The Bose Gas in a Box with Neumann Boundary Conditions

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Abstract

We consider a gas of bosonic particles confined in a box with Neumann boundary conditions. We prove Bose-Einstein condensation in the Gross-Pitaevskii regime, with an optimal bound on the condensate depletion. Our lower bound for the ground state energy in the box implies (via Neumann bracketing) a lower bound for the ground state energy of the Bose gas in the thermodynamic limit.

Contents

1 Introduction and main results

We describe a system of N interacting bosonic particles in a box $\Lambda = [-L/2, L/2]^3$ through the Hamiltonian

$$H_N = -\sum_{i=1}^{N} \Delta_i + \kappa \sum_{i<j}^{N} V(x_i - x_j) \tag{1.1}$$

acting on $L^2_s(\Lambda^N)$. This is the space of symmetrized L^2 functions, defined as

$$L^2_s(\Lambda^N) = \{\psi \in L^2(\Lambda^N) : \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = \psi(x_1, \dots, x_N) \text{ for every } \sigma \in S_N\},$$

where S_N is the set of all permutations of N objects. In (1.1), Δ_i indicates the Laplacian with Neumann boundary conditions acting on particle i. The interaction potential V is a multiplication operator and we will assume it to be a nonnegative, spherically symmetric, compactly supported and bounded (κ is a coupling constant). We denote $\mathfrak{a}$ the scattering length of the interaction potential κV. The scattering length is defined through the zero-energy scattering equation

$$\left[-\Delta + \frac{\kappa}{2} V(x)\right] f_0(x) = 0 \tag{1.2}$$

with the boundary condition that $f_0(x) \to 1$, as $|x| \to \infty$. Here Δ denotes the Laplacian on $\mathbb{R}^3$. For $|x|$ large enough (outside the support of V), we have

$$f_0(x) = 1 - \frac{\mathfrak{a}}{|x|} \tag{1.3}$$

where $\mathfrak{a}$ is the scattering length of κV. Equivalently, $\mathfrak{a}$ can be obtained as

$$8\pi\mathfrak{a} = \int_{\mathbb{R}^3} \kappa V(x) f_0(x) dx. \tag{1.4}$$

We are interested in static properties of the Bose gas. The ground state energy per particle in the thermodynamic limit, i.e., the limit $N, |\Lambda| \to \infty$ with $\rho = N/|\Lambda|$ fixed, is given by

$$e(\rho) = \lim_{N,L\to\infty} \frac{E(N,L)}{N} \tag{1.5}$$

where $E(N,L)$ is the ground state energy of H_N, defined as

$$E(N,L) = \inf_{\psi \in L^2_s(\Lambda^N),\, ||\psi||=1} \langle \psi, H_N \psi \rangle.$$

For dilute gases, i.e., when the density ρ is small, the ground state energy per particle in the thermodynamic limit is described by the Lee-Huang-Yang formula [20, 21]

$$e(\rho) = \lim_{\substack{N,L\to\infty \\ \rho = N/|\Lambda|}} \frac{E(N,L)}{N} = 4\pi\rho\mathfrak{a}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + o((\rho\mathfrak{a}^3)^{1/2})\right], \tag{1.6}$$

proved in [32, 16, 4]. One of the main characteristics of (1.6) is the universality of the first two orders, where only the scattering length appears and other details of the interaction potential do not matter.

To compute thermodynamic quantities such as the ground state energy $e(\rho)$, a standard method (see for example [26]) consists in dividing the box Λ into M^3 cells of size $\ell = L/M$ and reducing the problem to the study of the localized system to each cell. The choice of the boundary conditions on the cells is therefore very important, and while Dirichlet boundary condition are suited to compute upper bounds, lower bounds require for example Neumann boundary conditions. In particular, to compute a lower bound for $e(\rho)$, we distribute the N particles in the M^3 cells (so that the k-th box has n_k particles) and neglect interactions between particles in different cells, exploiting the positivity of the interaction potential. The lower bound is then obtained by adding the lower bounds in the different cells and minimize over all the possible ways of distributing the particles in the cells, i.e.,

$$E(N,L) \geq \inf_{\{n_k\}:\sum_k n_k = N} \sum_{k=1}^{M^3} E(n_k, \ell). \tag{1.7}$$

Here $E(n,\ell)$ is the ground state energy of H_n (defined in (1.1), with N substituted by n), acting on $L^2_s(\Lambda_\ell^{3n})$, where $\Lambda_\ell = [-\ell/2, \ell/2]^3$, with Neumann boundary conditions. Rescaling lengths, the Hamiltonian (1.1) takes the form

$$H_{n,\ell} = -\sum_{i=1}^n \Delta_i + \kappa \sum_{i<j}^n \ell^2 V\big(\ell(x_i - x_j)\big) \tag{1.8}$$

and acts on $L^2_s(\Lambda_1^{3n})$, with $\Lambda_1 = [-1/2, 1/2]^3$. Up to a factor ℓ^2, H_n and $H_{n,\ell}$ are unitarily equivalent, i.e. there exists a unitary[1] $\mathcal{U}$ such that $\mathcal{U}^* H_{n,\ell} \mathcal{U} = \ell^2 H_n$. Denoting with $e_{n,\ell}$ the ground state energy of (1.8), we have clearly $e_{n,\ell} = \ell^2 E(n,\ell)$.

[1]The unitary transformation $\mathcal{U}$ acts as

$$\begin{aligned} \mathcal{U}: \qquad & L^2(\Lambda_\ell^n) \longrightarrow L^2(\Lambda_1^n) \\ \varphi(x_1,\ldots,x_n) \to (\mathcal{U}\varphi)&(x_1,\ldots,x_n) = \ell^{3n/2}\varphi(\ell x_1,\ldots,\ell x_n) \end{aligned}$$

In the case $n = \ell = N$, (1.8) describes the well known Gross-Pitaevskii regime. Here the density is proportional to N^{-2}, and hence the energy per particle is of the same order as the spectral gap of the Laplacian. In particular, in this regime the large volume and large particles number limit is simultaneous to the low density limit. The Gross-Pitaevskii regime has been studied for the translation invariant Bose gas, where periodic boundary conditions are imposed on Λ_1, and for the trapped Bose gas, where particles move in $\mathbb{R}^3$ and are confined by an external potential. In these cases, Bose-Einstein condensation has been proved [23, 24, 28] with optimal rate [5, 7, 27, 11, 18]. In the translation invariant case, the ground state energy has been shown in [6] to be

$$e_N = 4\pi(N-1)\mathfrak{a} + b_\Lambda \mathfrak{a}^2 - \frac{1}{2}\sum_{p\in\Lambda_1^*}\left[p^2 + 8\pi\mathfrak{a} - \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2}\right] + \mathcal{O}(N^{-1/4}), \quad (1.9)$$

where $b_\Lambda = 2 - \lim_{M\to\infty}\sum_{p\in\mathbb{Z}^3\setminus\{0\},\,|p|\le M}\frac{\cos(|p|)}{p^2}$ is a boundary contribution. In addition in [6] the excitation spectrum has been derived (these results have been also revisited in [19]). The result has then later been generalized to the trapped Bose gas [29, 12].

In this paper we consider the Bose gas with Neumann boundary conditions in the Gross-Pitaevskii regime. In Theorem 1.1 below we prove Bose-Einstein condensation with optimal rate and we give a bound on the ground state energy for the system described by (1.8).

Theorem 1.1. *Let V be positive, compactly supported, spherically symmetric and bounded, and assume that κ is a fixed, small enough constant independent of all parameters and $n\ell^{-1} \le 1$. Then, the ground state energy $e_{n,\ell}$ of $H_{n,\ell}$ defined in* (1.8) *is such that*

$$\Big|e_{n,\ell} - 4\pi\mathfrak{a}\frac{n^2}{\ell}\Big| \le C\Big(\frac{n}{\ell} + \frac{n^2}{\ell^2}\ln(\ell)\Big) \quad (1.10)$$

for a constant $C > 0$ depending only on V.

Furthermore, let $\psi_n \in L^2_s(\Lambda_1^n)$ be a normalized wave function, with

$$\langle\psi_n, H_{n,\ell}\psi_n\rangle \le e_{n,\ell} + \zeta$$

for some $\zeta > 0$. Let $\gamma_n^{(1)} = \mathrm{tr}_{2,\dots,n}|\psi_n\rangle\langle\psi_n|$ be the one-particle reduced density associated with ψ_n. Then there exists a constant $C > 0$ depending only on V such that

$$1 - \langle\varphi_0, \gamma_n^{(1)}\varphi_0\rangle \le C\Big(\frac{\zeta}{n} + \frac{1}{\ell}\Big) \quad (1.11)$$

where $\varphi_0(x) = 1$ for all $x \in \Lambda_1$.

Remarks.

1. For $n = \ell = N$ we recover in (1.11) the condensate depletion rate N^{-1}, as shown for example in [7, Theorem 1.1] for periodic boundary conditions. However, the ground state energy is different from the translation invariant case and for the trapped case, since here we have
$$\Big|e_N - 4\pi\mathfrak{a}N\Big| \le C\Big(1 + \ln(N)\Big) \quad (1.12)$$
The logarithmic behavior of the error bound is actually sharp and is specific to the Neumann boundary conditions.
2. We need the requirement that κ is small to prove certain properties (see (2.18) below) of the ground state of the two-body problem in a box with Neumann boundary conditions.

To prove Theorem (1.1), the main novelty of our analysis is the control of the Neumann boundary conditions. To do so, we consider the energy functional for the two-body problem (see (2.11) below) which naturally lives in a six-dimensional space, and we study the properties of its minimizer. We use then the minimizer to describe two-body correlations arising from interactions. In this part, we follow the ideas of [5]: after transforming the Hamiltonian (1.8) with a unitary operator (taken from [22]) which maps $L^2_s(\Lambda_1^n)$ to Fock space and extracts the contribution of the factorized part of wave functions, we act with a (generalized) Bogoliubov transformation. We define its integral kernel $\eta(x,y)$ as a function of the minimizer of the two-body problem (projected outside the space spanned by the constant in $L^2(\Lambda_1) \times L^2(\Lambda_1)$). In comparison to the case with periodic boundary condition and the case where the system in $\mathbb{R}^3$ is trapped by an external potential, the choice of Neumann boundary conditions makes the problem considerably more involved from the technical point of view. In the former cases the kernel of the Bogoliubov transformation $\tilde{\eta}(x,y)$ can be chosen proportional to $(1-f_0(x-y))\varphi_0^2(x+y)$ (before projecting it outside the space spanned by the constant in $L^2 \times L^2$), where f_0 has been defined in (1.3) and φ_0 represents the minimizer of the Gross-Pitaevskii functional. In our case instead the integral kernel $\eta(x,y)$ does not have such a simple structure; the center of mass and relative coordinate do not decouple and ground state of the two-body problem is not explicitly known. While the properties of (1.3) can be studied by reducing the problem to a one-dimensional problem (depending only on a radial coordinate), here we need instead to study a full six-dimensional problem on $L^2(\Lambda_1) \times L^2(\Lambda_1)$. Moreover the Neumann boundary conditions set a non-translation invariant problem with no conserved momentum (this of course rules out also the use of Fourier series and Fourier transforms).

As mentioned above, the Neumann boundary conditions allow us to deduce very easily a lower bound for the leading order of ground state energy of the Bose gas in the thermodynamic limit, for the system described by (1.1), for a small coupling constant $\kappa > 0$. This is the result of Corollary 1.2.

Corollary 1.2. *Let V satisfy the same assumptions as in Theorem 1.1 and κ be small enough. Then there exists a constant $C > 0$ such that $e(\rho)$ as defined in (1.5) satisfies*

$$e(\rho) \geq 4\pi\mathfrak{a}\rho\Big(1 - C(\rho\mathfrak{a}^3)^{1/2}\ln(1/\rho)\Big) \tag{1.13}$$

for ρ small enough.

Remarks.

1. The bound (1.13) is not optimal, as evident from (1.6). The optimal result has been proved in [13, 16] with a different localization method which allows to avoid the explicit use of boundary conditions, at the price of dealing with a modified kinetic energy.
2. To obtain Corollary 1.2 we take ℓ proportional to $\rho^{-1/2}$. Larger lengths ℓ would allow for a better precision in (1.13), as achieved in [16] mentioned above. However, this requires a more precise study of (1.8), with larger n/ℓ. In the translation invariant setting, on a torus with length slightly larger than $\rho^{-1/2}$, Bose-Einstein condensation has been shown in [1, 15], while [9] also derives the excitation spectrum of (1.8).

Even though the lower bound (1.13) is not optimal, we believe that our method can be extended to allow for larger n/ℓ (which would yield the Lee-Huang-Yang formula in the thermodynamic limit) as well as to give the excitation spectrum in the cells, which would allow for giving precise bounds for the free energy at low temperature. We plan to return to this question in a subsequent work. Bounds for the free energy are up to now restricted to leading order [30, 33].

The paper is organized as follows. In Section 2 we introduce the setting for the analysis of (1.8), while the detailed estimates are done in Section 3. In Section 4 we prove Theorem 1.1 and Corollary 1.2. In Appendix A we study the two-body problem.

2 Excitation Hamiltonians

In this section we focus on the study of $H_{n,\ell}$, defined as in (1.8). The Hamiltonian $H_{n,\ell}$ acts on $L^2_s(\Lambda_1^n)$, which consists of square-integrable functions on Λ_1^n that are symmetric with respect to permutation of the variables. It is convenient to enlarge the space and work on Fock space, defined as

$$\mathcal{F} = \bigoplus_m L^2_s(\Lambda_1^m).$$

We call vacuum the vector $\Omega = \{1, 0, \dots\} \in \mathcal{F}$. We define, for $g \in L^2(\Lambda_1)$, the creation operator $a^*(g)$ and the annihilation operator $a(g)$ as

$$(a^*(g)\Psi)^{(m)}(x_1, \dots, x_m) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} g(x_j) \Psi^{(m-1)}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_m)$$
$$(a(g)\Psi)^{(m)}(x_1, \dots, x_m) = \sqrt{m+1} \int_\Lambda \bar{g}(x) \Psi^{(m+1)}(x, x_1, \dots, x_m)\, dx$$

The creation operator $a^*(g)$ is the adjoint of the annihilation operator $a(g)$ and they satisfy the canonical commutation relations: for $g, h \in L^2(\Lambda_1)$,

$$[a(g), a^*(h)] = \langle g, h \rangle, \quad [a(g), a(h)] = [a^*(g), a^*(h)] = 0$$

We introduce operator valued distributions $\check{a}_x, a_x^*$ defined by

$$a(g) = \int \bar{g}(x)\, a_x\, dx, \quad a^*(g) = \int g(x)\, a_x^*\, dx$$

for $g \in L^2(\Lambda_1)$. It will be convenient to work in the basis of the eigenfunctions of the Laplacian on the cube Λ_1 with Neumann boundary conditions. We denote with $\{\varphi_p\}$, for $p \in \pi\{0, 1, 2, 3, \dots\}^3$ such an orthonormal basis, which is given by $\varphi_p(x) = 1$ for $p = 0$ and, for $p \neq 1$,

$$\varphi_p(x) = \big(1/2\big)^{3/2} \cos(p^{(1)}(x^{(1)} + 1/2)) \cos(p^{(2)}(x^{(2)} + 1/2)) \cos(p^{(3)}(x^{(3)} + 1/2))$$

where we used the notation $(x^{(1)}, x^{(2)}, x^{(3)})$ for the three dimensional vector x. We call $\Lambda_1^* = \pi\{0, 1, 2, \dots\}^3$ the dual space to Λ_1. We introduce the space $\Lambda_{1,+}^* = \Lambda_1^* \backslash \{0\}$, where the zero momentum is removed. We adopt the notation

$$\hat{a}_p^* = a^*(\varphi_p), \quad \text{and} \quad \hat{a}_p = a(\varphi_p). \tag{2.1}$$

We call the number of particles operator on $\mathcal{F}$ the operator

$$\mathcal{N} = \sum_{p \in \Lambda_1^*} \hat{a}_p^* \hat{a}_p = \int a_x^* a_x\, dx.$$

Creation and annihilation operators are bounded with respect to $\mathcal{N}$; it is easy to check that, for all $g \in L^2(\Lambda_1)$,

$$\|a(g)\Psi\| \leq \|g\| \|\mathcal{N}^{1/2}\Psi\|, \quad \|a^*(g)\Psi\| \leq \|g\| \|(\mathcal{N}+1)^{1/2}\Psi\|.$$

The Hamiltonian (1.8) lifted to Fock space takes the form

$$H_{n,\ell} = \sum_{p \in \Lambda_1^*} p^2 \hat{a}_p^* \hat{a}_p + \frac{1}{2} \sum_{p,q,r,s \in \Lambda_1^*} V_{\ell,pqrs} \hat{a}_p^* \hat{a}_q^* \hat{a}_r \hat{a}_s, \tag{2.2}$$

with

$$V_{\ell,pqrs} = \langle \varphi_p \otimes \varphi_q, \kappa \ell^2 V(\ell \cdot)\, \varphi_r \otimes \varphi_s \rangle = \int_{\Lambda_1} dx \int_{\Lambda_1} dy\ \kappa \ell^2 V(\ell(x-y)) \varphi_p(x) \varphi_q(y) \varphi_r(x) \varphi_s(y). \tag{2.3}$$

The eigenfunction of the Laplacian $\varphi_0(x) = 1$ corresponding to the lowest eigenvalue $p^2 = 0$ represents the condensate wave function. It is convenient to separate the contribution of the zero mode and consider a modified Fock space describing excitations. We define

$$\mathcal{F}_+^{\leq n} = \bigoplus_{j=0}^{n} L_+^2(\Lambda_1)^{\otimes_s j}, \tag{2.4}$$

where $L_+^2(\Lambda_1)$ is the orthogonal complement to the one dimensional space spanned by φ_0 in $L^2(\Lambda_1)$. Additionally, in definition (2.4), we truncated the Fock space up to the sector with n

particles. A vector $\Psi = \{\psi^{(0)}, \psi^{(1)}, \ldots, \psi^{(n)}, 0, 0, \ldots\} \in \mathcal{F}$ lies in $\mathcal{F}_+^{\leq n}$, if $\psi^{(m)}$ is orthogonal to φ_0, in each of its coordinates, for all $m = 1, \ldots, n$, i.e. if

$$\int \bar{\varphi}_0(x)\, \psi^{(m)}(x, y_1, \ldots, y_{m-1}) dx = 0$$

for all $m = 1, \ldots, n$. On $\mathcal{F}_+^{\leq n}$, we denote the number of particles operator with $\mathcal{N}_+ = \mathcal{N}|_{\mathcal{F}_+^{\leq n}}$. We will use modified creation and annihilation operators

$$b(f) = \sqrt{\frac{n - \mathcal{N}_+}{n}}\, a(f), \qquad \text{and} \qquad b^*(f) = a^*(f) \sqrt{\frac{n - \mathcal{N}_+}{n}}.$$

If $f \in L^2_+(\Lambda_1)$, $b(f)$, $b^*(f)$ map $\mathcal{F}_+^{\leq n}$ into itself. Moreover, for $g \in L^2(\Lambda_1)$ and $Q = 1 - |\varphi_0\rangle\langle\varphi_0|$, $b(g) = b(Qg)$ on $\mathcal{F}_+^{\leq n}$. Analogously as before, we define operator valued distributions b_x, b_x^* as

$$b(f) = \int \bar{f}(x)\, b_x\, dx, \qquad \text{and} \qquad b^*(f) = \int f(x) b_x^*\, dx$$

satisfying modified canonical commutation relations

$$\begin{aligned} [b_x, b_y^*] &= \left(1 - \frac{\mathcal{N}_+}{n}\right) \delta(x - y) - \frac{1}{n} a_y^* a_x \\ [b_x, b_y] &= [b_x^*, b_y^*] = 0 \end{aligned} \tag{2.5}$$

and we define

$$\hat{b}_p^* = b^*(\varphi_p), \quad \text{and} \quad \hat{b}_p = b(\varphi_p). \tag{2.6}$$

Every n-particle wave function $\psi_n \in L^2(\Lambda_1^n)$ can be decomposed uniquely as

$$\psi_n = \sum_{m=0}^{n} \alpha^{(m)} \otimes_s \varphi_0^{\otimes(n-m)}$$

where $\alpha^{(m)} \in L^2_+(\Lambda_1)^{\otimes_s m}$ for all $m = 1, \ldots, n$. Following [22], we define a unitary operator $U_n : L^2_s(\Lambda_1^n) \to \mathcal{F}_+^{\leq n}$ such that

$$U_n \psi_n = \{\alpha^{(0)}, \alpha^{(1)}, \ldots, \alpha^{(n)}\},$$

i.e., the unitary map U_n removes the condensate contribution from $\psi_n \in L^2_s(\Lambda_1^n)$ and returns the excitations over the condensate. As shown in [22], when we conjugate couples of creation and annihilation operators with U_n, we obtain, for $p, q \in \Lambda_{1,+}^*$,

$$\begin{aligned} U_n\, \hat{a}_0^* \hat{a}_0\, U_n^* &= N - \mathcal{N}_+ \\ U_n\, \hat{a}_p^* \hat{a}_0\, U_n^* &= \hat{a}_p^* \sqrt{N - \mathcal{N}_+} \\ U_n\, \hat{a}_0^* \hat{a}_p\, U_n^* &= \sqrt{N - \mathcal{N}_+}\, \hat{a}_p \\ U_n\, \hat{a}_p^* \hat{a}_q\, U_n^* &= \hat{a}_p^* \hat{a}_q \end{aligned} \tag{2.7}$$

The operator $\mathcal{N}_+ = \mathcal{N} - a_0^* a_0$ counts the number of excitations. Using the properties of U_n, it is easy to see that $U_n^* \Omega = \varphi^{\otimes N}$.

With the transformation U_n we define the excitation Hamiltonian

$$\mathcal{L}_n := U_n H_{n,\ell} U_n^* : \mathcal{F}_+^{\leq n} \to \mathcal{F}_+^{\leq n} \tag{2.8}$$

As shown in [22], $\mathcal{L}_n$ consists of the sum

$$\mathcal{L}_{n,\ell} = \mathcal{L}_{n,\ell}^{(0)} + \mathcal{L}_{n,\ell}^{(1)} + \mathcal{L}_{n,\ell}^{(2)} + \mathcal{L}_{n,\ell}^{(3)} + \mathcal{L}_{n,\ell}^{(4)} \tag{2.9}$$

with

$$
\begin{aligned}
\mathcal{L}^{(0)}_{n,\ell} &= \frac{1}{2} V_{\ell,0000} (n - \mathcal{N}_+)(n - \mathcal{N}_+ - 1) \\
\mathcal{L}^{(1)}_{n,\ell} &= \sqrt{n} \sum_{p \in \Lambda^*_{1,+}} V_{\ell,000p} (n - \mathcal{N}_+ - 1) \hat{b}_p + \text{h.c.} \\
\mathcal{L}^{(2)}_{n,\ell} &= \sum_{p \in \Lambda^*_{1,+}} p^2 \hat{a}^*_p \hat{a}_p + \sum_{p,q \in \Lambda^*_{1,+}} (V_{\ell,0p0q} + V_{\ell,0pq0}) \hat{a}^*_p \hat{a}_q (n - \mathcal{N}_+) \\
&\quad + \frac{1}{2} \sum_{p,q \in \Lambda^*_{1,+}} (n V_{\ell,pq00} \hat{b}^*_p \hat{b}^*_q + \text{h.c.}) \\
\mathcal{L}^{(3)}_{n,\ell} &= \sum_{p,q,r \in \Lambda^*_{1,+}} (n^{1/2} V_{\ell,0pqr} \hat{a}^*_p \hat{a}_q \hat{b}_r + \text{h.c.}) \\
\mathcal{L}^{(4)}_{n,\ell} &= \frac{1}{2} \sum_{p,q,r,s \in \Lambda^*_{1,+}} V_{\ell,pqrs} \hat{a}^*_p \hat{a}^*_q \hat{a}_r \hat{a}_s
\end{aligned}
\tag{2.10}
$$

Conjugation with the map U_n does not extract from $H_{n,\ell}$ all the leading order contributions to the energy (by taking the vacuum expectation value); it extracts the contribution of the condensate part of wave functions, but it does not extract the contribution due to correlations (recall that $\langle \Omega, \mathcal{L}^{(0)}_{n,\ell} \Omega \rangle = \langle \varphi^{\otimes N}, H_{n,\ell} \varphi^{\otimes N} \rangle$). In fact, the ground state wave function is far from being factorized and correlations among particles play a crucial role. In order to describe the correlation structure of the ground state wave function we need to transform $\mathcal{L}_n$ further.

To model correlations we use the solution of the two-body problem with potential V: this describes the simplest scattering process. We find it more natural to work now on the rescaled double box $\Lambda_\ell \times \Lambda_\ell$, and impose Neumann boundary conditions (recall that $\Lambda_\ell = [-\ell/2, \ell/2]$). We look for the minimizer of the functional

$$
F[g] = \int_{\Lambda_\ell \times \Lambda_\ell} dxdy \left[\kappa V(x-y) |g(x,y)|^2 + |\nabla_x g(x,y)|^2 + |\nabla_y g(x,y)|^2 \right] \tag{2.11}
$$

among functions $g \in H^1(\Lambda_\ell \times \Lambda_\ell)$ with $\|g\|_{L^2(\Lambda_\ell \times \Lambda_\ell)} = 1$. In the next proposition we state the properties of the minimizer we shall need.

Proposition 2.1. *Let $\ell > 1$ and $\Lambda_\ell = [-\ell/2, \ell/2]^3 \subset \mathbb{R}^3$. Let the functional $F : H^1(\Lambda_\ell \times \Lambda_\ell) \to \mathbb{R}$ be defined in* (2.11)*. Then, in the subclass of functions such that*

$$
\|g\|_2^2 = \int_{\Lambda_\ell \times \Lambda_\ell} dxdy\, |g(x,y)|^2 = 1,
$$

there is a unique function f (up to a constant phase factor) that minimizes F. If $\mathfrak{a}$ is the scattering length of the potential V (defined in (1.4)*), we have, for ℓ sufficiently large,*

$$
\lambda_\ell := \inf_{g \in H^1(\Lambda_\ell \times \Lambda_\ell)} \left\{ F[g] : \int_{\Lambda_\ell \times \Lambda_\ell} dxdy\, |g(x,y)|^2 = 1, \right\} = \frac{8\pi\mathfrak{a}}{\ell^3} \Big(1 + \mathcal{O}\Big(\frac{\mathfrak{a}}{\ell} \ln(\ell/\mathfrak{a}) \Big) \Big) \tag{2.12}
$$

Moreover, the following properties of the minimizer f hold.

i) We have

$$
\int_{\Lambda_\ell \times \Lambda_\ell} dxdy \left[|\nabla_x f(x,y)|^2 + |\nabla_y f(x,y)|^2 \right] \leq C\kappa \ell^{-3} \tag{2.13}
$$

ii) There exists a constant $C > 0$ such that

$$
|f(x,y)| \leq C \ell^{-3} \tag{2.14}
$$

for every $x, y \in \Lambda_\ell$.

iii) There exists a constant $C>0$ such that

$$\int_{\Lambda_\ell\times\Lambda_\ell} dxdy\,\big|\ell^{-3}-f(x,y)\big|^2 \le C^2\kappa^2\ell^{-2} \tag{2.15}$$

and

$$\int_{\Lambda_\ell\times\Lambda_\ell} dxdy\,\big|\ell^{-3}-f(x,y)\big| \le C\kappa\ell^2 \tag{2.16}$$

iv) There exists a constant $C>0$ such that

$$|1-\ell^3 f(x,y)| \le C\kappa\left(\frac{1}{|x-y|+1}\right) \tag{2.17}$$

v) For κ small enough, there exists a constant $C>0$ such that

$$|\nabla_{x+y} f(x,y)| \le C\kappa\ell^{-3}\big(d(\tfrac{x+y}{2})^{5/3}+1\big)^{-1} \tag{2.18}$$

where $d(x)$ is the distance of x to the boundary of the box Λ_ℓ.

We postpone the proof of Prop. 2.1 to Appendix A. The minimizer of (2.11) satisfies the eigenvalue equation

$$\Big[-(\Delta_x+\Delta_y)+\kappa V(x-y)\Big]f(x,y)=\lambda_\ell f(x,y), \tag{2.19}$$

for $x,y\in\Lambda_\ell$. We define $f_\ell(x,y)=f(\ell x,\ell y)$; by scaling, $f_\ell(x,y)$ satisfies

$$\Big[-(\Delta_x+\Delta_y)+\kappa\ell^2 V(\ell(x-y))\Big]f_\ell(x,y)=\ell^2\lambda_\ell f_\ell(x,y), \tag{2.20}$$

for $x,y\in\Lambda_1$. We set $w_\ell=1-\ell^3 f_\ell$, which solves

$$(\Delta_x+\Delta_y)w_\ell(x,y)+\kappa\ell^5 V(\ell(x-y))f_\ell(x,y)=\ell^5\lambda_\ell f_\ell(x,y), \tag{2.21}$$

for $x,y\in\Lambda_1$. Using the function w_ℓ, we construct a Hilbert-Schmidt operator $\eta: L^2(\Lambda_1)\to L^2(\Lambda_1)$. We set

$$\eta=(1-|\varphi_0\rangle\langle\varphi_0|)k(1-|\varphi_0\rangle\langle\varphi_0|) \tag{2.22}$$

where $k: L^2(\Lambda_1)\to L^2(\Lambda_1)$ is the Hilbert-Schmidt operator with integral kernel

$$k(x,y)=-nw_\ell(x,y) \tag{2.23}$$

It will be useful to decompose $\eta=k+\mu$, with

$$\mu=-|\varphi_0\rangle\langle\varphi_0|k-k|\varphi_0\rangle\langle\varphi_0|+|\varphi_0\rangle\langle\varphi_0|k|\varphi_0\rangle\langle\varphi_0| \tag{2.24}$$

Therefore, we can express the integral kernel of the operator η as

$$\eta(x,y)=k(x,y)+\mu(x,y) \tag{2.25}$$

with

$$\mu(x,y)=n\int dz\,w_\ell(z,y)+n\int dz\,w_\ell(x,z)-n\int dz_1dz_2\,w_\ell(z_1,z_2)$$

Using (2.21) and (2.25) we have

$$(\Delta_x+\Delta_y)\eta(x,y)=n\ell^5(\kappa V(\ell(x-y))-\lambda_\ell)f_\ell(x,y)+n\int dz\,\Delta_x w_\ell(x,z)+n\int dz\,\Delta_y w_\ell(z,y) \tag{2.26}$$

We collect in Proposition 2.2 below properties of the operators η, k and μ (we postpone the proof of Proposition 2.2 to the end of Appendix A).

Proposition 2.2. *Let η be defined as in (2.22) and let κ be small enough and $n/\ell \leq 1$. Then the following estimates hold true.*

i) We have

$$\int_{\Lambda_1\times\Lambda_1} dxdy \left|\eta(x,y)\right|^2 = \|\eta\|_2^2 \leq C\kappa^2 n^2 \ell^{-2} \tag{2.27}$$

and

$$\int_{\Lambda_1\times\Lambda_1} dxdy \left[\left|\nabla_x \eta(x,y)\right|^2 + \left|\nabla_y \eta(x,y)\right|^2\right] \leq C\kappa n^2 \ell^{-1} \tag{2.28}$$

for a constant $C > 0$. Moreover, for any $x, y \in \Lambda_1$,

$$|\eta(x,y)| \leq Cn \tag{2.29}$$

and

$$|\eta(x,y)| \leq C\frac{\kappa n}{\ell}\left[\frac{1}{|x-y|+\ell^{-1}}\right] \tag{2.30}$$

for a constant $C > 0$.

ii) We indicate with $\eta_x(y)$ the function $\eta(y,x)$. For any $x \in \Lambda_1$

$$\|\eta_x\|_2 \leq C\kappa n \ell^{-1} \tag{2.31}$$

for a constant $C > 0$.

iii) Decomposing[2] $\sigma := \sinh(\eta) = \eta + r$ and $\gamma := \cosh(\eta) = 1 + p$, there exists a $C > 0$ such that

$$\|\sigma\|_2, \|p\|_2 \leq C\|\eta\|_2 \tag{2.32}$$

Moreover

$$|r(x,y)| \leq C\|\eta\|_2\|\eta_x\|_2\|\eta_y\|_2, \quad |p(x,y)| \leq C\|\eta_x\|_2\|\eta_y\|_2 \tag{2.33}$$

for every $x, y \in \Lambda_1$. This implies that

$$\|r_x\|_2 \leq C\|\eta\|_2^2\|\eta_x\|_2, \quad \|p_x\| \leq C\|\eta\|_2\|\eta_x\|_2 \tag{2.34}$$

With η introduced above, we define the generalized Bogoliubov transformation

$$e^B = \exp\left[\frac{1}{2}\int_{\Lambda_1\times\Lambda_1} dxdy\, \eta(x,y)\, b_x^* b_y^* - \text{h.c.}\right] \tag{2.35}$$

Equivalently we can express it as

$$e^B = \exp\left[\frac{1}{2}\sum_{p,q\in\Lambda_{1,+}^*}\left(\eta_{pq}\hat{b}_p^*\hat{b}_q^* - \text{h.c.}\right)\right] \tag{2.36}$$

with

$$\eta_{pq} = \langle \varphi_p \otimes \varphi_q, \eta\rangle \tag{2.37}$$

Note that $e^B : \mathcal{F}_+^{\leq n} \to \mathcal{F}_+^{\leq n}$ is unitary. In Section 3.1 below we present some key properties of e^B. With the generalized Bogoliubov transformation e^B we define a new excitation Hamiltonian $\mathcal{G}_{n,\ell} : \mathcal{F}_+^{\leq n} \to \mathcal{F}_+^{\leq n}$ as

$$\mathcal{G}_{n,\ell} = e^{-B}\mathcal{L}_{n,\ell}e^B = e^{-B}U_n H_{n,\ell} U_n^* e^B \tag{2.38}$$

Proposition 2.3 (which will be proved at the end of Section 3) presents our main estimates of $\mathcal{G}_{n,\ell}$.

[2] As we did for η, we are going to use the symbols σ, r and p to indicate both the operators and their integral kernels.

Proposition 2.3. *Let V be positive, compactly supported, spherically symmetric and bounded. Moreover, define*

$$\mathcal{K} = \sum_{p \in \Lambda_{1,+}^*} p^2 \hat{a}_p^* \hat{a}_p \qquad \text{and} \qquad \mathcal{V}_\ell = \frac{1}{2} \sum_{p,q,r,s \in \Lambda_{1,+}^*} V_{\ell,pqrs} \hat{a}_p^* \hat{a}_q^* \hat{a}_r \hat{a}_s. \tag{2.39}$$

where we defined $V_{\ell,pqrs}$ in (2.3)*. For κ be small enough and $n/\ell \leq 1$, we have*

$$\mathcal{G}_{n,\ell} = C_{n,\ell} + \mathcal{K} + \mathcal{V}_\ell + \mathcal{E}_{n,\ell} \tag{2.40}$$

where $C_{n,\ell}$ is given by

$$\begin{aligned} C_{n,\ell} = \frac{n^2}{2} \int dxdy \, \kappa \ell^2 V(\ell(x-y)) - \frac{1}{2} \langle \eta, (\Delta_1 + \Delta_2) \eta \rangle \\ + n \sum_{p,q \in \Lambda_{1,+}^*} V_{\ell,pq00} \langle \eta, \varphi_p \otimes \varphi_q \rangle + \frac{1}{2} \sum_{p,q,r,s \in \Lambda_{1,+}^*} V_{\ell,pqrs} \langle \varphi_s \otimes \varphi_r, \eta \rangle \langle \eta, \varphi_p \otimes \varphi_q \rangle, \end{aligned} \tag{2.41}$$

and the error $\mathcal{E}_{n,\ell}$ is such that for any $\delta > 0$ there exists a constant $C > 0$ so that

$$\pm \mathcal{E}_{n,\ell} \leq \delta(\mathcal{K} + \mathcal{V}_\ell) + C\kappa \frac{n}{\ell}(\mathcal{N}_+ + 1) \tag{2.42}$$

3 Analysis of the excitation Hamiltonian

In this section we analyze the excitation Hamiltonian $\mathcal{G}_{n,\ell}$ defined in (2.38). We decompose it as

$$\mathcal{G}_{n,\ell} = \mathcal{G}_{n,\ell}^{(0)} + \mathcal{G}_{n,\ell}^{(1)} + \mathcal{G}_{n,\ell}^{(2)} + \mathcal{G}_{n,\ell}^{(3)} + \mathcal{G}_{n,\ell}^{(4)}$$

with

$$\mathcal{G}_{n,\ell}^{(j)} = e^{-B} \mathcal{L}_{n,\ell}^{(j)} e^B$$

where $\mathcal{L}_{n,\ell}^{(j)}$ was defined in (2.10), for $j \in \{0,1,2,3,4\}$. We examine $\mathcal{G}_{n,\ell}$ and identify its main contributions. The goal of this section is to prove Proposition 2.3. While the analysis is similar to [5, Section 4], special care needs to be taken due to the Neumann boundary conditions. In Subsections 3.2, 3.3, 3.4, 3.5, 3.6 we extract from $\mathcal{G}_{n,\ell}^{(0)}$, $\mathcal{G}_{n,\ell}^{(1)}$, $\mathcal{G}_{n,\ell}^{(2)}$, $\mathcal{G}_{n,\ell}^{(3)}$ and $\mathcal{G}_{n,\ell}^{(4)}$ the main contributions which will be expressions that are constant, linear and quadratic in creation and annihilation operators, and we prove that cubic and quartic contributions are small. In Subsection 3.7 we bound the linear and quadratic contributions, obtaining Proposition 2.3. Throughout the whole section we will use some properties of the generalized Bogoliubov transformation e^B, which we review in Subsection 3.1.

3.1 Generalized Bogoliubov transformation

The generalized Bogoliubov transformation in the form (2.35) has been introduced in [10]; we refer to [10, Section 3] for a detailed discussion about it; we mention below only the results that are relevant in our analysis.

As proved in [31, 10], e^B does not change substantially the number of excitations. This is the content of the following Lemma.

Lemma 3.1. *Let $\eta \in L^2(\Lambda_1 \times \Lambda_1)$ be such that $\eta(x,y) = \eta(y,x)$ and let B be defined as in (2.35). Then, for every $m_1, m_2 \in \mathbb{Z}$, there exists a constant $C > 0$ such that, on $\mathcal{F}_+^{\leq n}$,*

$$e^{-B}(\mathcal{N}_+ + 1)^{m_1}(n + 1 - \mathcal{N}_+)^{m_2} e^B \leq C e^{C\|\eta\|_2} (\mathcal{N}_+ + 1)^{m_1}(n + 1 - \mathcal{N}_+)^{m_2}$$

The action of e^B on creation and annihilation operators can be expressed as follows. We define

$$\begin{aligned} \gamma_x(y) &= \cosh_\eta(y,x) = \sum_{n \geq 0} \frac{1}{(2n)!} \, \eta^{2n}(y,x) \, , \\ \sigma_x(y) &= \sinh_\eta(y,x) = \sum_{n \geq 0} \frac{1}{(2n+1)!} \eta^{2n+1}(y,x) \, , \end{aligned} \tag{3.1}$$

where η^m indicates the product in the sense of operators (the symbol η denotes the Hilbert-Schmidt operator whose kernel is $\eta(x,y)$). Note that $\eta^0(y,x)$ has to be interpreted as a δ distribution. With these definitions, we write

$$e^{-B} b_x e^B = b(\gamma_x) + b^*(\sigma_x) + d_x, \qquad e^{-B} b_x^* e^B = b^*(\gamma_x) + b(\sigma_x) + d_x^* \tag{3.2}$$

for a remainder operator d_x. Lemma 3.2 below states that d_x is a bounded operators on $\mathcal{F}_+^{\leq n}$ and it is small on states with a small number of excitations; the main contributions in the right hand sides of (3.2) correspond to those of the usual Bogoliubov transformation. Lemma 3.2 is a generalization of [6, Lemma 2.3], and can be proved in the same way.

Lemma 3.2. *Let $\eta \in L^2(\Lambda_1 \times \Lambda_1)$ be such that $\eta(x,y) = \eta(y,x)$ and let $j \in \mathbb{Z}$. Let the remainder operator d_x be defined as in* (3.2)*. Then, if $\|\eta\|$ is small enough, there exists a $C > 0$ such that*

$$\|(\mathcal{N}_+ + 1)^{j/2} d_x \xi\| \leq n^{-1} C \left[\|\eta_x\| \|(\mathcal{N}_+ + 1)^{(j+3)/2} \xi\| + \|\eta\| \|b_x (\mathcal{N}_+ + 1)^{(j+2)/2} \xi\| \right] \tag{3.3}$$

$$\begin{aligned} \|(\mathcal{N}_+ + 1)^{j/2} a_y d_x \xi\| \leq n^{-1} C \Big[& \|\eta_x\| \|\eta_y\| \|(\mathcal{N}_+ + 1)^{(j+2)/2} \xi\| + |\eta(y,x)| \|(\mathcal{N}_+ + 1)^{(j+2)/2} \xi\| \\ & + \|\eta_y\| \|b_x (\mathcal{N}_+ + 1)^{(j+1)/2} \xi\| + \|\eta_x\| \|a_y (\mathcal{N}_+ + 1)^{(j+3)/2} \xi\| \\ & + \|\eta\| \|a_y a_x (\mathcal{N}_+ + 1)^{(j+2)/2} \xi\| \Big] \end{aligned} \tag{3.4}$$

$$\begin{aligned} \|(\mathcal{N}_+ + 1)^{j/2} d_x d_y \xi\| \leq n^{-2} C \Big[& \|\eta_x\| \|\eta_y\| \|(\mathcal{N}_+ + 1)^{(j+6)/2} \xi\| + \|\eta\| \|\eta_x\| \|a_y (\mathcal{N}_+ + 1)^{(j+5)/2} \xi\| \\ & + \|\eta\| |\eta(y,x)| \|(\mathcal{N}_+ + 1)^{(j+4)/2} \xi\| + \|\eta\| \|\eta_y\| \|a_x (\mathcal{N}_+ + 1)^{(j+5)/2} \xi\| \\ & + \|\eta\| \|a_y a_x (\mathcal{N}_+ + 1)^{(j+4)/2} \xi\| \Big] \end{aligned} \tag{3.5}$$

for all $\xi \in \mathcal{F}_+^{\leq n}$. Moreover, for any $g \in L^2(\Lambda_1 \times \Lambda_1)$ such that $g(x,y) = g(y,x)$,

$$\begin{aligned} \|(\mathcal{N}_+ + 1)^{j/2} \int dx\, g(x,y) d_x \xi\| &\leq n^{-1} C \|g_y\| \|(\mathcal{N}_+ + 1)^{(j+3)/2} \xi\| \\ \|(\mathcal{N}_+ + 1)^{j/2} \int dx\, g(x,y) d_x^* \xi\| &\leq n^{-1} C \|g_y\| \|(\mathcal{N}_+ + 1)^{(j+3)/2} \xi\| \end{aligned} \tag{3.6}$$

3.2 Analysis of $\mathcal{G}_{n,\ell}^{(0)}$

Recall from (2.10) that

$$\mathcal{L}_{n,\ell}^{(0)} = \frac{1}{2} \int dx dy\, \kappa \ell^2 V(\ell(x-y)) (n - \mathcal{N}_+)(n - \mathcal{N}_+ - 1) \tag{3.7}$$

We define the error operator $\mathcal{E}_{n,\ell}^{(0)}$ through

$$\mathcal{G}_{n,\ell}^{(0)} = \frac{n^2}{2} \int dx dy\, \kappa \ell^2 V(\ell(x-y)) + \mathcal{E}_{n,\ell}^{(0)} \tag{3.8}$$

and we estimate it in the next proposition.

Proposition 3.3. *Let $\mathcal{E}_{n,\ell}^{(0)}$ be as defined in* (3.8)*. Then, under the same assumptions as in Proposition 2.3, there exists a $C > 0$ such that*

$$\pm \mathcal{E}_{n,\ell}^{(0)} \leq C \kappa n \ell^{-1} \mathcal{N}_+ \tag{3.9}$$

as operator inequalities on $\mathcal{F}_+^{\leq n}$.

Proof. Equation (3.8) implies that

$$\mathcal{E}_{n,\ell}^{(0)} = -\ e^{-B} \big(n + n\mathcal{N}_+ + \mathcal{N}_+/2 - \mathcal{N}_+^2/2\big) e^B \int dx dy\, \kappa \ell^2 V(\ell(x-y)) \tag{3.10}$$

The bounds in (3.9) follow from $\int dx dy\, \kappa \ell^3 V(\ell(x-y)) \leq \kappa \int dx\, V(x)$, Lemma 3.1 and (2.27). $\square$

3.3 Analysis of $\mathcal{G}^{(1)}_{n,\ell}$

On $\mathcal{F}_+^{\leq n}$ we can write (2.10) as

$$\mathcal{L}^{(1)}_{n,\ell} = \sqrt{n}(n-\mathcal{N}_+-1)\int dxdy\,\kappa\ell^2 V(\ell(x-y))b_x + \text{h.c.} \tag{3.11}$$

We define the error $\mathcal{E}^{(1)}_n$ by

$$\mathcal{G}^{(1)}_{n,\ell} = e^{-B}\mathcal{L}^{(1)}_{n,\ell}e^{B} = n^{3/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\big[b(\gamma_x)+b^*(\sigma_x)+\text{h.c.}\big] + \mathcal{E}^{(1)}_{n,\ell} \tag{3.12}$$

where γ_x and σ_x were defined in (3.1). We estimate $\mathcal{E}^{(1)}_{n,\ell}$ in the next proposition.

Proposition 3.4. *Let $\mathcal{E}^{(1)}_{n,\ell}$ be defined as in (3.12). Then, under the same assumptions as Proposition 2.3, there exists a $C>0$ such that*

$$\pm\,\mathcal{E}^{(1)}_{n,\ell} \leq C\kappa n\ell^{-1}(\mathcal{N}_++1) \tag{3.13}$$

as operator inequalities on $\mathcal{F}_+^{\leq n}$.

Proof. Comparing (3.11) and (3.12) we obtain

$$\begin{aligned}\mathcal{E}^{(1)}_{n,\ell} &= -n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\left[e^{-B}(\mathcal{N}_++1)b_x e^{B} + \text{h.c.}\right]\\ &\quad + n^{3/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\Big[e^{-B}b_x e^{B} - \big(b(\gamma_x)+b^*(\sigma_x)\big) + \text{h.c.}\Big]\\ &=: \mathrm{D}_1+\mathrm{D}_2\end{aligned} \tag{3.14}$$

We analyze D_1 first. Using the identity $(\mathcal{N}_++1)^{1/2}b_x = b_x\mathcal{N}_+^{1/2}$, we write it as

$$\mathrm{D}_1 = -n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\left[e^{-B}(\mathcal{N}_++1)^{1/2}b_x\mathcal{N}_+^{1/2}e^{B} + \text{h.c.}\right] \tag{3.15}$$

For any $\xi\in\mathcal{F}_+^{\leq n}$ we have

$$\begin{aligned}|\langle\xi,\mathrm{D}_1\xi\rangle| &\leq Cn^{1/2}\ell^{-1}\int dx\,|\langle\xi, e^{-B}(\mathcal{N}_++1)^{1/2}b_x\mathcal{N}_+^{1/2}e^{B}\xi\rangle|\int dy\,\kappa\ell^3 V(\ell(x-y))\\ &\leq C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}e^{B}\xi\|\int dx\,\|b_x\mathcal{N}_+^{1/2}e^{B}\xi\|\end{aligned}$$

With Lemma 3.1 and Cauchy-Schwarz we obtain

$$|\langle\xi,\mathrm{D}_1\xi\rangle| \leq C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\|(\mathcal{N}_++1)\xi\| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|^2$$

We consider now D_2. Using (3.2), we have

$$\mathrm{D}_2 = n^{3/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\big[d_x+\text{h.c.}\big] \tag{3.16}$$

By (3.3) (with $j=-1$) and Cauchy-Schwarz, we conclude that

$$\begin{aligned}|\langle\xi,\mathrm{D}_2\xi\rangle| &\leq n^{3/2}\ell^{-1}\int dx\,|\langle(\mathcal{N}_++1)^{1/2}\xi,(\mathcal{N}_++1)^{-1/2}d_x\xi\rangle|\int dy\,\kappa\ell^3 V(\ell(x-y))\\ &\leq C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\int dx\,\Big[\|\eta_x\|\|(\mathcal{N}_++1)\xi\| + \|\eta\|\|b_x(\mathcal{N}_++1)^{1/2}\xi\|\Big]\\ &\leq C\kappa n^{1/2}\ell^{-1}\|\eta\|\|(\mathcal{N}_++1)^{1/2}\xi\|\|(\mathcal{N}_++1)\xi\|\end{aligned} \tag{3.17}$$

This concludes the proof of estimate (3.13) if we use bound (2.27) for the norm of η. □

3.4 Analysis of $\mathcal{G}^{(2)}_{n,\ell}$

Recall, from (2.10) and (2.39), that

$$\mathcal{L}^{(2)}_{n,\ell} = \mathcal{K} + \mathcal{L}^{(2,V)}_{n,\ell}$$

with

$$\mathcal{L}^{(2,V)}_{n,\ell} = \sum_{p,q\in\Lambda^*_{1,+}} (V_{\ell,0p0q} + V_{\ell,0pq0})\hat{a}^*_p\hat{a}_q(n-\mathcal{N}_+) + \frac{1}{2}\sum_{p,q\in\Lambda^*_{1,+}} (nV_{\ell,pq00}\hat{b}^*_p\hat{b}^*_q + \text{h.c.}) \tag{3.18}$$

We consider now

$$\mathcal{G}^{(2)}_{n,\ell} = e^{-B}\mathcal{L}^{(2)}_{n,\ell}e^{B} = e^{-B}\mathcal{K}e^{B} + e^{-B}\mathcal{L}^{(2,V)}_{n,\ell}e^{B} \tag{3.19}$$

To prove Proposition 3.6 and Proposition 3.7 below, we will use the bounds contained in the following lemma, taken from [8, Lemma 3.6].

Lemma 3.5. *Let $V \in L^1(\mathbb{R}^3)$, $V \geq 0$. Let $j_1, j_2 \in L^2(\Lambda_1\times\Lambda_1)$. Consider the operators*

$$\begin{aligned} A_1 &= \int dxdy\, \kappa\ell^3 V(\ell(x-y))a^\sharp(j_{1,x})a^\sharp(j_{2,y}) \\ A_2 &= \int dxdy\, \kappa\ell^3 V(\ell(x-y))a^\sharp(j_{1,x})a_y \end{aligned} \tag{3.20}$$

where $a^\sharp$ indicates either a or a^*. Then, for every $\xi\in\mathcal{F}^{\leq n}_+$, we have

$$\begin{aligned} |\langle\xi, A_1\xi\rangle| &\leq \kappa\|V\|_1\|j_1\|_2\|j_2\|_2\|(\mathcal{N}+1)^{1/2}\xi\|^2 \\ |\langle\xi, A_2\xi\rangle| &\leq \kappa\|V\|_1\|j_1\|_2\|(\mathcal{N}+1)^{1/2}\xi\|^2 \end{aligned} \tag{3.21}$$

Proof. By Cauchy-Schwarz, we have

$$\begin{aligned} |\langle\xi, A_1\xi\rangle| &= \int dxdy\,\kappa\ell^3 V(\ell(x-y))\|a^\sharp(j_{1,x})\xi\|\|a^\sharp(j_{2,y})\xi\| \\ &\leq \int dxdy\,\kappa\ell^3 V(\ell(x-y))\|j_{1,x}\|\|j_{2,y}\|\|(\mathcal{N}_++1)^{1/2}\xi\|^2 \\ &\leq \|(\mathcal{N}_++1)^{1/2}\xi\|^2\left[\int dxdy\,\kappa\ell^3V(\ell(x-y))\|j_{1,x}\|^2\right]^{1/2}\left[\int dxdy\,\kappa\ell^3V(\ell(x-y))\|j_{2,y}\|^2\right]^{1/2} \\ &\leq \kappa\,\|V\|_1\|j_1\|_2\|j_2\|_2\|(\mathcal{N}+1)^{1/2}\xi\|^2. \end{aligned} \tag{3.22}$$

Similarly we obtain the second estimate in (3.21).

□

3.4.1 Analysis of $e^{-B}\mathcal{K}e^{B}$

We define the error operator $\mathcal{E}^{(2,K)}_{n,\ell}$ through

$$\begin{aligned} e^{-B}\mathcal{K}e^{B} = \mathcal{K} &- \frac{1}{2}\langle\eta, (\Delta_1+\Delta_2)\eta\rangle - \frac{1}{2}\sum_{p,r\in\Lambda^*_{1,+}}\langle\varphi_p\otimes\varphi_r, \big(\Delta_1+\Delta_2\big)\eta\rangle\hat{b}^*_p\hat{b}^*_r \\ &- \frac{1}{2}\sum_{p,r\in\Lambda^*_{1,+}}\langle\big(\Delta_1+\Delta_2\big)\eta, \varphi_p\otimes\varphi_r\rangle\hat{b}_p\hat{b}_r + \mathcal{E}^{(2,K)}_{n,\ell}. \end{aligned} \tag{3.23}$$

We estimate it in the following proposition.

Proposition 3.6. *Let $\mathcal{E}^{(2,K)}_{n,\ell}$ be defined as in (3.23). Then, under the same assumptions as Proposition 2.3, for every $\delta > 0$ there exists a $C > 0$ such that*

$$\pm\mathcal{E}^{(2,K)}_{n,\ell} \leq \delta\mathcal{V}_\ell + C\kappa n\ell^{-1}(\mathcal{N}_++1) \tag{3.24}$$

as operator inequalities on $\mathcal{F}^{\leq N}_+$.

Proof. We write

$$e^{-B}\mathcal{K}e^{B} = \mathcal{K} + \int_0^1 ds\, e^{-sB}[\mathcal{K}, B]e^{sB} \tag{3.25}$$

With definition (2.36) we have

$$[\mathcal{K}, B] = \frac{1}{2}\sum_{p,q,r\in\Lambda^*_{1,+}} r^2\langle\varphi_p\otimes\varphi_q,\eta\rangle[\hat{a}^*_r\hat{a}_r,\hat{b}^*_p\hat{b}^*_q] - \frac{1}{2}\sum_{p,q,r\in\Lambda^*_{1,+}} r^2\langle\eta,\varphi_p\otimes\varphi_q\rangle[\hat{a}^*_r\hat{a}_r,\hat{b}_p\hat{b}_q] \tag{3.26}$$

We use now

$$[\hat{a}^*_r\hat{a}_r,\hat{b}^*_p\hat{b}^*_q] = \hat{b}^*_p[\hat{a}^*_r\hat{a}_r, b^*_q] + [\hat{a}^*_r\hat{a}_r,\hat{b}^*_p]\hat{b}^*_q = \delta_{rq}\hat{b}^*_p\hat{b}^*_r + \delta_{rp}\hat{b}^*_r\hat{b}^*_q$$

to obtain

$$\begin{aligned}[\mathcal{K}, B] &= -\frac{1}{2}\sum_{p,r\in\Lambda^*_{1,+}}\langle\varphi_p\otimes\varphi_r,\big(\Delta_1+\Delta_2\big)\eta\rangle\hat{b}^*_p\hat{b}^*_r + \text{h.c.}\\ &= -\frac{1}{2}\int dxdy\,\big[\big(\Delta_y+\Delta_y\big)\eta(x,y)\big]b_x b_y + \text{h.c.}\end{aligned} \tag{3.27}$$

With relations (3.2), we decompose

$$\begin{aligned}\int_0^1 ds\, e^{-sB}[\mathcal{K},B]e^{sB} &= -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]e^{-sB}b_y e^{sB}e^{-sB}b_x e^{sB} + \text{h.c.}\\ &= \Big(\mathrm{E}_1+\mathrm{E}_2+\mathrm{E}_3\Big) + \text{h.c.}\end{aligned}$$

with

$$\begin{aligned}\mathrm{E}_1 &= -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]\big(b(\gamma^{(s)}_y)+b^*(\sigma^{(s)}_y)\big)\big(b(\gamma^{(s)}_x)+b^*(\sigma^{(s)}_x)\big)\\ \mathrm{E}_2 &= -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]\big(b(\gamma^{(s)}_y)+b^*(\sigma^{(s)}_y)\big)d^{(s)}_x\\ &\quad -\frac{1}{2}\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]d^{(s)}_y\big(b(\gamma^{(s)}_x)+b^*(\sigma^{(s)}_x)\big)\\ \mathrm{E}_3 &= -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]d^{(s)}_y d^{(s)}_x\end{aligned} \tag{3.28}$$

where $\gamma^{(s)}_x = \cosh(s\eta_x)$, $\sigma^{(s)}_x = \sinh(s\eta_x)$ (recall the notation $\eta_x(y) = \eta(y,x)$) and $d^{(s)}_y$ is defined as in (3.2) with η in B, γ and σ substituted by $s\eta$. We expand E_1 as

$$\begin{aligned}\mathrm{E}_1 = &-\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]\big(b(\gamma^{(s)}_y)b(\gamma^{(s)}_x) + b^*(\sigma^{(s)}_y)b(\gamma^{(s)}_x)\\ &+ b(\gamma^{(s)}_y)b^*(\sigma^{(s)}_x) + b^*(\sigma^{(s)}_y))b^*(\sigma^{(s)}_x)\big)\\ &= \mathrm{E}_{11}+\mathrm{E}_{12}+\mathrm{E}_{13}+\mathrm{E}_{14}\end{aligned}$$

Writing $\gamma^{(s)} = 1 + p^{(s)}$ we express E_{11} as

$$\mathrm{E}_{11} = -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]b_y b_x + \tilde{\mathrm{E}}_{11} \tag{3.29}$$

with

$$\tilde{\mathrm{E}}_{11} = -\frac{1}{2}\int_0^1 ds\int dxdy\,\big[(\Delta_x+\Delta_y)\eta(x,y)\big]\big(b_y b(p^{(s)}_x) + b(p^{(s)}_y)b_x + b(p^{(s)}_y)b(p^{(s)}_x)\big)$$

The first term in (3.29) contributes to (3.23); with equation (2.26) we write $\tilde{\mathrm{E}}_{11}$ as

$$\tilde{\mathrm{E}}_{11} = \frac{n}{2}\int_0^1 ds\int dxdy\,\big[\ell^5\lambda_\ell - \kappa\ell^5 V(\ell(x-y))\big]f_\ell(x,y)\big(b_y b(p^{(s)}_x) + b(p^{(s)}_y)b_x + b(p^{(s)}_y)b(p^{(s)}_x)\big)$$

(Here we also used that the last two terms in (2.26) are zero when projected onto the orthogonal subspace to φ_0.) To estimate $\tilde{\mathrm{E}}_{11}$ we bound f_ℓ using (2.14) and Cauchy-Schwarz; for the term proportional to λ_ℓ we use (2.12), Cauchy-Schwarz and (2.32), while for the term proportional to V we use Lemma 3.5 and (2.32). This leads to

$$|\langle \xi, \tilde{\mathrm{E}}_{11}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 \tag{3.30}$$

Similarly we estimate E_{12} and E_{14}, with the result that

$$|\langle \xi, \tilde{\mathrm{E}}_{12}\xi\rangle|, |\langle \xi, \tilde{\mathrm{E}}_{14}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2. \tag{3.31}$$

We consider now E_{13}. Here we cannot use Lemma 3.5 directly (since the L^2 norm of $\gamma^{(s)}$ is not finite); in fact, this is not an error term and we will extract from it an important contribution to (3.23). We write $b(\gamma_y^{(s)})b^*(\sigma_x^{(s)}) = b_y b^*(\sigma_x^{(s)}) + b(p_y^{(s)})b^*(\sigma_x^{(s)})$ and we put the product $b_y b^*(\sigma_x^{(s)})$ in normal order. Splitting $\sigma^{(s)} = \eta^{(s)} + r^{(s)}$ we arrive at

$$\begin{aligned}\mathrm{E}_{13} &= -\frac{1}{2}\int_0^1 ds \int dxdy\, \big[(\Delta_x + \Delta_y)\eta(x,y)\big] b(\gamma_y^{(s)})b^*(\sigma_x^{(s)}) \\ &= -\frac{1}{2}\int_0^1 ds\, s \int dxdy\, \big[(\Delta_x + \Delta_y)\eta(x,y)\big]\eta(y,x) + \tilde{\mathrm{E}}_{13}\end{aligned} \tag{3.32}$$

with

$$\begin{aligned}\tilde{\mathrm{E}}_{13} = -\frac{1}{2}\int_0^1 ds \int dxdy\, &\big[(\Delta_x + \Delta_y)\eta(x,y)\big]\big(r^{(s)}(y,x) \\ &+ b^*(\sigma_x^{(s)})b_y - n^{-1}a^*(\sigma_x^{(s)})a_y - n^{-1}\sigma^{(s)}(y,x)\mathcal{N}_+ + b(p_y^{(s)})b^*(\sigma_x^{(s)})\big).\end{aligned}$$

The first contribution in (3.32) appears in (3.23) (the integration over s gives an additional factor 1/2, but we still need to add its hermitian conjugate, which is equal to the term itself), while $\tilde{\mathrm{E}}_{13}$ is now an error term. As we did for $\tilde{\mathrm{E}}_{11}$, in $\tilde{\mathrm{E}}_{13}$ we plug in equation (2.26) and we use estimates (2.14) and (2.12). For the term proportional to $r^{(s)}(y,x)$ we use (2.33), Cauchy-Schwarz and (2.27), while for the term proportional to $\sigma^{(s)}(y,x) = s\eta(y,x) + r^{(s)}(y,x)$ we use additionally (2.29). For all the other contributions in $\tilde{\mathrm{E}}_{13}$ we use Lemma 3.5, (2.32) and (2.27). This way we obtain

$$|\langle \xi, \tilde{\mathrm{E}}_{13}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\|^2. \tag{3.33}$$

We consider now E_2, which we split in $\mathrm{E}_2 = \mathrm{E}_{21} + \mathrm{E}_{22}$ with

$$\begin{aligned}\mathrm{E}_{21} &= -\frac{1}{2}\int_0^1 ds \int dxdy\, \big[(\Delta_x + \Delta_y)\eta(x,y)\big]\big(b(\gamma_y^{(s)}) + b^*(\sigma_y^{(s)})\big)d_x^{(s)} \\ \mathrm{E}_{22} &= -\frac{1}{2}\int_0^1 ds \int dxdy\, \big[(\Delta_x + \Delta_y)\eta(x,y)\big]d_y^{(s)}\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)})\big)\end{aligned} \tag{3.34}$$

We focus on E_{21} first. As before, using equation (2.26) and observing that only the first term contributes on the orthogonal subspace to φ_0, we get

$$\mathrm{E}_{21} = \frac{n}{2}\int_0^1 ds \int dxdy\, \Big[\ell^5\lambda_\ell - \kappa\ell^5 V(\ell(x-y))\Big] f_\ell(x,y)\big(b(\gamma_y^{(s)}) + b^*(\sigma_y^{(s)})\big)d_x^{(s)}$$

We write it as

$$\begin{aligned}\mathrm{E}_{21} &= \frac{n}{2}\int_0^1 ds \int dxdy\, \Big[\ell^5\lambda_\ell - \kappa\ell^5 V(\ell(x-y))\Big] f_\ell(x,y) b_y d_x^{(s)} \\ &+ \frac{n}{2}\int_0^1 ds \int dxdy\, \Big[\ell^5\lambda_\ell - \kappa\ell^5 V(\ell(x-y))\Big] f_\ell(x,y)\big(b(p_y^{(s)}) + b^*(\sigma_y^{(s)})\big)d_x^{(s)} \\ &= \mathrm{E}_{211} + \mathrm{E}_{212}\end{aligned}$$

To estimate E_{212} we use (3.3) (with $j = 0$ and the factors s bounded by 1, together with the bound $\mathcal{N}_+^2 \leq n^2$) and Proposition 2.2 to obtain

$$\begin{aligned}|\langle \xi, \mathrm{E}_{212}\xi\rangle| \leq Cn \int dxdy\, &\Big|\ell^5\lambda_\ell f_\ell(x,y) - \kappa\ell^5 V(\ell(x-y)) f_\ell(x,y)\Big| \\ &\times \int_0^1 ds \|\big(b^*(p_y^{(s)}) + b(\sigma_y^{(s)})\big)\xi\| \Big[\|\eta_x\|\|(\mathcal{N}_+ + 1)^{1/2}\xi\| + \|\eta\|\|b_x\xi\|\Big].\end{aligned}$$

With the aid of the Cauchy-Schwarz inequality and estimates (2.14) and (2.12) we obtain

$$
\begin{aligned}
|\langle \xi, \mathrm{E}_{212}\xi\rangle| \leq Cn &\left[\int dxdy \left|\ell^{-1} - \kappa\ell^2 V(\ell(x-y))\right| \int_0^1 ds \big(\|p_y^{(s)}\|^2 + \|\sigma_y^{(s)}\|^2\big)\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2\right]^{1/2} \\
&\times \left[\int dxdy \left|\ell^{-1} - \kappa\ell^2 V(\ell(x-y))\right| \Big(\|\eta_x\|^2 \|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 + \|\eta\|^2\|b_x\xi\|^2\Big)\right]^{1/2}.
\end{aligned}
$$

Using estimates (2.34) and (2.27) to bound the norm of p, σ and η we get

$$
|\langle \xi, \mathrm{E}_{212}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2.
$$

To estimate E_{211} we use the second bound in Lemma 3.2

$$
\begin{aligned}
|\langle \xi, \mathrm{E}_{211}\xi\rangle| &\leq \frac{n}{2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \int_0^1 ds \int dxdy \left|\ell^5\lambda_\ell f_\ell(x,y) + \kappa\ell^5 V(\ell(x-y))f_\ell(x,y)\right| \\
&\qquad \|(\mathcal{N}_+ + 1)^{-1/2} b_y d_x^{(s)}\xi\| \\
&\leq C\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \int dxdy \left|\ell^5\lambda_\ell f_\ell(x,y) - \kappa\ell^5 V(\ell(x-y))f_\ell(x,y)\right| \\
&\qquad \Big[\|\eta_x\|\|\eta_y\|\|(\mathcal{N}_+ + 1)^{1/2}\xi\| + |\eta(y,x)|\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \\
&\qquad + \|\eta_y\|\|b_x\xi\| + \|\eta_x\|\|a_y(\mathcal{N}_+ + 1)\xi\| + \|\eta\|\|a_y a_x(\mathcal{N}_+ + 1)^{1/2}\xi\| \Big] \\
&\leq Cn\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 \\
&\quad + C\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \Big[\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|a_y a_x(\mathcal{N}_+ + 1)^{1/2}\xi\|^2\Big]^{1/2}.
\end{aligned}
$$

In the last step we used (2.14), Cauchy-Schwarz (similarly as above) and additionally (2.29) for the term containing $|\eta(x,y)|$. With (2.27) we conclude that

$$
|\langle \xi, \mathrm{E}_{211}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|.
$$

Therefore

$$
|\langle \xi, \mathrm{E}_{21}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\| \tag{3.35}
$$

The second term in (3.34) can be estimated as follows

$$
\begin{aligned}
|\langle \xi, \mathrm{E}_{22}\xi\rangle| \leq &\frac{1}{2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \int_0^1 ds \int dxdy\, |(\Delta_x + \Delta_y)\eta(x,y)| \\
&\times \|(\mathcal{N}_+ + 1)^{-1/2} d_y^{(s)}\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)})\big)\xi\| \\
\leq Cn^{-1} &\int_0^1 ds \int dxdy\, |(\Delta_x + \Delta_y)\eta(x,y)|\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \\
\times &\Big[\|\eta_y\|\|\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)})\big)(\mathcal{N}_+ + 1)\xi\| + \|\eta\|\|b_y\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)})\big)(\mathcal{N}_+ + 1)^{1/2}\xi\|\Big]
\end{aligned} \tag{3.36}
$$

Substituting (2.26) for $(\Delta_x + \Delta_y)\eta(x,y)$ and arguing as before we obtain

$$
|\langle \xi, \mathrm{E}_{22}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\| \tag{3.37}
$$

Finally we examine E_3 in (3.28); with the third estimate in Lemma 3.2 we have

$$
\begin{aligned}
|\langle \xi, \mathrm{E}_3\xi\rangle| &\leq C\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \int_0^1 ds \int dxdy\, |(\Delta_x + \Delta_y)\eta(x,y)|\|(\mathcal{N}_+ + 1)^{-1/2} d_y^{(s)} d_x^{(s)}\xi\| \\
&\leq Cn^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \int dxdy\, |(\Delta_x + \Delta_y)\eta(x,y)| \Big[\|\eta_x\|\|\eta_y\|\|(\mathcal{N} + 1)^{3/2}\xi\| \\
&\quad + \|\eta_x\|\|b_y(\mathcal{N} + 1)\xi\| + |\eta(y,x)|\|(\mathcal{N} + 1)^{1/2}\xi\| + \|\eta_y\|\|a_x(\mathcal{N}_+ + 1)\xi\| + \|a_y a_x(\mathcal{N} + 1)^{1/2}\xi\| \Big]
\end{aligned} \tag{3.38}
$$

leading to

$$|\langle \xi, \mathrm{E}_3 \xi\rangle| \leq C\kappa n \ell^{-1} \|(\mathcal{N}_+ +1)^{1/2}\xi\|^2 + C\kappa^{1/2} n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ +1)^{1/2}\xi\| \|\mathcal{V}_\ell^{1/2}\xi\| \tag{3.39}$$

The estimates (3.30), (3.31), (3.33), (3.35), (3.37) and (3.39) prove (3.24). □

3.4.2 Analysis of $e^{-B}\mathcal{L}^{(2,V)}_{n,\ell} e^B$

With $\mathcal{L}^{(2,V)}_{n,\ell}$ introduced in (3.18), we define the error operator $\mathcal{E}^{(2,V)}_{n,\ell}$ through

$$e^{-B}\mathcal{L}^{(2,V)}_{n,\ell} e^B = n \sum_{p,q\in\Lambda^*_{1,+}} V_{\ell,pq00} \langle \eta, \varphi_p \otimes \varphi_q\rangle + \frac{1}{2}\sum_{p,q\in\Lambda^*_{1,+}} (nV_{\ell,pq00}\hat{b}^*_p \hat{b}^*_q + \text{h.c.}) + \mathcal{E}^{(2,V)}_{n,\ell} \tag{3.40}$$

Proposition 3.7 provides an estimate for $\mathcal{E}^{(2,V)}_{n,\ell}$.

Proposition 3.7. *Let $\mathcal{E}^{(2,V)}_{n,\ell}$ be defined as in (3.40). Then, under the same assumptions as Proposition 2.3, for every $\delta>0$ there exists a $C>0$ such that*

$$\pm\, \mathcal{E}^{(2,V)}_{n,\ell} \leq \delta \mathcal{V}_\ell + C\kappa n\ell^{-1}(\mathcal{N}_+ +1) \tag{3.41}$$

as operator inequalities on $\mathcal{F}^{\leq N}_+$.

Proof of Proposition 3.7. We split $e^{-B}\mathcal{L}^{(2,V)}_{n,\ell} e^B$ as

$$e^{-B}\mathcal{L}^{(2,V)}_{n,\ell} e^B = \mathrm{F}_1 + \mathrm{F}_2 + \mathrm{F}_3$$

with

$$\begin{aligned} \mathrm{F}_1 &= \sum_{p,q\in\Lambda^*_{1,+}} V_{\ell,0p0q}\, e^{-B}\hat{a}^*_p \hat{a}_q (n-\mathcal{N}_+) e^B \\ \mathrm{F}_2 &= \sum_{p,q\in\Lambda^*_{1,+}} V_{\ell,0pq0}\, e^{-B}\hat{a}^*_p \hat{a}_q (n-\mathcal{N}_+) e^B \\ \mathrm{F}_3 &= \frac{1}{2}\sum_{p,q\in\Lambda^*_{1,+}} (nV_{\ell,pq00}\, e^{-B}\hat{b}^*_p\hat{b}^*_q e^B + \text{h.c.}) \end{aligned} \tag{3.42}$$

It is convenient to rewrite

$$\mathrm{F}_1 = \kappa n \int dxdy\, \ell^2 V(\ell(x-y))\, e^{-B}\Big(b^*_y b_y - \frac{1}{n} a^*_y a_y\Big) e^B$$

The expectation of F_1 on any $\xi \in \mathcal{F}^{\leq n}_+$ can be estimated as

$$|\langle \xi, \mathrm{F}_1\xi\rangle| \leq \kappa n \int dy\, |\langle \xi, e^{-B}\Big(b^*_y b_y - n^{-1}a^*_y a_y\Big)e^B\xi\rangle| \int dx\, \ell^2 V(\ell(x-y)) \;\leq C\kappa n\ell^{-1}\langle \xi, \mathcal{N}_+\xi\rangle \tag{3.43}$$

where we used Lemma 3.1. Similarly we have

$$|\langle \xi, \mathrm{F}_2\xi\rangle| \leq \kappa n \int dxdy\, \ell^2 V(\ell(x-y))\, |\langle \xi, e^{-B}\Big(b^*_y b_x - \frac{1}{n}a^*_y a_x\Big)e^B\xi\rangle| \leq C\kappa n\ell^{-1}\langle \xi, \mathcal{N}_+\xi\rangle \tag{3.44}$$

We focus now on on the last contribution in (3.42).

$$\mathrm{F}_3 = \frac{\kappa n}{2}\int dxdy\, \ell^2 V(\ell(x-y))\big(e^{-B}b_x b_y e^B + \text{h.c.}\big) \tag{3.45}$$

Using equations (3.2), we get

$$
\begin{aligned}
\mathrm{F}_3 &= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[(b(\gamma_x)+b^*(\sigma_x)+d_x)(b(\gamma_y)+b^*(\sigma_y)+d_y)+\text{h.c.}\big]\\
&= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[(b(\gamma_x)+b^*(\sigma_x))(b(\gamma_y)+b^*(\sigma_y))+\text{h.c.}\big]\\
&\quad+\frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[(b(\gamma_x)+b^*(\sigma_x))d_y+d_x(b(\gamma_y)+b^*(\sigma_y))+\text{h.c.}\big]\\
&\quad+\frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[d_xd_y+\text{h.c.}\big]\\
&= \mathrm{F}_{31}+\mathrm{F}_{32}+\mathrm{F}_{33}
\end{aligned}
\tag{3.46}
$$

We start analyzing F_{31}. After normal ordering, a simple calculation (similar to the one done in (3.32)) gives

$$
\mathrm{F}_{31} = \kappa n\int dxdy\,\ell^2 V(\ell(x-y))\eta(x,y)+\frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[b_xb_y+\text{h.c.}\big]+\mathcal{E}_{31} \tag{3.47}
$$

with

$$
\begin{aligned}
\mathcal{E}_{31} = \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[&r(x,y)-\eta(x,y)n^{-1}\mathcal{N}_+\\
&+b^*(r_y)b_x+b^*(\eta_y)b_x+n^{-1}a^*(\eta_y)a_x+b(p_x)b^*(\eta_y)+b(p_x)b^*(r_y)\\
&+b(p_x)b_y+b(\gamma_x)b(p_y)+b^*(\sigma_x)b(\gamma_y)+b^*(\sigma_x)b^*(\sigma_y)+\text{h.c.}\big]
\end{aligned}
\tag{3.48}
$$

where again we used the notation $\gamma_x = \delta_x + p_x$ and $\sigma_x = \eta_x + r_x$. Lemma 3.5 and Proposition 2.2 show that $\mathcal{E}_{31}$ satisfies

$$
|\langle\xi,\mathcal{E}_{31}\rangle\xi| \le C\kappa n\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|^2 \tag{3.49}
$$

Next we consider F_{32}. Again splitting $\gamma = 1+p$ and $\sigma = \eta + r$, we write

$$
\mathrm{F}_{32} =: \mathrm{F}_{321}+\mathrm{F}_{322}+\mathrm{F}_{323}+\text{h.c.} \tag{3.50}
$$

with

$$
\begin{aligned}
\mathrm{F}_{321} &= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))b_xd_y\\
\mathrm{F}_{322} &= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))d_xb_y\\
\mathrm{F}_{323} &= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[(b(p_x)+b^*(\sigma_x))d_y+d_x(b(p_y)+b^*(\sigma_y))\big]
\end{aligned}
\tag{3.51}
$$

To bound F_{321}, we use (3.4) and Proposition 2.2:

$$
\begin{aligned}
|\langle\xi,\mathrm{F}_{321}\rangle\xi| &\le C\kappa\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\Big[\,\|\eta_x\|\|\eta_y\|\|(\mathcal{N}_++1)^{1/2}\xi\|\\
&\quad+|\eta(y,x)|\|(\mathcal{N}+1)^{1/2}\xi\|+\|\eta_y\|\|b_x\xi\|+\|\eta_x\|\|a_y(\mathcal{N}_++1)\xi\|\Big]\\
&\quad+C\kappa n^{1/2}\|\eta\|_2\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\|a_yb_x\xi\|\\
&\le C\kappa n\ell^{-1}\|\eta\|_2\|(\mathcal{N}_++1)^{1/2}\xi\|^2+C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|\eta\|_2\|(\mathcal{N}_++1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|
\end{aligned}
\tag{3.52}
$$

The estimate for F_{322} follows from (3.3):

$$
\begin{aligned}
|\langle\xi,\mathrm{F}_{322}\xi\rangle| &\le \kappa n\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\|(\mathcal{N}_++1)^{-1/2}d_xb_y\xi\|\\
&\le C\kappa n\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\|\eta_x\|\|b_y\xi\|\\
&\quad+C\kappa n^{1/2}\|\eta\|\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\|b_xb_y\xi\|\\
&\le C\kappa n\ell^{-1}\|\eta\|_2\|(\mathcal{N}_++1)^{1/2}\xi\|^2+C\kappa^{1/2}n^{1/2}\ell^{1/2}\|\eta\|_2\|(\mathcal{N}_++1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|
\end{aligned}
\tag{3.53}
$$

and similarly the estimate for F_{323}:

$$
\begin{aligned}
|\langle \xi, \mathrm{F}_{323}\xi\rangle| &= \frac{\kappa n}{2}\int dxdy\,\ell^2 V(\ell(x-y))\big[(b(p_x)+b^*(\sigma_x))d_y + d_x(b(p_y)+b^*(\sigma_y))\big] \\
&\leq \kappa n \int dxdy\,\ell^2 V(\ell(x-y))\|(b^*(p_x)+b(\sigma_x))\xi\|\|d_y\xi\| \\
&\quad + \kappa n\,\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\|(\mathcal{N}_++1)^{-1/2}d_x(b(p_y)+b^*(\sigma_y))\xi\| \\
&\leq C\kappa n^{1/2}\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\big(\|p_x\|_2+\|\sigma_x\|_2\big) \\
&\qquad\qquad \times\Big[\,\|\eta_y\|\|(\mathcal{N}_++1)^{1/2}\xi\| + \|\eta\|\|b_y\xi\|\Big] \\
&\quad + C\kappa\,\|(\mathcal{N}_++1)^{1/2}\xi\|\int dxdy\,\ell^2 V(\ell(x-y))\Big[\,\|\eta_x\|\|(\mathcal{N}_++1)(b(p_y)+b^*(\sigma_y))\xi\| \\
&\qquad\qquad + \|\eta\|\|b_x(\mathcal{N}_++1)^{1/2}(b(p_y)+b^*(\sigma_y))\xi\|\Big]
\end{aligned}
\tag{3.54}
$$

We normal order the last term and use estimates (2.27), (2.29) and (2.33) to get

$$
|\langle \xi, \mathrm{F}_{323}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|^2 \tag{3.55}
$$

Finally we consider the last contribution in (3.46). With estimate (3.5) and Proposition 2.2 we conclude that

$$
\begin{aligned}
|\langle \xi, \mathrm{F}_{33}\xi\rangle| &\leq C\kappa n\ell^{-1}\|\eta\|^2\|(\mathcal{N}_++1)^{1/2}\xi\|^2 \\
&\quad + C\kappa n^{1/2}\ell^{-1/2}\|\eta\|^2\|(\mathcal{N}_++1)^{1/2}\xi\|\Big[\int dxdy\,\ell^2 V(\ell(x-y))\|a_y a_x\xi\|^2\Big]^{1/2} \\
&\leq C\kappa n\ell^{-1}\|\eta\|^2\|(\mathcal{N}_++1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|\eta\|^2\|(\mathcal{N}_++1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|
\end{aligned}
\tag{3.56}
$$

Estimates (3.43), (3.44), (3.49), (3.52), (3.53), (3.55) and (3.56) prove (3.41). □

3.5 Analysis of $\mathcal{G}^{(3)}_{n,\ell}$

As defined in (2.10),

$$
\begin{aligned}
\mathcal{L}^{(3)}_{n,\ell} &= \sum_{p,q,r\in\Lambda^*_{1,+}} (n^{1/2}V_{\ell,qr0p}\hat{b}^*_r\hat{a}^*_q\hat{a}_p + \text{h.c.}) \\
&= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\Big[b^*_x a^*_y a_x + \text{h.c.}\Big]
\end{aligned}
$$

We define $\mathcal{E}^{(3)}_{n,\ell}$ through

$$
\mathcal{G}^{(3)}_{n,\ell} = e^{-B}\mathcal{L}^{(3)}_{n,\ell}e^{B} = n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(y,x)\big[b(\gamma_x)+b^*(\sigma_x)+\text{h.c.}\big] + \mathcal{E}^{(3)}_{n,\ell}. \tag{3.57}
$$

Proposition 3.8. *Let $\mathcal{E}^{(3)}_{n,\ell}$ be defined as in (3.57). Then, under the same assumptions as Proposition 2.3, for any $\delta>0$ there exists a constant $C>0$ such that*

$$
\pm\,\mathcal{E}^{(3)}_{n,\ell} \leq \delta\mathcal{V}_\ell + C\kappa n\ell^{-1}(\mathcal{N}_++1) \tag{3.58}
$$

as operator inequalities on $\mathcal{F}^{\leq n}_+$.

To prove Proposition 3.8, we need the following lemma, taken from [8, Lemma 3.8].

Lemma 3.9. *Let $V\in L^1(\mathbb{R}^3)$, $V\geq 0$. Let $j_1, j_2\in L^2(\Lambda_1\times\Lambda_1)$ with*

$$
M_i := \max\left\{\sup_x\int dy|j_i(x,y)|^2, \sup_y\int dx|j_i(x,y)|^2\right\} < \infty
$$

for $i = 1,2$. Then we have

$$\int dxdy\,\kappa\ell^3 V(\ell(x-y))\|a^\sharp(j_{1,x})a^\sharp(j_{2,y})\xi\|^2 \leq C\kappa\min(M_1\|j_2\|_2^2, M_2\|j_1\|_2^2)\|(\mathcal{N}_+ +1)\xi\|^2$$
$$\int dxdy\,\kappa\ell^3 V(\ell(x-y))\|a^\sharp(j_{1,x})a_y\xi\|^2 \leq C\kappa M_1\|(\mathcal{N}_+ +1)\xi\|^2$$

for all $\xi \in \mathcal{F}$ (with $a^\sharp$ we indicate either a or a^*).

Proof. The first inequality simply follows from Cauchy-Schwarz

$$\begin{aligned}\int dxdy\,\kappa\ell^3 V(\ell(x-y))\|a^\sharp(j_{1,x})a^\sharp(j_{2,y})\xi\|^2 &\leq \int dxdy\,\kappa\ell^3 V(\ell(x-y))\|j_{1,x}\|_2^2\|j_{2,y}\|_2^2\|(\mathcal{N}_+ +1)\psi\|^2\\ &\leq C\kappa\min(M_1\|j_2\|_2^2, M_2\|j_1\|_2^2)\|(\mathcal{N}_+ +1)\psi\|^2\end{aligned}$$

The second inequality can be obtained similarly. □

Proof of Proposition 3.8. We compute

$$e^{-B}a_y^*a_xe^B = a_y^*a_x + \int_0^1 ds\,e^{-sB}[a_y^*a_x, B]e^{sB} = a_y^*a_x + \int_0^1 ds\,e^{-sB}\big(b(\eta_y)b_x + b^*(\eta_x)b_y^*\big)e^{sB} \tag{3.59}$$

We have therefore

$$\begin{aligned}\mathcal{G}_{n,\ell}^{(3)} &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\Big[e^{-B}b_x^*e^Ba_y^*a_x + \text{h.c.}\Big]\\ &\quad + n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\Big[e^{-B}b_x^*e^B\int_0^1 ds\,e^{-sB}b^*(\eta_x)b_y^*e^{sB} + \text{h.c.}\Big]\\ &\quad + n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\Big[e^{-B}b_x^*e^B\int_0^1 ds\,e^{-sB}b(\eta_y)b_xe^{sB} + \text{h.c.}\Big]\\ &=: \text{G}_1 + \text{G}_2 + \text{G}_3 + \text{h.c.}\end{aligned} \tag{3.60}$$

We start analyzing G_1. Using (3.2) and

$$b(\sigma_x)a_y^*a_x = \int dz\,\sigma(x,z)b_za_y^*a_x = a_y^*a_xb(\sigma_x) + \sigma(x,y)b_x \tag{3.61}$$

we write it as (adopting always the notation $\sigma = \eta + r$)

$$\begin{aligned}\text{G}_1 &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\big(b^*(\gamma_x) + b(\sigma_x) + d_x^*\big)a_y^*a_x\\ &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)b_x + \text{G}_{11} + \text{G}_{12} + \text{G}_{13} + \text{G}_{14}\end{aligned} \tag{3.62}$$

with

$$\begin{aligned}\text{G}_{11} &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))r(x,y)b_x\\ \text{G}_{12} &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))b^*(\gamma_x)a_y^*a_x\\ \text{G}_{13} &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))a_y^*a_xb(\sigma_x)\\ \text{G}_{14} &= n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))d_x^*a_y^*a_x\end{aligned} \tag{3.63}$$

With (2.33) and Cauchy-Schwarz we see that for any normalized $\xi \in \mathcal{F}_+^{\leq n}$

$$\begin{aligned}|\langle\xi,\text{G}_{11}\xi\rangle| &\leq Cn^{1/2}\|\eta\|\int dxdy\,\kappa\ell^2 V(\ell(x-y))\|\eta_x\|\|\eta_y\|\|b_x\xi\|\\ &\leq Cn^{1/2}\|\eta\|\Big[\int dxdy\,\kappa\ell^2 V(\ell(x-y))\|b_x\xi\|^2\Big]^{1/2}\Big[\int dxdy\,\kappa\ell^2 V(\ell(x-y))\|\eta_x\|^2\|\eta_y\|^2\Big]^{1/2}.\end{aligned} \tag{3.64}$$

In the last factor we use (2.31) and we arrive at

$$|\langle\xi, \mathrm{G}_{11}\xi\rangle| \leq C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2. \tag{3.65}$$

To bound G_{12} we split $\gamma = 1 + p$ and use estimate (2.34) and (2.31), so that

$$\begin{aligned}|\langle\xi, \mathrm{G}_{12}\xi\rangle| &\leq n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|a_y b_x\xi\|\|a_x\xi\| \\ &\quad + n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|\mathcal{N}_+^{-1/2}a_y b(p_x)\xi\|\|\mathcal{N}_+^{1/2}a_x\xi\| \\ &\leq Cn^{1/2}\kappa^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\| + C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2.\end{aligned} \tag{3.66}$$

In the last step we used the Cauchy-Schwarz inequality and note that the first term is proportional to $\mathcal{V}_\ell$, as defined in (2.39). Similarly

$$\begin{aligned}|\langle\xi, \mathrm{G}_{13}\xi\rangle| &\leq n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|\mathcal{N}_+^{-1/2}a_x b(\sigma_x)\xi\|\|\mathcal{N}_+^{1/2}a_y\xi\| \\ &\leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2\end{aligned} \tag{3.67}$$

In order to bound G_{14}, we use (3.4) to estimate

$$\begin{aligned}|\langle\xi, \mathrm{G}_{14}\xi\rangle| &\leq n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|\mathcal{N}_+^{-1/4}a_y d_x\xi\|\|\mathcal{N}_+^{1/4}a_x\xi\| \\ &\leq n^{1/2}\kappa^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{3/4}\xi\|\left[\int dxdy\, \kappa\ell^2 V(\ell(x-y))\|d_x(\mathcal{N}_+ + 1)^{1/4}\xi\|^{1/2}\right]^{1/2} \\ &\leq Cn^{1/2}\kappa^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{3/4}\xi\| \\ &\quad\times\left[\int dxdy\, \kappa\ell^2 V(\ell(x-y))\Big(\|\eta_x\|\|(\mathcal{N}_+ + 1)^{3/4}\xi\| + \|\eta\|\|b_x(\mathcal{N}_+ + 1)^{1/4}\xi\|\Big)\right]^{1/2} \\ &\leq Cn^{1/2}\kappa\ell^{-1}\|(\mathcal{N}_+ + 1)^{3/4}\xi\|^2\end{aligned} \tag{3.68}$$

Next we consider G_2. With (3.2), we have

$$\mathrm{G}_2 = n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\big(b^*(\gamma_x) + b(\sigma_x) + d_x^*\big)\int_0^1 ds\, e^{-sB}b_y^* b^*(\eta_x)e^{sB} \tag{3.69}$$

and we split $\mathrm{G}_2 = \mathrm{G}_{21} + \mathrm{G}_{22} + \mathrm{G}_{23}$, where

$$\begin{aligned}\mathrm{G}_{21} &= n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))b(\sigma_x)\int_0^1 ds\, e^{-sB}b_y^* b^*(\eta_x)e^{sB} \\ \mathrm{G}_{22} &= n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))b^*(\gamma_x)\int_0^1 ds\, e^{-sB}b_y^* b^*(\eta_x)e^{sB} \\ \mathrm{G}_{23} &= n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))d_x^*\int_0^1 ds\, e^{-sB}b_y^* b^*(\eta_x)e^{sB}\end{aligned} \tag{3.70}$$

In G_{21} we expand further

$$\mathrm{G}_{21} = n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))b(\sigma_x)\int_0^1 ds\, \big(b_y^* + b^*(p_y^{(s)}) + b(\sigma_y^{(s)}) + (d_y^{(s)})^*\big)e^{-sB}b^*(\eta_x)e^{sB} \tag{3.71}$$

where we denote again $\sigma^{(s)} = \sinh(s\eta)$, $p^{(s)} = \cosh(s\eta) - 1$ and $(d_y^{(s)})^*$ is defined as d_y^* in (3.2) with η in B, γ and σ substituted with $s\eta$. We commute b_y to the left using (2.5), so that

$$\begin{aligned}b(\sigma_x)b_y^* &= \int dw\, \sigma(w,x)b_w b_y^* = \int dw\, \sigma(w,x)\big(b_y^* b_w + \delta(y-w)(1-\mathcal{N}_+/n) - n^{-1}a_y^* a_w\big) \\ &= \sigma(y,x)(1-\mathcal{N}_+/n) + b_y^* b(\sigma_x) - n^{-1}a_y^* a(\sigma_x)\end{aligned} \tag{3.72}$$

Hence

$$
\begin{aligned}
\mathrm{G}_{21} =&n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\sigma(y,x)\int_0^1 ds\, e^{-sB}b^*(\eta_x)e^{sB}\\
&+n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\\
&\qquad\qquad \times\big(-\sigma(y,x)\mathcal{N}_+/n+b_y^*b(\sigma_x)-n^{-1}a_y^*a(\sigma_x)\big)\int_0^1 ds\, e^{-sB}b^*(\eta_x)e^{sB}\\
&+n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))b(\sigma_x)\\
&\qquad\qquad \times\int_0^1 ds\,\big(b^*(p_y^{(s)})+b(\sigma_y^{(s)})+(d_y^{(s)})^*\big)e^{-sB}b^*(\eta_x)e^{sB}\\
&=: \mathrm{G}_{211}+\mathrm{G}_{212}+\mathrm{G}_{213}
\end{aligned}
\tag{3.73}
$$

We use that

$$
\int_0^1 ds\int dz\,\eta(z,x)\cosh_{s\eta}(w,z)=\sinh_\eta(x,w)
$$

and

$$
\int_0^1 ds\int dz\,\eta(z,x)\sinh_{s\eta}(w,z)=(\cosh_\eta-1)(x,w),
$$

resulting in

$$
\begin{aligned}
\mathrm{G}_{211} =&n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\sigma(y,x)\int dz\,\eta(z,x)\int_0^1 ds\big(b^*(\gamma_z^{(s)})+b(\sigma_z^{(s)})\big)\\
&+n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\sigma(y,x)\int dz\,\eta(z,x)\int_0^1 ds(d_z^{(s)})^*\\
=&n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\sigma(y,x)\big(b^*(\sigma_x)+b(p_x)\big)\\
&+n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\sigma(y,x)\int dz\,\eta(z,x)\int_0^1 ds(d_z^{(s)})^*\\
=&:\mathrm{G}_{2111}+\mathrm{G}_{2112}
\end{aligned}
\tag{3.74}
$$

In G_{2111} we split $\sigma=\eta+r$ and write

$$
\mathrm{G}_{2111} =n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(y,x)\big(b^*(\sigma_x)+b(p_x)\big)+\mathcal{E}_1 \tag{3.75}
$$

The first contribution plus its hermitian conjugate adds up to the first term in the second line of (3.62) plus its hermitian conjugate to give the first contribution in (3.57), while

$$
\begin{aligned}
|\langle\xi,\mathcal{E}_1\xi\rangle| &\le n^{1/2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))|r(y,x)|\|\big(b^*(\sigma_x)+b(p_x)\big)\xi\|\\
&\le C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\|\xi\|
\end{aligned}
\tag{3.76}
$$

where we used (2.33) and (2.31). We estimate G_{2112} using estimate (2.29), (2.33) and (2.31) to bound $\sigma(y,x)$, and then estimates (3.3) and (2.31)

$$
\begin{aligned}
|\langle\xi,\mathrm{G}_{2112}\xi\rangle| \le\,& Cn^{3/2}\|(\mathcal{N}_++1)^{1/2}\xi\|\\
&\times\int dxdy\,\kappa\ell^2 V(\ell(x-y))\int dz\,|\eta(z,x)|\|(\mathcal{N}_++1)^{-1/2}d_z\xi\|\\
\le\,& Cn^{3/2}\|(\mathcal{N}_++1)^{1/2}\xi\|\left(\int dxdy\,\kappa\ell^2 V(\ell(x-y))\int dz\,|\eta(z,x)|^2\right)^{1/2}\\
&\times\left(\int dxdy\,\kappa\ell^2 V(\ell(x-y))\int dz\,\|(\mathcal{N}_++1)^{-1/2}d_z\xi\|^2\right)^{1/2}\\
\le\,& C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\|(\mathcal{N}_++1)\xi\|
\end{aligned}
\tag{3.77}
$$

Next we analyze G_{212} in (3.73). Using (2.29), (2.33) and (2.31) to bound $\sigma(y,x)$, as well as η_x, Lemma 3.1 and Lemma 3.9, we estimate

$$\begin{aligned}|\langle\xi,\mathrm{G}_{212}\xi\rangle| &\le n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))\\ &\qquad\times\|\big(-\sigma(y,x)\mathcal{N}_+/n+b(\sigma_x)^*b_y-n^{-1}a^*(\sigma_x)a_y\big)\xi\|\int_0^1 ds\,\|b^*(\eta_x)e^{sB}\xi\|\\ &\le \kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)\xi\|\|(\mathcal{N}_++1)^{1/2}\xi\|\end{aligned}\tag{3.78}$$

Similar arguments lead to the estimate for the last term in (3.73):

$$\begin{aligned}|\langle\xi,\mathrm{G}_{213}\xi\rangle| &\le n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))\\ &\qquad\times\int_0^1 ds\,\|\big(b(p_y^{(s)})+b^*(\sigma_y^{(s)})+d_y^{(s)}\big)b^*(\sigma_x)\xi\|\|b^*(\eta_x)e^{sB}\xi\|\\ &\le \kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)\xi\|\|(\mathcal{N}_++1)^{1/2}\xi\|\end{aligned}\tag{3.79}$$

We consider G_{22} in (3.70) next. We expand it as

$$\mathrm{G}_{22}=n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))b^*(\gamma_x)\int_0^1 ds\,\big(b^*(\gamma_y^{(s)})+b(\sigma_y^{(s)})+(d_y^{(s)})^*\big)e^{-sB}b^*(\eta_x)e^{sB}\tag{3.80}$$

and estimate it as

$$\begin{aligned}|\langle\xi,\mathrm{G}_{22}\xi\rangle| &\le n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))\\ &\qquad\times\int_0^1 ds\,\|\big(b_y+b(p_y^{(s)})+b^*(\sigma_y^{(s)})+(d_y^{(s)})\big)\big(b_x+b(p_x)\big)\xi\|\|b^*(\eta_x)e^{sB}\xi\|\\ &\le n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))\int_0^1 ds\,\|b^*(\eta_x)e^{sB}\xi\|\Big[\|b_yb_x\xi\|\\ &\qquad+\|b_yb(p_x)\xi\|+\|\big(b(p_y^{(s)})+b^*(\sigma_y^{(s)})+d_y^{(s)}\big)\big(b_x+b(p_x)\big)\xi\|\Big]\\ &\le C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_++1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|+C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\|(\mathcal{N}_++1)\xi\|\end{aligned}\tag{3.81}$$

where we used Lemma 3.1, Lemma 3.9 and Lemma 3.2. In order to bound the last contribution in (3.70), we estimate, similarly as we did for G_{22},

$$\begin{aligned}|\langle\xi,\mathrm{G}_{23}\xi\rangle| &\le n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))\int_0^1 ds\,\|\big(b(\gamma_y^{(s)})+b^*(\sigma_y^{(s)})+(d_y^{(s)})\big)d_x\xi\|\|b^*(\eta_x)e^{sB}\xi\|\\ &\le C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_++1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|+C\kappa n^{1/2}\ell^{-1}\|(\mathcal{N}_++1)^{1/2}\xi\|\|(\mathcal{N}_++1)\xi\|\end{aligned}\tag{3.82}$$

We analyze finally the last contribution in (3.60), given by

$$\begin{aligned}\mathrm{G}_3 &= n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))e^{-B}b_x^*e^B\\ &\qquad\times\int_0^1 ds\,\big(b((\eta\gamma^{(s)})_y)+b^*((\eta\sigma^{(s)})_y)\big)\big(b(\gamma_x^{(s)})+b^*(\sigma_x^{(s)})+d_x^{(s)}\big)\\ &\quad+n^{1/2}\int dxdy\,\kappa\ell^2V(\ell(x-y))e^{-B}b_x^*e^B\\ &\qquad\times\int_0^1 ds\int dz\,\eta(z,y)d_z^{(s)}\big(b(\gamma_x^{(s)})+b^*(\sigma_x^{(s)})+d_x^{(s)}\big)\\ &=:\mathrm{G}_{31}+\mathrm{G}_{32}\end{aligned}\tag{3.83}$$

With Lemma 3.1, Lemma 3.9 and Lemma 3.2 and the bounds (2.31) and (2.32) we get

$$\begin{aligned}|\langle \xi, \mathrm{G}_{31}\xi\rangle| \le n^{1/2} \int dxdy\, \kappa\ell^2 V(\ell(x-y)) \|b_x e^B \xi\| \\ \times \int_0^1 ds\, \big\| \big(b((\eta\gamma^{(s)})_y) + b^*((\eta\sigma^{(s)})_y)\big)\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)}) + d_x^{(s)}\big)\xi\big\| \\ \le C\kappa n^{1/2}\ell^{-1} \|(\mathcal{N}_+ +1)^{1/2}\xi\| \|(\mathcal{N}_+ +1)\xi\|;\end{aligned} \tag{3.84}$$

and

$$\begin{aligned}|\langle \xi, \mathrm{G}_{32}\xi\rangle| \le n^{1/2} \int dxdy\, \kappa\ell^2 V(\ell(x-y)) \|b_x e^B \xi\| \\ \times \int_0^1 ds \int dz\, |\eta(z,y)| \big\|d_z^{(s)}\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)}) + d_x^{(s)}\big)\xi\big\| \\ \le C\kappa n^{1/2}\ell^{-1} \|(\mathcal{N}_+ +1)^{1/2}\xi\| \|(\mathcal{N}_+ +1)\xi\|\end{aligned} \tag{3.85}$$

Putting together (3.65), (3.66), (3.67), (3.68), (3.76), (3.77), (3.78), (3.79), (3.81), (3.82), (3.84) and (3.85) we arrive at (3.58). □

3.6 Analysis of $\mathcal{G}_{n,\ell}^{(4)}$

Recall the definition of $\mathcal{L}_{n,\ell}^{(4)}$ in (2.10). We define the error $\mathcal{E}_n^{(4)}$ by

$$\begin{aligned}\mathcal{G}_{n,\ell}^{(4)} = e^{-B}\mathcal{L}_{n,\ell}^{(4)} e^B = \mathcal{V}_\ell + \frac{1}{2}\sum_{p,q,r,s\in\Lambda_{1,+}^*} V_{\ell,pqrs} \langle \varphi_s \otimes \varphi_r, \eta\rangle \langle \eta, \varphi_p \otimes \varphi_q\rangle \\ + \frac{1}{2}\sum_{p,q,r,s\in\Lambda_{1,+}^*} \big(V_{\ell,pqrs}\langle \varphi_s\otimes\varphi_r,\eta\rangle \hat{b}_p^* \hat{b}_q^* + \text{h.c.}\big) \\ + \mathcal{E}_n^{(4)}\end{aligned} \tag{3.86}$$

It can be estimated as in the Proposition below.

Proposition 3.10. *Let $\mathcal{E}_n^{(4)}$ be defined as in (3.86). Then, under the same assumptions as Proposition 2.3 for every $\delta > 0$ there exists a $C > 0$ such that*

$$\pm\, \mathcal{E}_{n,\ell}^{(4)} \le \delta \mathcal{V}_\ell + C\kappa n \ell^{-1}(\mathcal{N}_+ + 1) \tag{3.87}$$

as operator inequalities on $\mathcal{F}_+^{\le N}$.

Proof. The proof of (3.87) follows closely [10, Section 5.6] and [5, Section 4.5]. We write

$$\begin{aligned}e^{-B}\mathcal{L}_n^{(4)} e^B &= \frac{1}{2}\int dxdy\, \kappa\ell^2 V(\ell(x-y)) e^{-B} a_x^* a_y^* a_x a_y e^B \\ &= \mathcal{V}_\ell + \frac{1}{2}\int dxdy\, \kappa\ell^2 V(\ell(x-y)) \int_0^1 ds\, e^{-sB}[a_x^* a_y^* a_x a_y, B] e^{sB} \\ &= \mathcal{V}_\ell + \frac{1}{2}\int dxdy\, \kappa\ell^2 V(\ell(x-y)) \int_0^1 ds\, e^{-sB} b_x^* b_y^* \big(a_x a^*(\eta_y) + a^*(\eta_x) a_y + \text{h.c.}\big) e^{sB}\end{aligned} \tag{3.88}$$

We expand $e^{-sB}\big(a_x a^*(\eta_y) + a^*(\eta_x)a_y\big)e^{sB}$ further and get

$$e^{-B}\mathcal{L}_n^{(4)} e^B - \mathcal{V}_\ell = (\mathrm{W}_1 + \mathrm{W}_2 + \mathrm{W}_3 + \mathrm{W}_4) + \text{h.c.} \tag{3.89}$$

with

$$\begin{aligned}
\mathrm{W}_1 &= \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\, e^{-sB} b_x^* b_y^* e^{sB} \\
\mathrm{W}_2 &= \int dxdy\,\kappa\ell^2 V(\ell(x-y))\int_0^1 ds\, e^{-sB} b_x^* b_y^* e^{sB} a^*(\eta_x) a_y \\
\mathrm{W}_3 &= \int dxdy\,\kappa\ell^2 V(\ell(x-y))\int_0^1 ds\, e^{-sB} b_x^* b_y^* e^{sB}\int_0^s dt\, e^{-tB} b(\eta_x^2) b_y e^{tB} \\
\mathrm{W}_4 &= \int dxdy\,\kappa\ell^2 V(\ell(x-y))\int_0^1 ds\, e^{-sB} b_x^* b_y^* e^{sB}\int_0^s dt\, e^{-tB} b^*(\eta_y) b^*(\eta_x) e^{tB}
\end{aligned} \tag{3.90}$$

The term W_1 results from normal ordering of $a_x a^*(\eta_y)$; in W_3 the notation $\eta_x^2(w)$ stands for $\int dz\,\eta(w,z)\eta(z,x)$. We start with analyzing W_1. With the relations (3.2) we further expand it as

$$\begin{aligned}
\mathrm{W}_1 =& \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\,\big(b^*(\gamma_x^{(s)}) + b(\sigma_x^{(s)})\big)\big(b^*(\gamma_y^{(s)}) + b(\sigma_y^{(s)})\big) \\
&+ \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\,\big(d_x^{(s)}\big)^*\big(b^*(\gamma_y^{(s)}) + b(\sigma_y^{(s)})\big) \\
&+ \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\,\big(b^*(\gamma_x^{(s)}) + b(\sigma_x^{(s)})\big)\big(d_y^{(s)}\big)^* \\
&+ \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\,\big(d_x^{(s)}\big)^*\big(d_y^{(s)}\big)^* \\
=:& \ \mathrm{W}_{11} + \mathrm{W}_{12} + \mathrm{W}_{13} + \mathrm{W}_{14},
\end{aligned} \tag{3.91}$$

where, for $x,y\in\Lambda_1$, $\gamma_x^{(s)}(y)$, $\sigma_x^{(s)}(y)$ and $d_x^{(s)}$ are defined as in (3.1) and (3.2) respectively, with η substituted by $s\eta$. Multiplying out the product in W_{11} and normal ordering the term $b(\sigma_x^{(s)})b^*(\gamma_y^{(s)})$ leads to

$$\begin{aligned}
\mathrm{W}_{11} =& \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y) ds\,\Big(b_x^* b_y^* + \frac{1}{2}\eta(x,y)\Big) \\
&+ \mathrm{W}_{112}
\end{aligned} \tag{3.92}$$

with

$$\begin{aligned}
\mathrm{W}_{112} =& \frac{1}{2}\int dxdy\,\kappa\ell^2 V(\ell(x-y))\eta(x,y)\int_0^1 ds\,\Big[b_y^* b(\sigma_x) - n^{-1}a_y^* a(\sigma_x) + r^{(s)}(x,y) \\
&- \mathcal{N}_+ n^{-1}\sigma^{(s)}(x,y) + b_x^* b^*(p_y^{(s)}) + b^*(p_x^{(s)})\big(b_y^* + b^*(p_y^{(s)})\big) + \big(b_x^* + b^*(p_x^{(s)})\big)b(\sigma_y^{(s)}) \\
&+ b(\sigma_x^{(s)})\big(b^*(p_y^{(s)}) + b^*(\sigma_y^{(s)})\big)\Big]
\end{aligned} \tag{3.93}$$

where $p_x^{(s)}(y) = \gamma_x^{(s)}(y) - \delta(x-y)$ and $r_x^{(s)}(y) = \sigma_x^{(s)}(y) - s\eta_x(y)$. The first line in (3.92), together with its hermitian conjugate, gives the main terms in (3.86). To estimate W_{112} we first use (2.29) and then apply Lemma 3.5 with estimate (2.32) (for the term proportional to $r^{(s)}$ we use (2.33) and for the term proportional to $\sigma^{(s)}$ we use (2.29) and (2.33)). This way we obtain

$$|\langle \xi, \mathrm{W}_{112}\xi\rangle| \leq C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 \tag{3.94}$$

To control W_{12} we use Lemma 3.2 and (2.29):

$$\begin{aligned}
|\langle \xi, \mathrm{W}_{12}\xi\rangle| \leq& C\int dxdy\,\kappa\ell^2 V(\ell(x-y))|\eta(x,y)|\int_0^1 ds\,\|d_x^{(s)}\xi\|\|\big(b^*(p_y^{(s)}) + b(\sigma_y^{(s)})\big)\xi\| \\
&+ C\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\int dxdy\,\kappa\ell^2 V(\ell(x-y))|\eta(x,y)|\int_0^1 ds\,\|(\mathcal{N}_+ + 1)^{-1/2} b_y d_x^{(s)}\xi\| \\
\leq& C\kappa n\ell^{-1}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 + C\kappa^{1/2} n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|
\end{aligned} \tag{3.95}$$

Similarly, for W_{13} and for W_{14} we have

$$\begin{aligned}|\langle \xi, \mathrm{W}_{13}\xi\rangle| &\leq C\|(\mathcal{N}_+ +1)^{1/2}\xi\| \int dxdy\, \kappa\ell^2 V(\ell(x-y))|\eta(x,y)| \\ &\quad \int_0^1 ds\, \|(\mathcal{N}_+ +1)^{-1/2} d_y^{(s)}\big(b(\gamma_x^{(s)}) + b^*(\sigma_x^{(s)})\big)\xi\| \\ &\leq C\kappa n \ell^{-1}\|(\mathcal{N}_+ +1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ +1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|\end{aligned} \tag{3.96}$$

and

$$\begin{aligned}|\langle \xi, \mathrm{W}_{14}\xi\rangle| &\leq C\|(\mathcal{N}_+ +1)^{1/2}\xi\| \int dxdy\, \kappa\ell^2 V(\ell(x-y))|\eta(x,y)| \int_0^1 ds\, \|(\mathcal{N}_+ +1)^{-1/2} d_y^{(s)} d_x^{(s)}\xi\| \\ &\leq C\kappa n \ell^{-1}\|(\mathcal{N}_+ +1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ +1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|\end{aligned} \tag{3.97}$$

Next we consider W_2. By using (3.2) and Lemma 3.2, wee observe that

$$\begin{aligned}\|(\mathcal{N}_+ +1)^{1/2} e^{-sB} b_x b_y e^{sB}\xi\| &\leq C\Big[\|a_x a_y(\mathcal{N}_+ +1)^{1/2}\xi\| + \|\eta\|\|\eta_y\|\|a_x(\mathcal{N}_+ +1)\xi\| \\ &\quad + |\eta(x,y)|\|(\mathcal{N}_+ +1)^{1/2}\xi\| + \|\eta\|\|\eta_x\|\|a_y(\mathcal{N}_+ +1)\xi\| + \|\eta\|\|\eta_x\|\|\eta_y\|\|(\mathcal{N}_+ +1)^{3/2}\xi\|\Big],\end{aligned} \tag{3.98}$$

Combining this with estimate (2.31) we conclude that

$$\begin{aligned}&|\langle \xi, \mathrm{W}_2\xi\rangle| \\ &\leq C\int dxdy\, \kappa\ell^2 V(\ell(x-y)) \int_0^1 ds\, \|(\mathcal{N}_+ +1)^{1/2} e^{-sB} b_x b_y e^{sB}\xi\|\|(\mathcal{N}_+ +1)^{-1/2} a^*(\eta_x) a_y\xi\| \\ &\leq C\kappa n \ell^{-1}\|(\mathcal{N}_+ +1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ +1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|\end{aligned} \tag{3.99}$$

With similar arguments to those used to prove (3.98) (in particular, using the last two estimates in Lemma 3.2), we also obtain

$$\begin{aligned}\|(\mathcal{N}_+ +1)^{-1/2} e^{-sB} b(\eta_x^{(2)}) b_y e^{sB}\xi\| &= \|(\mathcal{N}_+ +1)^{-1/2} \int dz\, \eta^{(2)}(x,z) e^{-sB} b_z b_y e^{sB}\xi\| \\ &\leq C\Big[\|\eta\|\|\eta_x\|\|a_y\xi\| + \|\eta\|\|\eta_x\|\|\eta_y\|\|(\mathcal{N}_+ +1)^{1/2}\xi\|\Big]\end{aligned} \tag{3.100}$$

and

$$\begin{aligned}\|(\mathcal{N}_+ +1)^{-1/2} e^{-sB} b(\eta_x^{(2)}) b(\eta_y) e^{sB}\xi\| &= \|(\mathcal{N}_+ +1)^{-1/2} \int dzdt\, \eta(x,z)\eta(y,t) e^{-sB} b_z b_t e^{sB}\xi\| \\ &\leq C\|\eta\|\|\eta_x\|\|\eta_y\|\|(\mathcal{N}_+ +1)^{1/2}\xi\|\end{aligned} \tag{3.101}$$

leading to

$$|\langle \xi, \mathrm{W}_3\xi\rangle|, |\langle \xi, \mathrm{W}_4\xi\rangle| \leq C\kappa n \ell^{-1}\|(\mathcal{N}_+ +1)^{1/2}\xi\|^2 + C\kappa^{1/2}n^{1/2}\ell^{-1/2}\|(\mathcal{N}_+ +1)^{1/2}\xi\|\|\mathcal{V}_\ell^{1/2}\xi\|. \tag{3.102}$$

Estimate (3.102), together with (3.94), (3.95), (3.96), (3.97) and (3.99) conclude the proof of (3.87). □

3.7 Proof of Proposition 2.3

Proof of Prop. 2.3. From Propositions 3.3, 3.4, 3.6, 3.7, 3.8 and 3.10 we conclude that the excitation Hamiltonian $\mathcal{G}_{n,\ell}$ can be written as

$$e^{-B}\mathcal{L}_{n,\ell}e^B = C_{n,\ell} + L_{n,\ell} + \mathcal{K} + Q_{n,\ell} + \mathcal{V}_\ell + \mathcal{E}_{n,\ell}$$

where the operators $\mathcal{K}$ and $\mathcal{V}_\ell$ are defined as in (2.39), the constant contribution (i.e. the term not depending on operators) $C_{n,\ell}$ is given by (2.41), the linear terms are given by

$$\begin{aligned} L_{n,\ell} = n^{3/2} &\int dxdy\, \kappa\ell^2 V(\ell(x-y))\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big] \\ &+ n^{1/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\eta(y,x)\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big] \end{aligned} \tag{3.103}$$

and the quadratic terms are

$$\begin{aligned} Q_{n,\ell} = &-\frac{1}{2}\sum_{p,r\in\Lambda^*_{1,+}} \Big(\langle \varphi_p\otimes\varphi_r, (\Delta_1+\Delta_2)\eta\rangle \hat{b}^*_p\hat{b}^*_r + \text{h.c.}\Big) \\ &+ \frac{1}{2}\sum_{p,q\in\Lambda^*_{1,+}} \Big(nV_{\ell,pq00}\hat{b}^*_p\hat{b}^*_q + \text{h.c.}\Big) \\ &+ \frac{1}{2}\sum_{p,q,r,s\in\Lambda^*_{1,+}} \Big(V_{\ell,pqrs}\langle\varphi_s\otimes\varphi_r,\eta\rangle\hat{b}^*_p\hat{b}^*_q + \text{h.c.}\Big) \end{aligned} \tag{3.104}$$

The error term $\mathcal{E}_{n,\ell}$ satisfies

$$\pm\mathcal{E}_{n,\ell} \le \delta(\mathcal{K}+\mathcal{V}_\ell) + C\kappa n\ell^{-1}(\mathcal{N}_+ + 1).$$

We first consider the linear terms in (3.103). Decomposing η in the second line of (3.103) with the aid of (2.25), we have

$$L_{n,\ell} = \mathrm{L}_1 + \mathrm{L}_2 + \mathrm{L}_3 \tag{3.105}$$

with

$$\begin{aligned} \mathrm{L}_1 &= n^{3/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\ell^3 f_\ell(x,y)\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big] \\ \mathrm{L}_2 &= n^{3/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\int dz\big(w_\ell(z,y) + w_\ell(x,z)\big)\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big] \\ \mathrm{L}_3 &= -n^{3/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\int dz_1dz_2\, w_\ell(z_1,z_2)\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big] \end{aligned} \tag{3.106}$$

By estimates (2.16) and (2.32), it follows that for any $\xi\in\mathcal{F}_+^{\le n}$

$$\begin{aligned} |\langle\xi,\mathrm{L}_3\xi\rangle| &\le Cn^{3/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))|\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle|\int dz_1dz_2\,|w_\ell(z_1,z_2)| \\ &\le C\kappa n^{3/2}\ell^{-2}\int dx|\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle|\int dy\,\kappa\ell^3 V(\ell(x-y)) \\ &\le C\kappa n^{1/2}\ell^{-1}\|\mathcal{N}_+^{1/2}\xi\|\|\xi\|. \end{aligned} \tag{3.107}$$

For the term L_2 we estimate

$$\begin{aligned} |\langle\xi,\mathrm{L}_2\xi\rangle| &\le n^{3/2}\int dxdy\, \kappa\ell^2 V(\ell(x-y))\int dz\,|w_\ell(z,y)+w_\ell(x,z)||\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle| \\ &\le n^{3/2}\int dx|\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle|\int dy\,\kappa\ell^2 V(\ell(x-y))\int dz\,|w_\ell(z,y)| \\ &\quad + n^{3/2}\int dzdx\,|w_\ell(x,z)||\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle|\int dy\,\kappa\ell^2 V(\ell(x-y)) \end{aligned}$$

Using (2.15), (2.17) and (2.32), we get

$$\begin{aligned} |\langle\xi,\mathrm{L}_2\xi\rangle| &\le \kappa\frac{n^{3/2}}{\ell^2}\int dx|\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle| \\ &\quad + \frac{n^{3/2}}{\ell}\int dzdx\,|w_\ell(x,z)||\langle\xi,\big(b(\gamma_x)+b^*(\sigma_x)\big)\xi\rangle|\int dy\,\kappa\ell^3 V(\ell(x-y)) \\ &\le C\kappa n^{3/2}\ell^{-2}\|\mathcal{N}_+^{1/2}\xi\|\|\xi\| \le C\kappa n^{1/2}\ell^{-1}\|\mathcal{N}_+^{1/2}\xi\|\|\xi\| \end{aligned} \tag{3.108}$$

In order to control L_1 in (3.106), we write it as

$$\begin{aligned} \mathrm{L}_1 &= n^{3/2}\ell^{-1}c\int dx\,\big[b_x + b(p_x) + b^*(\sigma_x) + \text{h.c.}\big] \\ &\quad + n^{3/2}\ell^{-1}\int dx\,\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big]\left[\int dy\,\kappa\ell^3 V(\ell(x-y))\ell^3 f_\ell(x,y) - c\right] \\ &=: \mathrm{L}_{11} + \mathrm{L}_{12} \end{aligned} \tag{3.109}$$

for a constant $c \in \mathbb{R}$. The expectation on $\xi \in \mathcal{F}_+^{\leq n}$ of L_{11} in (3.109) vanishes for any c, since $\sigma, p \in L^2_+(\mathbb{R}^3) \times L^2_+(\mathbb{R}^3)$. We define

$$h_\ell(x) = \int dy\,\kappa\ell^3 V(\ell(x-y))\ell^3 f_\ell(x,y)$$

and we set $c = h_\ell(0)$, where $h_\ell(0)$ is the function h_ℓ evaluated at the center of the box. Let $d(x)$ denote the distance of x from the boundary of the box. We denote with $S_{4/\ell}$ the set of all $x \in \Lambda_1$ with $d(x) < 4R_0/\ell$, where R_0 is the diameter of the support of V. We call $\chi_{S_{4/\ell}}$ the characteristic function of this set. We split L_{12} as

$$\begin{aligned} \mathrm{L}_{12} &= n^{3/2}\ell^{-1}\int dx\,\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big]\,[h_\ell(x) - h_\ell(0)]\,\chi_{S^c_{4/\ell}}(x) \\ &\quad + n^{3/2}\ell^{-1}\int dx\,\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big]\,[h_\ell(x) - h_\ell(0)]\,\chi_{S_{4/\ell}}(x) \\ &= \mathrm{L}_{121} + \mathrm{L}_{122} \end{aligned} \tag{3.110}$$

From (2.14) it follows that $\sup_{x\in\Lambda_1} h_\ell(x) \leq C\kappa$, for a constant $C > 0$; therefore

$$\begin{aligned} |\langle \xi, \mathrm{L}_{122}\xi\rangle| &\leq C\kappa n^{3/2}\ell^{-1}\|\xi\|\int dx\,\|(b(\gamma_x) + b^*(\sigma_x))\xi\|\,\chi_{S_{4/\ell}}(x) \\ &\leq C\kappa n^{3/2}\ell^{-1}\|\xi\|\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\left(\int dx\,\chi_{S_{4/\ell}}(x)\right)^{1/2} \\ &\leq C\kappa n^{3/2}\ell^{-3/2}\|\xi\|\|(\mathcal{N}_+ + 1)^{1/2}\xi\| \end{aligned} \tag{3.111}$$

where we used Cauchy-Schwarz, (2.32) and (2.27). Using the same bounds, we obtain for L_{121}

$$\begin{aligned} |\langle \xi, \mathrm{L}_{121}\xi\rangle| &\leq Cn^{3/2}\ell^{-1}\|\xi\|\int dx\,\|\big[b(\gamma_x) + b^*(\sigma_x) + \text{h.c.}\big]\xi\||h_\ell(x) - h_\ell(0)|\chi_{S^c_{4/\ell}}(x) \\ &\leq Cn^{3/2}\ell^{-1}\|\xi\|\|(\mathcal{N}_+ + 1)^{1/2}\xi\|\||h_\ell - h_\ell(0)|\chi_{S^c_{4/\ell}}\|_2 \end{aligned} \tag{3.112}$$

Calling $h(x) = \int_{\Lambda_\ell} dy\,\kappa V(x-y)f(x,y)$, we have

$$\begin{aligned} \int_{S^c_{4/\ell}} dx\,|h_\ell(x) - h_\ell(0)|^2 &= \int_{S^c_{4/\ell}} dx\left|\int dy\,\kappa\ell^3 V(\ell(x-y))\ell^3 f_\ell(x,y) - h_\ell(0)\right|^2 \\ &= \ell^{-3}\int_{S^c_4} dx\,\big|\ell^3 h(x) - \ell^3 h(0)\big|^2 \end{aligned} \tag{3.113}$$

where S^c_4 is the set of points in Λ_ℓ whose coordinates are at a distance bigger than $4R_0$ from the boundary. We write

$$h(x) - h(0) = \int_0^1 dt\,\nabla h(tx)\,x$$

and it remains to calculate ∇h. We have

$$\begin{aligned} \partial_{x_i} h(x) &= -\int_{\Lambda_\ell} dy\,\kappa\partial_{y_i} V(x-y)f(x,y) + \int_{\Lambda_\ell} dy\,\kappa V((x-y)\partial_{x_i} f(x,y) \\ &= -\int_{\partial\Lambda_\ell} d\sigma_y\,\kappa V(x-y)f(x,y)\nu_i + \int_{\Lambda_\ell} dy\,\kappa V(x-y)(\partial_{x_i} + \partial_{y_i})f(x,y) \end{aligned}$$

The boundary contribution above vanishes for $x \in S_4^c$. Moreover, using (2.18) and the fact that V is bounded and compactly supported we obtain

$$|\nabla_x h(x)| \leq C\kappa \ell^{-3}\big(d(x)+1\big)^{-5/3}. \tag{3.114}$$

Therefore

$$\ell^3 |h(x) - h(0)| \leq C\kappa \Big[\int_0^1 dt \,\big(d(tx)+1\big)^{-5/3} |x| \Big]$$

To compute the integral, assume that $x^{(3)} \geq \max\{|x^{(1)}|, |x^{(2)}|\}$. Than $d(tx) = \ell/2 - tx^{(3)}$, and hence

$$\int_0^1 dt\,\big(d(tx)+1\big)^{-5/3} = \frac{3}{2x^{(3)}} \left(\frac{1}{\big(\ell/2+1-x^{(3)}\big)^{2/3}} - \frac{1}{(\ell/2+1)^{2/3}} \right) \leq \frac{3\sqrt{3}}{2|x|} \frac{1}{(d(x)+1)^{2/3}}$$

where we used that $|x|^2 \leq 3\,|x^{(3)}|^2$. In particular,

$$\ell^3|h(x)-h(0)| \leq \frac{C\kappa}{(d(x)+1)^{2/3}} \tag{3.115}$$

from which it easily follows that

$$\int_{S_4^c} dx\, \big|\ell^3\big(h(x)-h(0)\big)\big|^2 \leq C\kappa^2 \ell^2 \tag{3.116}$$

We have therefore proved that

$$|\langle \xi, \mathrm{L}_{121}\xi\rangle| \leq C\kappa n^{3/2}\ell^{-3/2} \|(\mathcal{N}_+ + 1)^{1/2}\xi\| \|\xi\|. \tag{3.117}$$

We examine now the quadratic contributions in (3.104), given by

$$Q_{n,\ell} = \frac{n}{2}\int dxdy\ \big[(\Delta_x+\Delta_y)w_\ell(x,y) + \kappa\ell^2 V(\ell(x-y))\big(1-w_\ell(x,y)\big)\big]\,[b_x b_y + b_x^* b_y^*]$$

By equation (2.21) and $1 - w_\ell(x,y) = \ell^3 f_\ell(x,y)$, we have

$$Q_{n,\ell} = \frac{n\ell^5}{2}\lambda_\ell \int dxdy\, f_\ell(x,y)[b_x b_y + b_x^* b_y^*]$$

For any $\xi \in \mathcal{F}_+^{\leq n}$ we estimate

$$\begin{aligned} |\langle \xi, Q_{n,\ell}\xi\rangle| &\leq C\kappa n \ell^2 \int dy\, |\langle b^*(f_\ell(\cdot,y))\xi, b_y\xi\rangle| \\ &\leq C\kappa n\ell^2 \|f_\ell\|_2 \|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 \leq C\kappa\frac{n}{\ell}\|(\mathcal{N}_+ + 1)^{1/2}\xi\|^2 \end{aligned}$$

where we used (2.12) and the fact that f is normalized to 1 in $\Lambda_\ell \times \Lambda_\ell$, so $\|f_\ell\|_2 = \ell^{-3}$. This concludes the proof of Prop. 2.3. □

4 Proof of Theorem 1.1 and Corollary 1.2

We shall now use Proposition 2.3 and Lemma 3.1 in order to prove Theorem 1.1.

Proof of Theorem 1.1. Using the bounds $\mathcal{K} = \sum_{p\in\Lambda_{1,+}^*} p^2 a_p^* a_p \geq \pi^2 \sum_{p\in\Lambda_{1,+}^*} a_p^* a_p = \pi^2 \mathcal{N}_+$, $\mathcal{V}_\ell \geq 0$ and setting $\delta = 1/3$, we have, from (2.40),

$$\mathcal{G}_{n,\ell} \geq C_{n,\ell} + (1-\delta)(\mathcal{K}+\mathcal{V}_\ell) - \kappa C\frac{n}{\ell}(\mathcal{N}_+ + 1) \geq C_{n,\ell} + \Big(\frac{2}{3} - \kappa\frac{C}{\pi^2}\frac{n}{\ell}\Big)\mathcal{K} - C\kappa\frac{n}{\ell} \tag{4.1}$$

Assuming $\kappa n/\ell$ small enough we get

$$\mathcal{G}_{n,\ell} \geq C_{n,\ell} + \frac{\pi^2}{2}\mathcal{N}_+ - C\kappa\frac{n}{\ell} \geq C_{n,\ell} - C\kappa\frac{n}{\ell} \tag{4.2}$$

Equation (2.40) also implies (taking $\delta = 1$) the upper bound

$$\mathcal{G}_{n,\ell} \leq C_{n,\ell} + 2(\mathcal{K} + \mathcal{V}_\ell) + C\kappa \frac{n}{\ell}(\mathcal{N}_+ + 1) \tag{4.3}$$

From (4.3) (evaluated on the vacuum) and (4.2) it follows that

$$|e_{n,\ell} - C_{n,\ell}| \leq C\kappa \frac{n}{\ell} \tag{4.4}$$

Using equation (2.41), the definition of η (in equation (2.22)) and the fact that it is orthogonal to the condensate wave function φ_0 we write

$$C_{n,\ell} = \frac{n^2}{2\ell^4} \int_{\Lambda_\ell \times \Lambda_\ell} dxdy \left[\kappa V(x-y)|1 - w(x,y)|^2 + |\nabla_x w(x,y)|^2 + |\nabla_y w(x,y)|^2\right] + R_{n,\ell} \tag{4.5}$$

where

$$R_{n,\ell} = -\frac{n^2}{2} \int dxdydz \left[w_\ell(z,y) + w_\ell(x,z) - \int dt\, w_\ell(z,t)\right](\Delta_x + \Delta_y) w_\ell(x,y) \tag{4.6}$$

Recalling the definition $1 - w = \ell^3 f$, where f is the minimizer of (2.11) in Proposition 2.1, we conclude that

$$C_{n,\ell} = 4\pi\mathfrak{a}\frac{n^2}{\ell}\Big(1 + \mathcal{O}\Big(\frac{\mathfrak{a}}{\ell}\ln(\ell/\mathfrak{a})\Big)\Big) + R_{n,\ell} \tag{4.7}$$

The error $R_{n,\ell}$ can be controlled by substituting equation (2.21) for $(\Delta_x + \Delta_y)w_\ell(x,y)$ and using estimates (2.14) for f_ℓ and (2.16) for w_ℓ. This gives $|R_{n,\ell}| \leq C\kappa n^2 \ell^{-2}$. Equations (4.4) and (4.7) imply (1.10).

Let now $\psi_n \in L^2_s(\Lambda_1^n)$ be a normalized wave function, with

$$\langle \psi_n, H_{n,\ell}\psi_n\rangle \leq e_{n,\ell} + \zeta$$

for some $\zeta > 0$ and $e_{n,\ell}$ the ground state energy of H_n. We define $\xi_n = e^{-B}U_n\psi_n \in \mathcal{F}_+^{\leq n}$. Therefore

$$\langle \xi_n, \mathcal{G}_{n,\ell}\xi_n\rangle = \langle \psi_n, H_n\psi_n\rangle \leq e_{n,\ell} + \zeta$$

From (4.2) and (4.4) we have

$$\frac{\pi^2}{2}\langle \xi_n, \mathcal{N}_+\xi_n\rangle \leq \zeta + C\kappa\frac{n}{\ell} \tag{4.8}$$

Using (2.7), Lemma 3.1 and (2.27) we have

$$n - \langle \psi_n, \hat{a}_0^*\hat{a}_0\psi_n\rangle = \langle \psi_n, U_n^*\mathcal{N}_+U_n\psi_n\rangle \leq C\langle \xi_n, \mathcal{N}_+\xi_n\rangle \leq \frac{2C}{\pi^2}(\zeta + \kappa n\ell^{-1}) \tag{4.9}$$

which implies (1.11). □

Corollary 1.2 follows from Theorem 1.1.

Proof of Corollary 1.2. Inequality (1.10) implies that for $n < \frac{c}{\kappa}\ell =: p$ (where c is a small enough number) there exists a $C > 0$ such that

$$E(n,\ell) \geq 4\pi\mathfrak{a}\Big[\frac{n^2}{\ell^3} - C\frac{n}{\ell^3} - C\mathfrak{a}\frac{n^2}{\ell^4}\ln(\ell/\mathfrak{a})\Big]. \tag{4.10}$$

We need now a bound in the case $n \geq p$. Following [26], we observe that since V is non-negative,

$$E(n+n',\ell) \geq E(n,\ell) + E(n',\ell),$$

where we dropped the interactions between the n particles and the n' particles. It follows that

$$E(n,\ell) \geq \left[\frac{n}{p}\right] E(p,\ell) \geq \frac{n}{2p}E(p,\ell) \tag{4.11}$$

where $\left[\frac{n}{p}\right]$ is the largest integer smaller than $\frac{n}{p}$. We use the latter estimate for $n \geq p$. Calling c_n the relative number of cells containing n particles, we have that

$$\begin{aligned}\frac{E(N,L)}{N} \geq& \frac{4\pi\mathfrak{a}}{\rho\ell^6}\inf\Big\{\sum_{n<p} c_n\Big(n^2 - Cn - C\mathfrak{a}\frac{n^2}{\ell}\ln(\ell/\mathfrak{a})\Big)\\ &+\frac{1}{2}\sum_{n\geq p} c_n n\Big(p - C - C\mathfrak{a}\frac{p}{\ell}\ln(\ell/\mathfrak{a})\Big)\Big\}\end{aligned} \tag{4.12}$$

Defining $A = 1 - C\mathfrak{a}\frac{\ln(\ell/\mathfrak{a})}{\ell}$, we need therefore to minimize

$$\sum_{n<p} c_n\big(n^2A - nC\big) + \frac{1}{2}\sum_{n\geq p} c_n n\big(pA - C\big) \tag{4.13}$$

with the constraints

$$\sum_{n\geq 0} c_n = 1, \qquad \sum_{n\geq 0} c_n n = \rho\ell^3.$$

We define the variable

$$t = \sum_{n<p} c_n n \leq \rho\ell^3;$$

we have therefore, by Cauchy-Schwarz,

$$\sum_{n<p} c_n\big(n^2A - nC\big) + \frac{1}{2}\sum_{n\geq p} c_n n\big(pA - C\big) \geq t^2A - tC + \frac{1}{2}(\rho\ell^3 - t)(pA - C) \tag{4.14}$$

which we minimize for $1 \leq t \leq \rho\ell^3$. If p is large enough, for example $p \geq 4\rho\ell^3$ (note that this imposes that $\ell^2 \geq c(4\kappa\rho)^{-1}$), we obtain that $t = \rho\ell^3$ and the minimum of (4.14) is $(\rho\ell^3)^2A - \rho\ell^3C$. This means that

$$\frac{E(N,L)}{N} \geq 4\pi\mathfrak{a}\rho\Big[1 - C\mathfrak{a}\frac{\ln(\ell/\mathfrak{a})}{\ell} - \frac{C}{\rho\ell^3}\Big] \tag{4.15}$$

We set $\ell = (c/4)^{1/2}(\kappa\rho)^{-1/2}$ and we obtain, for a new constant $C > 0$,

$$\frac{E(N,L)}{N} \geq 4\pi\mathfrak{a}\rho\Big[1 - C(\rho\mathfrak{a}^3)^{1/2}\ln(\rho/\mathfrak{a}) - C(\rho\mathfrak{a}^3)^{1/2}\Big] \tag{4.16}$$

□

A The two-body problem in the Neumann box

This Appendix is devoted to proving Propositions 2.1 and 2.2. We will use the following Lemma.

Lemma A.1. *Let $\Omega = [-\ell/2, \ell/2]^6$ and let ε be such that $0 < \varepsilon\ell^2 \leq 1$. For $y \in \Omega$ let $G_\varepsilon(x,y)$ be the solution of*

$$\big(-\Delta_x + \varepsilon\big)G_\varepsilon(x,y) = \delta_y(x) \tag{A.1}$$

on Ω with Neumann boundary conditions. There exists a constant $C > 0$ (independent of ε and ℓ) such that

$$G_\varepsilon(x,y) \leq C\Big(\frac{1}{|x-y|^4} + \frac{1}{\ell^6\varepsilon}\Big) \tag{A.2}$$

for every $x, y \in \Omega$. Moreover, let $\tilde{G}_\varepsilon$ be the unique solution of

$$\big(-\Delta_x + \varepsilon\big)\tilde{G}_\varepsilon(x-y) = \delta_y(x) \tag{A.3}$$

on $\mathbb{R}^6$ decaying at infinity. Then there exists a constant $C > 0$ such that for $1 \leq i \leq 6$

$$|\partial_{x^{(i)}}G_\varepsilon(x,y) - \partial_{x^{(i)}}\tilde{G}_\varepsilon(x-y)| \leq C\left[\sum_n \frac{1}{|x-y_n|^5} + \frac{1}{\varepsilon^{1/2}\ell^6}\right] \tag{A.4}$$

where the y_n are the (at most $3^6 - 1$) points obtained by reflecting y, y_n with respect to the planes generated by the sides of the box, whose distance from y is less than ℓ (each reflected point is counted only once, and among the y_n we don't include y itself).

Proof. The solution $\tilde{G}_\varepsilon$ to (A.3) can be expressed as

$$\tilde{G}_\varepsilon(x) = \frac{\varepsilon}{2^3\pi^3}\frac{\mathrm{K}_2(\sqrt{\varepsilon}|x|)}{|x|^2} \tag{A.5}$$

where K_2 is the modified Bessel function of the third kind of order 2 (see [2]). From the properties of K_2 we deduce that for large $\varepsilon^{1/2}|x|$

$$\tilde{G}_\varepsilon(x) = \frac{\varepsilon^{3/4}e^{-\sqrt{\varepsilon}|x|}}{|x|^{2+1/2}}\Big(1+\mathcal{O}((\sqrt{\varepsilon}|x|)^{-1})\Big) \tag{A.6}$$

while for small $\varepsilon^{1/2}|x|$ there exists a constant $C_1 > 0$ such that

$$\tilde{G}_\varepsilon(x) = \frac{C_1}{|x|^4} + \mathcal{O}(\varepsilon|x|^{-2}) \tag{A.7}$$

We obtain the Green function G_ε on Ω with Neumann boundary conditions as follows. For $x, y \in \Omega$,

$$G_\varepsilon(x,y) = \tilde{G}_\varepsilon(x-y) + \sum_{n\in\mathbb{Z}^6\setminus\{0\}} \tilde{G}_\varepsilon(x-y_n) \tag{A.8}$$

where the positions y_n are all possible reflections (each counted only once) of y and y_n with respect to the infinite planes obtained by extending the sides of the box Ω and their periodic replicas over all $\mathbb{R}^6$. This operation gives rise to a grid, and each six-dimensional cell contains one and only one y_n (therefore the label $n \in \mathbb{Z}^6\setminus\{0\}$ also identifies the cell where y_n belongs). The positions y_n can be thought as positions of image charges, whose contributions cancels the normal derivative of G_ε on $\partial\Omega$. Given a point $y = (y^{(1)}, \ldots, y^{(6)}) \in \Omega$, the coordinates of its image charges are, for $j = 1, \ldots, 6$,

$$y_n^{(j)} = n^{(j)}\ell + (-1)^{n^{(j)}} y^{(j)}.$$

In order to estimate (A.8), we deduce from (A.6) and (A.7) that for any $0 < \lambda < 1$ there exists a $C_\lambda > 0$ such that

$$\tilde{G}_\varepsilon(x) \le \frac{C_\lambda e^{-\lambda\sqrt{\varepsilon}|x|}}{|x|^4}. \tag{A.9}$$

Using the estimate above, for the charges that are such that $|x - y_n| \ge \ell$ we bound the contribution in the second term on the right-hand side of (A.8) as

$$\left|\sum_{n\in\mathbb{Z}^6\setminus\{0\}} \frac{e^{-\lambda\sqrt{\varepsilon}|x-y_n|}}{|x-y_n|^4}\right| \le \frac{C_\lambda}{\ell^4}\sum_{n\in\mathbb{Z}^6\setminus\{0\}}\frac{e^{-\lambda\sqrt{\varepsilon}|n|\ell}}{|n|^4}$$

We estimate the sum with an integral (this can be done since the summand is a continuous decreasing function of n on $\mathbb{R}^6\setminus B_1(0)$, where $B_1(0)$ is the ball or radius one centered in zero), so that

$$\sum_{n\in\mathbb{Z}^6\setminus\{0\}}\frac{e^{-\lambda\sqrt{\varepsilon}|n|\ell}}{|n|^4} \le \int_{\mathbb{R}^6\setminus B_1(0)} dn \frac{e^{-\lambda\sqrt{\varepsilon}n\ell}}{|n|^4} = \frac{1}{(\lambda\sqrt{\varepsilon}\ell)^2}\int_{\mathbb{R}^6\setminus B_1(0)} dn\frac{e^{-|n|}}{|n|^4}$$

and therefore

$$\left|\sum_{n\in\mathbb{Z}^6\setminus\{0\}} \frac{e^{-\lambda\sqrt{\varepsilon}|x-y_n|}}{|x-y_n|^4}\right| \le \frac{C_\lambda}{\varepsilon\ell^6} \tag{A.10}$$

Only a finite number of y_n are such that $|x - y_n| < \ell$, and for those we bound $|x-y| \le |x-y_n|$. We thus obtain (A.2).

We consider now $\partial_{x_i}\tilde{G}_\varepsilon(x)$, given by

$$\partial_{x^{(i)}}\tilde{G}_\varepsilon(x) = -x_i\frac{\varepsilon^{3/2}}{2^3\pi^3}\frac{\mathrm{K}_3(\sqrt{\varepsilon}|x|)}{|x|^3} \tag{A.11}$$

(see [2, Chapter 3] for properties of the Bessel function of the third kind). For large $\varepsilon^{1/2}|x|$,

$$\partial_{x^{(i)}}\tilde{G}_\varepsilon(x) \simeq C x_i \frac{\varepsilon^{5/4}}{|x|^{3+1/2}} e^{-\sqrt{\varepsilon}|x|} \tag{A.12}$$

For small $\varepsilon^{1/2}|x|$,

$$\partial_{x^{(i)}}\tilde{G}_\varepsilon(x) \simeq C \frac{x_i}{|x|^6} \tag{A.13}$$

The two equations above imply that for any $0 < \lambda < 1$ there exists a $C_\lambda > 0$ such that

$$|\partial_{x^{(i)}}\tilde{G}_\varepsilon(x)| \leq \frac{C_\lambda}{|x|^5} e^{-\lambda\sqrt{\varepsilon}|x|}. \tag{A.14}$$

Similarly as above, we sum the contribution from charges such that $|x - y_n| > \ell$, so that

$$\Big| \sum_{|x-y_n|>\ell} \partial_{x^{(i)}}\tilde{G}_\varepsilon(x - y_n)\Big| \leq C_\lambda \sum_{n\in\mathbb{Z}^6\setminus\{0\}} \frac{1}{|x-y_n|^5} e^{-\lambda\sqrt{\varepsilon}|x-y_n|} \leq \frac{C_\lambda}{\varepsilon^{1/2}\ell^6} \tag{A.15}$$

Therefore

$$|\partial_{x^{(i)}}G_\varepsilon(x,y) - \partial_{x^{(i)}}\tilde{G}_\varepsilon(x-y)| \leq \sum_{n\neq 0,\, |x-y_n|<\ell} \frac{C}{|x-y_n|^5} + \frac{C}{\varepsilon^{1/2}\ell^6} \tag{A.16}$$

for a constant $C > 0$. □

Proof of Proposition 2.1. Existence and uniqueness of minimizers can be proved by standard methods. We start by proving (2.12). Let f_0 be the zero-energy scattering solution defined in (1.2), and $f(x_1, x_2) = f_0(x_1 - x_2)$ for $x_1, x_2 \in \Lambda_\ell$. We write $\psi = fg$ and integrate by parts. Calling $\Lambda_\ell \times \Lambda_\ell = \Omega$ and writing ∇ for ∇_x, with $x = (x_1, x_2)$, we have

$$\int_\Omega \left(|\nabla\psi|^2 + \kappa V|\psi|^2\right) = \int_\Omega f^2|\nabla g|^2 + \int_{\partial\Omega} g^2 f\hat{n}\cdot\nabla f$$

where $\hat{n}$ is the unit outward normal vector, and we use the shorthand notation $V(x) = V(x_1 - x_2)$ for simplicity. Note that $\hat{n} \cdot \nabla f > 0$ since f_0 is an increasing function. By assumption V is regular enough such that $f_0 \geq c_0 > 0$ (see [14, Lemma 5.1] for properties of the zero energy scattering equation). Let us write $\tau = \delta_{\partial\Omega} f\hat{n} \cdot \nabla f$, so that the second term is simply $\int g^2\tau$. We thus have

$$\int_\Omega \left(|\nabla\psi|^2 + \kappa V|\psi|^2\right) \geq c_0^2 \int_\Omega |\nabla g|^2 + \int_\Omega g^2\tau \tag{A.17}$$

Let us look for the lowest eigenvalue of the right-hand side, i.e., the largest λ such that

$$c_0^2 \int_\Omega |\nabla g|^2 + \int_\Omega g^2\tau \geq \lambda \int_\Omega g^2$$

Since $f \leq 1$, this is also a lower bound to the eigenvalue we are looking for, i.e.,

$$\int_\Omega \left(|\nabla\psi|^2 + \kappa V|\psi|^2\right) \geq \lambda \int_\Omega g^2 \geq \lambda \int_\Omega \psi^2$$

Clearly $\lambda \leq \ell^{-6} \int \tau$. Using that $f \leq 1$ we have

$$\int \tau \leq \int_{\partial\Omega} \hat{n} \cdot \nabla f = \int_\Omega \Delta f \leq 2 \int_{\Lambda_\ell\times\mathbf{R}^3} dx_1 dx_2 (\Delta f_0)(x_1 - x_2) = 8\pi\mathfrak{a}\ell^3$$

We may assume that g shares the symmetries of Ω, in which case

$$\int_\Omega g^2\tau = 12 \int_\Omega g^2\tau_1$$

$$= 12 \int_{\Lambda_\ell} dx_2 \int_{[-\ell/2,\ell/2]^2} dx_1^\perp g(-\ell/2, x_1^\perp, x_2)^2 f(-\ell/2, x_1^\perp, x_2) \frac{\left(-\ell/2 - x_2^{(1)}\right)}{|(-\ell/2, x_1^\perp) - x_2|} f_0'((-\ell/2, x_1^\perp) - x_2)$$

where we write the vector x_j as $(x_j^{(1)}, x_j^\perp)$, and denote the radial derivative of f_0 by f_0'. Using the Schur complement formula, we have, with Q the projection orthogonal to the constant function on Ω,

$$\lambda \geq \ell^{-6} \int \tau - \frac{12^2}{\ell^6} \langle \tau_1, Q[Q(-c_0^2 \Delta - 8\pi \mathfrak{a} \ell^{-3})Q]^{-1} Q\, \tau_1 \rangle .$$

Since the spectral gap of $-\Delta$ equals $(\pi/\ell)^2$ we can further bound

$$Q(-c_0^2\Delta - 8\pi a \ell^{-3})Q \geq \frac{c_0^2}{2} Q\left(-\Delta + \ell^{-2}\right) Q \geq \frac{c_0^2}{2} Q\left(-\Delta_{x_1} + \ell^{-2}\right) Q$$

as long as $c_0^2(\pi^2-1)/2 \geq 8\pi\mathfrak{a}/\ell$, which we assume henceforth. In particular,

$$Q\left[Q(-c_0^2\Delta - 8\pi a\ell^{-3})Q\right]^{-1} Q \leq \frac{2}{c_0^2} Q\left[-\Delta_{x_1} + \ell^{-2}\right]^{-1} Q = \frac{2}{c_0^2}\left[-\Delta_{x_1} + \ell^{-2}\right]^{-1} - \frac{2\ell^2}{c_0^2} P$$

with $P = 1 - Q$ the projection onto the constant function. Observing that $-2\ell^2 c_0^{-2} P$ can be dropped for an upper bound, we thus have

$$\lambda \geq \ell^{-6} \int \tau - \frac{2\cdot 12^2}{c_0^2 \ell^6} \langle \tau_1, [-\Delta_{x_1} + 1/\ell^2]^{-1} \tau_1 \rangle$$

An analysis similar to Lemma A.1 shows that the integral kernel of $[-\Delta_{x_1} + \ell^{-2}]^{-1}$ on $[-\ell/2, \ell/2]^3$ is bounded above by $c_1 |x_1 - y_1|^{-1}$, hence

$$\langle \tau_1, [-\Delta_{x_1} + 1/\ell^2]^{-1} \tau_1 \rangle \leq c_1 \int_{\Lambda_\ell^3} dx_1 dy_1 dx_2 \frac{\tau_1(x_1,x_2)\tau_1(y_1,x_2)}{|x_1 - y_1|}$$

Using that $f \leq 1$ as well as $f_0'(x_1) \leq \mathfrak{a}/|x_1|^2$, we have, for fixed x_2,

$$\begin{aligned}
&\int_{\Lambda_\ell^2} dx_1 dy_1 \frac{\tau_1(x_1,x_2)\tau_1(y_1,x_2)}{|x_1 - y_1|} \\
&\leq \left(\mathfrak{a}\big(\ell/2 + x_2^{(1)}\big)\right)^2 \int_{[-\ell/2,\ell/2]^4} dx_1^\perp dy_1^\perp \frac{1}{|x_1^\perp - y_1^\perp|} \frac{1}{|(-\ell/2, x_1^\perp) - x_2|^3} \frac{1}{|(-\ell/2, y_1^\perp) - x_2|^3} \\
&\leq \frac{\mathfrak{a}^2}{\ell/2 + x_2^{(1)}} \int_{\mathbb{R}^4} dx_1^\perp dy_1^\perp \frac{1}{|x_1^\perp - y_1^\perp|} \frac{1}{(1 + (x_1^\perp)^2)^{3/2}} \frac{1}{(1+(y_1^\perp)^2)^{3/2}}
\end{aligned}$$

where $\ell/2 + x_2^{(1)}$ has been scaled out after extending the integral to $\mathbb{R}^4$. The final integral is finite by the Hardy-Littlewood-Sobolev inequality. In order to obtain a better bound for $x_2^{(1)}$ close to $-\ell/2$, we use in addition that f_0' is bounded, and hence that $f_0'(x) \leq c_2 \mathfrak{a}^{1/2}/|x|^{3/2}$ for some $c_2 > 0$. Thus

$$\begin{aligned}
&\int_{\Lambda_\ell^2} dx_1 dy_1 \frac{\tau_1(x_1,x_2)\tau_1(y_1,x_2)}{|x_1 - y_1|} \\
&\leq \mathfrak{a}\, c_2^2 (\ell/2 + x_2^{(1)})^2 \int_{[-\ell/2,\ell/2]^4} dx_1^\perp dy_1^\perp \frac{1}{|x_1^\perp - y_1^\perp|} \frac{1}{|(-\ell/2, x_1^\perp) - x_2|^{5/2}} \frac{1}{|(-\ell/2, y_1^\perp) - x_2|^{5/2}} \\
&\leq \mathfrak{a}\, c_2^2 \int_{\mathbb{R}^4} dx_1^\perp dy_1^\perp \frac{1}{|x_1^\perp - y_1^\perp|} \frac{1}{(1+(x_1^\perp)^2)^{5/4}} \frac{1}{(1+(y_1^\perp)^2)^{5/4}}
\end{aligned}$$

where the integral is again finite by the Hardy-Littlewood-Sobolev inequality.

Altogether, we have thus shown that

$$\int_\Omega dx_1 dy_1 \frac{\tau_1(x_1,x_2)\tau_1(y_1,x_2)}{|x_1 - y_1|} \leq C\mathfrak{a}^2 \min\left\{ \frac{1}{\ell/2 + x_2^{(1)}}, \frac{1}{\mathfrak{a}} \right\}$$

Integrating this over x_2 yields

$$\int_{\Lambda_\ell} dx_2 \int_\Omega dx_1 dy_1 \frac{\tau_1(x_1,x_2)\tau_1(y_1,x_2)}{|x_1 - y_1|} \leq C\mathfrak{a}^2 \ell^2 \ln\frac{\ell}{\mathfrak{a}}$$

and thus

$$\lambda \geq \ell^{-6} \int \tau - C \frac{\mathfrak{a}^2}{\ell^4} \ln \frac{\ell}{\mathfrak{a}}$$

To complete the lower bound on λ, we need a lower bound on $\int \tau$. We have

$$\int \tau = \frac{1}{2} \int_{\partial\Omega} \hat{n} \cdot \nabla f^2 = \frac{1}{2} \int_{\Omega} \Delta f^2 = \int_{\Omega} (|\nabla f|^2 + \kappa V f^2) = 8\pi \mathfrak{a} \ell^3 - \int_{\Lambda_\ell} dx_1 \int_{\Lambda_\ell^c} (|\nabla f|^2 + \kappa V f^2) \tag{A.18}$$

Using that $\Delta f^2 = 2(|\nabla f|^2 + \kappa V f^2) \leq C \min\{\mathfrak{a}^{-2}, \mathfrak{a}^2/|x_1 - x_2|^4\}$, the error term is bounded by

$$C\mathfrak{a}^2 \int_{\Lambda_\ell} dx_1 \min\{(\ell/2 + x_1^1)^{-1}, 1/\mathfrak{a}\} = C\mathfrak{a}^2 \ell^2 \ln \frac{\ell}{\mathfrak{a}}$$

We thus conclude that

$$\lambda \geq 8\pi \mathfrak{a} \ell^3 - C\mathfrak{a}^2 \ell^2 \ln \frac{\ell}{\mathfrak{a}}$$

and from (A.17)

$$\int_{\Omega} \big(|\nabla \psi|^2 + \kappa V |\psi|^2\big) \geq \lambda \int_{\Omega} |g|^2 \geq \lambda \int_{\Omega} |\psi|^2 \tag{A.19}$$

since $f_0 \leq 1$. In particular, $\lambda_\ell \geq \lambda$, and this concludes the lower bound. The upper bound follows by taking the trial function $\psi = f$ corresponding to $g = 1$ and using again (A.18) together with

$$\|f\|_2^2 \geq \ell^6 - C\mathfrak{a}\ell^5,$$

where the latter follows from (1.3). This completes the proof of (2.12).

The estimate (2.13) in point i) clearly follows from (2.12). We proceed with point ii). The minimizer satisfies the eigenvalue equation on Ω with Neumann boundary conditions

$$\Big[-\Delta_x + \kappa V(x) \Big] f(x) = \lambda_\ell f(x), \tag{A.20}$$

with $\lambda_\ell = 8\pi \mathfrak{a} \ell^{-3}\big(1 + \mathcal{O}(\mathfrak{a}\ell^{-1} \ln(\ell/\mathfrak{a}))\big)$. As before $x = (x_1, x_2) \in \Lambda_\ell \times \Lambda_\ell = \Omega$ and $\Delta_x = \Delta_{x_1} + \Delta_{x_2}$. Abusing notation we wrote $V(x) = V(x_1 - x_2)$. It is useful to introduce a parameter $0 < \varepsilon \leq \ell^{-2}$ and write (A.20) as

$$\big(-\Delta_x + \varepsilon \big) f(x) = \big(\lambda_\ell + \varepsilon - \kappa V(x)\big) f(x). \tag{A.21}$$

We can express the solution to (A.21) as

$$f(x) = \int_{\Omega} dy\, G_\varepsilon(x, y) \big(\lambda_\ell + \varepsilon - \kappa V(y)\big) f(y)$$

with $G_\varepsilon(x, y)$ defined in (A.1). Lemma A.1 and the positivity of the minimizer f, of $G_\varepsilon(x, y)$ and of the potential V imply that

$$f(x) \leq C(\lambda_\ell + \varepsilon) \int_{\Omega} dy\, \frac{f(y)}{|x - y|^4} + \frac{C(\lambda_\ell + \varepsilon)}{\ell^6 \varepsilon} \int_{\Omega} dy\, f(y) \tag{A.22}$$

The last term can be bounded as

$$\int_{\Omega} dy\, f(y) \leq \|f\|_2 \|\chi_\Omega\|_2 = \ell^3$$

We split the first integral in (A.22) as

$$\int_{\Omega} dy\, \frac{f(y)}{|x - y|^4} = \int_{\Omega \cap B_\delta(x)} dy\, \frac{f(y)}{|x - y|^4} + \int_{\Omega \setminus B_\delta(x)} dy\, \frac{f(y)}{|x - y|^4} \tag{A.23}$$

for $0 < \delta \leq \ell$ and $B_\delta(x) = \{y \in \mathbb{R}^6 : |x - y| \leq \delta\}$. We have

$$\int_{B_\delta(x)} dy\, \frac{f(y)}{|x - y|^4} \leq C\delta^2 \|f\|_\infty \tag{A.24}$$

and

$$\int_{\Omega\setminus B_\delta(x)} dy\,\frac{f(y)}{|x-y|^4} \le \|f\|_2 \left(\int_{\mathbb{R}^6\setminus B_\delta(x)} dy\,\frac{1}{|x-y|^8}\right)^{1/2} = \frac{C}{\delta} \tag{A.25}$$

Hence

$$\|f\|_\infty \le C(\lambda_\ell+\varepsilon)\Big[\delta^2\|f\|_\infty + \frac{1}{\delta} + \frac{1}{\ell^3\varepsilon}\Big]. \tag{A.26}$$

We set $\varepsilon = \ell^{-2}$ and $\delta^2 = \big(2C(\lambda_\ell+\varepsilon)\big)^{-1}$, so that $\|f\|_\infty \le C'\ell^{-3}$, proving (2.14).

In order to prove (2.15) in point *iii*), we decompose f as $f = c+g$, with $\int_\Omega g = 0$ and $c = \ell^{-6}\int f$. We shall show that

$$\|g\|_2 \le C\kappa\ell^{-1} \tag{A.27}$$

for a constant $C>0$. Since

$$\|f-1/\ell^3\|_2^2 \le 2\|f-c\|_2^2 + 2\|c-1/\ell^3\|_2^2 = 2\|g\|_2^2 + 2|\ell^3c-1|^2$$

and, since

$$\|f-c\|_2^2 = 1-c^2\ell^6 \ge |1-c\ell^3|^2,$$

we have

$$\|f-1/\ell^3\|_2^2 \le 4\|g\|_2^2$$

Hence (2.15) follows from (A.27). To prove (A.27) we write equation (A.21) as

$$\big(-\Delta_x+\varepsilon\big)g(x) = \big(\lambda_\ell-\kappa V(x)\big)f(x) + \varepsilon g(x) \tag{A.28}$$

for some $0<\varepsilon\le\ell^{-2}$. We have

$$g(x) = \int_\Omega dy\,G_\varepsilon(x,y)\big(\lambda_\ell-\kappa V(y)\big)f(y) + \varepsilon\int_\Omega dy\,G_\varepsilon(x,y)g(y) \tag{A.29}$$

By Lemma A.1 and the Hardy-Littlewood-Sobolev and Hölder inequalities we have

$$\begin{aligned}\Big\|\lambda_\ell\int_\Omega dy\,G_\varepsilon(\,\cdot\,,y)f(y)\Big\|_2 &\le C\lambda_\ell\Big\|\int_\Omega dy\,\Big(\frac{1}{|\,\cdot\,-y|^4}+\frac{1}{\ell^6\varepsilon}\Big)f(y)\Big\|_2\\ &\le C\lambda_\ell\|f\|_{6/5} + C\frac{\lambda_\ell}{\ell^3\varepsilon}\|f\|_1 \le \frac{C\kappa}{\ell^3\varepsilon}\end{aligned} \tag{A.30}$$

To bound the contribution proportional to V in (A.29), we use (2.14) and estimate

$$\int_\Omega dy\,\Big(\frac{1}{|x-y|^4}+\frac{1}{\ell^6\varepsilon}\Big)V(y)f(y) \le \frac{C}{\ell^3}\int_\Omega dy\,\frac{1}{|x-y|^4}V(y) + \frac{C}{\ell^9\varepsilon}\int_\Omega dy\,V(y)$$

Using the notation $y=(y_1,y_2)\in\Lambda_\ell\times\Lambda_\ell$, we observe that

$$\begin{aligned}&\int_{\Lambda_\ell\times\Lambda_\ell} dy_1dy_2\,\frac{V(y_1-y_2)}{\big[|x_1-y_1|^2+|x_2-y_2|^2\big]^2}\\ &\quad\le \int_{\mathbb{R}^3} dy_2\,V(y_2)\int_{\mathbb{R}^3} dy_1\frac{1}{\big[|x_1-y_1|^2+|x_2-y_1+y_2|^2\big]^2}\\ &\quad= C\int_{\mathbb{R}^3} dy_2\,\frac{V(y_2)}{|x_1-x_2-y_2|} \le \frac{C}{|x_1-x_2|}\int_{\mathbb{R}^3} dy\,V(y)\end{aligned} \tag{A.31}$$

where we have used Newton's theorem in the last step. The L^2 norm of the last expression is thus bounded by $(\int V)\ell^2$, and we conclude that

$$\Big\|\int_\Omega dy\,G_\varepsilon(\,\cdot\,,y)V(y)f(y)\Big\|_2 \le \frac{C}{\varepsilon\ell^3}\|V\|_1 \tag{A.32}$$

We are left with the last contribution in (A.29). Since g is orthogonal to the constant function, we can use the spectral gap $(\pi/\ell)^2$ of the Laplacian to obtain the bound

$$\varepsilon\|G_\varepsilon g\|_2 \le \varepsilon\frac{\ell^2}{\pi^2}\|g\|_2 \tag{A.33}$$

By (A.30), (A.32) and (A.33) and with the choice $\varepsilon = \ell^{-2}$ (so that $\varepsilon\frac{\ell^2}{\pi^2} < 1$) we therefore arrive at (A.27), proving (2.15). The estimate (2.16) follows by Cauchy-Schwarz.

Next we examine point *iv*). Again, we decompose f as $f = c + g$, with $\int_\Omega g = 0$ and c a positive constant. We observe that

$$|1 - \ell^3 f(x_1, x_2)| \leq |1 - \ell^3 c| + \ell^3 |g(x_1, x_2)| \leq \|g\|_2 + \ell^3 |g(x_1, x_2)|$$

Hence, if we show that

$$\sup_{x \in \Omega} (|x_1 - x_2| + 1)|g(x_1, x_2)| \leq C\kappa \ell^{-3}, \tag{A.34}$$

the bound (2.17) follows. To show (A.34), we multiply (A.29) by $|x_1 - x_2| + 1$ to obtain

$$\begin{aligned}
&(|x_1 - x_2| + 1) g(x_1, x_2) \\
&\quad = \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) \big(\lambda_\ell - \kappa V(y_1 - y_2)\big) f(y_1, y_2) \\
&\quad\quad + \varepsilon \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) g(y_1, y_2)
\end{aligned} \tag{A.35}$$

We use Lemma A.1 to estimate G_ε and (2.14) as well as (2.12) to get

$$\begin{aligned}
&\lambda_\ell \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) f(y_1, y_2) \\
&\qquad \leq \frac{C}{\ell^6} \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) \left[\frac{1}{\big[|x_1 - y_1|^2 + |x_2 - y_2|^2\big]^2} + \frac{1}{\ell^6 \varepsilon} \right] \\
&\qquad \leq C\kappa \ell^{-3} + C\kappa \varepsilon^{-1} \ell^{-5}.
\end{aligned}$$

Moreover, with (A.31) and (2.14), we have

$$\begin{aligned}
&\int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) \kappa V(y_1 - y_2) f(y_1, y_2) \\
&\qquad \leq \frac{C\kappa}{\ell^3} \int_{\mathbb{R}^3} dy_2\, (|x_1 - x_2| + 1) \frac{V(y_2)}{|x_1 - x_2 - y_2|} + \frac{C\kappa}{\varepsilon \ell^5} \int_{\mathbb{R}^3} V(y_2) dy_2
\end{aligned}$$

By Newton's theorem we see that

$$\begin{aligned}
&\int_{\mathbb{R}^3} dy_2\, (|x_1 - x_2| + 1) \frac{\kappa V(y_2)}{|x_1 - x_2 - y_2|} \\
&\quad \leq C \int_{\mathbb{R}^3} dy_2\, \kappa V(y_2) + \frac{1}{|x_1 - x_2|} \int_{|y_2| \leq |x_1 - x_2|} dy_2\, \kappa V(y_2) + \int_{|y_2| > |x_1 - x_2|} dy_2\, \frac{\kappa V(y_2)}{|y_2|} \\
&\quad \leq C\kappa,
\end{aligned} \tag{A.36}$$

where we used that $\int dx\, V(x)|x|^{-1}$ is finite. We conclude that

$$\int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) \kappa V(y_1 - y_2) f(y_1, y_2) \leq C\kappa(\ell^{-3} + \varepsilon^{-1} \ell^{-5})$$

We are left with the last contribution in (A.35). We write, using (2.16),

$$\begin{aligned}
&\varepsilon \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) G_\varepsilon(x_1, x_2, y_1, y_2) g(y_1, y_2) \\
&\qquad \leq C\varepsilon \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, (|x_1 - x_2| + 1) \left[\frac{1}{|x - y|^4} + \frac{1}{\varepsilon \ell^6} \right] g(y_1, y_2) \\
&\qquad \leq C\varepsilon \int_{\Lambda_\ell \times \Lambda_\ell} dy_1 dy_2\, \frac{(|x_1 - x_2| + 1)}{|x - y|^4} g(y_1, y_2) + \frac{C\kappa}{\ell^3}
\end{aligned} \tag{A.37}$$

We bound the first term above as follows

$$\begin{aligned}C\varepsilon\int_{\Lambda_\ell\times\Lambda_\ell}dy\,\frac{(|x_1-x_2|+1)}{|x-y|^4}\frac{(|y_1-y_2|+1)g(y)}{(|y_1-y_2|+1)}\\ \le C\varepsilon\Big[\sup_{y\in\Lambda_\ell\times\Lambda_\ell}(|y_1-y_2|+1)g(y)\Big]\int_{\Lambda_\ell\times\Lambda_\ell}dy\,\frac{|x_1-x_2|+1}{|y_1-y_2|+1}\frac{1}{|x-y|^4}\end{aligned}\tag{A.38}$$

Similarly as we did in (A.31) we estimate

$$\begin{aligned}&\int_{\Lambda_\ell\times\Lambda_\ell}dy\,\frac{1}{|y_1-y_2|+1}\frac{1}{|x-y|^4}\\ &\quad\le\int_{[-\ell,\ell]^3}dy_2\,\frac{1}{|y_2|+1}\int_{\mathbb{R}^3}dy_1\frac{1}{\big[|x_1-y_1|^2+|x_2-y_1+y_2|^2\big]^2}\\ &\quad\le\int_{|y_2|\le\sqrt{3}\ell}dy_2\,\frac{1}{|y_2|}\frac{1}{|x_1-x_2-y_2|}\le C\frac{\ell^2}{|x_1-x_2|+\ell}\end{aligned}\tag{A.39}$$

where we again applied Newton's theorem in the last step. Thus

$$\int_{\Lambda_\ell\times\Lambda_\ell}dy\,\frac{|x_1-x_2|+1}{|y_1-y_2|+1}\frac{1}{|x-y|^4}\le C\ell^2\tag{A.40}$$

In conclusion, we have

$$(|x_1-x_2|+1)|g(x_1,x_2)|\le\frac{C\kappa}{\varepsilon\ell^5}\int_{\mathbb{R}^3}dy\,V(y)+\frac{C\kappa}{\ell^3}+C\varepsilon\ell^2\Big[\sup_{y\in\Lambda_\ell\times\Lambda_\ell}(|y_1-y_2|+1)|g(y)|\Big]$$

therefore, by setting $\varepsilon=(2C\ell^2)^{-1}$, we obtain (A.34).

Finally we investigate point v). As above, we decompose $f=c+g$ with $c=\ell^{-6}\int f$. We shall prove that

$$\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]|\nabla_{x_1+x_2}g(x)|\le C\kappa\ell^{-3}\tag{A.41}$$

where $d(x)$ is the distance of x from the boundary of the box Λ_ℓ. By (A.29), we have

$$\begin{aligned}\nabla_{x_1+x_2}g(x)=&-\int_\Omega dy\,\nabla_{y_1+y_2}\tilde G_\varepsilon(x-y)\big(\lambda_\ell-V(y)\big)f(y)-\varepsilon\int_\Omega dy\,\nabla_{y_1+y_2}\tilde G_\varepsilon(x-y)g(y)\\ &+\int_\Omega dy\,\nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big]\big(\lambda_\ell-\kappa V(y)\big)f(y)\\ &+\varepsilon\int_\Omega dy\,\nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big]g(y)\end{aligned}\tag{A.42}$$

We integrate by parts in the first line, and obtain

$$\begin{aligned}\nabla_{x_1+x_2}g(x)=&\int_\Omega dy\,\tilde G_\varepsilon(x-y)\big(\lambda_\ell-\kappa V(y)\big)\nabla_{y_1+y_2}f(y)+\varepsilon\int_\Omega dy\,\tilde G_\varepsilon(x-y)\nabla_{y_1+y_2}g(y)\\ &+\int_{\partial\Omega}d\sigma_y\,\hat n\,\tilde G_\varepsilon(x-y)\big(\lambda_\ell-\kappa V(y)\big)f(y)+\varepsilon\int_{\partial\Omega}d\sigma_y\,\hat n\,\tilde G_\varepsilon(x-y)g(y)\\ &+\int_\Omega dy\,\nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big]\big(\lambda_\ell-\kappa V(y)\big)f(y)\\ &+\varepsilon\int_\Omega dy\,\nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big]g(y)=\sum_{j=1}^6\mathrm{D}_j(x)\end{aligned}\tag{A.43}$$

where $d\sigma_y$ is the surface element of the boundary of the box $\partial\Omega$ and $\hat n$ is the unit vector pointing outwards. We start by considering D_2. Using (A.9), we can bound, for every $x\in\Omega$,

$$\begin{aligned}&\big|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_2(x)\big|\\ &\le C\varepsilon\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\int_\Omega dy\,\frac{\big|\big[d(y_1+y_2)^{5/3}+1\big]\nabla_{y_1+y_2}g(y)\big|}{|x-y|^4\big[d(\frac{y_1+y_2}{2})^{5/3}+1\big]}\\ &\le C\varepsilon\sup_{y\in\Omega}\big|\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2}g(y)\big|\int_\Omega dy\,\frac{d(\frac{x_1+x_2}{2})^{5/3}+1}{|x-y|^4\big[d(\frac{y_1+y_2}{2})^{5/3}+1\big]}\end{aligned}\tag{A.44}$$

In the following we shall show that

$$\int_\Omega dy\, \frac{1}{|x-y|^4\big[d(\frac{y_1+y_2}{2})^{5/3}+1\big]} \le \frac{C\ell^2}{d(\frac{x_1+x_2}{2})^{5/3}+1}$$

Since

$$\frac{1}{d(\frac{x_1+x_2}{2})^{5/3}+1} \le \sum_{i=1}^{3}\sum_{j=1}^{2} \frac{1}{2^{-5/3}|x_1^{(i)}+x_2^{(i)}-(-1)^j\ell|^{5/3}+1} \le \frac{6}{d(\frac{x_1+x_2}{2})^{5/3}+1} \tag{A.45}$$

it is sufficient to prove that

$$\int_\Omega dy\, \frac{1}{|x-y|^4\big[|y_1^{(1)}+y_2^{(1)}-\ell|^{5/3}+1\big]} \le \frac{C\ell^2}{|x_1^{(1)}+x_2^{(1)}-\ell|^{5/3}+1} \tag{A.46}$$

For this purpose, we shall write

$$|x_1-y_1|^2+|x_2-y_2|^2 = \frac{1}{2}\big|(x_1+x_2)-(y_1+y_2)\big|^2+\frac{1}{2}\big|(x_1-x_2)-(y_1-y_2)\big|^2; \tag{A.47}$$

with the change of variable $y_1+y_2=b$, $y_1-y_2=a$ we have

$$\begin{aligned}&\int_\Omega dy\, \frac{|x_1^{(1)}+x_2^{(1)}-\ell|^{5/3}+1}{|x-y|^4\big[|y_1^{(1)}+y_2^{(1)}-\ell|^{5/3}+1\big]}\\ &\quad = \frac{1}{2}\int_{[-\ell,\ell]^3} db \int_{\omega(b)} da\, \frac{|x_1^{(1)}+x_2^{(1)}-\ell|^{5/3}+1}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1-x_2)-a\big|^2\big]^2\big[|b^{(1)}-\ell|^{5/3}+1\big]}\end{aligned} \tag{A.48}$$

where $\omega(b)=[|b^{(1)}|-\ell,\ell-|b^{(1)}|]\times[|b^{(2)}|-\ell,\ell-|b^{(2)}|]\times[|b^{(3)}|-\ell,\ell-|b^{(3)}|]$. Let us introduce the notation $a=(a^{(1)},a^\perp)$ and $b=(b^{(1)},b^\perp)$. To bound (A.48) we bound the numerator with $2(2\ell)^{5/3}$ (assuming $2\ell\ge 1$) and extend the integration domain of the variable $a^\perp$ to $[-\ell,\ell]^2$; dropping the term involving $a^{(1)}$ in the denominator, we can integrate over $a^{(1)}$ to obtain the bound

$$\begin{aligned}&\int_{[-\ell,\ell]^3} db \int_{\omega(b)} da\, \frac{|x_1^{(1)}+x_2^{(1)}-\ell|^{5/3}+1}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1-x_2)-a\big|^2\big]^2\big[|b^{(1)}-\ell|^{5/3}+1\big]}\\ &\le 2(2\ell)^{5/3}\int_{[-\ell,\ell]} db^{(1)} \frac{1}{|b^{(1)}-\ell|^{2/3}}\int_{[-\ell,\ell]^4} db^\perp da^\perp\, \frac{1}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1^\perp-x_2^\perp)-a^\perp\big|^2\big]^2}\end{aligned}$$

We estimate

$$\begin{aligned}\int_{[-\ell,\ell]^4} db^\perp da^\perp\, \frac{1}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1^\perp-x_2^\perp)-a^\perp\big|^2\big]^2} &\le C\int_{|(x_1^{(1)}+x_2^{(1)})-b^{(1)}|}^{3\ell} dz\,\frac{1}{z}\\ &= C\ln\left(\frac{3\ell}{|(x_1^{(1)}+x_2^{(1)})-b^{(1)}|}\right)\end{aligned}$$

and

$$\int_{[-\ell,\ell]} db^{(1)} \frac{1}{|b^{(1)}-\ell|^{2/3}}\ln\left(\frac{3\ell}{|(x_1^{(1)}+x_2^{(1)})-b^{(1)}|}\right) \le (2\ell)^{1/3}\sup_{0<s<1}\int_0^1 dt\, t^{-2/3}\ln\frac{3/2}{t-s} \le C\ell^{1/3}$$

This proves (A.46). We have thus shown that

$$\big|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_2(x)\big| \le C\varepsilon\ell^2\sup_{y\in\Omega}\big|\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2}g(y)\big| \tag{A.49}$$

We proceed with D_1, which we write as $\mathrm{D}_1=\mathrm{D}_{11}+\mathrm{D}_{12}$, with

$$\mathrm{D}_{11}(x) = \lambda_\ell\int_\Omega dy\, \tilde{G}_\varepsilon(x-y)\nabla_{y_1+y_2}f(y) \tag{A.50}$$

and

$$\mathrm{D}_{12}(x) = -\int_\Omega dy\,\tilde G_\varepsilon(x-y)\kappa V(y)\nabla_{y_1+y_2} f(y) \tag{A.51}$$

Using the same method as above we estimate

$$|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{11}(x)| \le C\lambda_\ell \ell^2 \sup_{y\in\Omega} |\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2} g(y)|. \tag{A.52}$$

For D_{12} we have

$$\begin{aligned} &|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{12}(x)| \\ &\quad\le \sup_{y\in\Omega} |\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2} g(y)| \int_\Omega dy\, \frac{\kappa V(y)\big[d(\frac{x_1+x_2}{2})^{5/3}+1\big]}{|x-y|^4\big[d(\frac{y_1+y_2}{2})^{5/3}+1\big]} \end{aligned} \tag{A.53}$$

Because of (A.45) it again suffices to bound the last integral with $d(z)$ replaced by $|z^{(1)}-\ell|$ for both $z = x_1+x_2$ and $z = y_1+y_2$. With the same change of variables as in (A.48) we have

$$\begin{aligned} &\int_\Omega dy\, \frac{\kappa V(y)}{|x-y|^4\big[\big(y_1^{(1)}+y_2^{(1)}\big)^{5/3}+1\big]} \\ &\quad\le \frac12 \int_{\mathbb{R}^3} da \int_{\mathbb{R}^3} db\, \frac{\kappa V(a)}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1-x_2)-a\big|^2\big]^2\big[|b^{(1)}-\ell|^{5/3}+1\big]} \end{aligned} \tag{A.54}$$

where we extended integration domain to $\mathbb{R}^6$. Integrating first in the variable $b^\perp$ we have

$$\begin{aligned} &\int_{\mathbb{R}^3} da \int_{\mathbb{R}^3} db\, \frac{\kappa V(a)}{\big[\big|(x_1+x_2)-b\big|^2+\big|(x_1-x_2)-a\big|^2\big]^2\big[|b^{(1)}-\ell|^{5/3}+1\big]} \\ &\quad= C\int_{\mathbb{R}} db^{(1)} \frac{1}{|b^{(1)}-\ell|^{5/3}+1} \int_{\mathbb{R}^3} da \frac{\kappa V(a)}{\big|\big(x_1^{(1)}+x_2^{(1)}\big)-b^{(1)}\big|^2+\big|(x_1-x_2)-a\big|^2} \end{aligned} \tag{A.55}$$

Using that V is bounded and of compact support, one readily checks that

$$\int_{\mathbb{R}^3} da \frac{V(a)}{X+|Y-a|^2} \le \frac{C}{X+|Y|^2+1} \tag{A.56}$$

for all $X \ge 0$ and $Y \in \mathbb{R}^3$. Hence we find that

$$\begin{aligned} \int_\Omega dy\, \frac{\kappa V(y)}{|x-y|^4\big[|y_1^{(1)}+y_2^{(1)}-\ell|^{5/3}+1\big]} &\le C\kappa \int_{\mathbb{R}} db^{(1)} \frac{1}{|b^{(1)}-\ell|^{5/3}+1} \frac{1}{|(x_1^{(1)}+x_2^{(1)})-b^{(1)}|^2+1} \\ &\le \frac{C\kappa}{\big[|x_1^{(1)}+x_2^{(1)}-\ell|^{5/3}+1\big]} \end{aligned} \tag{A.57}$$

which is the desired bound, allowing us to conclude that

$$|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{12}(x)| \le C\kappa \sup_{y\in\Omega} |\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2} g(y)|. \tag{A.58}$$

In order to bound D_5 we split it into

$$\mathrm{D}_{51}(x) = \lambda_\ell \int_\Omega dy\, \nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big] f(y) \tag{A.59}$$

and

$$\mathrm{D}_{52}(x) = -\int_\Omega dy\, \nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde G_\varepsilon(x-y)\Big]\kappa V(y) f(y) \tag{A.60}$$

We easily bound

$$\begin{aligned} &|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{51}(x)| \\ &\qquad\le \lambda_\ell\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big] \int_\Omega dy\, \Big[\sum_n \frac{1}{|x-y_n|^5}+\frac{1}{\varepsilon^{1/2}\ell^6}\Big] f(y) \\ &\qquad\le C\kappa(\ell^{-3-1/3}+\ell^{-4-1/3}\varepsilon^{-1/2}) \end{aligned} \tag{A.61}$$

where we used (A.4), (2.12) and (2.14) and we estimated $d(\frac{x_1+x_2}{2}) \leq \ell/2$. For D_{52}, we use again (A.4) and (2.14) to estimate

$$|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{52}(x)| \leq \frac{C\big[d(\frac{x_1+x_2}{2})^{5/3}+1\big]}{\ell^3}\int_\Omega dy\,\Big[\sum_n \frac{1}{|x-y_n|^5}+\frac{1}{\varepsilon^{1/2}\ell^6}\Big]\kappa V(y). \tag{A.62}$$

For the second contribution we have

$$\frac{\big[d(\frac{x_1+x_2}{2})^{5/3}+1\big]}{\varepsilon^{1/2}\ell^9}\int_\Omega dy\,\kappa V(y) \leq \frac{C\kappa}{\varepsilon^{1/2}\ell^{4+1/3}} \tag{A.63}$$

For the first contribution in (A.62), among the image charges y_n we start considering the one that has all coordinates equal to those of y except the first one. We rename it as $\tilde{y}$, and we have $\tilde{y}_1^{(1)} = -\ell - y_1^{(1)}$. We write

$$\begin{aligned}\int_\Omega dy\,\frac{1}{|x-\tilde{y}|^5}V(y) &= \int_\Omega dy_1 dy_2\,\frac{V(y_1-y_2)}{(|x_1-\tilde{y}_1|^2+|x_2-\tilde{y}_2|^2)^{5/2}}\\ &= \int_{[-3\ell/2,-\ell/2]\times[-\ell/2,\ell/2]^5} d\tilde{y}_1 d\tilde{y}_2\,\frac{V(\tilde{y}_1^{(1)}+\tilde{y}_2^{(1)}+\ell,\tilde{y}_1^\perp-\tilde{y}_2^\perp)}{(|x_1-\tilde{y}_1|^2+|x_2-\tilde{y}_2|^2)^{5/2}}\end{aligned} \tag{A.64}$$

The denominator can be expressed as in (A.47); with the change of variables $\tilde{y}_1+\tilde{y}_2 = b$, $\tilde{y}_1-\tilde{y}_2 = a$, we have (extending the integration domain to $\mathbb{R}^6$)

$$\begin{aligned}\int_\Omega dy\,\frac{1}{|x-\tilde{y}|^5}V(y) &\leq \frac{1}{\sqrt{2}}\int_{\mathbb{R}^3} db^{(1)}da^\perp\,V(b^{(1)}+\ell,a^\perp)\\ &\quad\times\int_{\mathbb{R}^3} da^{(1)}db^\perp\,\frac{1}{\big(|x_1+x_2-b|^2+|x_1-x_2-a|^2\big)^{5/2}}\\ &= C\int_{\mathbb{R}^3} db^{(1)}da^\perp\frac{V(b^{(1)}+\ell,a^\perp)}{\big(x_1^{(1)}+x_2^{(1)}-b^{(1)}\big)^2+\big(x_1^\perp-x_2^\perp-a^\perp\big)^2}\end{aligned} \tag{A.65}$$

Using now again (A.56), we arrive at

$$\frac{1}{\ell^3}\left|\int_\Omega dy\,\frac{1}{|x-\tilde{y}|^5}\kappa V(y)\right| \leq \frac{C}{\ell^3}\frac{\kappa}{|x_1^{(1)}+x_2^{(1)}-\ell|^2+1} \leq \frac{C}{\ell^3}\frac{\kappa}{d(x_1+x_2)^2+1} \tag{A.66}$$

The contribution from the other image charges can be estimated similarly, and we omit the details. We conclude that

$$|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_{52}(x)| \leq \frac{C\kappa}{\varepsilon^{1/2}\ell^{4+1/3}}+\frac{C\kappa}{\ell^3} \tag{A.67}$$

Next we investigate D_6. With (A.4) and (A.34) we have

$$\begin{aligned}|\mathrm{D}_6(x)| &= \left|\varepsilon\int_\Omega dy\,\nabla_{x_1+x_2}\Big[G_\varepsilon(x,y)-\tilde{G}_\varepsilon(x-y)\Big]g(y)\right|\\ &\leq \frac{C\varepsilon^{1/2}}{\ell^6}\int_\Omega dy\,|g(y)| + \frac{\varepsilon\kappa}{\ell^3}\sum_n\int_\Omega dy\,\frac{1}{|x-y_n|^5}\frac{1}{|y_1-y_2|+1}\end{aligned} \tag{A.68}$$

To bound the first term we can also use (A.34), which gives $\int|g| \leq C\kappa\ell^2$. To estimate the second term in (A.68) we start, as above, by considering the image charge $\tilde{y}$ such that $\tilde{y}_1^{(1)} = -\ell - y_1^{(1)}$, $\tilde{y}_1^{(i)} = y_1^{(i)}$ for $i = 2,3$ and $\tilde{y}_2^{(j)} = y_2^{(j)}$ for $j = 1,2,3$. We perform again the change of variables $\tilde{y}_1+\tilde{y}_2 = b$, $\tilde{y}_1-\tilde{y}_2 = a$ and extend the integration domains so that

$$\begin{aligned}&\int_\Omega dy\,\frac{1}{|x-\tilde{y}|^5}\frac{1}{|y_1-y_2|+1}\\ &\leq \frac{1}{\sqrt{2}}\int_{[-\ell,\ell]^2} da^\perp\int_{\mathbb{R}^4} db^{(1)}db^\perp da^{(1)}\\ &\quad\times\frac{1}{\big[|x_1+x_2-b|^2+|x_1-x_2-a|^2\big]^{5/2}}\frac{1}{\big[|b^{(1)}+\ell|^2+|a^\perp|^2\big]^{1/2}+1}\\ &\leq C\int_{[-\ell,\ell]^2} da^\perp\,\frac{1}{|a^\perp|+1}\frac{1}{|x_1^\perp-x_2^\perp-a^\perp|}\end{aligned}$$

where we dropped the term $|b^{(1)}+\ell|^2$ in the last step in order to be able to explicitly integrate over $b^{(1)}$. It is easy to see that the remaining integral is bounded by $\ln \ell$, uniformly in $x_1^\perp - x_2^\perp$. The same estimate can be applied to the other imaged charges, with the result that

$$|\mathrm{D}_6(x)| \le C\kappa\varepsilon^{1/2}\ell^{-4} + C\kappa\varepsilon\ell^{-3}\ln(\ell)$$

In particular,

$$\big|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_6(x)\big| \le C\kappa\varepsilon^{1/2}\ell^{-7/3} + C\kappa\varepsilon\ell^{-4/3}\ln(\ell) \tag{A.69}$$

We are left with considering D_3 and D_4. With the aid of (A.9) and (A.34) we can bound

$$|\mathrm{D}_4(x)| = \Big|\varepsilon\int_{\partial\Omega} d\sigma_y\,\hat{n}\,\tilde{G}_\varepsilon(x-y)g(y)\Big| \le \frac{C\varepsilon\kappa}{\ell^3}\int_{\partial\Omega} d\sigma_y \frac{1}{|x-y|^4}\frac{1}{|y_1-y_2|+1} \tag{A.70}$$

It clearly suffices to consider the contribution to the boundary integral coming from $y_1^{(1)} = -\ell/2$. With the change of variables $y_1^\perp + y_2^\perp = b^\perp$, $y_1^\perp - y_2^\perp = a^\perp$ we have, similarly as above,

$$\begin{aligned}
&\int_{\partial\Omega} d\sigma_y \frac{1}{|x-y|^4}\frac{1}{|y_1-y_2|+1}\\
&\le \int_{\mathbb{R}} dy_2^{(1)} \int_{[-\ell,\ell]^2} da^\perp \frac{1}{\big[|y_2^{(1)}+\ell/2|^2+|a^\perp|^2\big]^{1/2}+1}\\
&\quad\times\int_{\mathbb{R}^2} db^\perp \frac{1}{\Big[\big|x_1^\perp+x_2^\perp-b^\perp\big|^2+\big|x_1^\perp-x_2^\perp-a^\perp\big|^2+2\big|x_1^{(1)}+\ell/2\big|^2+2\big|x_2^{(1)}-y_2^{(1)}\big|^2\Big]^2}\\
&\le C\int_{[-\ell,\ell]^2} da^\perp \frac{1}{|a^\perp|+1}\frac{1}{|x_1^\perp-x_2^\perp-a^\perp|} \le C\ln\ell
\end{aligned}$$

and thus

$$\big|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_4(x)\big| \le C\kappa\varepsilon\ell^{-4/3}\ln(\ell) \tag{A.71}$$

In D_3 we estimate the contribution proportional to λ_ℓ as

$$\lambda_\ell\int_{\partial\Omega} d\sigma_y\,\tilde{G}_\varepsilon(x-y)f(y) \le C\frac{\lambda_\ell}{\ell^3}\int_{\partial\Omega} d\sigma_y\frac{1}{|x-y|^4} \le \frac{C\kappa}{\ell^5},$$

where we used (2.14) and (2.12). For the contribution proportional to V, we use again (2.14) to bound it as

$$\int_{\partial\Omega} d\sigma_y\,\tilde{G}_\varepsilon(x-y)\kappa V(y)f(y) \le \frac{C}{\ell^3}\int_{\partial\Omega} d\sigma_y\,\frac{\kappa V(y)}{|x-y|^4}$$

To estimate the first term on the right-hand side, we perform the same change of variables as in D_4. Extending the domain of integration to $\mathbb{R}^5$ and doing the integration over $b^\perp$ we have

$$\begin{aligned}
\int_{\partial\Omega,\,y_1^{(1)}=-\ell/2} d\sigma_y\,\frac{V(y)}{|x-y|^4} &\le C\int_{\mathbb{R}^3} dy_2^{(1)}da^\perp \frac{V(y_2^{(1)}+\ell/2,a^\perp)}{\big|x_1^\perp-x_2^\perp-a^\perp\big|^2+\big|x_1^{(1)}+x_2^{(1)}+\ell/2-y_2^{(1)}\big|^2}\\
&\le C\frac{1}{|x_1^{(1)}+x_2^{(1)}-\ell|^2+1}
\end{aligned}$$

where we used again (A.56) in the last step. Hence

$$\big|\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]\mathrm{D}_3(x)\big| \le C\kappa\ell^{-3} \tag{A.72}$$

By combining (A.43), (A.49), (A.52), (A.58), (A.61), (A.67), (A.69), (A.71) and (A.72) we have thus shown that

$$\begin{aligned}
\big[d(\tfrac{x_1+x_2}{2})^{5/3}+1\big]|\nabla_{x_1+x_2}g(x)| &\le C\kappa\Big(\ell^{-3}+\varepsilon\ell^{-4/3}\ln(\ell)\Big)\\
&\quad + C\left(\varepsilon\ell^2+\lambda_\ell\ell^2+\kappa\right)\sup_{y\in\Omega}\Big|\big[d(\tfrac{y_1+y_2}{2})^{5/3}+1\big]\nabla_{y_1+y_2}g(y)\Big|.
\end{aligned}$$

We choose $\varepsilon = c\ell^{-2}$ with small enough c so that the factor $C(\varepsilon\ell^2+\lambda_\ell\ell^2+\kappa)$ is smaller than one for large ℓ and small κ, concluding the proof of (2.18). □

Proof of Proposition 2.2. From (2.13) it follows that

$$\int_{\Lambda_1\times\Lambda_1} dxdy \left[|\nabla_x w_\ell(x,y)|^2 + |\nabla_y w_\ell(x,y)|^2\right] \leq \frac{C\kappa}{\ell}, \tag{A.73}$$

estimate (2.14) implies

$$|w_\ell(x,y)| \leq C \tag{A.74}$$

and from (2.15) it follows that

$$\int_{\Lambda_1\times\Lambda_1} dxdy \left|w_\ell(x,y)\right|^2 \leq \frac{C\kappa^2}{\ell^2}, \tag{A.75}$$

while (2.16) shows that

$$\int_{\Lambda_1\times\Lambda_1} dxdy \, |w_\ell(x,y)| \leq \frac{C\kappa}{\ell}. \tag{A.76}$$

By equation (2.24) and bounds (A.75), (A.73) we find

$$\begin{aligned} \int_{\Lambda_1\times\Lambda_1} dxdy \left|\mu(x,y)\right|^2 &\leq C\kappa\frac{n^2}{\ell^2} \\ \int_{\Lambda_1\times\Lambda_1} dxdy \left[\left|\nabla_x \mu(x,y)\right|^2 + \left|\nabla_y \mu(x,y)\right|^2\right] &\leq C\kappa\frac{n^2}{\ell} \end{aligned}$$

which imply (2.27) and (2.28). By (2.14) we have

$$|\eta(x,y)| \leq n|w_\ell(x,y)| + |\mu(x,y)| \leq Cn \tag{A.77}$$

which proves (2.29). Estimate (2.30) follows from (2.17). Point *ii*) follows from (2.30).
We consider now point *iii*). From the definition of r, we find

$$\begin{aligned} r(x,y) &= \sum_{n=1}^{\infty} \frac{1}{(2n+1)!}\eta^{2n+1}(x,y) \\ &= \sum_{n=1}^{\infty} \frac{1}{(2n+1)!} \int dzdw \, \eta(x,z)\, \eta^{2n-1}(z,w)\, \eta(w,y); \end{aligned} \tag{A.78}$$

using (2.27), which implies $\|\eta\|_2 \leq C$, we arrive at

$$\begin{aligned} |r(x,y)| &\leq \sum_{n=1}^{\infty} \frac{1}{(2n+1)!} \left[\int dwdz |\eta(x,z)|^2 |\eta(w,y)|^2\right]^{1/2} \left[\int dwdz \, |\eta^{2n-1}(z,w)|^2\right]^{1/2} \\ &\leq \sum_{n=1}^{\infty} \frac{1}{(2n+1)!} \|\eta\|_2^{2n-1} \, \|\eta(x,\cdot)\|_2 \|\eta(\cdot,y)\|_2 \leq C\|\eta\|_2 \|\eta(x,\cdot)\|_2 \|\eta(\cdot,y)\|_2 \end{aligned} \tag{A.79}$$

for every $x, y \in \Lambda_1$. The bound for p can be proven analogously. This proves (2.33) and consequently (2.34) and (2.32). □

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References

[1] A. Adhikari, C. Brennecke, B. Schlein. Bose-Einstein condensation beyond the Gross-Pitaevskii regime. *Ann. Henri Poincare.* **22** (2021), 1163–1233.

[2] N. Aronszajn, K.T. Smith. Theory of Bessel potentials. I. *Annales de l'institut Fourier*, tome 11 (1961), 385–475

[3] N. Benedikter, G. de Oliveira, B. Schlein. Quantitative derivation of the Gross-Pitaevskii equation. *Comm. Pure Appl. Math.* **68** (2014), 1399–1482.

[4] G. Basti, S. Cenatiempo, B. Schlein. A new second order upper bound for the ground state energy of dilute Bose gases.*Forum Math. Sigma* **9**(2021), e74.

[5] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein. Complete Bose-Einstein condensation in the Gross-Pitaevskii regime. *Commun. Math. Phys.* **359** (2018), 975–1026.

[6] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein. Bogoliubov theory in the Gross-Pitaevskii limit. *Acta Mathematica* **222** (2019), 219–335.

[7] C. Boccato, C. Brennecke, S. Cenatiempo, B. Schlein. Optimal rate for Bose-Einstein condensation in the Gross-Pitaevskii regime. *Commun. Math. Phys.* **376** (2020), 1311–1395.

[8] C. Boccato, S. Cenatiempo, B. Schlein. Quantum many-body fluctuations around nonlinear Schrödinger dynamics. *Ann. Henri Poincaré* **18** (2017), 113–191.

[9] C. Brennecke, M. Caporaletti, B. Schlein. Excitation spectrum for Bose Gases beyond the Gross-Pitaevskii regime. Preprint arXiv:2104.13003.

[10] C. Brennecke, B. Schlein. Gross-Pitaevskii dynamics for Bose-Einstein condensates. *Anal. PDE* **12** (2019), 1513–1596.

[11] C. Brennecke, B. Schlein, S. Schraven. Bose-Einstein condensation with optimal rate for trapped bosons in the Gross-Pitaevskii regime. *Math. Phys. Anal. Geom.* **25** (2022).

[12] C. Brennecke, B. Schlein, S. Schraven. Bogoliubov Theory for trapped bosons in the Gross-Pitaevskii regime. *Ann. Henri Poincaré* **23** (2022), 1583–1658.

[13] B. Brietzke, S. Fournais, J.P. Solovej. A simple 2nd order lower bound to the energy of dilute Bose gases. *Commun. Math. Phys.*, **376** (2020), 323-351.

[14] L. Erdős, B. Schlein, H.-T. Yau. Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate, *Annals of Math.* **172** (2010), no. 1, 291–370.

[15] S. Fournais. Length scales for BEC in the dilute Bose gas. *Partial Differential Equations, Spectral Theory, and Mathematical Physics*, EMS Series of Congress Reports (2021).

[16] S. Fournais, J.P. Solovej. The energy of dilute Bose gases. *Annals of Math.* **192** (2020), 893–976.

[17] P. Grech, R. Seiringer. The excitation spectrum for weakly interacting bosons in a trap. *Comm. Math. Phys.* **322** (2013), no. 2, 559–591.

[18] C. Hainzl. Another proof of BEC in the GP-limit. *J. Math. Phys.* **62** (2021), 051901.

[19] C. Hainzl, B. Schlein, A. Triay. Bogoliubov Theory in the Gross-Pitaevskii limit: a simplified approach. Preprint arXiv:2203.03440

[20] T.D. Lee, C.N. Yang. Many-body problem in quantum mechanics and in quantum statistical mechanics, *Phys. Rev.* **105** (1957), 1119–1120.

[21] T.D. Lee, K. Huang, C.N. Yang. Eigenvalues and eigenfunctions of a Bose system of hard spheres and its low-temperature properties, *Phys. Rev.* **106** (1957), 1135–1145.

[22] M. Lewin, P. T. Nam, S. Serfaty, J.P. Solovej. Bogoliubov spectrum of interacting Bose gases. *Comm. Pure Appl. Math.* **68** (2014), no. 3, 413–471

[23] E. H. Lieb and R. Seiringer. Proof of Bose-Einstein condensation for dilute trapped gases. *Phys. Rev. Lett.* **88** (2002), 170409.

[24] E. H. Lieb and R. Seiringer. Derivation of the Gross-Pitaevskii equation for rotating Bose gases. *Comm. Math. Phys.* **264**:2 (2006), 505–537.

[25] E. H. Lieb, R. Seiringer, J. P. Solovej, J. Yngvason. The mathematics of the Bose gas and its condensation. Oberwolfach Seminars **34** (2005), Birkhäuser Basel.

[26] E. H. Lieb, J. Yngvason. Ground state energy of the low density Bose Gas. *Phys. Rev. Lett.* **80** (1998), 2504–2507.

[27] P. T. Nam, M. Napiórkowski, J. Ricaud, A. Triay. Optimal rate of condensation for trapped bosons in the Gross-Pitaevskii regime. arXiv:2001.04364.

[28] P. T. Nam, N. Rougerie, R. Seiringer. Ground states of large bosonic systems: The Gross-Pitaevskii limit revisited. *Analysis and PDE.* **9** (2016), no. 2, 459–485.

[29] P. T. Nam, A. Triay. Bogoliubov excitation spectrum of trapped Bose gases in the Gross-Pitaevskii regime . Preprint arXiv:2106.11949.

[30] R. Seiringer. Free energy of a dilute Bose gas: Lower Bound. *Commun. Math. Phys.* **279** (2008), 595–636.

[31] R. Seiringer. The Excitation Spectrum for Weakly Interacting Bosons. *Comm. Math. Phys.* **306** (2011), 565–578.

[32] H.-T. Yau, J. Yin. The second order upper bound for the ground state energy of a Bose gas. *J. Stat. Phys.* **136** (2009), no. 3, 453–503.

[33] J. Yin. Free energies of dilute Bose Gases: upper bound. *J. Stat. Phys.* **141** (2010), 683–726.