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Dynamical Semigroup Description of Coherent and Incoherent Particle–Matter Interaction

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The meaning of statistical experiments with single microsystems in quantum mechanics is discussed and a general model in the framework of nonrelativistic quantum field theory is proposed to describe both coherent and incoherent interaction of a single microsystem with matter. Compactly developing the calculations with superoperators, it is shown that the introduction of a time scale linked to irreversibility of the reduced dynamics directly leads to a dynamical semigroup expressed in terms of quantities typical of scattering theory. Its generator consists of two terms, the first linked to a coherent wavelike behavior, the second related to an interaction having a measuring character, possibly connected to events the microsystem produces propagating inside matter. In case these events breed a measurement, an explicit realization of some concepts of modern quantum mechanics ("effects" and "operations") arises. The relevance of this description to a recent debate questioning the validity of ordinary quantum mechanics to account for such experimental situations as, e.g., neutron interferometry is briefly discussed.

1. INTRODUCTION

Consider a source emitting practically only one particle at a time, feeding an interferometer; one of the most impressive features of quantum mechanics is the fact that the record in a detector of the output of the interferometer during a suitable time interval shows an interference pattern. If the experimental setup allows detectable events to be produced during the time the particle takes to pass through the interferometer, thus showing which way the particle went, a two-component pattern is found, respectively affected and not affected by

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interference. Seemingly the interfering part can be strongly attenuated if the probability of detecting events is enhanced, though still retaining its visibility. A number of experiments of relevance to the question have been carried out (Rauch, 1990; Rauch *et al.*, 1990; Mittelstaedt *et al.*, 1987; Chapman *et al.*, 1995). It has sometimes been claimed, and also appears in textbooks, that the very possibility of such a detection forces the interference pattern to disappear; such a somewhat strange expectation is rooted in an exaggerated faith in the so-called state reduction postulate of quantum mechanics. This postulate is a strongly idealized description of what happens to a quantum system due to the interaction with a device measuring a given observable of the system; using this postulate, a short-hand explanation of measurement is usually given, based on the idea that a quantum system must be represented by a "state vector" $\psi(t)$. A much more comfortable situation is met if, instead of a state vector, a statistical operator $\rho(t)$ is taken as the basic mathematical representation of a quantum system (Lanz, 1994). This attitude is sometimes considered suitable for applications, e.g., quantum optics, but not fine enough for more fundamental problems; it is often implicitly assumed that a statistical operator applies only to the description of a statistical mixture of a large number of microsystems, while in modern experiments often only one or very few relevant microsystems are present together in the experimental device. In these single-particle experiments it is often argued (Namiki and Pascazio, 1991; Thomson, 1993) that the system is to be described by a state vector.

In our opinion, instead, one-particle quantum mechanics, no matter if one uses $\psi(t)$ or $\rho(t)$, refers in principle to a statistical experiment in which repeatedly a single particle is produced, prepared, and observed under fixed macroscopic conditions; this does not oppose the fact that a beam of particles whose interactions are negligible and whose correlations are irrelevant may be treated in many experimental situations as effectively equivalent to the former preparation. It is just the modalities of the statistical experiment, which remain unchanged during the different runs of the experiment, that are represented by the statistical operator (or by the state vector, when this higher idealization works); this is indeed the striking difference with classical mechanics, where to each run of the statistical experiment there corresponds a trajectory in phase space. In this context a completely different point of view seems to underlie the so-called many-Hilbert-space quantum mechanics that was recently proposed (Namiki and Pascazio, 1993). In this framework a wave function is associated to each single run of a statistical experiment and, for example, in a Young's interference experiment random phase shifts between the two branch waves may arise in the repeated experimental runs, due to interaction with matter along one of the two branches, leading to attenuation of the interference pattern (Namiki and Pascazio, 1991).

As is well known, state vectors $\psi \in \mathcal{H}$, via the one-dimensional projections P_ψ on $\mathcal{H}$, correspond to the subset of extreme points of the convex set $\mathcal{K}$ of statistical operators in $\mathcal{H}$; i.e., they cannot be interpreted as mixtures of other possible preparations and any $\rho \in \mathcal{K}$ can be represented as $\rho = \Sigma_j p_j P_{\psi_j}$. For this reason state vectors $\psi \in \mathcal{H}$ are also called "pure states." Let us recall a relevant mathematical result (Davies, 1976); any invertible affine mapping $\mathcal{M}$ on $\mathcal{K}$ onto $\mathcal{K}$ has the form

$$\mathcal{M}\rho = M\rho M^\dagger$$

where M is a unitary (or antiunitary) operator on $\mathcal{H}$; then, if time evolution is represented by such a mapping (Comi *et al.*, 1975), the basic role of pure states for the dynamics becomes obvious and consequently also the relevance of the Schrödinger equation, of the Hamilton operator, and finally the correspondence with classical mechanics and classical field theory. To summarize with the aid of formulas, we have

$$\rho_t = \mathcal{M}_{tt_0}\rho_{t_0} = U(t, t_0)\rho_{t_0}U^\dagger(t, t_0) = \sum_j p_j P_{\psi_j(t)}$$

$$\psi_t = U(t, t_0)\psi_{t_0}, \qquad i\hbar \frac{d\psi_t}{dt} = H_t\psi_t$$

In fact the main part of the physics of microsystems can be developed almost neglecting the concept of statistical operator [a noteworthy exception, however, is the definition of the quantum collision cross section (Taylor, 1972; Ludwig, 1976)].

Such a reversible dynamics is to be expected for an isolated system. If interaction with an environment is not negligible during the time evolution, the question to be raised is whether this evolution can be simply described by a mapping $\mathcal{M}_{tt_0}$ on $\mathcal{K}$; i.e., whether ρ_t is uniquely determined by ρ_{t_0} and not by the whole history $\{\rho_{t'}; t' \leq t_0\}$ before t_0, recorded via interaction by this environment. In this general situation the system becomes the whole complex of particle plus environment and no disentanglement of the particle's degrees of freedom is possible. On the contrary, a neat and extremely relevant simplification occurs if such a mapping $\mathcal{M}_{tt_0}$ exists: then the one-particle Hilbert space $\mathcal{H}$ and not the Fock space of the whole system is the relevant mathematical framework. Let us assume that this simplification occurs, typically due to the fact that the aforementioned history is forgotten during the time elapsed before ρ_t varies appreciably, as in the case of Markovian dynamics; nevertheless one can no longer expect $\mathcal{M}_{tt_0}$ to be invertible: then the statistical operator ρ_t acquires a primary role. In differential form the evolution equation for ρ_t is given by

$$\frac{d\rho_t}{dt} = \mathcal{L}_t\rho_t, \qquad \mathcal{L}_t = \lim_{\tau\to 0} \frac{\mathcal{M}(t+\tau, t) - \mathcal{I}}{\tau}$$

$$\mathcal{M}_{tt_0} = \mathcal{T}\left(\exp \int_{t_0}^{t} dt' \, \mathcal{L}(t')\right) \tag{1.1}$$

In Section 2 we explicitly construct the generator $\mathcal{L}_t$ of the temporal evolution for the microsystem showing in a general way how it can be obtained starting from the Hamiltonian describing the local interaction between microsystem and macrosystem. An essential step is the introduction of a time scale on which the system is to be described, linked to the irreversibility of the interaction. To develop the calculations we rely upon a reformulation of the theory of scattering based on superoperators, that is, mappings defined on the algebra generated by creation and destruction operators acting in the Fock space. Quantum statistics is readily accounted for and the mapping $\mathcal{T}(z)$ [see (2.6)], strictly connected to the transition operator of the quantum theory of scattering, plays a central role from the very beginning. The use of the Heisenberg picture, consistent with the concentration of one's attention on the microsystem's observables, allows one to take the whole complex structure of the macrosystem into account. The generator obtained is of the Lindblad type, though allowing for unbounded operators. The general structure of such generators, ensuring that $\mathcal{M}_{tt_0}$ maps $\mathcal{K}$ into $\mathcal{K}$, is the following:

$$\mathcal{L}_t\rho = -\frac{i}{\hbar}(H_t\rho - \rho H_t) - \frac{1}{\hbar}(A_t\rho + \rho A_t) + \frac{1}{\hbar}\sum_j L_{tj}\rho L_{tj}^{\dagger} \tag{1.2}$$

$$H_t = H_t^{\dagger}, \qquad A_t \geq 0, \qquad L_{tj} \text{ being operators in } \mathcal{H}$$

The relation

$$A_t = \frac{1}{2}\sum_j L_{tj}^{\dagger}L_{tj} \tag{1.3}$$

must be satisfied in order that Tr ρ_t be conserved. If the particle can be absorbed, (1.3) is replaced by

$$A_t \geq \frac{1}{2}\sum_j L_{tj}^{\dagger}L_{tj} \tag{1.4}$$

If the last term in (1.2) is neglected, for a pure state $\rho_t = |\psi_t\rangle\langle\psi_t|$, (1.1) yields the Schrödinger equation:

$$i\hbar \frac{d\psi_t}{dt} = (H_t - iA_t)\psi_t \tag{1.5}$$

This is the basis for the wavelike description of propagation of a particle inside matter. Setting $H_t - iA_t = p^2/(2m) + V(x, t)$, one can define

$$n(x, \nu, t) = \sqrt{1 - \frac{V(x, t)}{h\nu}} \tag{1.6}$$

as the refractive index of the medium, where $h\nu$ is to be identified with the energy of the incoming particle: such a description is usually adopted in interferometric experiments to explain how a block of matter whose properties are accounted for by the phenomenological macroscopic potential $V(x, t)$, when placed in one of the two branches, can induce a phase shift in the corresponding branch wave, or, in the case of an imaginary potential, cause absorption. Only in the very special case of $A_t = 0$, i.e., for a real "macroscopic" potential $V(x, t)$, does one have by (1.3) or (1.4) that $L_{tj} = 0$ and (1.5) is exactly equivalent to (1.2). In the presence of absorption $A_t \neq 0$ implies, by (1.3), $L_{tj} \neq 0$ for some j; but also in the absence of absorption one cannot expect that $L_{tj} = 0$. Notice that, if one is not aware of the basic role of (1.2) and of the importance of the last term in its r.h.s., by (1.5) one could be confirmed in the erroneous belief that the nonreality of the potential V is exclusively linked to absorption processes. To grasp the significance of the term $(1/\hbar)\Sigma_j L_{tj}\rho L_{tj}^\dagger$ for the dynamics of ρ, let us write the evolution of ρ due to it in a small time interval τ in the form

$$\Delta\rho = \frac{\tau}{\hbar} \operatorname{Tr}(2A_t\rho) \sum_j \tilde{L}_{tj}\rho\tilde{L}_{tj}^\dagger, \qquad \tilde{L}_{tj} = \frac{L_{tj}}{\sqrt{\operatorname{Tr}(2A_t\rho)}} \tag{1.7}$$

The statistical operator $\Sigma_j\tilde{L}_{tj}\rho\tilde{L}_{tj}^\dagger$ is a mixture of subcollections $\tilde{L}_{tj}\rho\tilde{L}_{tj}^\dagger$ related to outcome channels labeled by the index j; it bears some resemblance to the statistical operator $\Sigma_j P_j\rho P_j$ which represents, by the previously mentioned reduction postulate, the system after the measurement of an observable $A = \Sigma_j a_j P_j$; $(1/\hbar)\operatorname{Tr}(2A_t\rho)$ expresses the strength of the coupling to the incoherent regime. More generally a mapping whose infinitesimal generator is of the form (1.2) admits measuring decompositions that have been characterized in the context of "continuous measurement theory" initiated by Davies for the counting processes and developed later in full generality [for a recent review see Lanz and Melsheimer (1993) and Lanz (1994)]. These decompositions are related to the operators L_{tj} responsible for the irreversible dynamics, and clarify what is meant by the measuring character of a mapping describing the temporal evolution of a system. We will see in Section 3 that (1.2) couples very simply the typical wave dynamics, which is responsible for interference phenomena, with a "noncoherent" regime. Obviously in many instances the main interest is to put the wavelike behavior in major evidence; this amounts to making L_{ij} negligible, so that (1.5) is indeed suitable to describe the dynamics. On the contrary, more recent investigations, e.g., neutron interferometry in the presence of stray absorption in one path of the interferometer (Rauch, 1990; Rauch *et al.*, 1990), aim at investigating the competition between wavelike coherent behavior and which-way detection: then (1.1) and (1.2) must be considered. In Section 3 the physical interpretation of the dynamics thus obtained for the microsystem is discussed, showing the interplay between a "purely optical" regime [such as in (1.5) and (1.6)] and an "events-producing" one, strictly connected to the presence of the incoherent contribution in the r.h.s. of (1.2).

2. CONSTRUCTION OF THE GENERATOR

We assume for simplicity that the whole system is confined, e.g., in a box; eventually we can get rid of this confinement by letting the size of the box go to infinity. The microsystem is described in a Hilbert space $\mathcal{H}^{(1)}$; energy eigenvalues are E_f, energy eigenstates u_f, spanning the space $\mathcal{H}^{(1)}$. In this paper we use the formalism of nonrelativistic quantum field theory, which will play an essential role in obtaining a general procedure leading from the second-quantized Hamiltonian H of the whole system, acting in the global Fock space $\mathcal{H}_F$, to the generator of the semigroup $\mathcal{L}$ acting in $\mathcal{T}(\mathcal{H}^{(1)})$ (the set of trace-class operators in $\mathcal{H}^{(1)}$).

We shall set

$$H = H_0 + H_m + V$$

$$H_0 = \sum_f E_f a_f^\dagger a_f, \qquad [a_f, a_g^\dagger]_\mp = \delta_{fg}$$

where a_f is the destruction operator for the microsystem, either a Fermi or a Bose particle, in the state u_f; H_m is the Hamilton operator for the macrosystem ($[H_m, a_f] = 0$), also containing the potential determining the internal structure of the macrosystem; V represents the interaction between the two systems. We shall assume in this paper that no absorption process of the microsystem occurs: then $N = \Sigma_h a_h^\dagger a_h$ is a constant, $[N, H] = [N, V] = 0$. The present treatment is nonrelativistic due to the role played by particle number conservation.

We assume the following expression for the statistical operator:

$$\rho = \sum_{gf} a_g^\dagger \rho^m a_f \rho_{gf}^{(1)} \tag{2.1}$$

where ρ^m is a statistical operator in the subspace $\mathcal{H}_F^0$ of $\mathcal{H}_F$ in which $N = 0$, representing the macrosystem, and therefore

$$a_f \rho^m = 0, \qquad \rho^m a_f^\dagger = 0, \qquad \forall f$$

while ρ is a statistical operator in the subspace $\mathcal{H}_F^1$ of $\mathcal{H}_F$ in which $N = 1$. As far as the microsystem is concerned, the dynamics of the macrosystem is not appreciably perturbed by the presence of the microsystem itself, so we can assume that

$$\frac{d\rho^m(t)}{dt} = -\frac{i}{\hbar}[H_m, \rho^m(t)]$$

The coefficients $\rho_{gf}^{(1)}$ build a positive, trace-one matrix, which can be considered as the representative of a statistical operator $\rho^{(1)}$ in $\mathcal{H}^{(1)}$. In fact, since we are interested in the subdynamics of the microsystem and thus in observables of the form

$$A = \sum_{h,k} a_h^\dagger \mathsf{A}_{hk}^{(1)} a_k \tag{2.2}$$

where $\mathsf{A}_{hk}^{(1)}$ is the matrix element of the corresponding operator acting in $\mathcal{H}^{(1)}$, we will make use of the following reduction formula from $\mathcal{H}_F$ to $\mathcal{H}^{(1)}$ for the expectation value of an observable A of the form (2.2) in the state (2.1):

$$\mathrm{Tr}_{\mathcal{H}_F}(A\rho) = \sum_{h,k} \mathsf{A}_{hk}^{(1)} \rho_{kh}^{(1)} = \mathrm{Tr}_{\mathcal{H}^{(1)}}(\mathsf{A}^{(1)}\rho^{(1)})$$

Considering in particular the operator $A = a_f^\dagger a_g$, we have

$$\mathrm{Tr}_{\mathcal{H}_F}(A\rho) = \rho_{gf}^{(1)}$$

To specify the generator of the semigroup we will consider the evolution of the statistical operator on a time scale τ much longer than the correlation time for the macrosystem, thus approximating $d\rho_{gf}^{(1)}(t)/dt$ by

$$\begin{aligned}\frac{\Delta\rho_{gf}^{(1)}(t)}{\tau} &= \frac{1}{\tau}[\rho_{gf}^{(1)}(t+\tau) - \rho_{gf}^{(1)}(t)] \\ &= \frac{1}{\tau}[\mathrm{Tr}_{\mathcal{H}_F}(a_f^\dagger a_g e^{-(i/\hbar)H\tau}\rho(t)e^{(i/\hbar)H\tau}) - \rho_{gf}^{(1)}(t)]\end{aligned} \tag{2.3}$$

Exploiting the cyclicity of the trace, we will work in Heisenberg picture, shifting the action of the temporal evolution operator on the simple expression $a_f^\dagger a_g$, thus considerably simplifying the calculation without introducing restrictive assumptions on the structure of ρ^m or of the interaction. To proceed further, we introduce the superoperators

$$\mathcal{H} = \frac{i}{\hbar}[H, \cdot], \qquad \mathcal{H}_0 = \frac{i}{\hbar}[H_0 + H_m, \cdot], \qquad \mathcal{V} = \frac{i}{\hbar}[V, \cdot]$$

acting on the algebra generated by creation and destruction operators. Note that the operators

$$(a^\dagger_{h_1})^{n_1}(a^\dagger_{h_2})^{n_2}\cdots(a^\dagger_{h_r})^{n_r}(a_{k_1})^{m_1}(a_{k_2})^{m_2}\cdots(a_{k_s})^{m_s}$$

are "eigenstates" of the superoperator $\mathcal{H}_0$ with eigenvalues $(i/\hbar)(\Sigma_{i=1}^{r} n_i E_{h_i} - \Sigma_{i=1}^{s} m_i E_{k_i})$, in particular,

$$\mathcal{H}_0 a_h = -\frac{i}{\hbar} E_h a_h, \qquad \mathcal{H}_0 a^\dagger_h = +\frac{i}{\hbar} E_h a^\dagger_h$$

To calculate (2.3), we evaluate $e^{\mathcal{H}\tau}(a^\dagger_h a_k)$ with the help of the following integral representation:

$$\begin{aligned} e^{\mathcal{H}\tau}(a^\dagger_h a_k) &= (e^{\mathcal{H}\tau}a^\dagger_h)(e^{\mathcal{H}\tau}a_k) \\ &= \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{dz_1}{2\pi i}\, e^{z_1\tau}((z_1-\mathcal{H})^{-1}a^\dagger_h) \\ &\quad\times \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{dz_2}{2\pi i}\, e^{z_2\tau}((z_2-\mathcal{H})^{-1}a_k) \end{aligned} \tag{2.4}$$

Using twice the identity

$$\begin{aligned} (z-\mathcal{H})^{-1} &= (z-\mathcal{H}_0)^{-1}[1+\mathcal{V}(z-\mathcal{H})^{-1}] \\ &= [1+(z-\mathcal{H})^{-1}\mathcal{V}](z-\mathcal{H}_0)^{-1} \end{aligned} \tag{2.5}$$

we obtain

$$(z-\mathcal{H})^{-1} = (z-\mathcal{H}_0)^{-1} + (z-\mathcal{H}_0)^{-1}\mathcal{T}(z)(z-\mathcal{H}_0)^{-1} \tag{2.6}$$

$$\mathcal{T}(z) \equiv \mathcal{V} + \mathcal{V}(z-\mathcal{H})^{-1}\mathcal{V}$$

to be substituted in (2.4). Taking into account the fact that $[H, N] = 0$, one can see that the restriction to $\mathcal{H}^1_{\mathrm{F}}$ of the operator $\mathcal{T}(z)a_k$ has the simple general form

$$(\mathcal{T}(z)a_k)_{\mathcal{H}^1_{\mathrm{F}}} = \sum_h T^k_h(z)a_h \tag{2.7}$$

where $T^k_h(z)$ is an operator in the subspace $\mathcal{H}^0_{\mathrm{F}}$. This restriction is the only part of interest to us, since we are considering a single microsystem. One can also express $T^k_h(z)$ in terms of $\mathcal{T}(z)$ as

$$[(\mathcal{T}(z)a_k)a^\dagger_h]_{\mathcal{H}^0_{\mathrm{F}}} = T^k_h(z) \tag{2.8}$$

and, taking the adjoint, also

$$[a_h(\mathcal{T}(z)a_k^\dagger)]_{\mathcal{H}_F^0} = T_h^{\dagger k}(z^*) \tag{2.9}$$

Formulas (2.5) and (2.6) are clearly reminiscent of the usual identities satisfied by the resolvent operator in the theory of scattering. The mathematical framework is, however, quite different, since we are now dealing with superoperators. The quantity to be related to the usual T-matrix is the operator $T_h^k(z)$ of (2.8), acting in the subspace $\mathcal{H}_F^0$, that is, a second-quantized operator for the macrosystem. Its expectation value, which appears in the final equation (2.19) via the operator Q, may be linked to a refraction index, often used as a phenomenological description of the interactive of a single particle with matter (Vigué, 1995), as already mentioned in the first section. Since the index of refraction is an operator, it would also be possible to calculate fluctuations from the equilibrium value. On the same footing, neglecting the incoherent contribution to the dynamics, that is, the last term of the Lindblad equation (2.19), the usual description of neutron optics, still based on phenomenological potentials, may be recovered (Sears, 1989). In a future paper we intend to elucidate these possible connections to phenomenological expressions and concrete applications in detail.

Denoting by $|\lambda\rangle \equiv |0\rangle \otimes |\lambda\rangle$ the basis of eigenstates of H_m spanning $\mathcal{H}_F^0$, $H_m|\lambda\rangle = E_\lambda|\lambda\rangle$, we obtain the following explicit representation of $((z - \mathcal{H})^{-1}a_k)_{\mathcal{H}_F^1}$ as a mapping of $\mathcal{H}_F^1$ into $\mathcal{H}_F^0$:

$$((z - \mathcal{H})^{-1}a_k)_{\mathcal{H}_F^1} = \frac{a_k}{z + (i/\hbar)E_k} + \sum_{\substack{\lambda,\lambda' \\ f}} \frac{|\lambda'\rangle\langle\lambda'|T_f^k(z)|\lambda\rangle\langle\lambda|a_f}{(z + (i/\hbar)E_k)(z - (i/\hbar)(E_{\lambda'} - E_\lambda - E_f))}$$

Since $((z^* - \mathcal{H})^{-1}a_k)^\dagger = (z - \mathcal{H})^{-1}a_k^\dagger$ and by (2.1) one has easily

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}_F}[((z_1 - \mathcal{H})^{-1}a_h^\dagger)((z_2 - \mathcal{H})^{-1}a_k)\rho(t)] \\
&= \frac{\rho_{kh}^{(1)}(t)}{(z_1 - (i/\hbar)E_h)(z_2 + (i/\hbar)E_k)} \\
&+ \sum_{\substack{\lambda,\lambda' \\ g}} \frac{1}{z_2 + (i/\hbar)E_k}\rho_{kg}^{(1)}(t)\frac{\langle\lambda|T_g^{\dagger h}(z_1^*)|\lambda'\rangle\langle\lambda'|\rho^m(t)|\lambda\rangle}{(z_1 - (i/\hbar)E_h)(z_1 + (i/\hbar)(E_{\lambda'} - E_\lambda - E_g))} \\
&+ \sum_{\substack{\lambda,\lambda' \\ f}} \frac{\langle\lambda'|T_f^k(z_2)|\lambda\rangle\langle\lambda|\rho^m(t)|\lambda'\rangle}{(z_2 + (i/\hbar)E_k)(z_2 - (i/\hbar)(E_{\lambda'} - E_\lambda - E_f))}\rho_{fh}^{(1)}(t)\frac{1}{z_1 - (i/\hbar)E_h} \\
&+ \sum_{\substack{\lambda,\lambda',\lambda'' \\ f,g}} \frac{\langle\lambda''|T_f^k(z_2)|\lambda\rangle}{(z_2 + (i/\hbar)E_k)(z_2 - (i/\hbar)(E_{\lambda''} - E_\lambda - E_f))}
\end{aligned}$$

$$\times \langle \lambda | \rho^m(t) | \lambda' \rangle \frac{\langle \lambda' | T_g^{\dagger h}(z_1^*) | \lambda'' \rangle}{(z_1 - (i/\hbar)E_h)(z_1 + (i/\hbar)(E_{\lambda''} - E_{\lambda'} - E_g))} \rho_{fg}^{(1)}(t) \quad (2.10)$$

Since these expressions will be considered for values of the complex variables z, z_1, z_2 of the form $iy + \epsilon$, we can replace in (2.10) $E_h \to E_h - i\hbar\eta$, $E_k \to E_k + i\hbar\eta$, $E_f \to E_f + 2i\hbar\eta$, $E_g \to E_g - 2i\hbar\eta$, $\epsilon > \eta > 0$, without introducing singularities and obtaining expressions that depend smoothly on the parameter η and yield (2.10) in the limit $\eta \to 0$. Let us consider the expression

$$\mathbf{Q}_{gh}^{\dagger}(\tau, \eta) = \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{dz}{2\pi i} e^{(z-(i/\hbar)E_k+\eta)\tau}$$
$$\times \sum_{\lambda,\lambda'} \frac{\langle \lambda | T_g^{\dagger h}(z^*) | \lambda' \rangle \langle \lambda' | \rho^m(t) | \lambda \rangle}{(z - (i/\hbar)E_h - \eta)(z + (i/\hbar)(E_{\lambda'} - E_\lambda - E_g) - 2\eta)}$$

In the integration over z we will distinguish two different kinds of contributions: the first due to the denominators and strongly dependent on the indexes g, h; the second due to the singularities of $T_g^{\dagger h}(z^*)$ that are poles on the imaginary axis:

$$\mathbf{Q}_{gh}^{\dagger}(\tau, \eta) = \mathbf{Q}_{1gh}^{\dagger}(\tau, \eta) + \mathbf{Q}_{2gh}^{\dagger}(\tau, \eta)$$

We obtain

$$\mathbf{Q}_{1gh}^{\dagger}(\tau, \eta)$$
$$= \sum_{\lambda,\lambda'} \frac{e^{(i/\hbar)(E_h-E_k)\tau+2\eta\tau}}{(i/\hbar)(E_{\lambda'} + E_h - E_\lambda - E_g) - \eta} \langle \lambda | T_g^{\dagger h}\left(-\frac{i}{\hbar} E_h + \eta\right) | \lambda' \rangle \rho_{\lambda',\lambda}^m(t)$$
$$+ \sum_{\lambda,\lambda'} \frac{e^{-(i/\hbar)(E_{\lambda'}+E_k-E_\lambda-E_g)\tau+3\eta\tau}}{-(i/\hbar)(E_{\lambda'} + E_h - E_\lambda - E_g) + \eta}$$
$$\times \langle \lambda | T_g^{\dagger h}\left(\frac{i}{\hbar}(E_{\lambda'} - E_\lambda - E_g) + 2\eta\right) | \lambda' \rangle \rho_{\lambda'\lambda}^m(t)$$
$$= \sum_{\lambda,\lambda'} e^{(i/\hbar)(E_h-E_k)+2\eta\tau} \frac{1 - e^{-(i/\hbar)(E_{\lambda'}+E_h-E_\lambda-E_g)\tau+\eta\tau}}{(i/\hbar)(E_{\lambda'} + E_h - E_\lambda - E_g) - \eta}$$
$$\times \langle \lambda | T_g^{\dagger h}\left(-\frac{i}{\hbar} E_h + \eta\right) | \lambda' \rangle \rho_{\lambda'\lambda}^m(t)$$
$$+ \sum_{\lambda,\lambda'} e^{-(i/\hbar)(E_{\lambda'}+E_k-E_\lambda-E_g)\tau+3\eta\tau}$$
$$\times \frac{\langle \lambda | T_g^{\dagger h}(+(i/\hbar)(E_{\lambda'} - E_\lambda - E_g) + 2\eta) - T_g^{\dagger h}(-(i/\hbar)E_h + \eta) | \lambda' \rangle}{(-(i/\hbar)(E_{\lambda'} - E_\lambda - E_g) + 2\eta) - (+(i/\hbar)E_h + \eta)} \rho_{\lambda'\lambda}^m(t)$$
$$(2.11)$$

If we choose a time scale, dependent on the properties of the statistical operator, such that

$$|E_{\lambda'} + E_h - E_\lambda - E_g| \frac{\tau}{\hbar} << 1 \tag{2.12}$$

we can simply retain in the first factor the contribution linear in τ, which amounts to

$$\tau \sum_{\lambda,\lambda'} \langle \lambda | T_g^{\dagger h}\left(-\frac{i}{\hbar} E_h + \eta\right) | \lambda' \rangle \langle \lambda' | \rho^m(t) | \lambda \rangle$$

The second term is a superposition of a huge set of exponentials $\exp[-(i/\hbar)(E_{\lambda'} + E_k - E_\lambda - E_g)\tau]$ with amplitudes

$$\frac{\langle \lambda | T_g^{\dagger h}(+(i/\hbar)(E_{\lambda'} - E_\lambda - E_g) + 2\eta) - T_g^{\dagger h}(-(i/\hbar)E_h + \eta) | \lambda' \rangle}{-(i/\hbar)(E_{\lambda'} + E_h - E_\lambda - E_g) + \eta}$$

that are slowing varying over a range σ of the variable $(1/\hbar)(E_{\lambda'} + E_k - E_\lambda - E_g)$, as long as η is large with respect to the spacing between the values of this variable; then the second term of (2.11) is negligible for $\tau >> 1/\sigma$, where $1/\sigma$ may be identified with the correlation time for the macrosystem; we are thus working on a time scale long enough to ignore fluctuations from the nonperturbed state for the macrosystem. Since by (2.6) $\mathcal{T}(z)$ has poles on the imaginary axis at the points $(i/\hbar)(\xi_\lambda - \xi_{\lambda'})$, ξ_λ being the eigenvalues of H, and therefore by (2.9) $T_f^{\dagger k}(z^*)$ also has such poles, as we did before we shall assume that the superposition of this huge set of contributions makes $\mathbf{Q}_{2gh}^{\dagger}(\tau, \eta)$ negligible if $\tau >> 1/\sigma$; then we have the simple asymptotic result

$$\mathbf{Q}_{gh}^{\dagger}(\tau, \eta) = \tau \operatorname{Tr}_{\mathcal{H}_F}\left[a_g\left(\mathcal{T}\left(\frac{i}{\hbar} E_h + \eta\right) a_h^{\dagger}\right)\rho^m(t)\right],$$

$$\frac{1}{\sigma} << \tau << \tau_1, \quad \eta >> \delta \tag{2.13}$$

where δ is the spacing between the poles of $T(z)$ and τ_1 represents the typical variation time inside the reduced description; τ_1 must be large enough, i.e., the reduced dynamics must be slow enough, to justify (2.12). Correspondingly, the statistical operator of the microsystem must be such that

$$\rho_{gf}^{(1)} \simeq 0 \qquad \text{if} \quad \frac{E_g - E_f}{\hbar} \simeq \frac{1}{\tau_1} \tag{2.14}$$

and the statistical operator $\rho^m(t)$ must be close enough to an equilibrium statistical operator:

$$\rho^m(t)_{\lambda\lambda'} \simeq 0 \qquad \text{if} \quad \frac{E_\lambda - E_{\lambda'}}{\hbar} \geq \frac{1}{\tau_1} \tag{2.15}$$

Let us now concentrate on the expression

$$\begin{aligned}
\mathbf{L}_{kfgh}(\tau, \eta) &= \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{dz_1}{2\pi i} \int_{-i\infty+\epsilon}^{+i\infty+\epsilon} \frac{dz_2}{2\pi i}\, e^{(z_1+z_2)\tau} \\
&\quad \times \sum_{\substack{\lambda,\lambda' \\ \lambda''}} \frac{\langle \lambda'' | T_f^k(z_2) | \lambda \rangle}{(z_2 + (i/\hbar)E_k)(z_2 - (i/\hbar)(E_{\lambda''} - E_\lambda - E_f))} \\
&\quad \times \langle \lambda | \rho^m(t) | \lambda' \rangle \frac{\langle \lambda' | T_g^{\dagger h}(z_1^*) | \lambda'' \rangle}{(z_1 - (i/\hbar)E_h)(z_1 + (i/\hbar)(E_{\lambda''} - E_{\lambda'} - E_g))}
\end{aligned}$$

By a similar procedure, neglecting the singularities of $T(z)$ and taking into account the slow variability of $T_f^k(iy + \eta)$, one has

$$\begin{aligned}
&\mathbf{L}_{kfgh}(\tau, \eta) \\
&= \sum_{\lambda,\lambda',\lambda''} \frac{\hbar^2}{(E_h + E_{\lambda''} - E_g - E_{\lambda'} + i\hbar\eta)(E_k + E_{\lambda''} - E_f - E_\lambda - i\hbar\eta)} \\
&\quad \times \Bigg\{ e^{(i/\hbar)(E_h - E_k) + 2\eta\tau} \langle \lambda'' | T_f^k\left(-\frac{i}{\hbar} E_k + \eta\right) | \lambda \rangle \\
&\quad \times \rho^m_{\lambda\lambda'}(t) \langle \lambda' | T_g^{\dagger h}\left(-\frac{i}{\hbar} E_h + \eta\right) | \lambda'' \rangle \\
&\quad + e^{-(i/\hbar)(E_f - E_g)\tau + 4\eta\tau} \langle \lambda'' | T_f^k\left(\frac{i}{\hbar}(E_{\lambda''} - E_\lambda - E_f) + 2\eta\right) | \lambda \rangle \rho^m_{\lambda\lambda'}(t) \\
&\quad \times \langle \lambda' | T_g^{\dagger h}\left(\frac{i}{\hbar}(E_{\lambda''} - E_{\lambda'} - E_g) + 2\eta\right) | \lambda'' \rangle \\
&\quad - e^{(i/\hbar)(E_h + E_{\lambda''} - E_f - E_\lambda)\tau + 3\eta\tau} \langle \lambda'' | T_f^k\left(\frac{i}{\hbar}(E_{\lambda''} - E_\lambda - E_f) + 2\eta\right) | \lambda \rangle \rho^m_{\lambda\lambda'}(t) \\
&\quad \times \langle \lambda' | T_g^{\dagger h}\left(-\frac{i}{\hbar} E_h + \eta\right) | \lambda'' \rangle \\
&\quad - e^{(i/\hbar)(E_g + E_{\lambda'} - E_k - E_{\lambda''})\tau + 3\eta\tau} \langle \lambda'' | T_f^k\left(-\frac{i}{\hbar} E_k + \eta\right) | \lambda \rangle \rho^m_{\lambda\lambda'}(t) \\
&\quad \times \langle \lambda' | T_g^{\dagger h}\left(\frac{i}{\hbar}(E_{\lambda''} - E_{\lambda'} - E_g) + 2\eta\right) | \lambda'' \rangle \Bigg\}
\end{aligned}$$

Arguing as before, we can extract from this expression the dominant part:

$$\sum_{\lambda,\lambda',\lambda''} \hbar^2 \frac{\langle\lambda''|T_f^k(-(i/\hbar)E_k + \eta)|\lambda\rangle\rho^m_{\lambda\lambda'}(t)\langle\lambda'|T_g^{\dagger h}(-(i/\hbar)E_h + \eta)|\lambda''\rangle}{(E_h + E_{\lambda''} - E_g - E_{\lambda'} + i\hbar\eta)(E_k + E_{\lambda''} - E_f - E_\lambda - i\hbar\eta)}$$
$$\times [e^{(i/\hbar)(E_h - E_k)\tau + 2\eta\tau} - e^{(i/\hbar)(E_h + E_{\lambda''} - E_f - E_\lambda)\tau + 3\eta\tau}$$
$$- e^{(i/\hbar)(E_g + E_{\lambda'} - E_k - E_{\lambda''})\tau + 3\eta\tau} + e^{(i/\hbar)(E_g - E_f)\tau + 4\eta\tau}] \qquad (2.16)$$

The evaluations (2.13) and (2.16) hold for a finite value of the parameter η; in the limit $\eta \to 0$ singularities arise in these expressions that would be compensated by singularities coming from the neglected contributions: the splitting of $\mathbf{Q}^\dagger_{gh}(\tau, \eta)$ and $\mathbf{L}_{kfgh}(\tau, \eta)$ into a relevant and a negligible part therefore becomes meaningless. For a finite confined system this treatment unavoidably relies on an approximation. The situation can be improved by considering the limit of no confinement: then the set of eigenvalues $\{E_g\}$ and $\{E_\lambda\}$ becomes a continuum; expressions of the form $\langle\lambda|T_f^g(z)|\lambda'\rangle$ become analytic functions for Re $z > 0$, having a cut on the imaginary axis, and the existence of the limit $\delta \to 0$ can be reasonably assumed. The analytic continuation across the cut can be considered and one can assume that the singularities of this continuation are located in the left half-plane far enough from the imaginary axis to give contributions that rapidly decay for $\tau >> 1/\sigma$, thus providing the precise reason that makes the previously considered terms indeed negligible. In this way a further simplification of (2.16) becomes clear: if the sum over $E_{\lambda''}$ (or $E_{\lambda'}$) is eventually replaced by an integral and the integration path shifted inside the complex $E_{\lambda''}$ plane, the contribution of the term $\exp[(i/\hbar)(E_h + E_{\lambda''} - E_f - E_\lambda)\tau + 3\eta\tau]$ can be calculated by shifting the integration path for $E_{\lambda''}$ in the upper half-plane; then only the contribution of the singularity $1/(E_k + E_{\lambda''} - E_f - E_\lambda - i\hbar\eta)$ lying in the upper half-plane must be considered, so that replacing $E_{\lambda''}$ by $E_{\lambda''} = (E_\lambda + E_f - E_k + i\hbar\eta)$, the term becomes $\exp[(i/\hbar)(E_h - E_k)\tau + 2\eta\tau]$. Similarly, $\exp[(i/\hbar)(E_g + E_{\lambda'} - E_k - E_{\lambda''})\tau + 3\eta\tau]$, replacing $E_{\lambda''} = (E_{\lambda'} + E_g - E_h - i\hbar\eta)$, becomes $\exp[(i/\hbar)(E_h - E_k)\tau + 2\eta\tau]$. We thus obtain for the square bracket in (2.16)

$$[e^{(i/\hbar)(E_g - E_f)\tau + 4\eta\tau} - e^{(i/\hbar)(E_h - E_k)\tau + 2\eta\tau}] \simeq 2\eta\tau + \frac{i}{\hbar}(E_g - E_f + E_k - E_h)\tau$$

Keeping η finite and appealing to (2.14), we are led to keep only the first contribution. As mentioned previously, the limit $\eta \to 0$ cannot be taken at any arbitrary step of the calculation, which in its intermediate steps essentially relies upon the finiteness of η [see (2.13)]; anyway it is to be expected that this limit can be considered after taking the continuous limit on the set

$\{E_\alpha\}$. By this systematic asymptotic evaluation of (2.10) we come to the following result:

$$\rho^{(1)}_{kh}(t+\tau) = \mathrm{Tr}_{\mathcal{H}_F}[e^{\mathcal{H}\tau}(a^\dagger_h a_k)\rho(t)]$$

$$= \rho^{(1)}_{kh}(t) - \frac{i}{\hbar}\tau(E_k - E_h)\rho^{(1)}_{kh}(t)$$

$$+ \tau \sum_g \rho^{(1)}_{kg}(t)\, \mathrm{Tr}_{\mathcal{H}_F}\left[a_g\left(\mathcal{T}\left(\frac{i}{\hbar}E_h + \eta\right)a^\dagger_h\right)\rho^m(t)\right]$$

$$+ \tau \sum_g \mathrm{Tr}_{\mathcal{H}_F}\left[\left(\mathcal{T}\left(-\frac{i}{\hbar}E_k + \eta\right)a_k\right)a^\dagger_f \rho^m(t)\right]\rho^{(1)}_{fh}(t)$$

$$+ 2\eta\hbar^2\tau \sum_{\substack{\lambda,\lambda',\lambda''\\ f,g}} \rho^{(1)}_{fg}(t)\, \frac{\langle\lambda''|T^k_f(-(i/\hbar)E_k + \eta)|\lambda\rangle}{(E_k + E_{\lambda''} - E_f - E_\lambda - i\hbar\eta)}\langle\lambda|\rho^m(t)|\lambda'\rangle$$

$$\times \frac{\langle\lambda'|T^{\dagger h}_g(-(i/\hbar)E_h + \eta)|\lambda''\rangle}{(E_h + E_{\lambda''} - E_g - E_{\lambda'} + i\hbar\eta)}$$

and recalling (2.3), we have

$$\frac{d\rho^{(1)}_{kh}(t)}{dt}$$

$$= -\frac{i}{\hbar}(E_k - E_h)\rho^{(1)}_{kh}(t) + \frac{1}{\hbar}\sum_g \rho^{(1)}_{kg}(t)\mathbf{Q}^\dagger_{gh}$$

$$+ \frac{1}{\hbar}\sum_f \mathbf{Q}_{kf}\rho^{(1)}_{fh}(t) + \frac{1}{\hbar}\sum_{fg}\rho^{(1)}_{fg}(t)\mathbf{L}_{kfgh} \tag{2.17}$$

which shows the structure of the generator $\mathcal{L}$, where

$$\mathbf{Q}_{kf} = \hbar\, \mathrm{Tr}_{\mathcal{H}_F}\left[\left(\mathcal{T}\left(-\frac{i}{\hbar}E_k + \eta\right)a_k\right)a^\dagger_f\rho^m(t)\right]$$

$$\mathbf{Q}^\dagger_{gh} = \hbar\, \mathrm{Tr}_{\mathcal{H}_F}\left[a_g\left(\mathcal{T}\frac{i}{\hbar}E_h + \eta\right)a^\dagger_h\right)\rho^m(t)\right]$$

$$\mathbf{L}_{kfgh} = 2\eta\hbar^3 \sum_{\substack{\lambda,\lambda'\\ \lambda''}} \frac{\langle\lambda''|T^k_f(-(i/\hbar)E_k + \eta)|\lambda\rangle\rho^m_{\lambda\lambda'}(t)\langle\lambda'|T^{\dagger h}_g(-(i/\hbar)E_h + \eta)|\lambda''\rangle}{(E_k + E_{\lambda''} - E_f - E_\lambda - i\hbar\eta)(E_h + E_{\lambda''} - E_g - E_{\lambda'} + i\hbar\eta)}$$

By the splitting

$$\mathbf{L}_{kfgh} = \sum_{\xi,\lambda} \pi_\xi (\mathbf{L}_{\lambda\xi})_{kf}(\mathbf{L}_{\lambda\xi})^*_{hg}$$

where

$$(\mathsf{L}_{\lambda\xi})_{kf} = \sqrt{2\eta\hbar^3}\langle\lambda| \left[\left(\mathcal{T}\left(-\frac{i}{\hbar} E_k + \eta\right) a_k\right) a_f^\dagger\right] (E_k + E_\lambda - E_f - H_m - i\hbar\eta)^{-1} |\xi(t)\rangle \tag{2.18}$$

$\xi(t)$ being a complete system of eigenvectors of $\rho^m(t)$ [$\rho^m(t) = \sum_{\xi(t)} \tau_{\xi(t)} |\xi(t)\rangle\langle\xi(t)|$], and introducing in $\mathcal{H}^{(1)}$ the operators Q, $\mathsf{L}_{\lambda\xi}$,

$$\langle k|\mathsf{Q}|f\rangle = \mathsf{Q}_{kf}, \qquad \langle k|\mathsf{L}_{\lambda\xi}|f\rangle = (\mathsf{L}_{\lambda\xi})_{kf}$$

we get the desired expression:

$$\frac{d\rho^{(1)}(t)}{dt} = -\frac{i}{\hbar}[\mathsf{H}, \rho^{(1)}(t)] + \frac{1}{2\hbar}\{(\mathsf{Q} + \mathsf{Q}^\dagger), \rho^{(1)}(t)\} + \frac{1}{\hbar}\sum_{\xi,\lambda} \pi_\xi \mathsf{L}_{\lambda\xi}\rho^{(1)}(t)\mathsf{L}_{\lambda\xi}^\dagger \tag{2.19}$$

where

$$\mathsf{H} = \mathsf{H}_0 + \frac{i}{2}(\mathsf{Q} - \mathsf{Q}^\dagger)$$

There is still one most important check to be done, that is, we have to verify that conservation of the trace of the statistical operator has not been affected by the way we have extracted the completely positive evolution (2.19) from the Hamiltonian. Recalling (1.3), we have to check that the identity

$$\mathrm{Tr}_{\mathcal{H}^{(1)}}[\rho^{(1)}(t)(\mathsf{Q} + \mathsf{Q}^\dagger)] = -\mathrm{Tr}_{\mathcal{H}^{(1)}}[\rho^{(1)}(t)\sum_{\xi,\lambda} \pi_\xi \mathsf{L}_{\lambda\xi}^\dagger \mathsf{L}_{\lambda\xi}] \tag{2.20}$$

holds within the approximations so far introduced. Then we can replace the second term in the l.h.s. of (2.19) by $(1/2\hbar)\{\sum_{\xi,\lambda} \pi_\xi \mathsf{L}_{\lambda\xi}^\dagger \mathsf{L}_{\lambda\xi}, \rho^{(1)}(t)\}$. Equation (2.20) can be rewritten as

$$\sum_{kf} \rho_{fk}^{(1)}(t)(\mathsf{Q} + \mathsf{Q}^\dagger)_{kf} = -\sum_{\substack{\xi,\lambda \\ g,k,f}} \rho_{fk}^{(1)}(t)\pi_\xi(\mathsf{L}_{\lambda\xi}^\dagger)_{kg}(\mathsf{L}_{\lambda\xi})_{gf} \tag{2.21}$$

The part of the l.h.s. of (2.21) not containing the statistical operator is equal to

$$\mathrm{Tr}_{\mathcal{H}_F}\left\{\left[\left(\mathcal{T}\left(-\frac{i}{\hbar} E_k + \eta\right) a_k\right) a_f^\dagger + a_k\left(\mathcal{T}\left(\frac{i}{\hbar} E_f + \eta\right) a_f^\dagger\right)\right] \rho^m(t)\right\} \tag{2.22}$$

The r.h.s. demands a more complex calculation:

$$
\begin{aligned}
-\frac{1}{\hbar}\sum_{\substack{\xi,\lambda''\\ g}} \pi_\xi (\mathsf{L}^\dagger_{\lambda''\xi})_{kg}(\mathsf{L}_{\lambda''\xi})_{gf}
&= -2\eta \sum_{\substack{\lambda,\lambda',\lambda''\\ g}} \left\{ \langle\lambda''| \left(\mathcal{T}\left(-\frac{i}{\hbar}E_g+\eta\right)a_g\right) a_f^\dagger |\lambda\rangle \right.\\
&\quad \times \left. \rho^m_{\lambda\lambda'}(t)\langle\lambda'| a_k \left(\mathcal{T}\left(\frac{i}{\hbar}E_g+\eta\right)a_g^\dagger\right)|\lambda''\rangle \right\}\\
&\quad \times \left[\frac{1}{-(i/\hbar)E_g-\eta-(i/\hbar)(E_{\lambda''}-E_f-E_\lambda)} \right.\\
&\quad + \left. \frac{1}{(i/\hbar)E_g-\eta+(i/\hbar)(E_{\lambda''}-E_k-E_{\lambda'})} \right]\\
&\quad \times \frac{1}{-2\eta+(i/\hbar)(E_f+E_\lambda-E_k-E_{\lambda'})}
\end{aligned}
$$

[having in mind to demonstrate (2.21), we now relay on (2.14)]

$$
\begin{aligned}
&\simeq \sum_{\substack{\lambda,\lambda',\lambda''\\ g}} \langle\lambda''| \left[\left(-\frac{i}{\hbar}E_g-\eta-\mathcal{H}_0\right)^{-1} \right.\\
&\quad \times \left. \left(\mathcal{T}\left(-\frac{i}{\hbar}E_g+\eta\right)a_g\right)\right] |\lambda f\rangle \rho^m_{\lambda\lambda'}(t)\\
&\quad \times \langle\lambda' k| \left(\mathcal{T}\left(\frac{i}{\hbar}E_g+\eta\right)a_g^\dagger\right)|\lambda''\rangle\\
&\quad + \sum_{\substack{\lambda,\lambda',\lambda''\\ g}} \langle\lambda''| \left(\mathcal{T}\left(-\frac{i}{\hbar}E_g+\eta\right)a_g\right)|\lambda f\rangle \rho^m_{\lambda\lambda'}(t)\\
&\quad \times \langle\lambda' k| \left[\left(\frac{i}{\hbar}E_g-\eta-\mathcal{H}_0\right)^{-1} \left(\mathcal{T}\left(\frac{i}{\hbar}E_g+\eta\right)a_g^\dagger\right)\right]|\lambda''\rangle
\end{aligned}
$$

but using the identity

$$(z-\eta-\mathcal{H}_0)^{-1}\mathcal{T}(z+\eta) = (1+2\eta(z-\eta-\mathcal{H}_0)^{-1})((z+\eta-\mathcal{H})^{-1}\mathcal{V})$$

we get, to zeroth order in η,

$$\left(-\frac{i}{\hbar}E_g-\eta-\mathcal{H}_0\right)^{-1}\left(\mathcal{T}\left(-\frac{i}{\hbar}E_g+\eta\right)a_g\right) = a_g$$

and similarly

$$\left(+\frac{i}{\hbar}E_g - \eta - \mathcal{H}_0\right)^{-1}\left(\mathcal{T}\left(+\frac{i}{\hbar}E_g + \eta\right)a_g^\dagger\right) = a_g^\dagger$$

thus obtaining

$$-\frac{1}{\hbar}\sum_{\substack{\xi,\lambda\\ g}} \pi_\xi(\mathsf{L}_{\lambda\xi}^\dagger)_{kg}(\mathsf{L}_{\lambda\xi})_{gf}$$

$$= \mathrm{Tr}_{\mathcal{H}_F}\left\{\left[\left(\mathcal{T}\left(-\frac{i}{\hbar}E_k + \eta\right)a_k\right)a_f^\dagger + a_k\left(\mathcal{T}\left(\frac{i}{\hbar}E_f + \eta\right)a_f^\dagger\right)\right]\rho^m(t)\right\}$$

that is, the same expression as in (2.22).

3. PHYSICAL DISCUSSION AND CONCLUDING REMARKS

To elucidate how an equation of the form (2.19) or equivalently (2.17) may be well suited to describe an interplay between a "purely optical" (that is wavelike) dynamics and an interaction with a measurement character, let us introduce the reversible mappings $\mathcal{A}_{t''t'} = U_{t''t'}\cdot U_{t''t'}^\dagger$, where

$$U_{t''t'} = T\left(\exp\left[-\frac{i}{\hbar}\int_{t'}^{t''} d\tau\, (\mathsf{H}_0(t) + i\mathsf{Q}(t))\right]\right) \tag{3.1}$$

corresponding to a coherent contractive evolution of the microsystem during the time interval $[t', t'']$, and the completely positive mappings

$$\mathcal{L}_{\lambda\xi} = \mathsf{L}_{\lambda\xi}(t)\cdot \mathsf{L}_{\lambda\xi}^\dagger(t)\pi_{\xi(t)} \tag{3.2}$$

whose measurement character may be inferred from the discussion following (1.7). The structure of the operators $\mathsf{L}_{\lambda\xi}$ [see (2.18)] further shows that these mappings may be linked with a transition inside the macrosystem specified by the pair of indexes ξ, λ, as a result of scattering with the microsystem. Under very particular conditions, strongly enhancing the measurement character of the interaction (as would be the case for a detector), these transitions could be macroscopically detectable, thus leading to a localization of the particle. To indicate such interactions we will therefore use the word "event."

The solution of (2.19) can be written as

$$\rho_t = \mathcal{A}_{tt_0}\rho_{t_0} + \sum_{\lambda_1\xi_1}\int_{t_0}^{t} dt_1\, \mathcal{A}_{tt_1}\mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1t_0}\rho_{t_0}$$

$$+ \sum_{\substack{\lambda_1\xi_1\\ \lambda_2\xi_2}}\int_{t_0}^{t} dt_2\int_{t_0}^{t_2} dt_1\, \mathcal{A}_{tt_2}\mathcal{L}_{\lambda_2\xi_2}(t_2)\mathcal{A}_{t_2t_1}\mathcal{L}_{\lambda_2\xi_1}(t_1)\mathcal{A}_{t_1t_0}\rho_{t_0} + \cdots \tag{3.3}$$

which can be interpreted as a sum over subcollections corresponding to the realization of no event, one event, two events, and so on. To see this, let us perform a measurement on the microsystem at time t, associated with an eigenstate u_α of some observable A. Then by (3.2) and (3.3) the probability $p_\alpha(t)$ of the result α for this observable at time t has the following structure:

$$p_\alpha(t) = \langle u_\alpha | \mathcal{A}_{tt_0} \rho_{t_0} | u_\alpha \rangle + \sum_{\lambda_1 \xi_1} \int_{t_0}^{t} dt_1 \, \langle u_\alpha | \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \rho_{t_0} | u_\alpha \rangle$$

$$+ \sum_{\substack{\lambda_1 \xi_1 \\ \lambda_2 \xi_2}} \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1$$

$$\times \langle u_\alpha | \mathcal{A}_{tt_2} \mathcal{L}_{\lambda_2 \xi_2}(t_2) \mathcal{A}_{t_2 t_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \rho_{t_0} | u_\alpha \rangle + \cdots \qquad (3.4)$$

Let us assume for simplicity that the initial preparation ρ_{t_0} is a pure state $\rho_{t_0} = |\psi_{t_0}\rangle\langle\psi_{t_0}|$; then by (3.1), the first term in the l.h.s. of (3.4) has the form

$$\langle u_\alpha | \mathcal{A}_{tt_0} \rho_{t_0} | u_\alpha \rangle = |\langle u_\alpha | \psi(t) \rangle|^2$$

$$\psi(t) = T\left(\exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} d\tau \, (\mathsf{H}_0(t) + i\mathsf{Q}(t)) \right] \right) \psi_{t_0} \qquad (3.5)$$

and it gives the probability of measuring $A = \alpha$ at time t when no event is produced in between the preparation of the state ψ_{t_0} at time t_0 and the measurement of A at time t; the trace of the first subcollection

$$p_t^0 = \mathrm{Tr}_{\mathcal{H}^{(1)}} \mathcal{A}_{tt_0} \rho_{t_0} = \|\psi(t)\|^2$$

gives the probability that no event happens in the time interval $[t_0, t]$; then apart from the fact that $p_t^0 \leq 1$ (p_t^0 is a nonincreasing function), the usual statistical interpretation of the wave function is recovered. The integrand of the second term $\langle u_\alpha | \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \rho_{t_0} | u_\alpha \rangle$ can be interpreted as the probability of detecting $A = \alpha$ at time t, when the transition $\lambda_1 \xi_1$ happens in the time interval $[t', t' + dt']$, while no transition $\lambda\xi$ happens in the time intervals $[t_0, t']$, $[t' + dt', t]$; in other words, the expression

$$\int_{t_0}^{t} dt_1 \, \langle u_\alpha | \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \rho_{t_0} | u_\alpha \rangle$$

gives the probability of $A = \alpha$ at time t when one and only one event linked to the transition $\lambda_1 \xi_1$ happens in the time interval $[t_0, t]$, while

$$p_t^1 = \mathrm{Tr}_{\mathcal{H}^{(1)}} \left(\int_{t_0}^{t} dt_1 \, \mathcal{A}_{tt_1} \lambda_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \rho_{t_0} \right)$$

is just the probability for this sole event in the time interval $[t_0, t]$. While the first term in the l.h.s. of (3.3) is a pure state, provided ρ_{t_0} is, the second one, due to different transition times, is a mixture. The other terms of (3.3) provide the almost obvious generalization describing repeated production of events $\lambda\xi$.

If the macrosystem is an interferometer, the role of the first term is enhanced by the experimental situation; nevertheless, if one can monitor the path followed by the microsystem inside the interferometer, then the other terms also become relevant. If at the output of the interferometer an interference pattern is observed, some disturbance by an incoherent background due to these terms is unavoidable. Obviously such disturbance can be made negligible if the experimental setup is such as to "automatically" select only coherent contributions. This is the case if the disturbance originates in scattering and the acceptance along the whole path is small enough as in neutron interferometry; however, forward scattering cannot be eliminated, so, even simply relying on the present general theoretical framework, one should expect that the first term of (3.4) cannot account for the whole experimental evidence, and this should explain some difficulties that have been reported in the interpretation of neutron interference experiments, without resorting to a reformulation of quantum mechanics, as proposed by Namiki and Pascazio (1993). A more precise insight into the structure of the operators Q and L can be obtained by introducing the field operator

$$\psi(\mathbf{x}, \omega) = \sum_f a_f u_f(\mathbf{x}, \omega), \qquad a_f = \sum_\omega \int d^3x\, u_f^*(\mathbf{x}, \omega)\psi(\mathbf{x}, \omega)$$

and writing instead of (2.7)

$$(\mathcal{T}(z)\psi)(\mathbf{x}, \omega) = \sum_{\omega'} \int d^3x'\, T(\mathbf{x}, \omega, \mathbf{x}', \omega', z)\psi(\mathbf{x}', \omega')$$

Then (2.8) becomes

$$T_l^k(z) = \sum_{\omega,\omega'} \int d^3x\, d^3x'\, u_k^*(\mathbf{x}, \omega)T(\mathbf{x}, \mathbf{x}', \omega, \omega', z)u_l(\mathbf{x}', \omega')$$

and assuming translation invariance,

$$T_l^k(z) = \sum_{\omega,\omega'} \int d^3x\, d^3x'\, u_k^*(\mathbf{x}, \omega)T(\mathbf{x} - \mathbf{x}', \omega, \omega', z)u_l(\mathbf{x}', \omega')$$

$$= \int d^3X\, T_l^k(\mathbf{X}, z)$$

$$T_l^k(\mathbf{X}, z) = \sum_{\omega,\omega'} \int d^3r\, u_k^*\left(\mathbf{X} + \frac{\mathbf{r}}{2}, \omega\right)T(\mathbf{r}, \omega, \omega', z)u_l\left(\mathbf{X} - \frac{\mathbf{r}}{2}, \omega'\right) \quad (3.6)$$

Corresponding to the representation (3.6) of $T_f^k(z)$, one has a similar representation for $(\mathsf{L}_{\lambda\xi})_{kf}$:

$$(\mathsf{L}_{\lambda\xi})_{kf} = \int d^3X \, [\mathsf{L}_{\lambda\xi}(\mathbf{X})]_{kf} \tag{3.7}$$

simply obtained by substituting (3.6) into (2.18).

The set of variables $N_{\lambda\xi}(\tau)$, $\tau \geq t_0$, with $N_{\lambda\xi}(\tau)$ being the number of transitions $\lambda\xi$ up to time τ, defines a multicomponent classical stochastic process for which probability distributions and the description of statistical subcollections at times τ, conditioned by the values $N_{\lambda\xi}(\tau)$, can be given. This is a straightforward generalization of the typical "counting process" considered by Srinivas and Davies (1981); e.g., the probability that in a time interval $[\tau_1, \tau_2]$ there are N events related to transitions $\lambda_1\xi_1, \lambda_2\xi_2, \ldots, \lambda_N\xi_N(\boldsymbol{\lambda\xi})$, belonging, respectively, to certain subsets $\sigma_1 \in \Gamma_{t_1}, \sigma_2 \in \Gamma_{t_2}, \ldots, \sigma_N \in \Gamma_{t_N}$ [λ and $\xi(t)$ belong, respectively, to the spectra Λ of H_m and $\Xi(t)$ of $\rho^m(t)$, which are practically a continuum, and Γ_t is a σ-algebra on $\Lambda \times \Xi(t)$], when no event happens before τ_1, is given by

$$P_{\tau_1\tau_2}(N, \boldsymbol{\sigma}) = \mathrm{Tr}(\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})\mathcal{A}_{tt_0}\rho_{t_0})$$

where $\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})$ is an operation, i.e., a contractive positive mapping on $\mathcal{T}(\mathcal{H}^{(1)})$:

$$\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) = \sum_{(\boldsymbol{\lambda\xi})\in\boldsymbol{\sigma}} \int_{\tau_1}^{\tau_2} dt_N \cdots \int_{\tau_1}^{t_2} dt_1 \, \mathcal{A}_{\tau_2 t_N}\mathcal{L}_{\lambda_N\xi_N}(t_N)\mathcal{A}_{t_N t_{N-1}} \cdots \mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1\tau_1}$$

This flow of transitions accompanying the propagation of the microsystem in the medium could prime a measurement inside some suitable measuring device; then $P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})$ would be the probability for this device to be affected by the microsystem. In fact, writing $F(\boldsymbol{\sigma}) = \mathcal{F}'_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})I$, with $\mathcal{F}'$ the adjoint mapping on $\mathcal{B}(\mathcal{H}^{(1)})$ (the set of bounded operators on $\mathcal{H}^{(1)}$), one has

$$P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) = \mathrm{Tr}_{\mathcal{H}^{(1)}}(F(\boldsymbol{\sigma})\mathcal{A}_{tt_0}\rho_{t_0}) \tag{3.8}$$

where $F(\boldsymbol{\sigma})$ is a positive operator, $F(\boldsymbol{\sigma}) \leq 1$. Equation (3.8) is the typical probability rule of modern quantum mechanics in which the notion of an "effect-valued measure" $F(\boldsymbol{\sigma})$ on some σ-algebra of subsets generalizes the customary concept of a projection-valued measure, or equivalently of a self-adjoint operator, associated to an observable; these observables present an idealization that is very useful for understanding the basic structure of quantum mechanics, but is too strong for representing real measuring devices

(Ludwig, 1983; Kraus, 1983; Holevo, 1982; Davies, 1976). A similar situation is met if one considers the statistical operator

$$\rho_{\tau_2} = \frac{\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})\mathcal{A}_{tt_0}\rho_{t_0}}{P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})}$$

which represents the repreparation at time τ_2 of the statistical collection ρ_{t_0} under the condition that the aforementioned effect happens in the time interval $[\tau_1, \tau_2]$. Taking (3.2) into account, we see that ρ_{τ_2} bears an analogy with the highly idealized von Neumann state reduction rule

$$\rho_{\tau_2}^{(+)} = \frac{P\rho_{\tau_2}^{(-)}P}{\mathrm{Tr}(P\rho_{\tau_2}^{(-)})}$$

for the statistical operator $\rho_{\tau_2}^{(-)}$, when it is reprepared at time τ_2 taking a measurement into account, associated with the projection operator P.

Actually, by (3.3) a decomposition of ρ_t is given into subcollections related to all possible detection patterns of events primed by the elementary transitions $\lambda\xi$; mathematically this means that a decomposition of the evolution mapping $T(\exp \int_{t_0}^{t} dt' \ \mathcal{L}(t'))$ has been given on the space of the jump processes $N_{\lambda\xi}(\tau)$. In different physical contexts, e.g., optical heterodyne detection, more general decompositions of an evolution mapping can be given, as has been shown in the aforementioned theory of continuous measurement: then the variables involved are not only $N_{\lambda\xi}(\tau)$, but also the values of continuously measured variables related to the system.

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