)}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \right]. \end{aligned} \quad (4.84)$$

Recalling that the Dirichlet kernel and its derivatives are all regular at  $u = 0$ , the general zeta approach to renormalization (3.126) reduces in this case to

$$p_i^{ren}(\mathbf{x}) := p_i^u(\mathbf{x}) \Big|_{u=0} = -(\mathbf{v} | \hat{T}_{i1}^u(\mathbf{x}) \mathbf{v}) \Big|_{u=0}. \quad (4.85)$$

When dealing with the case  $d = 2$ , we will evaluate the pressure starting from Eq.s (4.84) (4.85) and substituting the functions  $\partial_{x^1 y^1} \mathcal{A}_{(\bullet)}^{-s}(\cdot, \cdot)$  therein with the truncations  $\partial_{x^1 y^1} \mathcal{A}_{(\bullet), N}^{-s}(\cdot, \cdot)$  of a sufficiently large order  $N$ ; the errors of these approximants will be evaluated using the analogues of Eq.s (4.75) and (4.77), holding for the derivatives of the Dirichlet kernel.

Before proceeding, let us mention a couple of facts about the renormalized pressure on the boundary; their proof are discussed in detail in our previous work [67].

i) Let us remark that at points on the edges of the box (i.e., on the corners which appear whenever  $d > 1$ ) the outer normal and, consequently, the pressure are both ill-defined. It can be proved that the renormalized pressure (4.85) evaluated at inner points of one side diverges in a non-integrable manner when moving towards anyone of the edges; this fact is of utmost importance when attempting to evaluate the total force acting on any side of the box, a topic we discussed in detail in [66].

ii) In accordance with the alternative definition (3.133), one could define the pressure at a boundary point  $\mathbf{x} \in \pi_{1,0}$  as

$$p_i^{ren}(\mathbf{x}) := \left( \lim_{\mathbf{x}' \in \Omega, \mathbf{x}' \rightarrow \mathbf{x}} (\mathbf{v} | \hat{T}_{i1}^u(\mathbf{x}') \mathbf{v})_{ren} \right) n^j(\mathbf{x}) = - \left( \lim_{\mathbf{x}' \in \Omega, \mathbf{x}' \rightarrow \mathbf{x}} (\mathbf{v} | \hat{T}_{i1}^u(\mathbf{x}') \mathbf{v})_{ren} \right). \quad (4.86)$$

<sup>10</sup>In the application of Eq. (3.109) to the present case, we use the following identities, holding for all  $\mathbf{x} \in \partial\Omega$  and suitable  $s \in \mathbb{C}$ :

$$\begin{aligned} \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= 0, \quad \partial_{x^i x^j} \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = 0 \quad \text{for all } i, j \in \{1, \dots, d\}; \\ \partial_{x^i y^j} \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= 0 \quad \text{for all } i, j \in \{1, \dots, d\} \text{ such that } i \neq 1 \text{ or } j \neq 1. \end{aligned}$$

These follow straightforwardly from the Dirichlet conditions prescribed on the boundary of  $\Omega$  and from item vi) of Proposition 2.64.

Simple but long computations allow to infer that the different prescriptions (4.85) and (4.86) are, in fact, equivalent for the configuration under analysis; therefore, no anomaly of the type mentioned in subsection 3.2 appears in this case for the VEV of the pressure at boundary points.

### The total energy.

First of all, let us point out that, by a slight generalization of Proposition 3.45, the zeta-regularized total energy  $\mathcal{E}^u$  can be expressed as the sum of both a bulk and a boundary contribution, respectively indicated with  $E^u$  and  $B^u$ . Since Dirichlet conditions are assumed on the boundary, according to the considerations of Remark 3.29 we have

$$B^u = 0 ; \quad (4.87)$$

therefore, we only have to discuss the regularized bulk term  $E^u$ . Recalling the general definition (3.118) and using the expression (4.61) for the Dirichlet kernel, we readily infer

$$E^u = E_{(>)}^u + E_{(<)}^u \quad \text{where} \\ E_{(\bullet)}^u := \frac{\kappa^u}{2} \int_{(0,a_1) \times \dots \times (0,a_d)} dx^1 \dots dx^d \mathcal{A}_{(\bullet)}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{x}) \quad \text{for } \bullet \in \{>, <\}. \quad (4.88)$$

*Series expansion for  $E_{(>)}^u$ .* Let us insert the expansion (4.62) for  $\mathcal{A}_{(>)}^{-s}$  into Eq. (4.88); then, exchanging the order of integration and summation and evaluating each single integral thus obtained in terms of incomplete gamma functions, we obtain

$$E_{(>)}^u = \frac{\kappa^u}{2\Gamma(\frac{u-1}{2})} \sum_{\mathbf{m} \in \mathbb{N}_*^d} \omega_{\mathbf{m}}^{1-u} \Gamma\left(\frac{u-1}{2}, \omega_{\mathbf{m}}^2 T\right). \quad (4.89)$$

The above series can be proved to converge for all  $u \in \mathbb{C}$ , thus giving the analytic continuation of  $E^{u,(>)}$  to the whole complex plane, in particular at  $u = 0$ .

*Series expansion for  $E_{(<)}^u$ .* Similarly, inserting the expansion (4.63) for  $\mathcal{A}_{(<)}^{-s}$  into Eq. (4.88), after some effort we obtain

$$E_{(<)}^u = \frac{\kappa^u T^{\frac{u-1}{2}}}{2^{d+1} \Gamma(\frac{u-1}{2})} \sum_{p=0}^d \frac{(-1)^{d-p}}{(d-p)! p!} \sum_{\sigma \in \mathbb{P}_d} \frac{\mathbf{a}_{\sigma,p}}{(\pi T)^{p/2}} \sum_{\mathbf{h} \in \mathbb{Z}^p} \mathcal{P}_{\frac{u-p-1}{2}}\left(\frac{B_{\sigma,p}(\mathbf{h})}{T}\right). \quad (4.90)$$

In the above  $\mathbb{P}_d$  indicates the symmetric group with  $d$  elements and we have put

$$\mathbf{a}_{\sigma,0} := 1, \quad \mathbb{Z}^0 := \{\mathbf{0}\}, \quad B_{\sigma,0}(\mathbf{0}) := 0, \\ \mathbf{a}_{\sigma,p} := \prod_{i=1}^p a_{\sigma(i)}, \quad B_{\sigma,p}(\mathbf{h}) := \sum_{i=1}^p (a_{\sigma(i)} h_i)^2 \quad \text{for } \sigma \in \mathbb{P}_d, p \in \{1, \dots, d\}; \quad (4.91)$$

note that the term with  $p = 0$  in Eq. (4.90) is just  $(-1)^d \mathcal{P}_{\frac{u-1}{2}}(0)$  and that all the functions  $\mathcal{P}_s$  must be evaluated according to Eq. (4.65). It can be shown that Eq. (4.90) gives

the analytic continuation of  $E_{(<)}^u$  to a meromorphic function on the whole complex plane, with simple poles at

$$u \in \{1, \dots, d+1\} ; \quad (4.92)$$

in particular, the series in Eq. (4.90) converges for all  $u \in \mathbb{C} \setminus \{1, \dots, d+1\}$  and explicit remainder estimates can be derived, as well.

Summing up,  $u = 0$  is a regular point for the analytic continuations of both  $E_{(>)}^u$  and  $E_{(<)}^u$  so that, the general prescription in Eq. (3.125) yields

$$E^{ren} = E_{(>)}^u \Big|_{u=0} + E_{(<)}^u \Big|_{u=0} \quad (4.93)$$

where the two addenda on the right-hand side simply indicate the expressions (4.89) and (4.90) evaluated at  $u = 0$ .

Before moving on, let us also mention that results analogous to those reported previously concerning the convergence rate of the expansions (4.62) (4.63) for the functions  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$  and  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$  can be derived for the series representations (4.89) (4.90) of  $E_{(>)}^u, E_{(<)}^u$ . In particular, quantitative remainder estimates can be derived for the truncation of these series at any order  $N \in \mathbb{N}$ ; we refer to [67] for more details.

### Scaling considerations.

Let us consider the  $d$ -tuple  $\mathbf{x}_*$  and the  $(d-1)$ -tuple  $\boldsymbol{\rho}$  with components, respectively,

$$x_*^i := \frac{x^i}{a_i} \in (0, 1) \quad \text{for } i \in \{1, \dots, d\}, \quad \rho_i := \frac{a_i}{a_1} \quad \text{for } i \in \{2, \dots, d\}. \quad (4.94)$$

Using the decomposition (4.61) of the Dirichlet kernel  $\mathcal{A}^{-s}(\cdot, \cdot)$  and recalling the series expansions (4.62), (4.63) for the functions  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$  and  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$ , it can be shown that

$$\mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = a_1^{-(d-2)s} \mathfrak{D}_s(\boldsymbol{\rho}; \mathbf{x}_*, \mathbf{y}_*), \quad (4.95)$$

for all  $\mathbf{x}, \mathbf{y} \in \Omega$  and for some suitable function  $\mathfrak{D}_s$  <sup>(11)</sup>. From the above relation it follows that, for any pair  $z, w$  of spatial variables, there also holds

$$\partial_{zw} \mathcal{A}^{-s}(\mathbf{x}, \mathbf{y}) = a_1^{-(d-2)s-2} \partial_{z_* w_*} \mathfrak{D}_s(\boldsymbol{\rho}; \mathbf{x}_*, \mathbf{y}_*). \quad (4.96)$$

Due to the above results, analogous considerations can be deduced for the zeta-regularized VEV of the observables mentioned in the previous paragraphs.

In particular, from Eq.s (4.78-4.81) it can be easily inferred the following relation for each component of the regularized stress-energy VEV ( $\mu, \nu \in \{0, \dots, d\}$ ):

$$(\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) = a_1^{u-d-1} T_{\mu\nu}^u(\boldsymbol{\rho}; \mathbf{x}_*), \quad (4.97)$$

---

<sup>11</sup>Let us point out that for  $d = 1$  the variables  $\rho_i$  are not defined and  $\mathfrak{D}_s(\boldsymbol{\rho}; \mathbf{x}_*, \mathbf{y}_*) \equiv \mathfrak{D}_s(\mathbf{x}_*, \mathbf{y}_*)$  only depends on the complex parameter  $s$  and on the rescaled spatial variables  $\mathbf{x}_*, \mathbf{y}_*$ .

where  $T_{\mu\nu}^u$  is a suitable function.

Similarly, for the regularized pressure acting on any point  $\mathbf{x}$  in the interior of the side  $\pi_{1,0}$ , we deduce from Eq.s (4.83) (4.97) that

$$p_i^u(\mathbf{x}) = a_1^{u-d-1} p_i^u(\boldsymbol{\rho}; \mathbf{x}_\star) \quad \text{for } i \in \{1, \dots, d\}, \quad (4.98)$$

where  $p_i^u$  are suitable functions and  $\mathbf{x}_\star$  is defined as in Eq. (4.94) at points on the boundary. Clearly, the same conclusions can be drawn for the pressure on any other side  $\pi_{p,\alpha}$  ( $p \in \{1, \dots, d\}$ ,  $\alpha \in \{0, 1\}$ ).

Analogous considerations hold for the regularized bulk energy  $E^u$ ; from the expansions (4.88-4.90), it can be easily inferred that (indicating with  $E^u$  a suitable function)

$$E^u = a_1^{u-1} E^u(\boldsymbol{\rho}). \quad (4.99)$$

By analytic continuation at  $u = 0$ , we obtain the renormalized counterparts of the above relations: more precisely, we have

$$\begin{aligned} (\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren} &= a_1^{-(d+1)} T_{\mu\nu}(\boldsymbol{\rho}; \mathbf{x}_\star), \\ p_i^{ren}(\mathbf{x}) &= a_1^{-(d+1)} p_i(\boldsymbol{\rho}; \mathbf{x}_\star), \quad E^{ren} = a_1^{-1} E(\boldsymbol{\rho}), \end{aligned} \quad (4.100)$$

where the right-hand sides of the above relations are obtained evaluating at  $u = 0$  the functions in the right-hand sides of Eq.s (4.97-4.99).

Due to the remarks of this paragraph, for any spatial dimension  $d$  the analysis of the renormalized stress-energy VEV, pressure and total energy can always be reduced to the case  $a_1 = 1$ ; we will use this fact in the next paragraph dealing with the case  $d = 2$ .

### The previous results in spatial dimension $d = 2$ .

As an application of the general framework developed in the previous paragraphs, let us consider the 2-dimensional case where

$$d = 2, \quad \Omega = (0, a_1) \times (0, a_2) \quad (a_1, a_2 > 0). \quad (4.101)$$

In our computations we fix

$$a_1 = 1 \quad (4.102)$$

and consider different values of  $a_2$ ; let us repeat that this choice causes no loss of generality due to the scaling considerations discussed in the previous paragraph. Moreover, we present the final results in terms of the rescaled coordinates  $x_\star^1 := x^1/a_1 \equiv x^1$ ,  $x_\star^2 := x^2/a_2 \in (0, 1)$ , defined in Eq. (4.94) <sup>(12)</sup>.

The basic elements to compute the renormalized stress-energy VEV and the pressure are the Dirichlet functions  $\mathcal{A}_{(>)}^{-s}(\cdot, \cdot)$ ,  $\mathcal{A}_{(<)}^{-s}(\cdot, \cdot)$ , along with their spatial derivatives, for

<sup>12</sup> Let us stress that, for  $a_1 = 1$ , the quantities  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$ ,  $p_i^{ren}$  and  $E^{ren}$  (to be discussed hereafter) do in fact coincide with the rescaled analogues  $T_{\mu\nu}^{ren}$ ,  $p_i^{ren}$ ,  $E^{ren}$  introduced in Eq.s (4.97) (4.98) (4.99). Besides, the length  $a_2$  of the second side is identified with the ratio  $\rho_2$  (see Eq. (4.94)).

which we use the truncated expansions (4.74), (4.76) and the remainder bounds of Eq.s (4.75), (4.77) (plus similar results for the derivatives; see [67]). Needless to say, analogous considerations also hold for the renormalized bulk energy.

*The renormalized stress-energy VEV.* As an example, we compute this observable for the two configurations with

$$a_2 = 1 \quad \text{and} \quad a_2 = 5 . \quad (4.103)$$

In these cases, for the parameter  $T$  of the decomposition into ( $>$ ) and ( $<$ ) parts and for the truncation order  $N$ , we make the following choices:

$$\begin{aligned} T = 1 , \quad N = 7 & \quad \text{for } a_2 = 1 ; \\ T = 1 , \quad N = 9 & \quad \text{for } a_2 = 5 . \end{aligned} \quad (4.104)$$

Furthermore, the truncation errors in Eq.s (4.75-4.77) are evaluated making for the parameter  $\alpha$  appearing therein the choice

$$\alpha = 0.04 . \quad (4.105)$$

The renormalized stress-energy VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$  is obtained setting  $u = 0$  in Eq.s (4.78-4.81). We separate the conformal and nonconformal parts, respectively indicated by the superscripts ( $\diamond$ ) and ( $\blacksquare$ ); recall that Eq. (3.127) gives, in the two-dimensional case,

$$\xi_2 = \frac{1}{8} . \quad (4.106)$$

In the following we present, as examples, the graphs for  $(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$  obtained from the previous truncated expansions; more precisely, Fig.s 4.3 and 4.4 show, respectively, the results obtained for the configurations with  $a_2 = 1$  and  $a_2 = 5$ . In the cited figures we refer to the variables  $x_\star^i := x^i/a_i \in (0, 1)$  and, keeping into account some obvious symmetry considerations (<sup>13</sup>), we only show the graphs for

$$x_\star^i \in (0, 1/2) \quad \text{for } i \in \{1, 2\} . \quad (4.107)$$

---

<sup>13</sup>Indeed, every component of the stress-energy VEV can be shown to be symmetric under the exchange  $x^i \leftrightarrow a_i - x^i$  (or  $x_\star^i \leftrightarrow 1 - x_\star^i$ ) for  $i \in \{1, 2\}$ .



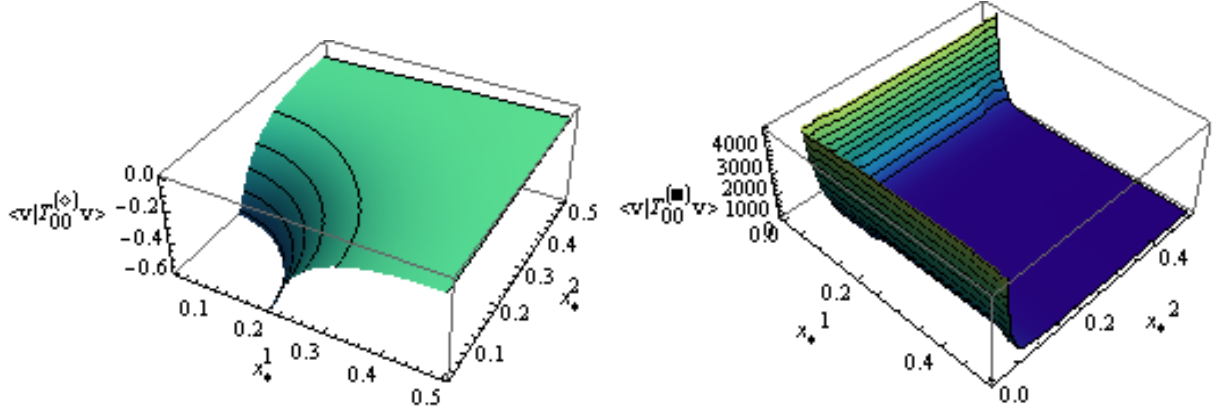


Figure 4.3: Graphs of  $(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$  for  $a_2 = 1$  ( $d = 2$ ).

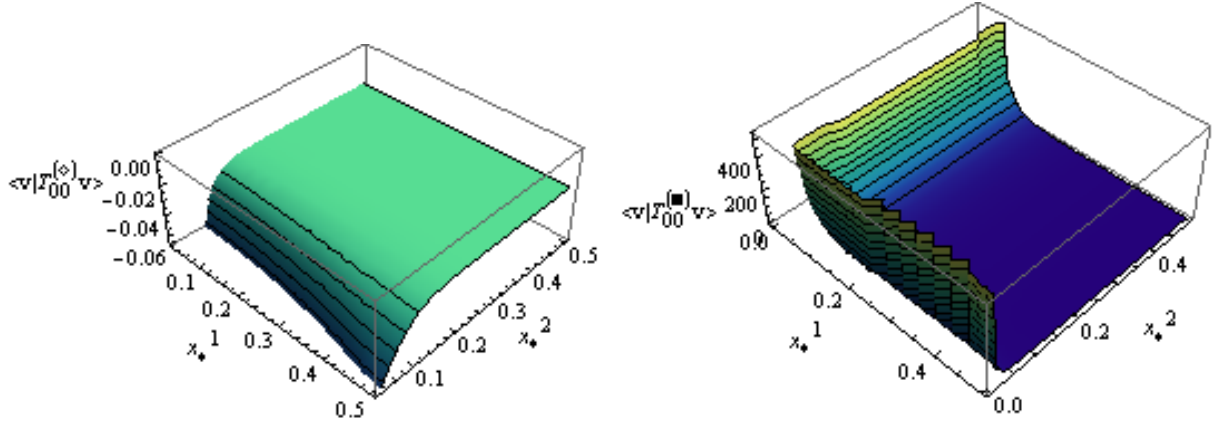


Figure 4.4: Graphs of  $(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$  for  $a_2 = 5$  ( $d = 2$ ).

Concerning the error estimates, for  $\mu, \nu \in \{0, 1, 2\}$  and  $\bullet \in \{\diamond, \blacksquare\}$ , let us introduce the following notation:

$$\mathcal{E}_{\mu\nu} := \begin{array}{l} \text{remainder corresponding to our approximation} \\ \text{by truncation of } (\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren} . \end{array} \quad (4.108)$$

On the one hand, for  $a_2 = 1$ , our choice  $N = 7$  ( $T = 1$ ,  $\alpha = 0.04$ ) yields the uniform bound

$$|\mathcal{E}_{\mu\nu}| \leq 3 \cdot 10^{-11} \quad \text{for } \mu, \nu \in \{0, 1, 2\} . \quad (4.109)$$

On the other hand, for  $a_2 = 5$ , our choice  $N = 9$  ( $T = 1$ ,  $\alpha = 0.04$ ) ensures

$$|\mathcal{E}_{\mu\nu}| \leq 8 \cdot 10^{-11} \quad \text{for } \mu, \nu \in \{0, 1, 2\} . \quad (4.110)$$

*The renormalized pressure on the boundary.* As in the construction of the general theory we consider, as an example, the pressure  $p_1^{ren}(\mathbf{x})$  at points  $\mathbf{x} \equiv (0, x^2)$  in the interior of the side  $\pi_{1,0}$ , making reference to the prescription (4.85). Fig. 4.5 shows the graphs obtained for  $p_1^{ren}(\mathbf{x})$  as a function of  $x_*^2 := x^2/a_2$  (again, choosing  $T = 1$  and truncating the related expansions to order  $N = 7$ , for  $a_2 = 1$ , and  $N = 9$ , for  $a_2 = 5$ ).

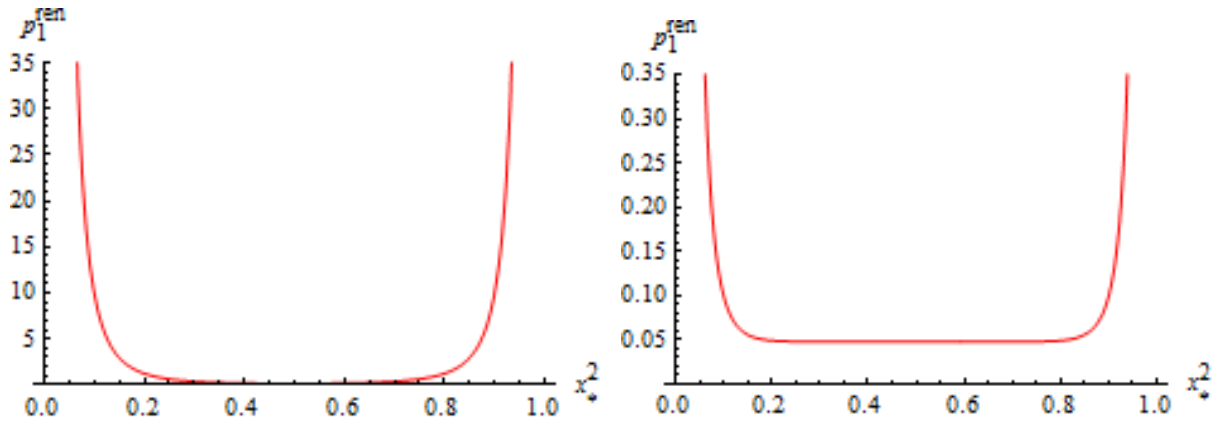


Figure 4.5: Graphs of  $p_1^{ren}$  for  $a_2 = 1$  (left) and  $a_2 = 5$  (right) ( $d = 2$ ).

As for the error, indicating with  $\epsilon_1$  the remainder associated to our approximation by truncation of  $p_1^{ren}$ , we obtain the following uniform estimates (setting  $\alpha = 0.04$ ):

$$\begin{aligned} |\epsilon_1| &\leq 2 \cdot 10^{-12} && \text{for } a_2 = 1 ; \\ |\epsilon_1| &\leq 5 \cdot 10^{-12} && \text{for } a_2 = 5 . \end{aligned} \quad (4.111)$$

Before moving on, let us mention that the renormalized pressure  $p_1^{ren}$  can be proved to possess the following asymptotic behaviour near the edge  $\mathbf{x} = \mathbf{0}$ , for all  $a_2 > 0$ :

$$p_1^{ren}(\mathbf{x}) = \frac{1}{32\pi(x^2)^3} + O((x^2)^2) \quad \text{for } \mathbf{x} = (0, x^2) \text{ and } x^2 \rightarrow 0^+ . \quad (4.112)$$

*The renormalized bulk energy.* Let us fix again  $a_1 = 1$  and consider this observable for different values of  $a_2$ . Using the decomposition into ( $>$ ) and ( $<$ ) parts and truncating the corresponding series at order  $N = 50$  (with  $T = 1$ ,  $\alpha = 0,04$ ), one can plot  $E^{ren}$  as a function of  $a_2$  (see Figure 4.6); with the choices made for the parameters  $a_1, T, N, \alpha$ , it can be proved that the error is smaller than  $2 \cdot 10^{-3}$  for any  $a_2 \in [0.05, 10]$ . Let us discuss some facts regarding the function  $a_2 \mapsto E^{ren}(a_2)$ , which can be read from the graph in Fig. 4.6 (the results reported hereafter are obtained using standard numerical methods, implemented in **Mathematica**).

i) There is only one point of maximum  $a_2^{\max}$ ; our approximation by truncation at order  $N = 50$  gives

$$a_2^{\max} = 0.72719110 \pm 10^{-8} , \quad E^{ren}(a_2^{\max}) = 0.04472675 \pm 10^{-8} . \quad (4.113)$$

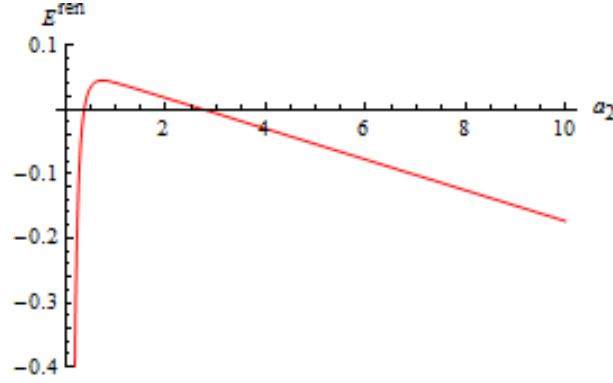


Figure 4.6: Graph of  $E^{ren}$  as function of  $a_2$  ( $d = 2$ ).

ii)  $E^{ren}$  vanishes for two values  $\bar{a}_2^{(1)} < \bar{a}_2^{(2)}$  of  $a_2$ ; these are found to be

$$\bar{a}_2^{(1)} = 0.36538151 \pm 10^{-8}, \quad \bar{a}_2^{(2)} = 2.73686534 \pm 10^{-8}. \quad (4.114)$$

$E^{ren}$  is positive for  $\bar{a}_2^{(1)} < a_2 < \bar{a}_2^{(2)}$  and negative elsewhere. This feature was also pointed out in [102]; therein it is stated that  $\bar{a}_2^{(2)} = (\bar{a}_2^{(1)})^{-1}$ , a relation (approximately) verified by the numerical values in Eq. (4.114).

iii) For  $a_2 \rightarrow 0^+$ ,  $E^{ren}$  has the asymptotic behaviour

$$E^{ren}(a_2) = \frac{e_0}{(a_2)^2} \left(1 + O(a_2)\right) \quad \text{with} \quad e_0 = -0.02391 \pm 10^{-5}. \quad (4.115)$$

iv) There are indications that  $E^{ren}$  approaches an asymptote for  $a_2 \rightarrow +\infty$ ; taking into account values of the abscissa up to  $a_2 = 100$ , we find that this asymptote is the straight line

$$y = m_E a_2 + q_E \quad \text{with} \quad \begin{cases} m_E = -0.02391416 \pm 10^{-8} \\ q_E = +0.06544985 \pm 10^{-8} \end{cases}. \quad (4.116)$$

Finally, let us mention that the numerical values of  $E^{ren}$  given by our previous analysis are in good agreement with those arising from the expansions in [25], a fact strongly indicating the equivalence between our approach and [25]. Let us also mention that the results of [25] about  $E^{ren}$  are equivalent to the ones of [11, 57, 77].

### 4.3 The case of parallel planes with Robin boundary conditions.

In the present conclusive section we consider a variant of the original setting studied by Casimir in his seminal paper [35], involving a massless field confined between two parallel planes. Let us recall that we already analyzed this type of configuration in our previous work [65] (see also [63] for the three-dimensional case with Dirichlet boundary conditions

and [64] for the one-dimensional analogue of a segment); therein, working in arbitrary odd spatial dimension  $d$  (also greater than  $d = 3$ ), we considered several kinds of boundary conditions, namely of Dirichlet, Neumann, mixed<sup>(14)</sup> and periodic type. For each one of these specific models we computed the renormalized VEVs of several observables. To this purpose, using the methods described in [64] and reformulated more rigorously in the present manuscript, in [65] we developed a series of general computational rules, independent of the boundary conditions prescribed on the (hyper-)planes; these general rules rely, in particular, on the fact that the configuration under analysis is of *slab type*<sup>(15)</sup> (so that it suffices to study the reduced one-dimensional problem of a segment) and on the fact that the corresponding cylinder kernel possesses some general suitable features. In the subsequent paragraphs we first recall briefly the above mentioned general rules and then use them to study the case of a massless field fulfilling a particular type of Robin conditions on the boundary planes. In the specific setting under analysis, it is possible to derive an explicit integral representation for the cylinder kernel corresponding to the reduced one-dimensional model; this representation allows to infer that the mentioned kernel fulfills the hypotheses of Theorem 2.93, so that the analytic continuation of the related Dirichlet kernel at the points of interest can be computed by means of the residue theorem (see, in particular, Eq. (2.361)). Finally, these facts are used to obtain exact expressions for the renormalized VEV of the stress-energy tensor (we plan to discuss the total vacuum energy per unit area and the pressure on the boundary elsewhere [68]).

Needless to say, the literature on the Casimir effect for the configuration with two parallel planes is immense, both regarding local and global aspects; following [65], here we only cite a few references. In his seminal paper [35], using an exponential cut-off regularization along with Abel-Plana resummation, Casimir was the first to compute the total energy and the boundary forces for the case of two parallel planes; concerning local aspects, the foremost derivation of the full stress-energy tensor VEV was given by Brown and Maclay [29], using a point-splitting technique. Computation of both global and local quantities for this model was later repropoed by several authors, using various regularization techniques: see, e.g., the monographies by Milton [110], Elizalde et al. [56, 57], Bordag et al. [25] (see, as well, the works cited therein).

The first to address the case of Robin boundary conditions were Romeo and Saharian [133], who used a generalized version of the Abel-Plana formula to obtain the renormalized

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<sup>14</sup>Here the nomenclature “mixed boundary conditions” is used to indicate the case where Dirichlet conditions are prescribed on one of the planes, while Neumann conditions are prescribed on the other.

<sup>15</sup>By definition, this means that

$$\Omega = \Omega_1 \times \mathbb{R}^{d_2} \ni \mathbf{x} \equiv (\mathbf{x}_1, \mathbf{x}_2), \quad V(\mathbf{x}) = V(\mathbf{x}_1),$$

with  $\Omega_1 \subset \mathbb{R}^{d_1}$  ( $d_1 + d_2 = d$ ) a suitable domain, and that the boundary conditions refer to  $\partial\Omega_1 \times \mathbb{R}^{d_2}$ . In this case the relevant operators are  $\mathcal{A}_1 := -\Delta_1 + V$  acting in  $\mathcal{H}_1 := L^2(\Omega_1)$ ,  $\mathcal{A}_2 := -\Delta_2$  acting in  $\mathcal{H}_2 := L^2(\mathbb{R}^{d_2})$  and  $\mathcal{A} = \mathcal{A}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \mathcal{A}_2 = -\Delta + V(\mathbf{x}_1)$  acting in  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 = L^2(\Omega)$  (with  $\mathbb{I}_1, \mathbb{I}_2$  indicating the identity operators on  $L^2(\Omega_1)$  and  $L^2(\mathbb{R}^{d_2})$ , respectively). See [64] for more details; we refer, in particular, to subsection 3.18 and to the related Appendix E.

stress-energy VEV and zeta techniques to compute the renormalized total vacuum energy. Analogous configurations were later considered by Saharian et al. [137] (dealing with uniformly accelerated plates, described using Rindler coordinates) and by Setare [144] (treating a case with de Sitter background spacetime); see also [9]. All these works use primarily regularization techniques different from the zeta approach; on the contrary, the analysis we present hereafter only relies on ZR in the general formulation described in the previous chapters of the present manuscript.

### Introducing the problem.

We consider the  $d$ -dimensional configuration where

$$\Omega := (0, a) \times \mathbb{R}^{d-1} \quad (a > 0), \quad V = 0; \quad (4.117)$$

the above choices correspond to a massless scalar field confined between two parallel hyperplanes set at a distance  $a$ , with no background potential. The boundary  $\partial\Omega$  of the spatial domain is composed by the planes

$$\pi_0 = \{\mathbf{x} \in \mathbb{R}^d \mid x^1 = 0\}, \quad \pi_a = \{\mathbf{x} \in \mathbb{R}^d \mid x^1 = a\}. \quad (4.118)$$

Boundary conditions of Robin type are generically established setting, for some given parameters  $\beta_0, \beta_a \in \mathbb{R}$ ,

$$(1 + \beta_0 \partial_{\mathbf{n}}) \hat{\varphi} \Big|_{\pi_0} = 0, \quad (1 + \beta_a \partial_{\mathbf{n}}) \hat{\varphi} \Big|_{\pi_a} = 0 \quad (4.119)$$

(here, as usual,  $\partial_{\mathbf{n}}$  indicates the derivative in the outer direction normal to the boundary). The case where  $\beta_0 \neq -\beta_a$  can only be treated by perturbation theory<sup>(16)</sup>; on the contrary, in the following we focus the attention to the specific setting where

$$\beta_0 = -\beta_a \equiv \beta \in (0, +\infty), \quad (4.120)$$

since in this case it is possible to perform a fully explicit analysis. In view of the above considerations, the boundary conditions (4.119) reduce to

$$(1 - \beta \partial_{x^1}) \hat{\varphi} \Big|_{\pi_0} = 0, \quad (1 - \beta \partial_{x^1}) \hat{\varphi} \Big|_{\pi_a} = 0. \quad (4.121)$$

In passing, let us point out that the above constraints correspond to the usual Dirichlet conditions for  $\beta = 0$ , while they formally reduce to Neumann conditions in the limit of large  $\beta$ <sup>(17)</sup>. Moreover, the case with  $\beta < 0$  can be recovered at the end by obvious symmetry arguments, making the replacement  $x^1 \mapsto a - x^1$ .

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<sup>16</sup>In fact, in this case, only implicit expressions can be derived for the eigenvalues of the Laplacian, which are a main ingredient for the following developments.

<sup>17</sup>By elementary dimensional analysis arguments, it appears that this statement must be interpreted in terms of the adimensional ratio  $\beta/a$ , meaning that the limit  $\beta/a \rightarrow +\infty$  has to be considered.

Keeping into account the boundary conditions (4.121), also in this case we put

$$\mathcal{A} := -\Delta ; \quad (4.122)$$

this is strictly positive and self-adjoint on  $\mathcal{H} = L^2(\Omega)$ , with domain  $\mathcal{D}_{\mathcal{A}} := \{f \in L^2(\Omega) \mid (1 - \beta \partial_{x^1})f \in H^1(\Omega), \Delta f \in L^2(\Omega) \text{ and } (1 - \beta \partial_{x^1})f \upharpoonright \pi_0 = (1 - \beta \partial_{x^1})f \upharpoonright \pi_a = 0\}$  <sup>(18)</sup>. Again,  $\mathcal{A}$  is an *admissible operator* in the sense of definition 2.37; moreover, its spectrum can be explicitly determined and is given by

$$\sigma(\mathcal{A}) = \left\{ \omega_{\mathbf{k},n}^2 := |\mathbf{k}|^2 + \frac{n^2 \pi^2}{a^2} \mid \mathbf{k} \in \mathbb{R}^{d-1}, n \in \{1, 2, 3, \dots\} \right\} \quad (4.123)$$

<sup>(19)</sup>. In view of the above considerations, the general framework of Chapter 2 can be employed also in this case; in particular, the Dirichlet kernel associated to  $\mathcal{A}$  and its derivatives are well-defined integral kernels.

Let us stress that the setting under analysis is, in fact, a *slab* configuration; we discussed in detail this type of configurations in our previous work [64] (see in particular subsection 3.18 therein), giving some general rules allowing to compute the Dirichlet kernel and its derivatives evaluated along the diagonal in terms of the integral kernels associated to a lower dimensional problem. In the subsequent paragraph we briefly recall the main tools related to the above considerations, required for the evaluation of the stress-energy VEV to be described in the following.

Before proceeding to this topic, let us point out the following fact.

*Remark 4.2.* Throughout this section we assume

$$d \text{ odd , } d \geq 3 ; \quad (4.124)$$

this hypothesis is purely technical and will be motivated later (see the comments before Eq. (4.142)). The case  $d = 1$ , here excluded, could be discussed using a slight variation of the computational rules presented here (compare also with the analysis described in Section 6 of [64]); for brevity, we defer this topic to a future work [68]. Let us also anticipate that at the end of the present section we will consider more in detail the case  $d = 3$ , performing the required computations explicitly.

### Reduction to a one-dimensional problem.

As mentioned previously, it appears from Eq. (4.117) that the configuration under analysis is of slab type (see the footnote 15 on page 184 and the references given therein). In particular, in the present setting, we have

$$\Omega = \Omega_1 \times \mathbb{R}^{d-1} \quad \text{with } \Omega_1 = (0, a) \subset \mathbb{R} \quad (\text{plus, } V = 0) ; \quad (4.125)$$

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<sup>18</sup>Similarly to what was said in the Footnote 7 of page 169, using the eigenfunction expansion of  $\mathcal{A}$ , it can be shown that there holds  $\mathcal{D}_{\mathcal{A}} = \{f \in H^2(\Omega) \mid (1 - \beta \partial_{x^1})f \upharpoonright \pi_0 = (1 - \beta \partial_{x^1})f \upharpoonright \pi_a = 0\}$ .

<sup>19</sup>In this case the the parameter  $\varepsilon > 0$  fulfilling  $\sigma(\mathcal{A}) \subset [\varepsilon, +\infty)$ , can be chosen to be  $\varepsilon := (\pi/a)^2$ .

therefore, the admissible operator  $\mathcal{A}$  on  $L^2(\Omega)$  can be expressed as (with the domain specifications provided by the subsequent considerations)

$$\mathcal{A} = \mathcal{A}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \mathcal{A}_2 , \quad (4.126)$$

where we have introduced the two operators

$$\begin{aligned} \mathcal{A}_1 &:= -\partial_{x^1 x^1} : \text{Dom}(\mathcal{A}_1) \subset L^2(0, a) \rightarrow L^2(0, a) , \\ \mathcal{A}_2 &:= -\sum_{i=2}^d \partial_{x^i x^i} : \text{Dom}(\mathcal{A}_2) \subset L^2(\mathbb{R}^{d-1}) \rightarrow L^2(\mathbb{R}^{d-1}) . \end{aligned} \quad (4.127)$$

Here the domains of definitions  $\text{Dom}(\mathcal{A}_1), \text{Dom}(\mathcal{A}_2)$  are determined by the boundary conditions described in Eq. (4.121); more precisely, we have

$$\begin{aligned} \text{Dom}(\mathcal{A}_1) &:= \{f \in L^2(0, a) \mid \partial_{x^1 x^1} f \in L^2(0, a), (1 - \beta \partial_{x^1})f(0) = (1 - \beta \partial_{x^1})f(a) = 0\} , \\ \text{Dom}(\mathcal{A}_2) &:= \{f \in L^2(\mathbb{R}^{d-1}) \mid \partial_{x^1 x^1} f \in L^2(\mathbb{R}^{d-1})\} . \end{aligned} \quad (4.128)$$

<sup>(20)</sup>. Let us stress that  $\mathcal{A}_1$  is itself an admissible operator in the sense of Definition 2.37. Furthermore, it has purely discrete spectrum

$$\sigma(\mathcal{A}_1) = \left\{ \omega_n^2 := \frac{n^2 \pi^2}{a^2} \mid n \in \{1, 2, 3, \dots\} \right\} , \quad (4.129)$$

and it possesses a complete orthonormal set of eigenfunctions in  $L^2(0, a)$ , corresponding to the eigenvalues  $(\omega_n^2)$  in Eq. (4.129), given by

$$F_n(x^1) := \sqrt{\frac{2}{a(1 + \beta^2 \omega_n^2)}} \left( \sin(\omega_n x^1) + \beta \omega_n \cos(\omega_n x^1) \right) \quad (x^1 \in (0, a)) . \quad (4.130)$$

In view of the above considerations, we can resort to the general framework of Chapter 2, to speak about the integral kernels associated to  $\mathcal{A}_1$  and about the related traces. In particular, in accordance with the general notations adopted in the present manuscript, we indicate the reduced Dirichlet and cylinder kernel with  $\mathcal{A}_1^{-s}(x^1, y^1)$  and  $e^{-t\sqrt{\mathcal{A}_1}}(x^1, y^1)$  (for  $x^1, y^1 \in (0, a)$ ), respectively; similarly, the corresponding traces will be denoted with  $\text{Tr } \mathcal{A}_1^{-s}$  and  $\text{Tr } e^{-t\sqrt{\mathcal{A}_1}}$ .

*General relations between  $\mathcal{A}^{-s}(\cdot, \cdot)$  and  $\mathcal{A}_1^{-s}(\cdot, \cdot)$ .* It can be proved that the Dirichlet kernel  $\mathcal{A}^{-s}(\mathbf{x}, \mathbf{y})$  evaluated along the diagonal  $\mathbf{y} = \mathbf{x}$  can be expressed in terms of the reduced kernel  $\mathcal{A}_1^{-s}(x^1, y^1)$  at  $y^1 = x^1$ ; analogous relations can be derived also for the

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<sup>20</sup>For any  $f \in \text{Dom}(\mathcal{A}_1)$  it follows that  $\partial_{x^1} f \in H^1(0, a)$ , so that  $\partial_{x^1} f(0)$  and  $\partial_{x^1} f(a)$  are well defined. Moreover, also in this case, using the eigenfunction expansion of  $\mathcal{A}_1$  and  $\mathcal{A}_2$  it can be shown that  $\text{Dom}(\mathcal{A}_1) = \{f \in H^2(0, a) \mid (1 - \beta \partial_{x^1})f(0) = (1 - \beta \partial_{x^1})f(a) = 0\}$ .

derivatives. Here, we are referring to Eq.s (3.115–3.118) of [64]; in the present setting, for any  $u \in \Sigma_d$ , these relations reduce to

$$\mathcal{A}^{-\frac{u-1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{\Gamma(\frac{u-d}{2})}{(4\pi)^{\frac{d-1}{2}} \Gamma(\frac{u-1}{2})} \mathcal{A}_1^{-\frac{u-d}{2}}(x^1, y^1) \Big|_{y^1=x^1} ; \quad (4.131)$$

$$\begin{aligned} \partial_{x^i y^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= \partial_{x^i x^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \partial_{y^i y^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = 0 \\ \text{for } i = 1 \text{ and } j \in \{2, \dots, d\} \text{ or } i \in \{2, \dots, d\} \text{ and } j = 1 ; \end{aligned} \quad (4.132)$$

$$\partial_{zw} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{\Gamma(\frac{u-d+2}{2})}{(4\pi)^{\frac{d-1}{2}} \Gamma(\frac{u+1}{2})} \partial_{zw} \mathcal{A}_1^{-\frac{u-d+2}{2}}(x^1, y^1) \Big|_{y^1=x^1} \text{ for } z, w \in \{x^1, y^1\}; \quad (4.133)$$

$$\begin{aligned} \partial_{x^i y^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} &= -\partial_{x^i x^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = -\partial_{y^i y^j} \mathcal{A}^{-\frac{u+1}{2}}(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \\ &= \delta_{ij} \frac{\Gamma(\frac{u-d}{2})}{2(4\pi)^{\frac{d-1}{2}} \Gamma(\frac{u+1}{2})} \mathcal{A}_1^{-\frac{u-d}{2}}(x^1, y^1) \Big|_{y^1=x^1} \text{ for } i, j \in \{2, 3, \dots, d\}. \end{aligned} \quad (4.134)$$

The reduced cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$ . With some computational effort (see the Appendix), it is possible to express this integral kernel as follows, for all  $x^1, y^1 \in (0, a)$  and all  $\mathbf{t} \in (0, +\infty)$ :

$$\begin{aligned} e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) &= T_0(\mathbf{t}; x^1, y^1) + T_1(\mathbf{t}; x^1, y^1) + T_2(\mathbf{t}; x^1, y^1) \quad \text{with} \\ T_0(\mathbf{t}; x^1, y^1) &= \frac{1}{2a} \left[ \frac{\cos(\frac{\pi}{a}(x^1 - y^1)) - e^{-\frac{\pi}{a}\mathbf{t}}}{\cosh(\frac{\pi}{a}\mathbf{t}) - \cos(\frac{\pi}{a}(x^1 - y^1))} - \frac{\cos(\frac{\pi}{a}(x^1 + y^1)) - e^{-\frac{\pi}{a}\mathbf{t}}}{\cosh(\frac{\pi}{a}\mathbf{t}) - \cos(\frac{\pi}{a}(x^1 + y^1))} \right], \\ T_1(\mathbf{t}; x^1, y^1) &= \int_0^{+\infty} d\mathbf{v} \cos \mathbf{v} S_1(\mathbf{t} + |\beta|\mathbf{v}; x^1, y^1), \\ T_2(\mathbf{t}; x^1, y^1) &= S_2(\mathbf{t}; x^1, y^1) - \int_0^{+\infty} d\mathbf{v} \sin \mathbf{v} S_2(\mathbf{t} + |\beta|\mathbf{v}; x^1, y^1), \end{aligned} \quad (4.135)$$

where the functions  $S_1, S_2$  are given by

$$S_1(\mathbf{t}; x^1, y^1) := \frac{1}{a} \left[ \frac{\sin(\frac{\pi}{a}(x^1 + y^1))}{\cosh(\frac{\pi}{a}\mathbf{t}) - \cos(\frac{\pi}{a}(x^1 + y^1))} \right], \quad (4.136)$$

$$S_2(\mathbf{t}; x^1, y^1) := \frac{1}{a} \left[ \frac{\cos(\frac{\pi}{a}(x^1 + y^1)) - e^{-\frac{\pi}{a}\mathbf{t}}}{\cosh(\frac{\pi}{a}\mathbf{t}) - \cos(\frac{\pi}{a}(x^1 + y^1))} \right]. \quad (4.137)$$

Before proceeding, let us point out some facts concerning the functions  $T_0, T_1, T_2$  introduced above to evaluate the reduced cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$ .



i)  $T_0$  is the cylinder kernel corresponding to the configuration of a segment  $(0, a)$  with Dirichlet boundary conditions (see [64], Eq. 6.20). Notice in particular that, for any fixed  $x^1, y^1 \in (0, a)$ , the map  $(0, +\infty) \ni \mathbf{t} \mapsto T_0(\mathbf{t}, x^1, y^1)$  extends to a function which is meromorphic in a complex neighbour of  $[0, +\infty)$ , with only a pole singularity in  $\mathbf{t} = 0$ , and which vanishes exponentially for  $\Re \mathbf{t} \rightarrow +\infty$ . Analogous considerations hold for its derivatives. ii) Making the change of integration variable  $\mathbf{v} = t + \beta \mathbf{w}$  and using some trivial trigonometric identities, the function  $T_1, T_2$  defined in Eq. (4.135) can be re-expressed as follows:

$$T_1(\mathbf{t}; x^1, y^1) = \tag{4.138}$$

$$\frac{1}{\beta} \left[ \cos\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \cos\left(\frac{\mathbf{w}}{\beta}\right) S_1(\mathbf{w}; x^1, y^1) + \sin\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \sin\left(\frac{\mathbf{w}}{\beta}\right) S_1(\mathbf{w}; x^1, y^1) \right]$$

$$T_2(\mathbf{t}; x^1, y^1) = S_2(\mathbf{t}; x^1, y^1) + \tag{4.139}$$

$$+ \frac{1}{\beta} \left[ \sin\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \cos\left(\frac{\mathbf{w}}{\beta}\right) S_2(\mathbf{w}; x^1, y^1) - \cos\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \sin\left(\frac{\mathbf{w}}{\beta}\right) S_2(\mathbf{w}; x^1, y^1) \right]$$

Using the above expressions, it can be shown (see the Appendix) that, for any fixed  $x^1, y^1 \in (0, a)$ , both the maps  $[0, +\infty) \ni \mathbf{t} \mapsto T_1(\mathbf{t}, x^1, y^1), T_2(\mathbf{t}, x^1, y^1)$  extend to functions which are analytic in a complex neighbour of  $[0, +\infty)$  and vanish exponentially for  $\Re \mathbf{t} \rightarrow +\infty$ ; moreover, their Taylor series in  $\mathbf{t} = 0$  can be determined explicitly (see Proposition .4 in the cited appendix). Analogous considerations hold for the spatial derivatives of  $T_1$  and  $T_2$ .

*The reduced Dirichlet kernel in terms of the reduced cylinder kernels.* In view of the features pointed out above for the reduced cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$  it appears that this function fulfills the assumptions of Theorem 2.93. Therefore, the analytic continuations of the related Dirichlet kernel  $\mathcal{A}_1^{-s}(\cdot, \cdot)$  and of its derivatives can be determined according to Eq. (2.360); in particular, we have

$$\mathcal{A}_1^{-\frac{u-d}{2}}(x^1, y^1) = \frac{e^{-i\pi(u-d)} \Gamma(d+1-u)}{2\pi i} \int_{\mathfrak{H}} d\mathbf{t} \mathbf{t}^{u-d-1} e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1); \tag{4.140}$$

$$\partial_{zw} \mathcal{A}_1^{-\frac{u-d+2}{2}}(x^1, y^1) = \frac{e^{-i\pi(u-d)} \Gamma(d-1-u)}{2\pi i} \int_{\mathfrak{H}} d\mathbf{t} \mathbf{t}^{u-d+1} \partial_{zw} e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) \tag{4.141}$$

for  $z, w \in \{x^1, y^1\}$

(let us recall that  $\mathfrak{H}$  denotes the Hankel contour).

### The stress-energy tensor.

Recall the expressions (3.107-3.109) giving the zeta-regularized stress-energy VEV in terms of the Dirichlet kernel and of its derivatives. Eq.s (4.131-4.134), along with the expressions (4.140) (4.141) for the reduced Dirichlet functions, allow to obtain integral representations for each component of the above mentioned VEV. These integral representations give the analytic continuation of the map  $\Sigma_{d+1} \ni u \mapsto (\mathbf{v} | \hat{T}_{\mu\nu}^u \mathbf{v})$  to the whole

complex plane; due to the assumption (4.124) on the spatial dimension  $d$ , this analytic continuation is regular at  $u = 0$ . So, the general prescription (3.124) reduces in the present setting to

$$(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren} := (\mathbf{v} | \hat{T}_{\mu\nu}^u(\mathbf{x}) \mathbf{v}) \Big|_{u=0}. \quad (4.142)$$

Due to the meromorphic nature of the reduced cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$  (and of its derivatives), the resulting integrals along the Hankel contour can be explicitly evaluated via the residue theorem; the final expressions for the non-vanishing components of the renormalized stress-energy VEV are ( $i \in \{2, \dots, d\}$ )

$$\begin{aligned} & (\mathbf{v} | \hat{T}_{00}(\mathbf{x}) \mathbf{v})_{ren} = - (\mathbf{v} | \hat{T}_{ii}(\mathbf{x}) \mathbf{v})_{ren} = \\ & - C_d \text{Res} \left( \mathbf{t}^{-(d+1)} \left[ \left( \xi - \frac{d-2}{4d} \right) d e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) + \right. \right. \\ & \quad \left. \left. + \frac{\mathbf{t}^2}{d-1} \left( \frac{1}{4} - \xi \right) \partial_{x^1 y^1} e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) \right]_{y^1=x^1}; 0 \right); \end{aligned} \quad (4.143)$$

$$\begin{aligned} & (\mathbf{v} | \hat{T}_{11}(\mathbf{x}) \mathbf{v})_{ren} = \\ & - C_d \text{Res} \left( \mathbf{t}^{-(d+1)} \left[ \left( \frac{1}{4} - \xi \right) d e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) + \right. \right. \\ & \quad \left. \left. + \frac{\mathbf{t}^2}{d-1} \left( \frac{1}{4} \partial_{x^1 y^1} - \xi \partial_{x^1 x^1} \right) e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(x^1, y^1) \right]_{y^1=x^1}; 0 \right); \end{aligned} \quad (4.144)$$

Here, for the sake of brevity, we have put

$$C_d := (-\pi)^{-\frac{d-1}{2}} \Gamma\left(\frac{d+1}{2}\right). \quad (4.145)$$

We repeat that, in the above,  $d$  is an arbitrary odd dimension  $> 1$ . In the following paragraph we will report the explicit expressions for the renormalized stress-energy components arising from Eq.s (4.143-4.144) in the case of spatial dimension  $d = 3$ ; again, we will give the final results in the form described in subsection 3.2, separating the conformal and non-conformal parts (see, in particular, Eq. (3.131)), noting that Eq. (3.127) gives

$$\xi_3 = \frac{1}{6}. \quad (4.146)$$

### The previous results in spatial dimension $d = 3$ .

As an example, let us compute the renormalized stress-energy VEV in the case where  $d = 3$ . To this purpose, recall the explicit expression (4.135) for the reduced cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$  (along with the results of the Appendix) regarding its Laurent series at  $\mathbf{t} = 0$ ; then, separating the conformal ( $\diamond$ ) and non-conformal ( $\blacksquare$ ) parts, in the present setting the general identities (4.143-4.144) yield

$$\begin{aligned}
 (\mathbf{v} | \hat{T}_{00}^{(\diamond)}(\mathbf{x}) \mathbf{v})_{ren} &= -(\mathbf{v} | \hat{T}_{22}^{(\diamond)}(\mathbf{x}) \mathbf{v})_{ren} = -(\mathbf{v} | \hat{T}_{33}^{(\diamond)}(\mathbf{x}) \mathbf{v})_{ren} = \\
 &= -\frac{\pi^2}{1440a^4} - \frac{1}{24\pi a^4} \left[ \left( \frac{a}{\beta} \right)^2 \frac{\pi}{2 \sin^2(\frac{\pi x^1}{a})} - \left( \frac{a}{\beta} \right)^3 \frac{\cos(\frac{\pi x^1}{a})}{\sin(\frac{\pi x^1}{a})} + \right. \\
 &\quad \left. + \left( \frac{a}{\beta} \right)^4 \int_0^{+\infty} dt (1 - \beta^2 \partial_{x^1 y^1}) \left( \cos\left(\frac{\mathbf{t}}{\beta}\right) S_2(\mathbf{t}; x^1, y^1) + \sin\left(\frac{\mathbf{t}}{\beta}\right) S_1(\mathbf{t}; x^1, y^1) \right) \right]_{y^1=x^1},
 \end{aligned} \tag{4.147}$$

$$\begin{aligned}
 (\mathbf{v} | \hat{T}_{00}^{(\blacksquare)}(\mathbf{x}) \mathbf{v})_{ren} &= -(\mathbf{v} | \hat{T}_{22}^{(\blacksquare)}(\mathbf{x}) \mathbf{v})_{ren} = -(\mathbf{v} | \hat{T}_{33}^{(\blacksquare)}(\mathbf{x}) \mathbf{v})_{ren} = \\
 &= -\frac{\pi^2(3-2\sin^2(\frac{\pi}{a}x^1))}{8a^4 \sin^4(\frac{\pi}{a}x^1)} + \frac{1}{2\pi a^4} \left[ \left( \frac{a}{\beta} \right) \frac{\pi^2 \cos(\frac{\pi}{a}x^1)}{\sin^3(\frac{\pi}{a}x^1)} - \left( \frac{a}{\beta} \right)^2 \frac{\pi}{2 \sin^2(\frac{\pi}{a}x^1)} + \left( \frac{a}{\beta} \right)^3 \frac{\cos(\frac{\pi}{a}x^1)}{\sin(\frac{\pi}{a}x^1)} + \right. \\
 &\quad \left. + \left( \frac{a}{\beta} \right)^4 \int_0^{+\infty} dt (1 + \beta^2 \partial_{x^1 y^1}) \left( \cos\left(\frac{\mathbf{t}}{\beta}\right) S_2(\mathbf{t}; x^1, y^1) + \sin\left(\frac{\mathbf{t}}{\beta}\right) S_1(\mathbf{t}; x^1, y^1) \right) \right]_{y^1=x^1},
 \end{aligned} \tag{4.148}$$

$$\begin{aligned}
 (\mathbf{v} | \hat{T}_{11}^{(\diamond)}(\mathbf{x}) \mathbf{v})_{ren} &= \\
 &= -\frac{3\pi^2}{1440a^4} - \frac{1}{24\pi a^4} \left[ \left( \frac{a}{\beta} \right)^2 \frac{\pi}{2 \sin^2(\frac{\pi x^1}{a})} - \left( \frac{a}{\beta} \right)^3 \frac{\cos(\frac{\pi x^1}{a})}{\sin(\frac{\pi x^1}{a})} + \right. \\
 &\quad \left. + \left( \frac{a}{\beta} \right)^4 \int_0^{+\infty} dt (1 - 3\beta^2 \partial_{x^1 y^1} + 2\beta^2 \partial_{x^1 x^1}) \left( \cos\left(\frac{\mathbf{t}}{\beta}\right) S_2(\mathbf{t}; x^1, y^1) + \sin\left(\frac{\mathbf{t}}{\beta}\right) S_1(\mathbf{t}; x^1, y^1) \right) \right]_{y^1=x^1},
 \end{aligned} \tag{4.149}$$

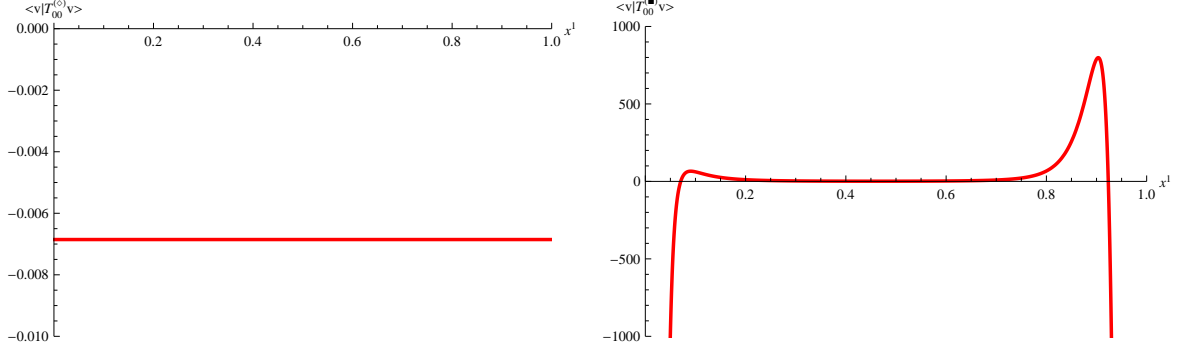
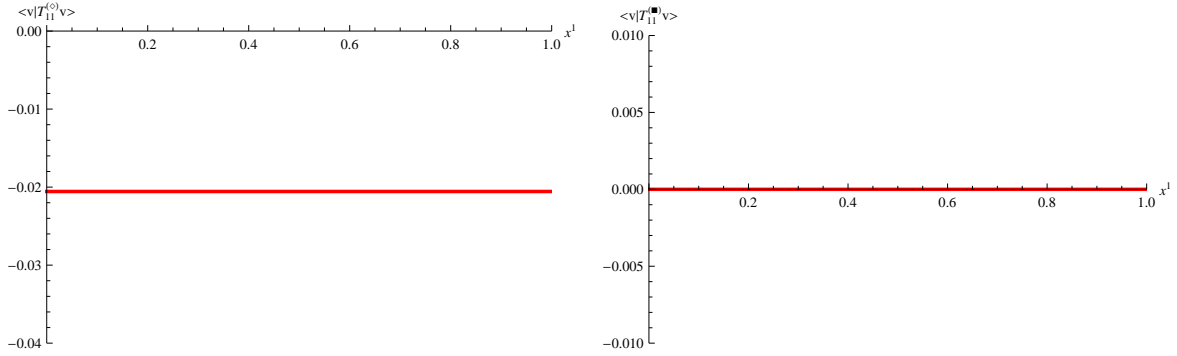
$$\begin{aligned}
 (\mathbf{v} | \hat{T}_{11}^{(\blacksquare)}(\mathbf{x}) \mathbf{v})_{ren} &= \\
 &= \frac{1}{2\pi a^4} \left[ \left( \frac{a}{\beta} \right)^2 \frac{\pi}{2 \sin^2(\frac{\pi}{a}x^1)} - \left( \frac{a}{\beta} \right)^3 \frac{\cos(\frac{\pi}{a}x^1)}{\sin(\frac{\pi}{a}x^1)} + \right. \\
 &\quad \left. + \left( \frac{a}{\beta} \right)^4 \int_0^{+\infty} dt (1 - \beta^2 \partial_{x^1 x^1}) \left( \cos\left(\frac{\mathbf{t}}{\beta}\right) S_2(\mathbf{t}; x^1, y^1) + \sin\left(\frac{\mathbf{t}}{\beta}\right) S_1(\mathbf{t}; x^1, y^1) \right) \right]_{y^1=x^1}
 \end{aligned} \tag{4.150}$$

(here  $S_1$  and  $S_2$  are the functions given in Eq.s (4.136) and (4.137), respectively).

Let us point out a couple of facts appearing from the expressions (4.147-4.150) obtained above for the renormalized stress-energy VEV components. On the one hand, as was to be expected due to clear symmetry considerations, the renormalized VEV  $(\mathbf{v} | \hat{T}_{\mu\nu} \mathbf{v})_{ren}$  only depends on the spatial coordinates  $x^1 \in (0, a)$ , corresponding to the direction orthogonal to the planes; so, with a slight abuse of notation, we put (for  $\mu, \nu \in \{0, \dots, 3\}$ )

$$(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren} \equiv (\mathbf{v} | \hat{T}_{\mu\nu}(x^1) \mathbf{v})_{ren} . \tag{4.151}$$

In fact, the same statement can be easily proven to hold for any spatial dimension  $d$  and for the regularized stress-energy VEV, as well. On the other hand, keeping only the contributions not depending on the parameter  $\beta$  in the above expressions (4.147-4.150), one recovers the renormalized stress-energy VEV corresponding to the case of Dirichlet boundary conditions for the same geometrical configuration with two parallel planes <sup>(21)</sup>.

Figure 4.7: Graphs of  $(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$ .Figure 4.8: Graphs of  $(\mathbf{v} | \hat{T}_{11}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{11}^{(\blacksquare)} \mathbf{v})_{ren}$ .

In conclusion, let us present, some results which can be obtained by numerical evaluation for the functions

$$(0, a) \ni x^1 \mapsto (\mathbf{v} | \hat{T}_{\mu\mu}^{(\bullet)}(x^1) \mathbf{v})_{ren} \quad \text{for } \mu \in \{0, 1\} \quad \text{and } \bullet \in \{\diamond, \blacksquare\}. \quad (4.152)$$

To this purpose, we fix

$$a = 1 \quad (4.153)$$

and consider several values for the parameter  $\beta \in (0, +\infty)$ . As an example, we report in Figs 4.7 and 4.8 the graphs obtained for  $\beta = 0.04$ , evaluating numerically the expressions

<sup>21</sup>In fact, the renormalized stress-energy VEV for a massless scalar field confined between two parallel planes with Dirichlet boundary conditions in spatial dimension  $d = 3$  is (see, e.g., [21, 59, 64, 75, 110])

$$(\mathbf{v} | \hat{T}_{\mu\nu}(\mathbf{x}) \mathbf{v})_{ren} = \frac{\pi^2}{1440a^4} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -3 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \left(\xi - \frac{1}{6}\right) \frac{\pi^2(3 - 2 \sin^2(\frac{\pi}{a} x^1))}{8a^4 \sin^4(\frac{\pi}{a} x^1)} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

(4.147-4.150) (including the integrals appearing therein) with the aid of *Matematica* <sup>(22)</sup>. In view of the above figures, all the functions  $(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren}$ ,  $(\mathbf{v} | \hat{T}_{11}^{(\diamond)} \mathbf{v})_{ren}$  and  $(\mathbf{v} | \hat{T}_{11}^{(\blacksquare)} \mathbf{v})_{ren}$  appear to be constant, assuming the approximate numerical values

$$\begin{aligned} (\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren} &\simeq -0.006853 \dots, \\ (\mathbf{v} | \hat{T}_{11}^{(\diamond)} \mathbf{v})_{ren} &\simeq -0.020561 \dots, \\ (\mathbf{v} | \hat{T}_{11}^{(\blacksquare)} \mathbf{v})_{ren} &\simeq 0. \end{aligned} \tag{4.154}$$

As a matter of fact, it can be checked by direct inspection that the above results continue to hold for any fixed  $\beta \in (0, +\infty)$ , so that all the components in Eq. (4.154) appear to be independent of the parameter  $\beta$ . Let us also stress that the above results agree with the exact results corresponding to both the limiting cases of Dirichlet ( $\beta \rightarrow 0^+$ ) and Neumann ( $\beta \rightarrow +\infty$ ) conditions <sup>(23)</sup>.

In view of the above considerations, it appears that the only term depending non-trivially on the parameter  $\beta$  (and on the coordinate  $x^1$ ) is  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$ ; in Fig. 4.9 we show the graph of this term as a function of  $x^1 \in (0, 1)$  and  $\beta \in (0, 1)$ .

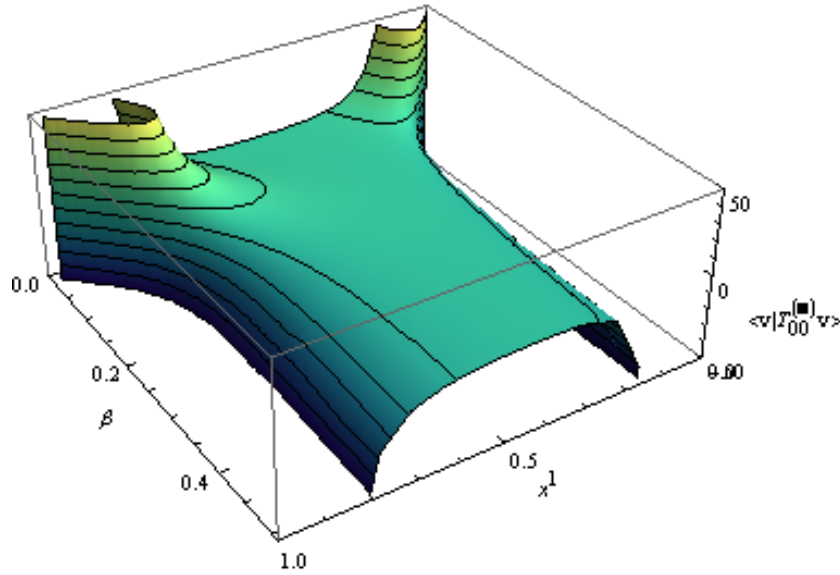


Figure 4.9: Graphs of  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$  as a function of  $x^1, \beta$ .

We plan to give a more detailed analysis of the present configuration, discussing also the total energy and the boundary pressure, in a future work [68].

<sup>22</sup>The lack of symmetry under the exchange  $x^1 \leftrightarrow a - x^1$  in the graph for  $(\mathbf{v} | \hat{T}_{00}^{(\blacksquare)} \mathbf{v})_{ren}$  (see Fig. 4.7) is due to the non-symmetric boundary conditions (4.121).

<sup>23</sup>In fact, in both these cases (with the present choice  $a = 1$ ), there holds (see, e.g., [65])

$$(\mathbf{v} | \hat{T}_{00}^{(\diamond)} \mathbf{v})_{ren} = -\frac{\pi^2}{1440} \simeq -0.006853 \dots, \quad (\mathbf{v} | \hat{T}_{11}^{(\diamond)} \mathbf{v})_{ren} = -\frac{3\pi^2}{1440} \simeq -0.020561 \dots, \quad (\mathbf{v} | \hat{T}_{11}^{(\blacksquare)} \mathbf{v})_{ren} = 0.$$



## Appendix. Some results for the cylinder kernel on a segment with Robin boundary conditions.

In the present appendix we collect some results which were mentioned and employed in Section 4.3, dealing with a massless scalar field confined between two parallel planes on which Robin boundary conditions of the type (4.119) of Robin type are prescribed (recall that  $\beta > 0$ ). Therein we argued that, since the configuration under analysis is a slab, it suffices to consider the reduced one-dimensional problem where  $\Omega_1 = (0, a)$  ( $a > 0$ ) and  $V = 0$ ; in particular, we have the admissible operator (see Eq. (4.127))

$$\mathcal{A}_1 := -\partial_{x^1 x^1} : \text{Dom}(\mathcal{A}_1) \subset L^2(0, a) \rightarrow L^2(0, a) , \quad (155)$$

$$\text{Dom}(\mathcal{A}_1) := \{f \in H^1(0, a) \mid \partial_{x^1 x^1} f \in L^2(0, a), (1 - \beta \partial_{x^1})f(0) = (1 - \beta \partial_{x^1})f(a) = 0\}$$

(notice that the domain  $\text{Dom}(\mathcal{A}_1)$  keeps into account the boundary conditions induced by those in Eq. (4.121)). We already mentioned (see Eq.s (4.123) (4.130)) that a complete orthonormal set of eigenfunctions of  $\mathcal{A}_1$  with corresponding eigenvalues is given by <sup>(24)</sup>

$$F_n(x^1) := \sqrt{\frac{2}{a(1 + \beta^2 \omega_n^2)}} \left( \sin(\omega_n x^1) + \beta \omega_n \cos(\omega_n x^1) \right) \quad (x^1 \in (0, a)) , \quad (156)$$

$$\omega_n^2 := \frac{n^2 \pi^2}{a^2} , \quad \text{for } n \in \{1, 2, 3, \dots\} .$$

---

<sup>24</sup>To prove this fact, it suffices to consider the differential problem

$$-\partial_{x^1 x^1} F_n = \omega_n^2 F_n , \quad F_n(0) - \beta F_n'(0) = 0 , \quad F_n(a) - \beta F_n'(a) = 0 , \quad \langle F_n | F_m \rangle_{L^2} = \delta_{nm} .$$

Considering the general solution  $F_n(x^1) = A_n \sin(\omega_n x^1) + B_n \cos(\omega_n x^1)$  and imposing the boundary conditions yields automatically the relations

$$B_n = \beta \omega_n A_n , \quad \omega_n = \frac{\pi n}{a} \quad (n \in \{1, 2, 3, \dots\}) .$$

Finally, the first identity can be used along with the normalization condition  $\langle F_n | F_m \rangle_{L^2} = \delta_{nm}$  to infer

$$A_n = \sqrt{\frac{2}{a(1 + \beta^2 \omega_n^2)}} .$$

In the following we will use these facts to compute explicitly the cylinder kernel  $e^{-t\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$  and to deduce the features possessed by this function, already mentioned in Section 4.3.

### Computation of $e^{-t\sqrt{\mathcal{A}_1}}(\cdot, \cdot)$ .

**Lemma .1.** *For any fixed  $t \in (0, +\infty)$ ,  $x^1, y^1 \in (0, a)$  and any fixed  $\beta \in (0, +\infty)$ , the cylinder kernel can be expressed as*

$$\begin{aligned}
 e^{-t\sqrt{\mathcal{A}_1}}(x^1, y^1) &= T_0(\mathbf{t}; x^1, y^1) + T_1(\mathbf{t}; x^1, y^1) + T_2(\mathbf{t}; x^1, y^1) \quad \text{where} \\
 T_0(\mathbf{t}; x^1, y^1) &:= \frac{1}{a} \sum_{n=1}^{+\infty} e^{-t\omega_n} \left( \cos(\omega_n(x^1 - y^1)) - \cos(\omega_n(x^1 + y^1)) \right), \\
 T_1(\mathbf{t}; x^1, y^1) &:= \frac{2}{a} \sum_{n=1}^{+\infty} e^{-t\omega_n} \frac{\beta\omega_n}{1 + \beta^2\omega_n^2} \sin(\omega_n(x^1 + y^1)), \\
 T_2(\mathbf{t}; x^1, y^1) &:= \frac{2}{a} \sum_{n=1}^{+\infty} e^{-t\omega_n} \frac{\beta^2\omega_n^2}{1 + \beta^2\omega_n^2} \cos(\omega_n(x^1 + y^1)),
 \end{aligned} \tag{157}$$

where  $\omega_n$  is given by (156). Moreover, all the series above are absolutely convergent.

*Proof.* It suffices to consider the eigenfunction expansion

$$e^{-t\sqrt{\mathcal{A}_1}}(x^1, y^1) = \sum_{n=1}^{+\infty} e^{-t\omega_n} F_n(x^1) \bar{F}_n(y^1)$$

along with the explicit expressions (156) for  $F_n$  and  $\omega_n$  (some elementary trigonometric identities must be used, as well). Absolute convergence can be easily proved recalling again that  $\omega_n = \frac{\pi n}{a}$ .  $\square$

**Lemma .2.** *There holds the relations of Eq. (4.135), i.e.,*

$$\begin{aligned}
 T_0(\mathbf{t}; x^1, y^1) &= \frac{1}{2a} \left[ \frac{\cos(\frac{\pi}{a}(x^1 - y^1)) - e^{-\frac{\pi}{a}t}}{\cosh(\frac{\pi}{a}t) - \cos(\frac{\pi}{a}(x^1 - y^1))} - \frac{\cos(\frac{\pi}{a}(x^1 + y^1)) - e^{-\frac{\pi}{a}t}}{\cosh(\frac{\pi}{a}t) - \cos(\frac{\pi}{a}(x^1 + y^1))} \right], \\
 T_1(\mathbf{t}; x^1, y^1) &= \int_0^{+\infty} d\mathbf{v} \cos \mathbf{v} S_1(\mathbf{t} + \beta\mathbf{v}; x^1, y^1), \\
 T_2(\mathbf{t}; x^1, y^1) &= S_2(\mathbf{t}; x^1, y^1) - \int_0^{+\infty} d\mathbf{v} \sin \mathbf{v} S_2(\mathbf{t} + \beta\mathbf{v}; x^1, y^1),
 \end{aligned}$$

where the functions  $S_1, S_2$  are as in Eq.s (4.136) (4.137).

*Proof.* We show how to compute the functions  $T_0, T_1, T_2$  in separate steps.

1 - *Computation of  $T_0$ .* Let us consider the corresponding series expansion given in Eq. (157); then, it suffices to express the trigonometric functions therein in terms of complex



exponentials, to sum the geometric series thus obtained and to perform some elementary algebraic manipulations.

2 - *Computation of  $T_1$ .* First notice that, for any  $\alpha > 0$ , there holds

$$\frac{\alpha}{1 + \alpha^2} = \int_0^{+\infty} d\mathbf{v} e^{-\alpha\mathbf{v}} \cos \mathbf{v} .$$

Using the above relation with  $\alpha = \beta\omega_k$ , the series expansion for  $T_1$  in Eq. (157) can be re-expressed as follows:

$$T_1(\mathbf{t}; x^1, y^1) = \frac{2}{a} \sum_{n=1}^{+\infty} \int_0^{+\infty} d\mathbf{v} e^{-(\mathbf{t}+\beta\mathbf{v})\omega_n} \cos \mathbf{v} \sin(\omega_n(x^1 + y^1)) . \quad (158)$$

Since  $|e^{-(\mathbf{t}+\beta\mathbf{v})\omega_n} \cos \mathbf{v} \sin(\omega_n(x^1 + y^1))| \leq e^{-(\mathbf{t}+\beta\mathbf{v})\omega_n}$ , by dominated convergence the sum and integral in the right-hand side of Eq. (158) can be interchanged; then, the thesis follows evaluating explicitly the sum over  $n = 1, 2, 3, \dots$  (again, this is a geometric series).

3 - *Computation of  $T_2$ .* First consider the identity

$$\frac{\alpha^2}{1 + \alpha^2} = 1 - \int_0^{+\infty} d\mathbf{v} e^{-\alpha\mathbf{v}} \sin \mathbf{v} ,$$

holding for any  $\alpha > 0$ . Then, the series expansion for  $T_2$  given in Eq. (157) can be reformulated as

$$T_2(\mathbf{t}; x^1, y^1) = \frac{2}{a} \sum_{n=1}^{+\infty} e^{-\mathbf{t}\omega_n} \cos(\omega_n(x^1 + y^1)) - \frac{2}{a} \sum_{n=1}^{+\infty} \int_0^{+\infty} d\mathbf{v} e^{-(\mathbf{t}+\beta\mathbf{v})\omega_n} \sin \mathbf{v} \cos(\omega_n(x^1 + y^1)) .$$

Again, the sum and the integral in the second term can be interchanged by dominated convergence theorem; also in this case the thesis follows evaluating explicitly the two sums over  $n = 1, 2, 3, \dots$  (once more, these are geometric series).  $\square$

### Regularity and asymptotic expansions for $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}}(, )$ .

Let us first state the following general result.

**Lemma .3.** *Let  $\mathcal{S} : [0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto \mathcal{S}(\mathbf{t})$  be an analytic function possessing the following properties:*

i.  *$\mathcal{S}$  has an analytic estension to a complex neighbour  $\mathcal{U} \subset \mathbb{C}$  of  $[0, +\infty)$ , with Laurent expansion in  $\mathbf{t} = 0$  of the form*

$$\mathcal{S}(\mathbf{t}) = \sum_{n=0}^{+\infty} \sigma_n \mathbf{t}^n . \quad (159)$$

ii. *there exist  $C, \alpha > 0$  such that, for all  $\mathbf{t} \in [0, +\infty)$ ,*

$$|\mathcal{S}(\mathbf{t})| \leq C e^{-\alpha\mathbf{t}} . \quad (160)$$

Then, the function

$$\mathcal{T} : [0, +\infty) \rightarrow \mathbb{R}, \quad \mathbf{t} \mapsto \mathcal{T}(\mathbf{t}) := \int_{\mathbf{t}}^{+\infty} dz \mathcal{S}(z), \quad (161)$$

is well defined and there hold the following results:

i)  $\mathcal{T}$  is analytic in  $\mathcal{U}$  and its Laurent expansion in  $\mathbf{t} = 0$  is given by

$$\mathcal{T}(\mathbf{t}) = \sum_{n=0}^{+\infty} \tau_n \mathbf{t}^n \quad \text{with} \quad (162)$$

$$\tau_0 := \int_0^{+\infty} dz \mathcal{S}(z), \quad \tau_n := -\frac{\sigma_{n-1}}{n} \quad \text{for } n \in \{1, 2, 3, \dots\};$$

ii) for all  $\mathbf{t} \in [0, +\infty)$ , there holds

$$|\mathcal{T}(\mathbf{t})| \leq \frac{C}{\alpha} e^{-\alpha \mathbf{t}}. \quad (163)$$

*Proof.* Let us first remark that the hypotheses on  $\mathcal{S}$  grant, in particular,  $\mathcal{S} \in C^0([0, +\infty))$  and  $\mathcal{S} \in L^1(0, +\infty) (\subset L^1(\mathbf{t}, +\infty))$ , for all  $\mathbf{t} \in [0, +\infty)$ ; then, the existence of the map (161) follows trivially. Hereafter we discuss in separate steps the proofs of statements i) and ii).

*Step 1 - Proof of item i).* Since  $\mathcal{S} \in C^0([0, +\infty)) \cap L^1(0, +\infty)$ , the map (161) is differentiable and  $\mathcal{T}'(\mathbf{t}) = -\mathcal{S}(\mathbf{t})$  for all  $\mathbf{t} \in [0, +\infty)$  (see, e.g., Thm.7.11 in [134]); then, hypothesis i. implies the analyticity of  $\mathcal{T}$  in  $\mathcal{U}$ . Moreover, by elementary results on power series, we have

$$\mathcal{T}(\mathbf{t}) = \mathcal{T}(0) + \sum_{m=0}^{+\infty} \left( -\frac{\sigma_m}{m+1} \right) \mathbf{t}^{m+1} \quad \text{for } \mathbf{t} \in \mathcal{U};$$

Eq. (162) follows relabeling the summation index ( $n := m + 1$ ) and noting that  $\tau_0 = \mathcal{T}(0) = \int_0^{+\infty} dz \mathcal{S}(z)$  by definition.

*Step 2 - Proof of item ii).* The bound (160) and the definition (161) imply, for all  $\mathbf{t} \in [0, +\infty)$ ,

$$|\mathcal{T}(\tau)| \leq C \int_{\mathbf{t}}^{+\infty} dz e^{-\alpha z};$$

evaluation of the elementary integral in the right-hand side above yields Eq. (163).  $\square$

To proceed, let us consider again the explicit expressions (4.136) (4.137) for the functions  $S_1, S_2$ ; in view of these expressions, it appears that

$$S_1, S_2 \in C^\infty([0, +\infty) \times (0, a) \times (0, a)). \quad (164)$$

Moreover, for any fixed  $x^1, y^1 \in (0, a)$ , both the maps  $[0, +\infty) \rightarrow \mathbb{R}, \mathbf{t} \mapsto S_1(\mathbf{t}; x^1, y^1), S_2(\mathbf{t}; x^1, y^1)$  are analytic and vanish exponentially; more precisely, for  $i = 1, 2$ , there exist constants  $C_i(x^1, y^1) > 0$  such that

$$|S_i(\mathbf{t}; x^1, y^1)| \leq C_i(x^1, y^1) e^{-\frac{\pi}{a}\mathbf{t}} \quad \text{for all } \mathbf{t} \in [0, +\infty). \quad (165)$$

The same considerations can be drawn for the derivatives  $\partial_{\mathbf{t}}^l \partial_{x^1}^m \partial_{y^1}^n S_i$  ( $i = 1, 2$ ), for any  $l, m, n \in \{0, 1, 2, \dots\}$ . Let us stress that, by Lebesgue's dominated convergence theorem, the differentiation and integration orders in the expressions for the derivatives of  $T_1, T_2$  (obtained starting from the relations in Eq. (4.135)) can be interchanged by Lebesgue dominated convergence theorem.

Then, we have the following result, mention in Section 4.3.

**Proposition .4.** *Consider the reduced cylinder kernel  $e^{-\bullet\sqrt{\mathcal{A}_1}(\cdot, \cdot)} : (0, +\infty) \times (0, a) \times (0, a), (\mathbf{t}, x^1, y^1) \mapsto e^{-\mathbf{t}\sqrt{\mathcal{A}_1}(x^1, y^1)}$ . There hold the following results:*

i)  $e^{-\bullet\sqrt{\mathcal{A}_1}(\cdot, \cdot)}$  is jointly smooth in all the variables, i.e.,  $e^{-\bullet\sqrt{\mathcal{A}_1}(\cdot, \cdot)} \in C^\infty((0, +\infty) \times (0, a) \times (0, a))$ ;

ii) for any  $l, m, n \in \{0, 1, 2, \dots\}$  and any fixed  $x^1 \in (0, a)$ , the map  $(0, +\infty) \rightarrow \mathbb{R}, \mathbf{t} \mapsto \partial_{\mathbf{t}}^l \partial_{x^1}^m \partial_{y^1}^n T(\mathbf{t}; x^1, y^1)|_{y^1=x^1}$  can be written in the form

$$\partial_{\mathbf{t}}^l \partial_{x^1}^m \partial_{y^1}^n T(\mathbf{t}; x^1, y^1) \Big|_{y^1=x^1} = \frac{1}{\mathbf{t}^q} J_{l,m,n}(\mathbf{t}; x^1) \quad (166)$$

where  $q \in \mathbb{N}$  (depending on  $l, m, n$ ) and the function  $J_{l,m,n}(\cdot; x^1) : [0, +\infty) \rightarrow \mathbb{R}, \mathbf{t} \mapsto J_{l,m,n}(\mathbf{t}; x^1)$  is analytic and vanishes exponentially<sup>(25)</sup>. In particular, there hold

$$T(\mathbf{t}; x^1, y^1) \Big|_{y^1=x^1} = \frac{1}{\mathbf{t}} J_{0,0,0}(\mathbf{t}; x^1), \quad (167)$$

$$\partial_{x^1}^m \partial_{y^1}^n T(\mathbf{t}; x^1, y^1) \Big|_{y^1=x^1} = \frac{1}{\mathbf{t}^3} J_{0,m,n}(\mathbf{t}; x^1) \quad \text{for } m, n \in \{0, 1, 2\} \text{ with } m+n = 2. \quad (168)$$

*Proof.* First of all, recall that Eq. (4.135) allows to express the cylinder kernel  $e^{-\mathbf{t}\sqrt{\mathcal{A}_1}(x^1, y^1)}$  as the sum of three functions, namely  $T_0(\mathbf{t}; x^1, y^1), T_1(\mathbf{t}; x^1, y^1)$  and  $T_2(\mathbf{t}; x^1, y^1)$ . Hereafter we discuss in separate steps their features, which in conclusion yield the thesis.

*Step 1 - The function  $T_0$ .* Consider the explicit expression given in Eq. (4.135); it can be easily checked by direct computations that, for any  $l, m, n \in \{0, 1, 2, \dots\}$  and any fixed  $x^1 \in (0, a)$ , there holds

$$\partial_{\mathbf{t}}^l \partial_{x^1}^m \partial_{y^1}^n T_0(\mathbf{t}; x^1, y^1) \Big|_{y^1=x^1} = \frac{1}{\mathbf{t}^q} J_{l,m,n}^{(0)}(\mathbf{t}; x^1)$$

---

<sup>25</sup>Explicit bounds could be derived but we will not report them here, since they involve cumbersome expressions and are not necessary for later developments

for some  $q \in \mathbb{N}$  and some function  $J_{l,m,n}^{(0)}(\cdot; x^1) : [0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto J_{l,m,n}(\mathbf{t}; x^1)$  which is analytic and vanishes exponentially. In particular, we have  $q = 1$  if  $(l, m, n) = (0, 0, 0)$  and  $q = 3$  if  $(l, m, n) \in \{(0, 2, 0), (0, 1, 1), (0, 0, 2)\}$ .

*Step 2 - The functions  $T_1, T_2$ .* We are going to show that, for any  $x^1, y^1 \in (0, a)$  (including the case  $y^1 = x^1$ ), the map  $[0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto T_1(\mathbf{t}; x^1, y^1)$  is analytic and exponentially decreasing for  $\mathbf{t} \rightarrow +\infty$ ; the very same arguments employed in the following can be used to derive analogous results for the function  $T_2$  and for any derivative of either  $T_1$  or  $T_2$ . Let us consider the representation for  $T_1$  given in Eq. (4.135); making the change of variable  $\mathbf{w} := \mathbf{t} + \beta\mathbf{v} \in [\mathbf{t}, +\infty)$  and using elementary trigonometric identities, this representation can be re-expressed as (see Eq. (4.138))

$$T_1(\mathbf{t}; x^1, y^1) = \frac{1}{\beta} \sin\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \sin\left(\frac{\mathbf{w}}{\beta}\right) S_1(\mathbf{w}; x^1, y^1) + \frac{1}{\beta} \cos\left(\frac{\mathbf{t}}{\beta}\right) \int_{\mathbf{t}}^{+\infty} d\mathbf{w} \cos\left(\frac{\mathbf{w}}{\beta}\right) S_1(\mathbf{w}; x^1, y^1).$$

The properties of  $S_1$  pointed out previously allow to infer that, for any fixed  $x^1, y^1 \in (0, a)$ , both the functions  $[0, +\infty) \rightarrow \mathbb{R}$ ,  $\mathbf{t} \mapsto \sin(\frac{\mathbf{t}}{\beta})S_1(\mathbf{t}; x^1, y^1)$ ,  $\cos(\frac{\mathbf{t}}{\beta})S_1(\mathbf{t}; x^1, y^1)$  fulfill the hypotheses of Lemma .3. In consequence of this, the integrals in the above equation are analytic functions for  $\mathbf{t} \in [0, +\infty)$  which vanish exponentially; then, it follows trivially that the function  $\mathbf{t} \mapsto T_1(\mathbf{t}; x^1, y^1)$  possesses the very same features.  $\square$

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