

SUBDYNAMICS OF RELEVANT OBSERVABLES: A FIELD THEORETICAL APPROACH

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An approach to the description of subdynamics inside the nonrelativistic quantum field theory is presented, in which the notions of relevant observable, time scale and complete positivity of the time evolution are stressed. A scattering theory derivation of the subdynamics of a microsystem interacting through collisions with a macrosystem is given, leading to a master equation expressed in terms of the operator-valued dynamic structure factor, a two-point correlation function which compactly takes the statistical mechanics properties of the macrosystem into account. For the case of a free quantum gas the dynamic structure factor can be exactly calculated and in the long wavelength limit a Fokker–Planck equation for the description of quantum dissipation and in particular quantum Brownian motion is obtained, where peculiar corrections due to quantum statistics can be put into evidence.

1. Introduction

A subject of major interest in recent research work in quantum mechanics is the study of time evolutions other than unitary, allowing for the description of irreversible dynamics. At the macroscopic level the motivation is partly shared with classical physics, lying in the manifest irreversibility of natural phenomena,¹ and partly rests on the quest for a clear connection between the extremely well working quantum mechanical description of physical systems at microphysical level and our classical perception of reality, hardly compatible with the superposition principle.² At microscopic level the phenomenon which now attracts most of the attention is decoherence,³ certainly because of its relevance in the understanding of the appearance of a classical world,² but perhaps even more because of its fundamental role in answering the question whether practically useful quantum computers will be feasible in a more or less distant future;⁴ besides this, nonunitary time evolutions are essential for the description of quantum dissipation and approach to equilibrium,⁵ issues whose relevance at the level of applications is increased thanks to the growing ability to deal experimentally with microphysical probes. The emergence of such irreversible dynamics is strictly linked to the study of subdynamics,

i.e. of the dynamics of a restricted set of degrees of freedom. In the case of a microsystem this corresponds to the usual procedure in which one takes the trace over the degrees of freedom of the environment, or more precisely of the macroscopic system with which the system of interest is interacting, often leading to a dynamics in which memory effects can be neglected, describable in terms of a master equation. More generally for a system with many degrees of freedom one considers a subset of relevant observables, suitably chosen with respect to the quantities that can be effectively measured on the system, and looks for the subdynamics of this restricted subset of degrees of freedom, determining the statistical operator significant for this coarse-grained physical description with reference to the relevant observables, typically obtaining kinetic equations.^{6,7} These effective descriptions should be meaningful on a coarse-grained time scale over which the considered observables are suitably slowly varying, typically being densities of conserved charges.^{8–10}

In this paper we shall review some recent work on the formulation of subdynamics in which the main emphasis lies in the field theoretical description of the relevant degrees of freedom both for macrosystems and microsystems, together with a scattering theory approach to the description of the interaction and a particular attention to the structural properties of the mappings describing the nonunitary time evolution, such as complete positivity^{11–13} or a less stringent generalization of it,^{9,10} viewpoints also considered in Ref. 14. The approach has already led to some new results in the treatment of the subdynamics of a microsystem, namely in the case of neutron optics,¹⁵ and most recently especially in connection with the description of quantum Brownian motion and of the so-called Rayleigh gas;^{16–20} it is presently under study for the treatment of subdynamics of relevant observables inside macroscopic systems,⁷ as to be discussed later on. The whole treatment is by now nonrelativistic, thus relying on a second quantization formalism where particle number conservation plays an important role; some work has however already been done along similar lines of thought for the generalization to the relativistic case.²¹ The use of quantum field theory is central in putting into evidence the interplay between the locality of the interactions and the confinement pertaining to any real physical system, expressed through suitable boundary conditions on the fields, which determine the relevant normal modes. Finiteness of any real physical system that can be prepared in the laboratory is in fact a fundamental evidence that can be removed through a thermodynamic limit, in order to recover more simple and elegant results which may have general validity, only as a final step, provided finite size effects are indeed negligible at the chosen level of description.

The paper is organized as follows. In Sec. 2 the formalism which leads to a general structure of master equation for the description of the subdynamics of a microsystem is outlined; in Sec. 3 its application to the case of the interaction of a test particle in a quantum gas is considered; in Sec. 4 the connection to quantum Brownian motion is discussed; in Sec. 5 we comment on the results and discuss future developments.

2. Field Theoretical Approach to the Derivation of Subdynamics

We consider a microsystem interacting through collisions with a macroscopic system, in other words a particle interacting with matter, both being confined in a finite region which may be taken for simplicity to be a box, looking for the subdynamics of the microsystem, essentially referring to Ref. 22, where a short derivation of the structure of the master equation is given, although a more thorough derivation based on the same physical approximations can be given and will appear shortly. In the absence of external potentials the Hamiltonian for the particle can be written

$$H_P = \sum_h E_h a_h^\dagger a_h, \quad [a_h, a_k^\dagger]_{\mp} = \delta_{hk},$$

where $[A, B]_{\mp} = AB \mp BA$, a_h and a_h^\dagger denote annihilation and creation operators for the particle (obeying either Bose or Fermi statistics) acting in the Fock-space $\mathcal{H}_P = \sum_{n=0}^{\infty} \oplus \mathcal{H}_P^n$ (where \mathcal{H}_P^n is the symmetrized or antisymmetrized n -particle Hilbert space) and the index f labels a complete set of states $\{u_f\}$ in \mathcal{H}_P^1 , the normal modes of the single-particle Hamiltonian with the suitable boundary conditions. The whole system is then described in the Fock-space $\mathcal{H}_{PM} = \mathcal{H}_P \otimes \mathcal{H}_M$ by the Hamiltonian

$$H_{PM} = H_P + H_M + V_{PM},$$

where H_M describes matter and satisfies

$$[H_M, a_f] = 0,$$

while V_{PM} is the interaction potential. We are interested in the description of a single microsystem (and therefore the statistics of the microsystem will not play any role), so that

$$N_P = \sum_h a_h^\dagger a_h$$

is a conserved quantity, $[V_{PM}, N_P] = 0$ and as a consequence $[H_{PM}, N_P] = 0$. We therefore only describe scattering without absorption or creation phenomena, according to the nonrelativistic treatment. Since we are considering a single particle we take for the statistical operator describing the whole system at the initial time the following uncorrelated expression:

$$\rho_{PM} = \sum_{gf} a_g^\dagger \varrho_M a_f \varrho_{gf}, \tag{1}$$

where ϱ_M is a statistical operator in $\mathcal{H}_{PM}^0 \equiv \mathcal{H}_P^0 \otimes \mathcal{H}_M$, the subspace of \mathcal{H}_{PM} in which $N_P = 0$, describing the macroscopic system alone, so that

$$a_f \varrho_M = \varrho_M a_f^\dagger = 0 \quad \forall f. \tag{2}$$

In terms of the conserved charge $Q = N_P$ Eq. (2) means that ϱ_M has charge zero, $Q\varrho_M = 0$, i.e. the microsystem is not part of the macrosystem, while (1) means that ρ_{PM} describes the system perturbed by a single microsystem, i.e.:

$$Q\rho_{PM} = \rho_{PM}.$$

We will assume that the macrosystem is not appreciably perturbed by the presence of the microsystem, so that its dynamics is given by

$$\frac{d\rho_M}{dt} = -\frac{i}{\hbar}[H_M, \rho_M].$$

The coefficients ϱ_{gf} in (1) build a positive, trace one matrix, to be seen as the representative of a statistical operator $\hat{\varrho}$ in \mathcal{H}_P^1 spanned by the states $\{u_f\}$ according to $\varrho_{gf} = \langle u_g | \hat{\varrho} | u_f \rangle$, so that ρ_{PM} is indeed a statistical operator. According to the general purpose we are only interested in the subdynamics of a subset of slowly varying observables, generally given by linear operators in \mathcal{H}_{PM} , and not in a dynamics to be considered reliable for any observable of the system. In this specific case the relevant degree of freedom is the particle, whose subdynamics we are looking for, so that we restrict to operators of the form

$$A = \sum_{hk} a_h^\dagger A_{hk} a_k = \sum_{hk} a_h^\dagger \langle u_h | \hat{A} | u_k \rangle a_k, \tag{3}$$

where \hat{A} can generally be an operator in $\mathcal{H}_{PM}^1 = \mathcal{H}_P^1 \otimes \mathcal{H}_M$ or equivalently A_{hk} can be operator-valued in \mathcal{H}_M . In order to determine the dynamics of the microsystem we consider the following simple reduction formula from \mathcal{H}_{PM} to \mathcal{H}_P^1 for the expectation value of observables of the form (3) in the state (1):

$$\text{Tr}_{\mathcal{H}_{PM}}(A\rho_{PM}) = \sum_{hk} \varrho_{kh} \text{Tr}_{\mathcal{H}_M}(A_{hk}\rho_M) = \sum_{hk} \varrho_{kh} \bar{A}_{hk} = \text{Tr}_{\mathcal{H}_P^1}(\hat{\varrho}\hat{A}), \tag{4}$$

where

$$\bar{A}_{hk} = \langle u_h | \text{Tr}_{\mathcal{H}_M}(A\rho_M) | u_k \rangle = \langle u_h | \hat{A} | u_k \rangle.$$

Let us note that even if A_{hk} is initially a *c*-number, it becomes operator-valued in \mathcal{H}_M due to the time evolution.

In order to obtain the subdynamics of the particle, given by the time dependence of the coefficients ϱ_{gf} , we are led to consider in particular the operator

$$A = a_f^\dagger a_g,$$

so that \hat{A} is given by the rank one operator $|u_f\rangle\langle u_g|$ and one has, according to (4)

$$\text{Tr}_{\mathcal{H}_{PM}}(A\rho_{PM}) = \varrho_{gf}.$$

The microsystem represents here the selected degree of freedom, with a characteristic variation time τ which is much longer than the relaxation time of the macrosystem, which is a microphysical time τ_0 , typically of the order the duration of a collision. The slow variability will naturally depend on the physical features of the normal modes $\{u_f\}$ and of the interaction V_{PM} . We determine the generator of the time evolution of the statistical operator for the microsystem, which according to

irreversibility will be generally given by a semigroup,^{23,13} on a time scale τ much longer than the correlation time for the macrosystem, approximating $d\rho_{gf}(t)/dt$ by:

$$\begin{aligned} \frac{\Delta\rho_{gf}(t)}{\tau} &= \frac{1}{\tau}[\rho_{gf}(t + \tau) - \rho_{gf}(t)] \\ &= \frac{1}{\tau}[\text{Tr}_{\mathcal{H}_{\text{PM}}}(a_f^\dagger a_g e^{-\frac{i}{\hbar}H_{\text{PM}}} \rho(t) e^{\frac{i}{\hbar}H_{\text{PM}}}) - \rho_{gf}(t)]. \end{aligned} \tag{5}$$

We then exploit the cyclic invariance of the trace, working in Heisenberg picture and shifting the action of the temporal evolution operator on the simple operator expression $a_f^\dagger a_g$, thus concentrating on the observables and considerably simplifying the calculation, without introducing restrictive assumptions on the structure of ρ_M or of the interaction. We have to study the expression $e^{+\frac{i}{\hbar}H_{\text{PM}}t} a_f^\dagger a_k e^{-\frac{i}{\hbar}H_{\text{PM}}t}$, relying on the slow variability of the considered observable, corresponding to the quasi-diagonality in the indexes h, k . To proceed further we introduce the following superoperators (the prime recalling the Heisenberg picture):

$$\mathcal{H}' = \frac{i}{\hbar}[H_{\text{PM}}, \cdot], \quad \mathcal{H}'_0 = \frac{i}{\hbar}[H_{\text{P}} + H_{\text{M}}, \cdot], \quad \mathcal{V}' = \frac{i}{\hbar}[V_{\text{PM}}, \cdot], \tag{6}$$

acting on the algebra generated by creation and annihilation operators. Note that the operators $(a_{h_1}^\dagger)^{n_1} (a_{h_2}^\dagger)^{n_2} \dots (a_{h_r}^\dagger)^{n_r} (a_{k_1})^{m_1} (a_{k_2})^{m_2} \dots (a_{k_s})^{m_s}$ are *eigenvectors* of the superoperator \mathcal{H}'_0 with eigenvalues $\frac{i}{\hbar}(\sum_{i=1}^r n_i E_{h_i} - \sum_{i=1}^s m_i E_{k_i})$, in particular:

$$\mathcal{H}'_0 a_h = -\frac{i}{\hbar} E_h a_h, \quad \mathcal{H}'_0 a_h^\dagger = +\frac{i}{\hbar} E_h a_h^\dagger.$$

In order to calculate (5) we set $\mathcal{U}'(t) = e^{\mathcal{H}'t}$ and evaluate $\mathcal{U}'(t)(a_h^\dagger a_k)$ by means of the following integral representation:

$$\mathcal{U}'(t)a_k = \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} e^{zt} (z - \mathcal{H}')^{-1} a_k, \quad \mathcal{U}'(t)(a_h^\dagger a_k) = (\mathcal{U}'(t)a_h^\dagger)(\mathcal{U}'(t)a_k).$$

For the mappings defined in (6) identities hold that are reminiscent of the usual ones in scattering theory:

$$(z - \mathcal{H}')^{-1} = (z - \mathcal{H}'_0)^{-1} [1 + \mathcal{V}'(z - \mathcal{H}')^{-1}] = [1 + (z - \mathcal{H}')^{-1} \mathcal{V}'] (z - \mathcal{H}'_0)^{-1}. \tag{7}$$

In particular we can introduce the superoperator $\mathcal{T}(z)$

$$\mathcal{T}(z) \equiv \mathcal{V}' + \mathcal{V}'(z - \mathcal{H}')^{-1} \mathcal{V}', \tag{8}$$

satisfying

$$(z - \mathcal{H}')^{-1} = (z - \mathcal{H}'_0)^{-1} + (z - \mathcal{H}'_0)^{-1} \mathcal{T}(z) (z - \mathcal{H}'_0)^{-1} \tag{9}$$

and

$$\mathcal{T}(z) = \mathcal{V}' + \mathcal{V}'(z - \mathcal{H}'_0)^{-1} \mathcal{T}(z), \tag{10}$$

corresponding to the Lippman–Schwinger equation for the T matrix. Exploiting $[H_{\text{PM}}, N_{\text{P}}] = 0$ the restriction to $\mathcal{H}_{\text{PM}}^1$ of the operator $\mathcal{T}(z)[a_k]$ has the simple general form:

$$i\hbar\overline{\mathcal{T}(z)[a_k]}|_{\mathcal{H}_{\text{PM}}^1} = \sum_f T_f^k(i\hbar z)a_f, \tag{11}$$

and similarly, taking the adjoint

$$-i\hbar\mathcal{T}(z^*)[a_k^\dagger]|_{\mathcal{H}_{\text{PM}}^0} = \sum_f [T_f^h(i\hbar z)]^\dagger a_f^\dagger \equiv \sum_f T_f^{h\dagger}(i\hbar z)a_f^\dagger,$$

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

$$\begin{aligned} i\hbar\mathcal{T}(z)[a_k]a_h^\dagger|_{\mathcal{H}_{\text{PM}}^0} &= T_h^k(i\hbar z), \\ -i\hbar a_h\mathcal{T}(z)[a_k^\dagger]|_{\mathcal{H}_{\text{PM}}^0} &= T_h^{k\dagger}(i\hbar z^*). \end{aligned} \tag{12}$$

Denoting by $|\lambda\rangle \equiv |0\rangle \otimes |\lambda\rangle$ the basis of eigenstates of H_{M} spanning $\mathcal{H}_{\text{PM}}^0$, $H_{\text{M}}|\lambda\rangle = E_\lambda|\lambda\rangle$, and exploiting (11) we obtain the following explicit representation of $\mathcal{U}'(t)a_k|_{\mathcal{H}_{\text{PM}}^1}$ as a mapping of $\mathcal{H}_{\text{PM}}^1$ into $\mathcal{H}_{\text{PM}}^0$:

$$\begin{aligned} \mathcal{U}'(t)a_k|_{\mathcal{H}_{\text{PM}}^1} &= \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} e^{zt} [(z - \mathcal{H}'_0)^{-1} + (z - \mathcal{H}'_0)^{-1}\mathcal{T}(z)(z - \mathcal{H}'_0)^{-1}] a_k|_{\mathcal{H}_{\text{PM}}^1} \\ &= \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} e^{zt} \frac{1}{z + \frac{i}{\hbar}E_k} \left[a_k + (z - \mathcal{H}'_0)^{-1} \frac{1}{i\hbar} \sum_f T_f^k(i\hbar z)a_f \right] \\ &= e^{-\frac{i}{\hbar}E_k t} a_k + \frac{1}{i\hbar} \sum_{\lambda\lambda'} \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} \\ &\quad \times e^{zt} \frac{|\lambda'\rangle\langle\lambda'|T_f^k(i\hbar z)|\lambda\rangle\langle\lambda|}{(z + \frac{i}{\hbar}E_k)(z + \frac{i}{\hbar}(E_f + E_\lambda - E_{\lambda'}))} a_f. \end{aligned} \tag{13}$$

The operator $\mathcal{T}(z)$ has poles on the imaginary axis for $z = (i/\hbar)(e_\alpha - e_\beta)$, e_α being the eigenvalues of H_{PM} . In the calculation we assume that the function $\mathcal{T}(z)$ for $\text{Re } z$ positive and much bigger than the typical spacing between the poles is smooth enough, so that the only relevant contribution stems from the singularities of $(z - \mathcal{H}'_0)^{-1}$: this smoothness property is linked to the fact that the set of poles of $(z - \mathcal{H}')^{-1}$ goes over to a continuum if the confinement is removed yielding an analytic function with a cut along the imaginary axis, that can be continued across the cut without singularities if no absorption of the microsystem occurs. The T

matrix will therefore be taken to depend very smoothly on energy. Evaluating the integral (13) becomes

$$\begin{aligned} \mathcal{U}'(t) a_k |_{\mathcal{H}_{\text{PM}}^1} &= +e^{-\frac{i}{\hbar} E_k t} a_k + \sum_{\substack{\lambda \lambda' \\ f}} |\lambda'\rangle \left[e^{-\frac{i}{\hbar} E_k t} \frac{\langle \lambda' | T_f^k(E_k) | \lambda \rangle}{E_k + E_{\lambda'} - E_f - E_\lambda} \right. \\ &\quad \left. + e^{-\frac{i}{\hbar} (E_f - E_\lambda - E_{\lambda'}) t} \frac{\langle \lambda' | T_f^k(E_f + E_\lambda - E_{\lambda'}) | \lambda \rangle}{E_f + E_\lambda - E_{\lambda'} - E_k} \right] \langle \lambda | a_f, \end{aligned}$$

and similarly for the adjoint mapping. On a time scale t , much longer than the collision time τ_0 , but still much shorter than the typical variation time inside the reduced description τ ($\tau_0 \ll t \ll \tau$), considering suitable slow variables, so that

$$\frac{|E_h - E_k|}{\hbar} \ll \frac{1}{\tau_0}, \quad \frac{|E_h + E_{\lambda'} - E_f - E_\lambda|}{\hbar} \ll \frac{1}{\tau_0},$$

one obtains the following expression for the generator of the time evolution in Heisenberg picture, denoted by \mathcal{L}' :

$$\begin{aligned} \mathcal{U}'(t)(a_h^\dagger a_k) |_{\mathcal{H}_{\text{PM}}^1} &= a_h^\dagger a_k + t \mathcal{L}'(a_h^\dagger a_k) \\ &= a_h^\dagger a_k + \frac{i}{\hbar} t (E_h - E_k) a_h^\dagger a_k \\ &\quad - \frac{i}{\hbar} t \sum_f a_h^\dagger T_f^k(E_k + i\varepsilon) a_f + \frac{i}{\hbar} t \sum_g a_g^\dagger T_g^{h\dagger}(E_h + i\varepsilon) a_k \\ &\quad + 2 \frac{\varepsilon}{\hbar} t \sum_{\substack{\lambda \alpha \alpha' \\ g f}} a_g^\dagger |\alpha\rangle \frac{\langle \alpha | T_g^{h\dagger}(E_h + i\varepsilon) | \alpha' \rangle}{E_g + E_\alpha - E_h - E_{\alpha'} - i\varepsilon} \\ &\quad \times \frac{\langle \alpha' | T_f^k(E_k + i\varepsilon) | \lambda \rangle}{E_f + E_\lambda - E_k - E_{\alpha'} + i\varepsilon} \langle \lambda | a_f, \end{aligned} \tag{14}$$

where ε is a positive quantity, which can tend to zero after the thermodynamic limit has been taken. In view of (14) let us define the operators

$$\begin{aligned} T^{[1]} &= \sum_{gr} a_r^\dagger T_g^r(E_r + i\varepsilon) a_g, \\ T^{[1]\dagger} &= \sum_{gr} a_r^\dagger T_r^{g\dagger}(E_g + i\varepsilon) a_g, \\ R_{k\lambda}^{[1]} &= \sum_f R_{k\lambda f} a_f \\ &= \sum_f [\sqrt{2\varepsilon} \langle \lambda | T_f^k(E_k + i\varepsilon) (E_f + H_M - E_k - E_\lambda + i\varepsilon)^{-1} | a_f], \\ R_{h\lambda}^{[1]\dagger} &= \sum_g a_g^\dagger R_{h\lambda g}^\dagger \\ &= \sum_g a_g^\dagger [\sqrt{2\varepsilon} (E_g + H_M - E_h - E_\lambda - i\varepsilon)^{-1} T_g^{h\dagger}(E_h + i\varepsilon) | \lambda], \end{aligned}$$

so that we can write

$$\begin{aligned} \mathcal{L}'(a_h^\dagger a_k) &= \frac{i}{\hbar}[H_0, a_h^\dagger a_k] + \frac{i}{\hbar}[T^{[1]\dagger}, a_h^\dagger]a_k \\ &\quad + \frac{i}{\hbar}a_h^\dagger[T^{[1]}, a_k] + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[1]\dagger}R_{k\lambda}^{[1]}. \end{aligned}$$

Introducing the following one-particle operators

$$\begin{aligned} V^{[1]} &= \sum_{gr} a_r^\dagger V_{rg} a_g = \frac{1}{2}[T^{[1]} + T^{[1]\dagger}], \\ \Gamma^{[1]} &= \sum_{gr} a_r^\dagger \Gamma_{rg} a_g = \frac{i}{2}[T^{[1]} - T^{[1]\dagger}] \end{aligned}$$

so that

$$T^{[1]} = V^{[1]} - i\Gamma^{[1]}, \quad V^{[1]} = V^{[1]\dagger}, \quad \Gamma^{[1]} = \Gamma^{[1]\dagger}$$

the generator of the time evolution may be written

$$\begin{aligned} \mathcal{L}'(a_h^\dagger a_k) &= \frac{i}{\hbar}[H_0 + V^{[1]}, a_h^\dagger a_k] \\ &\quad - \frac{1}{\hbar}\{[\Gamma^{[1]}, a_h^\dagger]a_k - a_h^\dagger[\Gamma^{[1]}, a_k]\} + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[1]\dagger}R_{k\lambda}^{[1]}. \end{aligned} \quad (15)$$

Let us observe that V_{rg} and Γ_{rg} are not c -number coefficients, but operators acting in the Fock-space for the macrosystem \mathcal{H}_M : they are connected respectively to the self-adjoint and anti-self-adjoint part of what can be considered as an operator valued T matrix. The last contribution displays a *bilinear structure* typical of the generators of completely positive time evolutions,¹⁰ directly connected to irreversibility, as we shall see in Subsec. 2.1.

2.1. Particle number conservation and complete positivity

It is worth mentioning that within the approximations exploited in its derivation (15) accounts for particle number conservation, that is to say $\mathcal{L}'(N_P) = 0$ and therefore $\mathcal{U}'(t)(N_P) = N_P$. Due to

$$\sum_h [\Gamma^{[1]}, a_h^\dagger]a_h = \Gamma^{[1]}, \quad \sum_h a_h^\dagger[\Gamma^{[1]}, a_h] = -\Gamma^{[1]}$$

we have

$$\mathcal{L}'(N_P) = -\frac{2}{\hbar}\Gamma^{[1]} + \frac{1}{\hbar}\sum_{h\lambda} R_{h\lambda}^{[1]\dagger}R_{h\lambda}^{[1]}$$

and therefore particle number conservation amounts to

$$\Gamma^{[1]} = \frac{1}{2}\sum_{h\lambda} R_{h\lambda}^{[1]\dagger}R_{h\lambda}^{[1]}. \quad (16)$$

The structure of (15) is moreover such that $\mathcal{U}'(t)$ satisfies a property analogous to, but weaker than complete positivity. We first briefly recall the definition of complete positivity.^{11–13} Consider a system described in a Hilbert space H and the set $B(H)$ of bounded linear operators on H , containing the observables. A mapping \mathcal{M}' defined on this set,

$$\mathcal{M}' : B(H) \rightarrow B(H),$$

e.g. a mapping giving the dynamics in Heisenberg picture, is said to be completely positive provided it satisfies the inequality

$$\sum_{i,j=1}^n \langle \psi_i | \mathcal{M}'(\hat{B}_i^\dagger \hat{B}_j) | \psi_j \rangle \geq 0 \quad \forall n \in \mathbf{N}, \quad \forall \{\psi_i\} \in H, \quad \forall \{\hat{B}_i\} \in B(H). \quad (17)$$

For $n = 1$ the usual notion of positivity is obtained, the condition $n \in \mathbf{N}$ implying that complete positivity is in general actually a stronger requirement. It is worthwhile observing that unitary evolutions are not only positive, but also completely positive. Equation (15) satisfies a weaker version of complete positivity^{9,10} in that an inequality like (17) only holds for a restricted subset of observables, bilinear in the creation and annihilation operators a and a^\dagger , that is to say

$$\sum_{i,j=1}^n \langle \psi_i | \mathcal{U}'(t) \left[\sum_{hk} a_h^\dagger \langle u_h | \hat{B}_i^\dagger \hat{B}_j | u_k \rangle a_k \right] | \psi_j \rangle \geq 0 \quad \forall n \in \mathbf{N} \quad (18)$$

with $\{\psi_i\}$ vectors in Fock-space and $\{\hat{B}_i\}$ operators in the one-particle Hilbert space \mathcal{H}_p^1 . Setting

$$[\Gamma^{[1]}, a_k] = -F_k, \quad [\Gamma^{[1]}, a_h^\dagger] = F_h^\dagger, \quad H_0 + V^{[1]} = C$$

we have in fact, at first order in t

$$\begin{aligned} & \sum_{i,j=1}^n \langle \psi_i | \mathcal{U}'(t) \left[\sum_{hk} a_h^\dagger \langle u_h | \hat{B}_i^\dagger \hat{B}_j | u_k \rangle a_k \right] | \psi_j \rangle \\ &= \sum_{i,j=1}^n \sum_{hk} \langle u_h | \hat{B}_i^\dagger \hat{B}_j | u_k \rangle \langle \psi_i | a_h^\dagger a_k + t \mathcal{L}'(a_h^\dagger a_k) | \psi_j \rangle \\ &= \sum_{i,j=1}^n \sum_{hk} \langle u_h | \hat{B}_i^\dagger \hat{B}_j | u_k \rangle \langle \psi_i | \left[a_h + t \frac{i}{\hbar} [C, a_h] - \frac{t}{\hbar} F_h \right]^\dagger \\ & \quad \times \left[a_k + t \frac{i}{\hbar} [C, a_k] - \frac{t}{\hbar} F_k \right] + \frac{t}{\hbar} \sum_{\lambda} R_{h\lambda}^{[1]\dagger} R_{k\lambda}^{[1]} | \psi_j \rangle \\ &= \sum_g \left(\sum_{i=1}^n \sum_h \langle u_h | \hat{B}_i^\dagger | u_g \rangle \langle \psi_i | \left[a_h + t \frac{i}{\hbar} [C, a_h] - \frac{t}{\hbar} F_h \right]^\dagger \right) \\ & \quad \times \left(\sum_{j=1}^n \sum_k \langle u_g | \hat{B}_j | u_k \rangle \left[a_k + t \frac{i}{\hbar} [C, a_k] - \frac{t}{\hbar} F_k \right] | \psi_j \rangle \right) \end{aligned}$$

$$\begin{aligned}
 & + \frac{t}{\hbar} \sum_{g\lambda} \left(\sum_{i=1}^n \sum_h \langle u_h | \hat{B}_i^\dagger | u_g \rangle \langle \psi_i | R_{h\lambda}^{[1]\dagger} \right) \left(\sum_{j=1}^n \sum_k \langle u_g | \hat{B}_j | u_k \rangle R_{k\lambda}^{[1]} | \psi_j \rangle \right) \\
 & = \sum_g \left\| \sum_{j=1}^n \sum_k \langle u_g | \hat{B}_j | u_k \rangle \left[a_k + t \frac{i}{\hbar} [C, a_k] - \frac{t}{\hbar} F_k \right] | \psi_j \rangle \right\|_{\mathcal{H}_{\text{PM}}}^2 \\
 & + \frac{t}{\hbar} \sum_{g\lambda} \left\| \sum_{j=1}^n \sum_k \langle u_g | \hat{B}_j | u_k \rangle R_{k\lambda}^{[1]} | \psi_j \rangle \right\|_{\mathcal{H}_{\text{PM}}}^2 \geq 0 \quad \text{for } t \geq 0. \tag{19}
 \end{aligned}$$

Note that according to (19) the condition in (18) holds provided t is a positive time, thus expressing the irreversibility of the obtained time evolution, which gives rise to a semigroup law.

2.2. The master equation

Exploiting the reduction formulas (4) and (5), together with (14), we come to the master equation for the statistical operator describing the microsystem

$$\begin{aligned}
 \frac{d}{dt} \varrho_{kh} & = \text{Tr}_{\mathcal{H}_{\text{PM}}} (\mathcal{L}'(a_h^\dagger a_k) \rho_{\text{PM}}) \\
 & = + \frac{i}{\hbar} (E_h - E_k) \sum_{pq} \text{Tr}_{\mathcal{H}_{\text{PM}}} (a_h^\dagger a_k a_p^\dagger \varrho_M a_q \varrho_{pq}) \\
 & \quad - \frac{i}{\hbar} \sum_{pqf} \text{Tr}_{\mathcal{H}_{\text{PM}}} (a_h^\dagger T_f^k (E_k + i\varepsilon) a_f a_p^\dagger \varrho_M a_q \varrho_{pq}) \\
 & \quad + \frac{i}{\hbar} \sum_{pqg} \text{Tr}_{\mathcal{H}_{\text{PM}}} (a_g^\dagger T_g^{h\dagger} (E_h + i\varepsilon) a_k a_p^\dagger \varrho_M a_q \varrho_{pq}) \\
 & \quad + 2 \frac{\varepsilon}{\hbar} \sum_{\substack{\lambda\alpha\alpha' \\ pqgf}} \text{Tr}_{\mathcal{H}_{\text{PM}}} \left(a_g^\dagger | \alpha \rangle \frac{\langle \alpha | T_g^{h\dagger} (E_h + i\varepsilon) | \alpha' \rangle}{E_g + E_\alpha - E_h - E_{\alpha'} - i\varepsilon} \right. \\
 & \quad \left. \times \frac{\langle \alpha' | T_f^k (E_k + i\varepsilon) | \lambda \rangle}{E_f + E_\lambda - E_k - E_{\alpha'} + i\varepsilon} \langle \lambda | a_f a_p^\dagger \varrho_M a_q \varrho_{pq} \right)
 \end{aligned}$$

which due to (2) and using the decomposition $\varrho_M = \sum_\xi \pi_\xi | \xi \rangle \langle \xi |$ becomes

$$\begin{aligned}
 \frac{d}{dt} \varrho_{kh} & = - \frac{i}{\hbar} (E_k - E_h) \varrho_{kh} - \frac{i}{\hbar} \sum_f \text{Tr}_{\mathcal{H}_{\text{PM}}} [T_f^k (E_k + i\varepsilon) \varrho_M] \varrho_{fh} \\
 & \quad + \frac{i}{\hbar} \sum_g \varrho_{kg} \text{Tr}_{\mathcal{H}_{\text{PM}}} [T_g^{h\dagger} (E_h + i\varepsilon) \varrho_M] \\
 & \quad + 2 \frac{\varepsilon}{\hbar} \sum_{\substack{\eta\xi \\ gf}} \frac{\langle \eta | T_f^k (E_k + i\varepsilon) | \xi \rangle}{E_f + E_\xi - E_k - E_\eta + i\varepsilon} \pi_\xi \varrho_{fg} \frac{\langle \xi | T_g^{h\dagger} (E_h + i\varepsilon) | \eta \rangle}{E_g + E_\xi - E_h - E_\eta - i\varepsilon}.
 \end{aligned}$$

The master equation describing the irreversible time evolution of the statistical operator on the chosen time scale can also be written:

$$\begin{aligned} \frac{d}{dt} \varrho_{kh} &= -\frac{i}{\hbar} (E_k - E_h) \varrho_{kh} - \frac{i}{\hbar} \sum_f Q_{kf} \varrho_{fh} + \frac{i}{\hbar} \sum_g \varrho_{kg} Q_{hg}^* \\ &+ \frac{1}{\hbar} \sum_{\substack{gf \\ \lambda\xi}} (L_{\lambda\xi})_{kf} \varrho_{fg} (L_{\lambda\xi})_{hg}^*, \end{aligned} \tag{20}$$

the quantities appearing in (20) being defined in the following way:

$$\begin{aligned} Q_{kf} &= \text{Tr}_{\mathcal{H}_{\text{PM}}} [T_f^k (E_k + i\varepsilon) \varrho_{\text{M}}], \\ Q_{hg}^* &= \text{Tr}_{\mathcal{H}_{\text{PM}}} [T_g^{h\dagger} (E_h + i\varepsilon) \varrho_{\text{M}}], \\ (L_{\lambda\xi})_{kf} &= \sqrt{2\varepsilon\pi\xi} \frac{\langle \lambda | T_f^k (E_k + i\varepsilon) | \xi(t) \rangle}{E_f + E_\xi - E_k - E_\lambda + i\varepsilon}. \end{aligned} \tag{21}$$

If we now introduce in \mathcal{H}_{P}^1 the operators \hat{H}_0 , \hat{Q} , $\hat{L}_{\lambda\xi}$ and $\hat{\varrho}$

$$\begin{aligned} \langle g | \hat{H}_0 | f \rangle &= E_f \delta_{gf}, & \langle g | \hat{Q} | f \rangle &= Q_{gf}, \\ \langle g | \hat{L}_{\lambda\xi} | f \rangle &= (L_{\lambda\xi})_{gf}, & \langle g | \hat{\varrho} | f \rangle &= \varrho_{gf}. \end{aligned}$$

Equation (20) takes the operator form:

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar} [\hat{H}_0 + \hat{V}, \hat{\varrho}] - \frac{1}{\hbar} \{\hat{\Gamma}, \hat{\varrho}\} + \frac{1}{\hbar} \sum_{\xi\lambda} \hat{L}_{\lambda\xi} \hat{\varrho} \hat{L}_{\lambda\xi}^\dagger,$$

where

$$\hat{V} = \frac{\hat{Q} + \hat{Q}^\dagger}{2}, \quad \hat{\Gamma} = i \frac{\hat{Q} - \hat{Q}^\dagger}{2}.$$

Verification of the conservation of the trace of the statistical operator leads according to (16) to the following relationship:

$$\hat{\Gamma} = \frac{1}{2} \sum_{\xi\lambda} \hat{L}_{\lambda\xi}^\dagger \hat{L}_{\lambda\xi},$$

and therefore to

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar} [\hat{H}_0 + \hat{V}, \hat{\varrho}] - \frac{1}{\hbar} \left\{ \frac{1}{2} \sum_{\xi\lambda} \hat{L}_{\lambda\xi}^\dagger \hat{L}_{\lambda\xi}, \hat{\varrho} \right\} + \frac{1}{\hbar} \sum_{\xi\lambda} \hat{L}_{\lambda\xi} \hat{\varrho} \hat{L}_{\lambda\xi}^\dagger. \tag{22}$$

We have thus obtained a general structure of master equation for the subdynamics of the microsystem, which we shall now apply to some specific example, making a suitable Ansatz for the T matrix appearing in (21) and describing the collisions which drive the interaction between microsystem and macrosystem. This matrix, obtained averaging over the state of the macrosystem the matrix (11), operator-valued in \mathcal{H}_{M} , takes the statistical mechanics properties of the macrosystem into account and is a natural place for fundamental or phenomenological Ansatz.

3. Master Equation for a Test Particle in a Quantum Gas

We now aim to apply the master equation (22) to the case of a test particle interacting through collisions with a quantum fluid considered in Ref. 18, a physical example corresponding to the so-called Rayleigh gas.²⁴ Exploiting the fact that interactions at microphysical level are translation invariant, a general Ansatz for the T matrix (12) is given by

$$T_h^k(z) = \int_{\omega} d^3\mathbf{x} \int_{\omega} d^3\mathbf{y} \psi^\dagger(\mathbf{x}) u_k^*(\mathbf{y}) t(z, \mathbf{x} - \mathbf{y}) u_h(\mathbf{y}) \psi(\mathbf{x}), \quad (23)$$

where the integrals are extended over the region in which the system is confined. We now only want to consider local dissipation effects, so that we will suppose the system to be homogeneous and use as quantum numbers momentum eigenvalues. This picture holds provided we are sufficiently far away from the boundaries and the peculiar features of the normal modes do not play a relevant role, which for a real confined system will generally be true only for a finite time. According to this picture at a later stage we will take a thermodynamic or continuum limit, thus obtaining an expression describing an idealized situation in which the confinement is completely removed, actual calculations are made easier through the introduction of integrals instead of sums and invariance properties with respect to symmetry transformations are more directly formulated and checked.¹⁹

Using as quantum numbers momentum eigenvalues and introducing creation and destruction operators b_η^\dagger , b_μ in the Fock-space of the macrosystem \mathcal{H}_M one obtains from (23) the following expression in terms of the Fourier transform of the translation and rotation invariant interaction kernel, which therefore only depends on the modulus of the momentum transfer

$$T_h^k = \sum_{\eta\mu} \delta_{p_\eta+p_k, p_h+p_\mu} \tilde{t}(|\mathbf{p}_\mu - \mathbf{p}_\eta|) b_\eta^\dagger b_\mu, \quad (24)$$

and where the slow energy dependence of the T -matrix has been neglected for simplicity, this in turn implying that the potential term in (22), expressible in terms of the forward scattering amplitude,¹⁶ is in fact a c -number, of relevance only for wave-like, coherent dynamics.¹⁵ Equation (22) then becomes

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] + \mathcal{L}[\hat{\rho}], \quad (25)$$

where \hat{H}_0 is the Hamiltonian for the free particle $\hat{H}_0 = \frac{\hat{p}^2}{2M}$ and according to (24)

$$\begin{aligned} \mathcal{L}[\hat{\rho}] = & + \frac{2\varepsilon}{\hbar} \sum_{\lambda\xi} \sum_{kf} \sum_{hg} |\mathbf{p}_f\rangle \frac{\sum_{\eta\mu} \delta_{p_\eta+p_f, p_k+p_\mu} \tilde{t}(|\mathbf{p}_\mu - \mathbf{p}_\eta|) \langle \lambda | b_\eta^\dagger b_\mu | \xi \rangle}{E_k - E_f + E_\xi - E_\lambda + i\varepsilon} \\ & \times \langle \mathbf{p}_k | \hat{\rho} | \mathbf{p}_h \rangle \pi_\xi \frac{\sum_{\eta'\mu'} \delta_{p_{\eta'}+p_g, p_h+p_{\mu'}} \tilde{t}^*(|\mathbf{p}_{\mu'} - \mathbf{p}_{\eta'}|) \langle \xi | b_{\mu'}^\dagger b_{\eta'} | \lambda \rangle}{E_h - E_g + E_\xi - E_\lambda - i\varepsilon} \langle \mathbf{p}_g | \end{aligned}$$

$$\begin{aligned}
 & -\frac{\varepsilon}{\hbar} \sum_{\lambda\xi} \sum_k \sum_{fg} \{|\mathbf{p}_f\rangle\langle\mathbf{p}_g|, \hat{\varrho}\} \frac{\sum_{\eta\mu} \delta_{p_\eta+p_k, p_g+p_\mu} \tilde{t}(|\mathbf{p}_\mu - \mathbf{p}_\eta\rangle) \langle\lambda|b_\eta^\dagger b_\mu|\xi\rangle}{E_f - E_k + E_\xi - E_\lambda - i\varepsilon} \\
 & \times \pi_\xi \frac{\sum_{\eta'\mu'} \delta_{p_{\eta'}+p_k, p_f+p_{\mu'}} \tilde{t}^*(|\mathbf{p}_{\mu'} - \mathbf{p}_{\eta'}\rangle) \langle\xi|b_{\mu'}^\dagger b_{\eta'}|\lambda\rangle}{E_g - E_k + E_\xi - E_\lambda + i\varepsilon}. \tag{26}
 \end{aligned}$$

Due to translation invariance of the interaction it is now natural and convenient to introduce as variables the momentum transfers $\mathbf{q} = \mathbf{p}_\mu - \mathbf{p}_\eta$, $\mathbf{q}' = \mathbf{p}_{\mu'} - \mathbf{p}_{\eta'}$ and accordingly the operators ρ_q

$$\rho_q = \sum_{\mu} b_{\mu}^\dagger b_{\mu+q}, \tag{27}$$

so that (26) becomes

$$\begin{aligned}
 \mathcal{L}[\hat{\varrho}] &= +\frac{2\varepsilon}{\hbar} \sum_{\lambda\xi} \sum_{pp'} \sum_{qq'} \tilde{t}(q) \tilde{t}^*(q') e^{\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} |\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar} \mathbf{q}' \cdot \hat{\mathbf{x}}} \\
 & \times \frac{1}{E_p - E_{p+q} + E_\xi - E_\lambda + i\varepsilon} \frac{1}{E_{p'} - E_{p'+q'} + E_\xi - E_\lambda - i\varepsilon} \\
 & \times \langle\lambda|\rho_q|\xi\rangle \pi_\xi \langle\xi|\rho_q^\dagger|\lambda\rangle - \frac{\varepsilon}{\hbar} \sum_{\lambda\xi} \sum_p \sum_{qq'} \tilde{t}(q) \tilde{t}^*(q') \{|\mathbf{p}\rangle\langle\mathbf{p} + \mathbf{q}' - \mathbf{q}|, \hat{\varrho}\} \\
 & \times \frac{1}{E_p - E_{p+q} + E_\xi - E_\lambda - i\varepsilon} \frac{1}{E_{p+q'-q} - E_{p+q'} + E_\xi - E_\lambda + i\varepsilon} \\
 & \times \langle\lambda|\rho_q|\xi\rangle \pi_\xi \langle\xi|\rho_q^\dagger|\lambda\rangle,
 \end{aligned}$$

where the contributions for $\mathbf{q} = \mathbf{q}' = 0$ have canceled out, as denoted by the primed sum. Expressing the denominators through a Laplace transform and denoting the energy transfer $E_{p+q} - E_p$ by $\Delta E_q(\mathbf{p})$, the ensemble average over ϱ_M by $\langle\cdots\rangle$, the Heisenberg operator $e^{+\frac{i}{\hbar} H_M t} \rho_q e^{-\frac{i}{\hbar} H_M t}$ by $\rho_q(t)$, we have

$$\begin{aligned}
 \mathcal{L}[\hat{\varrho}] &= +\frac{2\varepsilon}{\hbar} \sum_{pp'} \sum_{qq'} \tilde{t}(q) \tilde{t}^*(q') e^{\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} |\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar} \mathbf{q}' \cdot \hat{\mathbf{x}}} \frac{1}{\hbar^2} \int_0^\infty d\tau e^{-\frac{\varepsilon}{\hbar} \tau} \\
 & \times \int_0^\infty d\tau' e^{-\frac{\varepsilon}{\hbar} \tau'} e^{-\frac{i}{\hbar} \Delta E_q(\mathbf{p}) \tau} e^{+\frac{i}{\hbar} \Delta E_{q'}(\mathbf{p}') \tau'} \langle\rho_{q'}^\dagger \rho_q(\tau - \tau')\rangle \\
 & - \frac{\varepsilon}{\hbar} \sum_p \sum_{qq'} \tilde{t}(q) \tilde{t}^*(q') \{|\mathbf{p}\rangle\langle\mathbf{p} + \mathbf{q}' - \mathbf{q}|, \hat{\varrho}\} \frac{1}{\hbar^2} \int_0^\infty d\tau e^{-\frac{\varepsilon}{\hbar} \tau} \\
 & \times \int_0^\infty d\tau' e^{-\frac{\varepsilon}{\hbar} \tau'} e^{+\frac{i}{\hbar} \Delta E_{q'}(\mathbf{p}) \tau} e^{-\frac{i}{\hbar} \Delta E_q(\mathbf{p} + \mathbf{q}' - \mathbf{q}) \tau'} \langle\rho_{q'}^\dagger \rho_q(\tau - \tau')\rangle.
 \end{aligned}$$

Using the identity $1 = \int dt \delta(t - \alpha)$ and giving for the Dirac δ a Fourier representation one obtains

$$\begin{aligned} \mathcal{L}[\hat{\varrho}] = & + \frac{2\varepsilon}{\hbar} \sum_{pp'} \sum_q' |\tilde{t}(q)|^2 e^{\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} |\mathbf{p}\rangle \langle \mathbf{p} | \hat{\varrho} | \mathbf{p}'\rangle \langle \mathbf{p}' | e^{-\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} \frac{1}{\hbar^2} \int_0^\infty d\tau e^{-\frac{\varepsilon}{\hbar} \tau} \int_0^\infty d\tau' e^{-\frac{\varepsilon}{\hbar} \tau'} \\ & \times \int dE e^{-\frac{i}{\hbar} [\Delta E_q(\mathbf{p}) - E] \tau} e^{+\frac{i}{\hbar} [\Delta E_q(\mathbf{p}') - E] \tau'} \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle \\ & - \frac{\varepsilon}{\hbar} \sum_p \sum_q' |\tilde{t}(q)|^2 \{ |\mathbf{p}\rangle \langle \mathbf{p} |, \hat{\varrho} \} \frac{1}{\hbar^2} \int_0^\infty d\tau e^{-\frac{\varepsilon}{\hbar} \tau} \int_0^\infty d\tau' e^{-\frac{\varepsilon}{\hbar} \tau'} \\ & \times \int dE e^{-\frac{i}{\hbar} [\Delta E_q(\mathbf{p}) - E] \tau} e^{+\frac{i}{\hbar} [\Delta E_q(\mathbf{p}) - E] \tau'} \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle, \end{aligned}$$

where a major simplification has been given by the homogeneity of the macrosystem, implying $\mathbf{q} = \mathbf{q}'$. We can now undo the Laplace transform coming to

$$\begin{aligned} \mathcal{L}[\hat{\varrho}] = & + \frac{2\varepsilon}{\hbar} \sum_{pp'} \sum_q' |\tilde{t}(q)|^2 e^{\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} |\mathbf{p}\rangle \langle \mathbf{p} | \hat{\varrho} | \mathbf{p}'\rangle \langle \mathbf{p}' | e^{-\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} \\ & \times \int dE \frac{\varepsilon}{\pi} \frac{1}{E - \Delta E_q(\mathbf{p}) + i\varepsilon} \frac{1}{E - \Delta E_q(\mathbf{p}') - i\varepsilon} \\ & \times \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle \\ & - \frac{\varepsilon}{\hbar} \sum_p \sum_q' |\tilde{t}(q)|^2 \{ |\mathbf{p}\rangle \langle \mathbf{p} |, \hat{\varrho} \} \\ & \times \int dE \frac{\varepsilon}{\pi} \frac{1}{E - \Delta E_q(\mathbf{p}) - i\varepsilon} \frac{1}{E - \Delta E_q(\mathbf{p}) + i\varepsilon} \\ & \times \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle. \end{aligned}$$

As a last step we exploit the quasidegeneracy of $\hat{\varrho}$ in this representation, linked to its slow variability, and substitute in the denominators of the first term \mathbf{p} , \mathbf{p}' with the symmetric expression $\frac{1}{2}(\mathbf{p} + \mathbf{p}')$, so that we obtain the expression

$$\begin{aligned} \mathcal{L}[\hat{\varrho}] = & + \frac{2\varepsilon}{\hbar} \sum_{pp'} \sum_q' |\tilde{t}(q)|^2 e^{\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} |\mathbf{p}\rangle \langle \mathbf{p} | \hat{\varrho} | \mathbf{p}'\rangle \langle \mathbf{p}' | e^{-\frac{i}{\hbar} \mathbf{q} \cdot \hat{\mathbf{x}}} \\ & \times \int dE \delta\left(E - \Delta E_q\left(\frac{\mathbf{p} + \mathbf{p}'}{2}\right)\right) \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle \\ & - \frac{\varepsilon}{\hbar} \sum_p \sum_q' |\tilde{t}(q)|^2 \{ |\mathbf{p}\rangle \langle \mathbf{p} |, \hat{\varrho} \} \\ & \times \int dE \delta(E - \Delta E_q(\mathbf{p})) \frac{1}{2\pi\hbar} \int dt e^{\frac{i}{\hbar} Et} \langle \rho_q^\dagger \rho_q(t) \rangle. \end{aligned} \quad (28)$$

Apart from a factor N corresponding to the total number of particles in the macroscopic system the two-point correlation function appearing in (28) is the well-known dynamic structure factor,^{25,26} here given in terms of momentum \mathbf{q} and energy E transferred to the particle in the collision

$$S(\mathbf{q}, E) = \frac{1}{2\pi\hbar} \frac{1}{N} \int dt e^{\frac{i}{\hbar}Et} \langle \rho_{\mathbf{q}}^\dagger \rho_{\mathbf{q}}(t) \rangle, \quad (29)$$

and evaluated in (28) for energy transfers $\Delta E_q \left(\frac{\mathbf{p} + \mathbf{p}'}{2} \right)$ and $\Delta E_q(\mathbf{p})$. The master equation (25) obtained from (22) through the Ansatz (24) can therefore be generally expressed in terms of the dynamic structure factor of the macrosystem through

$$\begin{aligned} \frac{d\hat{\rho}}{dt} &= -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] + \mathcal{L}[\hat{\rho}] \\ &= -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] + \frac{2\pi}{\hbar} N \sum_q' |\tilde{t}(q)|^2 \\ &\quad \times \left[\sum_{pp'} e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} |\mathbf{p}\rangle \langle \mathbf{p} | \hat{\rho} | \mathbf{p}'\rangle \langle \mathbf{p}' | e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} S \left(\mathbf{q}, \Delta E_q \left(\frac{\mathbf{p} + \mathbf{p}'}{2} \right) \right) \right. \\ &\quad \left. - \frac{1}{2} \sum_p \{ |\mathbf{p}\rangle \langle \mathbf{p} |, \hat{\rho} \} S(\mathbf{q}, \Delta E_q(\mathbf{p})) \right]. \end{aligned} \quad (30)$$

In particular, provided an approximation of the form

$$S \left(\mathbf{q}, \frac{E + E'}{2} \right) \approx \sqrt{S(\mathbf{q}, E)} \sqrt{S(\mathbf{q}, E')} \quad (31)$$

can be assumed, Eq. (30) retains a Lindblad structure, typical of the generators of completely positive time evolutions,^{27,13} which in the continuum limit is given by

$$\begin{aligned} \frac{d\hat{\rho}}{dt} &= -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] + \mathcal{L}[\hat{\rho}] \\ &= -\frac{i}{\hbar} \left[\frac{\hat{\mathbf{p}}^2}{2M}, \hat{\rho} \right] + \frac{2\pi}{\hbar} (2\pi\hbar)^3 n \int d^3\mathbf{q} |\tilde{t}(q)|^2 \\ &\quad \times \left[e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} \sqrt{S(\mathbf{q}, \Delta E_q(\hat{\mathbf{p}}))} \hat{\rho} \sqrt{S(\mathbf{q}, \Delta E_q(\hat{\mathbf{p}}))} e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} - \frac{1}{2} \{ S(\mathbf{q}, \Delta E_q(\hat{\mathbf{p}})), \hat{\rho} \} \right]. \end{aligned} \quad (32)$$

Exploiting the fact that

$$\Delta E_q(\mathbf{p}) = E_{p+q} - E_p = \frac{q^2}{2M} + \frac{\mathbf{q} \cdot \mathbf{p}}{M}$$

we will use in the following the equivalent notations

$$S(\mathbf{q}, E) \equiv S(\mathbf{q}, \Delta E_q(\mathbf{p})) \equiv S(\mathbf{q}, \mathbf{p}), \quad (33)$$

so that one can put in major evidence in the master equation the relevant quantities: momentum transfer \mathbf{q} and the operators position and momentum for the microsystem \hat{x} and \hat{p} . In particular the dynamic structure factor is operator-valued due to its dependence on the momentum operator for the microsystem \hat{p} . According to (33), Eq. (32) therefore becomes

$$\begin{aligned} \frac{d\hat{\rho}}{dt} &= -\frac{i}{\hbar}[\hat{H}_0, \hat{\rho}] + \mathcal{L}[\hat{\rho}] \\ &= -\frac{i}{\hbar}\left[\frac{\hat{p}^2}{2M}, \hat{\rho}\right] + \frac{2\pi}{\hbar}(2\pi\hbar)^3 n \int d^3\mathbf{q} |\tilde{t}(q)|^2 \\ &\quad \times \left[e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}} \sqrt{S(\mathbf{q}, \hat{p})} \hat{\rho} \sqrt{S(\mathbf{q}, \hat{p})} e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}} - \frac{1}{2}\{S(\mathbf{q}, \hat{p}), \hat{\rho}\} \right]. \end{aligned} \quad (34)$$

Equation (34) is one of the main results presented in this paper, giving a general structure of master equation driving a completely positive time evolution for a test particle interacting through collisions with a fluid. In its expression only quantities with a direct physical meaning appear: the square modulus of the Fourier transform of the T matrix, stating the relevance of the single collisions, and the dynamic structure factor, which accounts for the statistical mechanics properties of the macrosystem, giving its response to external perturbations; both together, according to (35), essentially give the scattering rate, as appropriate in a master equation. The two-point correlation function S defined in (29) appears operator-valued, as to be expected in a quantum framework, thus determining the particular structure (34). In fact (34), as well as the general Lindblad structure,²⁷ would become meaningless if all operators appearing in it were c -numbers, thus all commuting and therefore losing their distinctive quantum feature.

We note in passing that (34) gives a physical example (to our knowledge the first one) of a recent general mathematical result on the structure of generators of translation covariant quantum dynamical semigroups.²⁸ The validity of the approximation (31), which is in any case well-defined because the dynamic structure factor is always a positive function, being related to the scattering cross-section as shown in (35), depends both on the energy dependence of the dynamic structure factor and on the quasi-diagonality of the statistical operator describing the microsystem, which can be safely assumed if the microsystem is not-too-far from equilibrium and correspondingly its dynamics are on a not-too-short time scale. For a discussion of this point in a specific physical application see Sec. 4 and also Ref. 29, where a master equation of the form (30) was considered for a free Bose or Maxwell-Boltzmann gas, as can be recognized keeping (38) and (39) into account. In any case the neglected terms are at least quadratic in the energy difference.

3.1. *Dynamic structure factor*

Let us now go back to the physical meaning of the dynamic structure factor. This two-point correlation function translates into the master equation driving

the subdynamics of the microsystem the statistical mechanics properties of the macrosystem, giving in particular its spectrum of spontaneous fluctuations. The relevance of the dynamic structure factor mainly lies in its direct experimental access, in fact as first shown by van Hove³⁰ it appears in the expression of the energy dependent scattering cross-section of a microscopic probe off the considered system, which gives the physical reason for its being always positive: in particular one has the result

$$\frac{d^2\sigma}{d\Omega_{p'}dE_{p'}} = (2\pi\hbar)^6 \left(\frac{M}{2\pi\hbar^2}\right)^2 \frac{p'}{p} |\tilde{t}(q)|^2 S(\mathbf{q}, E), \quad (35)$$

which gives the scattering cross-section per target particle, if the momentum of the incoming probe changes from \mathbf{p} to $\mathbf{p}' = \mathbf{p} + \mathbf{q}$.

The dynamic structure factor, apart from being accessible through experiments and a natural starting point for phenomenological expressions, can be exactly calculated in the case of a collection of free particles. In fact from the general expression (29) one has, denoting with b_η^\dagger , b_μ creation and destruction operators associated to the modes of the macrosystem

$$\begin{aligned} S(\mathbf{q}, E) &= \frac{1}{2\pi\hbar} \frac{1}{N} \int dt e^{\frac{i}{\hbar}Et} \langle \rho_q^\dagger \rho_q(t) \rangle \\ &= \frac{1}{2\pi\hbar} \frac{1}{N} \int dt e^{\frac{i}{\hbar}Et} \sum_{\mu, \eta} \langle b_\mu^\dagger b_{\mu-q} b_\eta^\dagger(t) b_{\eta+q}(t) \rangle \\ &= \frac{1}{2\pi\hbar} \frac{1}{N} \int dt e^{\frac{i}{\hbar}Et} \sum_{\mu, \eta} \text{Tr}_{\mathcal{H}_M} \left(\frac{e^{-\beta H_M}}{\mathcal{Z}} b_\mu^\dagger b_{\mu-q} e^{+\frac{i}{\hbar}H_M t} b_\eta^\dagger b_{\eta+q} e^{-\frac{i}{\hbar}H_M t} \right), \end{aligned}$$

and for free particles, setting $\mu \rightarrow p_\mu$, $\eta \rightarrow p_\eta$, $H_M \rightarrow \sum_\mu \frac{p_\mu^2}{2m} b_\mu^\dagger b_\mu$, where m is the mass of the particles, one has

$$S(\mathbf{q}, E) = \frac{1}{2\pi\hbar} \frac{1}{N} \sum_\mu \int dt e^{\frac{i}{\hbar} \left(E + \frac{p_\mu^2}{2m} - \frac{(p_\mu - \mathbf{q})^2}{2m} \right) t} \sum_\eta \langle b_\mu^\dagger b_{\mu-q} b_\eta^\dagger b_{\eta+q} \rangle_0,$$

where $\langle \cdots \rangle_0$ denotes the expectation value calculated with the free Hamiltonian. Using Wick's theorem at finite temperature one then has

$$\begin{aligned} \sum_\eta \langle b_\mu^\dagger b_{\mu-q} b_\eta^\dagger b_{\eta+q} \rangle_0 &= \langle n_\mu \rangle_0 \pm \sum_\eta \langle b_\mu^\dagger b_\eta^\dagger b_{\mu-q} b_{\eta+q} \rangle_0 \\ &= \langle n_\mu \rangle_0 \pm \sum_\eta \{ \langle b_\eta^\dagger b_{\mu-q} \rangle_0 \langle b_\mu^\dagger b_{\eta+q} \rangle_0 \pm \langle b_\mu^\dagger b_{\mu-q} \rangle_0 \langle b_\eta^\dagger b_{\eta+q} \rangle_0 \} \\ &= \langle n_\mu \rangle_0 \pm \langle n_\mu \rangle_0 \langle n_{\mu-q} \rangle_0 + \delta_{q,0} \langle n_\mu \rangle_0 \sum_\eta \langle n_\eta \rangle_0 \\ &= \langle n_\mu \rangle_0 (1 \pm \langle n_{\mu-q} \rangle_0) + \delta_{q,0} \langle n_\mu \rangle_0 N, \end{aligned}$$

where the + and – signs refer to Bose and Fermi statistics respectively. Denoting by $S_{B/F}(\mathbf{q}, E)$ the dynamic structure factor for a free quantum gas made up of Bose or Fermi particles one therefore has

$$S_{B/F}(\mathbf{q}, E) = \frac{1}{N} \sum_{\mu} \delta\left(E - \frac{q^2}{2m} + \frac{\mathbf{p}_{\mu} \cdot \mathbf{q}}{m}\right) \langle n_{\mu} \rangle_0 (1 \pm \langle n_{\mu-q} \rangle_0) + \delta_{q,0} \delta(E) N. \quad (36)$$

The last contribution in (36), physically corresponding to forward scattering (and often neglected in the very definition of dynamic structure factor) is of no relevance in the present context, since the contributions corresponding to zero transferred momentum cancel out in the master equation, as stressed by the primed sums in (30). In the continuum limit (36) can be further simplified evaluating the integral and thus obtaining¹⁹

$$S_{B/F}(\mathbf{q}, E) = \pm \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} \frac{e^{-\frac{\beta}{2}E}}{\sinh(\frac{\beta}{2}E)} \times \operatorname{arth} \left[\frac{\pm z e^{-\frac{\beta}{8m}q^2} e^{-\frac{\beta}{2} \frac{m}{q^2} E^2} \sinh(\frac{\beta}{2}E)}{1 \mp z e^{-\frac{\beta}{8m}q^2} e^{-\frac{\beta}{2} \frac{m}{q^2} E^2} \cosh(\frac{\beta}{2}E)} \right] \quad (37)$$

or equivalently

$$S_{B/F}(\mathbf{q}, E) = \mp \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} \frac{1}{1 - e^{\beta E}} \times \log \left[\frac{1 \mp z \exp\left[-\frac{\beta}{8m} \frac{(2mE+q^2)^2}{q^2}\right]}{1 \mp z \exp\left[-\frac{\beta}{8m} \frac{(2mE-q^2)^2}{q^2}\right]} \right], \quad (38)$$

where n is the particle density, β the inverse temperature and z the fugacity of the gas, expressed in terms of the chemical potential μ by $z = e^{\beta\mu}$. For a Bose gas at finite temperature $0 \leq z < 1$, while for a Fermi gas $z \geq 0$. If the statistical correction in (36) is left out, so that one is describing a collection of Maxwell–Boltzmann particles, the expression for the dynamic structure factor becomes much simpler and is given by

$$S_{MB}(\mathbf{q}, E) = \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z \exp \left[-\frac{\beta m}{2q^2} \left(E + \frac{q^2}{2m} \right)^2 \right]. \quad (39)$$

Note the presence of the recoil energy in (39), corresponding to the $\frac{q^2}{2m}$ contribution in the argument of the exponential, which is essential in order to give the correct dependence on E in (44), determining the exact factorization property (45) and the operator structure of (46), no matter how small the recoil energy in each single collision may actually be. For more complex systems a direct evaluation of the dynamic structure factor is of course an extremely complicated task, nevertheless, even if

a direct experimental determination is not available, approximated or phenomenological expressions can often be obtained, whose validity can be checked on the basis of general features such as detailed balance condition and sum rules.^{25,26}

An important property of the dynamic structure factor, valid in complete generality, is the fact that it can be expressed as a Fourier transform, with respect to transferred momentum and energy, of the time dependent density correlation function²⁵ according to

$$S(\mathbf{q}, E) = \frac{1}{2\pi\hbar} \frac{1}{N} \int dt \int d^3\mathbf{x} e^{\frac{i}{\hbar}(Et - \mathbf{q}\cdot\mathbf{x})} \int d^3\mathbf{y} \langle N(\mathbf{y})N(\mathbf{x} + \mathbf{y}, t) \rangle, \quad (40)$$

a property which as we shall see in Subsec. 4.1 will have an important physical interpretation in the case of the quantum description of Brownian motion.

4. Completely Positive Quantum Brownian Motion

We will now apply (34) to the description at quantum level of Brownian motion,³¹ i.e. the dynamics of a massive test particle interacting through collisions with a fluid of much lighter particles. This physical model, as a distinguished example of quantum dissipation, has been the subject of extensive research in the physical and chemical literature,^{32–34} and is still a very debated topic.^{16,17} On the one hand Brownian motion is a paradigmatic example of irreversible process and its correct description at fundamental quantum level should be a natural gateway to more complex irreversible phenomena; on the other hand quantum dissipative processes, among which the Brownian motion of a heavy test particle, play a crucial role in many fields of science, such as nuclear magnetic resonance,³⁵ quantum optics³⁶ and molecular dynamics in condensed phases,^{5,37} thus leading to a particular interest in physically and mathematically reliable structures for the description of quantum dissipation.

We here first consider the case of a fluid made up of noninteracting Maxwell–Boltzmann particles, where quantum statistics can be neglected. The relevant dynamic structure factor is given by (39), where the energy transfer E is actually given by

$$E = E_{p+q} - E_p = \frac{q^2}{2M} + \frac{\mathbf{q} \cdot \mathbf{p}}{M}, \quad (41)$$

with M the mass of the test particle. Writing $S_{\text{MB}}(\mathbf{q}, E)$ in the form

$$S_{\text{MB}}(\mathbf{q}, E) = \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z e^{-\frac{\beta}{8m}q^2} e^{-\frac{\beta}{2}E} e^{-\frac{\beta}{2} \frac{m}{q^2} E^2}$$

one immediately sees that the following identity holds:

$$S_{\text{MB}}\left(\mathbf{q}, \frac{E + E'}{2}\right) = \sqrt{S_{\text{MB}}(\mathbf{q}, E)} \sqrt{S_{\text{MB}}(\mathbf{q}, E')} e^{\frac{\beta}{8} \frac{m}{q^2} (E - E')^2}, \quad (42)$$

so that the terms violating the factorization (31) are in fact at least quadratic in the energy difference. Using (41) moreover (42) can be written

$$S_{\text{MB}}\left(\mathbf{q}, \frac{E + E'}{2}\right) = \sqrt{S_{\text{MB}}(\mathbf{q}, E)}\sqrt{S_{\text{MB}}(\mathbf{q}, E')}e^{\frac{\beta}{8m}\frac{\alpha^2}{q^2}[(\mathbf{p}-\mathbf{p}')\cdot\mathbf{q}]^2}, \quad (43)$$

where we have denoted by $\alpha = m/M$ the ratio between the mass m of the particles of the fluid and the mass M of the test particle. Considering (30) one now most directly sees that the term violating the factorization in (43) is indeed negligible provided the statistical operator is quasideagonal. In the Brownian case, when the test particle is much more massive than the other particles, the factorization is actually exact, in fact denoting by S_{MB}^∞ the dynamic structure factor evaluated in the limit $\alpha \ll 1$ one has

$$\begin{aligned} S_{\text{MB}}^\infty(\mathbf{q}, E) &= \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z e^{-\frac{\beta}{8m}q^2} e^{-\frac{\beta}{2}E} \\ &= \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z e^{-\frac{\beta}{8m}(1+2\alpha)q^2} e^{-\frac{\beta}{2M}\mathbf{q}\cdot\mathbf{p}}, \end{aligned} \quad (44)$$

and therefore the dynamic structure factor evaluated in the arithmetic mean of the energies is exactly equal to the geometric mean of the dynamic structure factor evaluated in the two different energies

$$S_{\text{MB}}^\infty\left(\mathbf{q}, \frac{E + E'}{2}\right) = \sqrt{S_{\text{MB}}^\infty(\mathbf{q}, E)}\sqrt{S_{\text{MB}}^\infty(\mathbf{q}, E')}. \quad (45)$$

Inserting (44) in (34) one has the following master equation, first obtained in Ref. 16:

$$\begin{aligned} \frac{d\hat{\rho}}{dt} &= -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2M}, \hat{\rho}\right] + \frac{2\pi}{\hbar}(2\pi\hbar)^3 n \int d^3\mathbf{q} |\tilde{t}(q)|^2 \\ &\quad \times \left[e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}}\sqrt{S_{\text{MB}}^\infty(\mathbf{q}, \hat{\mathbf{p}})}\hat{\rho}\sqrt{S_{\text{MB}}^\infty(\mathbf{q}, \hat{\mathbf{p}})}e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} - \frac{1}{2}\{S_{\text{MB}}^\infty(\mathbf{q}, \hat{\mathbf{p}}), \hat{\rho}\} \right] \\ &= -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2M}, \hat{\rho}\right] + z \frac{4\pi^2 m^2}{\beta\hbar} \int d^3\mathbf{q} \frac{|\tilde{t}(q)|^2}{q} e^{-\frac{\beta}{8m}(1+2\alpha)q^2} \\ &\quad \times \left[e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}}e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{\mathbf{p}}}\hat{\rho}e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{\mathbf{p}}}e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{\mathbf{x}}} - \frac{1}{2}\{e^{-\frac{\beta}{2M}\mathbf{q}\cdot\hat{\mathbf{p}}}, \hat{\rho}\} \right], \end{aligned} \quad (46)$$

where z for a free gas of Maxwell–Boltzmann particles is given by $n\lambda_m^3$, with $\lambda_m = \sqrt{2\pi\hbar^2\beta/m}$ the thermal de Broglie wavelength of the gas particles. Note that (46) has in fact the structure of the generator of a completely positive time evolution.²⁷ One can directly check that an operator of the form

$$\hat{w}_0(\hat{\mathbf{p}}) = e^{-\beta\frac{\hat{\mathbf{p}}^2}{2M}}, \quad (47)$$

where β is the inverse temperature of the macrosystem and M the mass of the microsystem, is a stationary solution of (46), in fact

$$\begin{aligned} & e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}}e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{p}}\hat{w}_0(\hat{p})e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{p}}e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}} - \frac{1}{2}\left\{e^{-\frac{\beta}{2M}\mathbf{q}\cdot\hat{p}}, \hat{w}_0(\hat{p})\right\} \\ &= e^{-\frac{\beta}{2M}\mathbf{q}\cdot(\hat{p}-\mathbf{q})}\hat{w}_0(\hat{p}-\mathbf{q}) - e^{-\frac{\beta}{2M}\mathbf{q}\cdot\hat{p}}\hat{w}_0(\hat{p}) \\ &= 2\sinh\left(\frac{\beta}{2M}\mathbf{q}\cdot\hat{p}\right)\hat{w}_0(\hat{p}), \end{aligned}$$

which is an odd function of \mathbf{q} , so that the integral over the whole space vanishes.

In order to go over from the master equation (46) to a Fokker–Planck structure describing quantum dissipation, corresponding to the quantum description of the classical Brownian motion,³¹ we consider the limit of small momentum transfer \mathbf{q} , corresponding through the physical interpretation of the dynamic structure factor to long wavelength fluctuations in the macrosystem. Expanding the exponentials containing the operators \hat{x} and \hat{p} up to second order in \mathbf{q} or equivalently keeping contributions at most bilinear in \hat{x} and \hat{p} one has

$$\begin{aligned} & e^{\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}}e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{p}}\hat{\varrho}e^{-\frac{\beta}{4M}\mathbf{q}\cdot\hat{p}}e^{-\frac{i}{\hbar}\mathbf{q}\cdot\hat{x}} - \frac{1}{2}\left\{e^{-\frac{\beta}{2M}\mathbf{q}\cdot\hat{p}}, \hat{\varrho}\right\} \\ &= +\frac{i}{\hbar}\sum_{i=1}^3\mathbf{q}_i[\hat{x}_i, \hat{\varrho}] + \left(\frac{\beta}{4M}\right)^2\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j\hat{p}_i\hat{p}_j \\ &+ \frac{1}{2}\left(\frac{\beta}{4M}\right)^2\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j\{\hat{p}_i\hat{p}_j, \hat{\varrho}\} \\ &- \frac{i}{\hbar}\left(\frac{\beta}{4M}\right)\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j[\hat{x}_i, \{\hat{p}_j, \hat{\varrho}\}] \\ &- \frac{1}{2}\frac{1}{\hbar^2}\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j[\hat{x}_i, [\hat{x}_j, \hat{\varrho}]] \\ &- \frac{1}{4}\left(\frac{\beta}{2M}\right)^2\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j\{\hat{p}_i\hat{p}_j, \hat{\varrho}\} \\ &= +\frac{i}{\hbar}\sum_{i=1}^3\mathbf{q}_i[\hat{x}_i, \hat{\varrho}] - \frac{1}{2}\sum_{i,j=1}^3\mathbf{q}_i\mathbf{q}_j\left\{\frac{1}{\hbar^2}[\hat{x}_i, [\hat{x}_j, \hat{\varrho}]]\right. \\ &\left.+ \left(\frac{\beta}{4M}\right)^2[\hat{p}_i, [\hat{p}_j, \hat{\varrho}]] + \frac{i}{\hbar}\left(\frac{\beta}{2M}\right)[\hat{x}_i, \{\hat{p}_j, \hat{\varrho}\}]\right\} \end{aligned} \tag{48}$$

and therefore (46) in this limit becomes

$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -\frac{i}{\hbar} \left[\frac{\hat{\mathbf{p}}^2}{2M}, \hat{\rho} \right] - z \frac{2\pi^2 m^2}{\beta \hbar} \int d^3 \mathbf{q} \frac{|\tilde{t}(q)|^2}{q} e^{-\frac{\beta}{8m} q^2} \sum_{i=1}^3 \mathbf{q}_i^2 \\ & \times \left\{ \frac{1}{\hbar^2} [\hat{x}_i, [\hat{x}_i, \hat{\rho}]] + \frac{\beta^2}{16M^2} [\hat{\mathbf{p}}_i, [\hat{\mathbf{p}}_i, \hat{\rho}]] + \frac{i}{\hbar} \frac{\beta}{2M} [\hat{x}_i, \{\hat{\mathbf{p}}_i, \hat{\rho}\}] \right\}, \end{aligned} \quad (49)$$

where again because of the integration only terms bilinear in the momentum transfer and with $i = j$ survive. Note that the result (49) heavily depends on an exact compensation of the different coefficients in (48), leading to the particularly simple structure of the last line of (48), which is a typical structure of generator of quantum Brownian motion.³² Supposing without loss of generality the scattering to be isotropic, we have $\mathbf{q}_i^2 = \frac{1}{3}q^2$, and the following coefficients related to diffusion and friction can be introduced:

$$\begin{aligned} D_{pp} &= z \frac{2\pi^2 m^2}{3\beta \hbar} \int d^3 \mathbf{q} |\tilde{t}(q)|^2 q e^{-\frac{\beta}{8m} q^2}, \\ D_{xx} &= \left(\frac{\beta \hbar}{4M} \right)^2 D_{pp}, \\ \gamma &= \left(\frac{\beta}{2M} \right) D_{pp}, \end{aligned} \quad (50)$$

so that the Fokker–Planck equation (49) can be more compactly written

$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] - \frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\hat{x}_i, [\hat{x}_i, \hat{\rho}]] \\ & - \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\hat{\mathbf{p}}_i, [\hat{\mathbf{p}}_i, \hat{\rho}]] - \frac{i}{\hbar} \gamma \sum_{i=1}^3 [\hat{x}_i, \{\hat{\mathbf{p}}_i, \hat{\rho}\}]. \end{aligned} \quad (51)$$

4.1. Structural features

We now consider some structural features of the mapping giving the dissipative part of (51), given by

$$\begin{aligned} \mathcal{L}^{\hat{x}, \hat{\mathbf{p}}}[\hat{\mathbf{w}}] \equiv \mathcal{L}[\hat{\mathbf{w}}] = & -\frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\hat{x}_i, [\hat{x}_i, \hat{\mathbf{w}}]] \\ & - \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\hat{\mathbf{p}}_i, [\hat{\mathbf{p}}_i, \hat{\mathbf{w}}]] - \frac{i}{\hbar} \gamma \sum_{i=1}^3 [\hat{x}_i, \{\hat{\mathbf{p}}_i, \hat{\mathbf{w}}\}], \end{aligned} \quad (52)$$

where the dependence on the operators \hat{x} and $\hat{\mathbf{p}}$ has been put in major evidence. The mapping $\mathcal{L}^{\hat{x}, \hat{\mathbf{p}}}$ is said to be covariant under the action of a unitary representation \mathcal{U}_g of a symmetry group G provided the identity

$$\mathcal{L}^{\hat{x}, \hat{\mathbf{p}}}[\mathcal{U}_g[\hat{\mathbf{w}}]] = \mathcal{U}_g[\mathcal{L}^{\hat{x}, \hat{\mathbf{p}}}[\hat{\mathbf{w}}]]$$

holds, where $\mathcal{U}_g[\hat{w}] = \hat{U}(g)\hat{w}\hat{U}^\dagger(g)$. Exploiting the simple relation

$$[\hat{A}, \hat{U}\hat{B}\hat{U}^\dagger]_{\mp} = \hat{U}[\hat{U}^\dagger\hat{A}\hat{U}, \hat{B}]_{\mp}\hat{U}^\dagger,$$

where \hat{U} is a unitary operator, and considering the explicit structure (52) of $\mathcal{L}^{\hat{x}, \hat{p}}$ we have

$$\mathcal{L}^{\hat{x}, \hat{p}}[\mathcal{U}_g[\hat{w}]] = \mathcal{U}_g[\mathcal{L}^{\hat{U}^\dagger(g)\hat{x}\hat{U}(g), \hat{U}^\dagger(g)\hat{p}\hat{U}(g)}[\hat{w}]],$$

so that covariance is granted if and only if the condition

$$\mathcal{L}^{\hat{U}^\dagger(g)\hat{x}\hat{U}(g), \hat{U}^\dagger(g)\hat{p}\hat{U}(g)} = \mathcal{L}^{\hat{x}, \hat{p}}$$

holds. Let us now consider the symmetry groups of relevance to our physical context. Under translations the operators position and momentum of the particle transform as

$$\hat{U}^\dagger(\mathbf{a})\hat{x}\hat{U}(\mathbf{a}) = \hat{x} + \mathbf{a}, \quad \hat{U}^\dagger(\mathbf{a})\hat{p}\hat{U}(\mathbf{a}) = \hat{p},$$

and one immediately has

$$\mathcal{L}^{\hat{x}+\mathbf{a}, \hat{p}} = \mathcal{L}^{\hat{x}, \hat{p}}.$$

Considering the group of rotations one has the following transformation laws:

$$\hat{U}^\dagger(R)\hat{x}\hat{U}(R) = R\hat{x}, \quad \hat{U}^\dagger(R)\hat{p}\hat{U}(R) = R\hat{p},$$

and according to the relation

$$\begin{aligned} \sum_{i=1}^3 [(R\hat{u})_i, [(R\hat{v})_i, \hat{w}]_{\mp}]_{\mp} &= \sum_{i,j,k=1}^3 R_{ij}R_{ik}[\hat{u}_j, [\hat{v}_k, \hat{w}]_{\mp}]_{\mp} \\ &= \sum_{j,k=1}^3 (R^t R)_{jk}[\hat{u}_j, [\hat{v}_k, \hat{w}]_{\mp}]_{\mp} \\ &= \sum_{j=1}^3 [\hat{u}_j, [\hat{v}_j, \hat{w}]_{\mp}]_{\mp} \end{aligned}$$

valid for any couple of vector operators \hat{u}, \hat{v} , one still has invariance

$$\mathcal{L}^{R\hat{x}, R\hat{p}} = \mathcal{L}^{\hat{x}, \hat{p}}.$$

One can also see that an operator with the expected canonical structure (47) is a stationary solution of (51) in that

$$\mathcal{L}[\hat{w}_0(\hat{p})] = 0,$$

due to the relationship

$$\frac{\gamma}{D_{pp}} = \frac{\beta}{2M} \tag{53}$$

obeyed by the coefficients defined in (50).

The relaxation properties of the dynamics driven by the Fokker–Planck equation (51) can be easily obtained considering the adjoint mapping \mathcal{L}' , which gives the time evolution of the single particle observables according to

$$\begin{aligned} \frac{d\hat{A}}{dt} &= +\frac{i}{\hbar}[\hat{H}_0, \hat{A}] + \mathcal{L}'[\hat{A}] \\ &= +\frac{i}{\hbar}[\hat{H}_0, \hat{A}] - \frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\hat{x}_i, [\hat{x}_i, \hat{A}]] \\ &\quad - \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\hat{p}_i, [\hat{p}_i, \hat{A}]] + \frac{i}{\hbar} \gamma \sum_{i=1}^3 \{\hat{p}_i, [\hat{x}_i, \hat{A}]\}. \end{aligned} \quad (54)$$

Considering the components of the momentum operator one has, setting in (54) $\hat{A} \rightarrow \hat{p}_k$

$$\frac{d\hat{p}_k}{dt} = -2\gamma\hat{p}_k, \quad (55)$$

while for the kinetic energy $\hat{E} = \frac{\hat{p}^2}{2M}$

$$\frac{d\hat{E}}{dt} = 3\frac{D_{pp}}{M} - 4\gamma\hat{E}, \quad (56)$$

and exploiting (53)

$$\frac{d\hat{E}}{dt} = -4\gamma\left(\hat{E} - \frac{3}{2\beta}\right). \quad (57)$$

Due to (55), setting $\eta = 2\gamma$, the mean value of the momentum relaxes exponentially to zero, on a typical time scale $1/\eta$, recovering a result strictly analogous to the classical one.⁶ Correspondingly (57) implies that the mean value of the kinetic energy of the microsystem reaches for long times the expected classical value

$$\langle \hat{E} \rangle = \frac{3}{2\beta} = \frac{3}{2}kT,$$

where T is the temperature of the macrosystem, the relaxation being also exponential with a rate $1/2\eta$.

Analogies and differences of (51) with the classical Fokker–Planck equations for the description of Brownian motion can be perhaps most easily seen writing it in terms of the Wigner function.³⁸ The Wigner function, related to the statistical operator by the identity

$$f_W(\mathbf{x}, \mathbf{p}) = \int \frac{d^3\mathbf{k}}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{k}} \langle \mathbf{p} + \mathbf{k}/2 | \hat{\rho} | \mathbf{p} - \mathbf{k}/2 \rangle, \quad (58)$$

allows for a phase-space description in quantum mechanics,³⁹ giving a phase space probability density.^a Using (58) Eq. (51) becomes

$$\begin{aligned} \frac{\partial}{\partial t} f_W(\mathbf{x}, \mathbf{p}) = & -\frac{\mathbf{p}}{M} \cdot \nabla_x f_W(\mathbf{x}, \mathbf{p}) + D_{pp} \Delta_p f_W(\mathbf{x}, \mathbf{p}) \\ & + D_{xx} \Delta_x f_W(\mathbf{x}, \mathbf{p}) + 2\gamma \nabla_p \cdot (\mathbf{p} f_W(\mathbf{x}, \mathbf{p})), \end{aligned} \quad (59)$$

that is to say a Fokker–Planck equation in which, apart from a dissipative contribution, terms corresponding to diffusion in both position and momentum appear. The appearance of both these contributions together is necessary in order that (51) exhibits a structure of generator of a completely positive time evolution,¹⁶ and therefore appears as a peculiar quantum feature.

Many other similar examples of Fokker–Planck equations describing dissipation can be found in the literature (for a review see Refs. 32–34), mainly relying on phenomenological approaches or on a characterization of the formal structures compatible with complete positivity. They differ in the definition of the coefficients, in their relative weight, and in the presence or absence of various dissipative contributions or of potential terms which determine the underlying free dynamics. All these factors determine the general properties such as the existence of a stationary solution, invariance under symmetry transformations and complete positivity.¹⁷ These properties for (51) and more generally for (34) are considered in some detail in Ref. 19. In particular a distinguishing feature of (34) is the existence of a canonical stationary solution provided the state of the macrosystem with which the microsystem is interacting is a β -KMS state.⁴¹

The unique feature of the Fokker–Planck equation (51) from a physical point of view is its derivation as a long wavelength limit of the master equation (34), which gives the subdynamics of the microsystem in terms of the dynamic structure factor of the medium: this corresponds to a Kramers–Moyal expansion in the small parameter \mathbf{q} characterizing the size of the fluctuations.^{37,42} This connection between (34) and (51) gives a profound justification for the selection of possible dissipative contributions appearing in (51) and for the exact expressions of the coefficients in (50). More than this, observing that the dynamic structure factor can also be expressed as a Fourier transform, with respect to transferred momentum and energy, of the time dependent density correlation function according to (40), one has a direct physical connection between Brownian motion of the test particle and density fluctuations in the medium. This physical intuition was in fact the starting point of Einstein’s approach to the classical description of Brownian motion, his key idea being that the random motion was due to the discrete nature

^aThe Wigner function defined in (58) is not actually a well-defined probability density, since its positivity is not granted. Well-defined probability densities can nevertheless be introduced in quantum mechanics, exploiting the more modern formulation in terms of POV measures.^{40,13} Here we are only interested in drawing some simple analogies with the classical case, so that we will use (58) because of its simplicity and popularity, together with the appeal of the compact expression (59).

of matter.⁴³ Equation (51) also has a mathematically distinguishing feature, since it can be written in explicit Lindblad form in terms of a single generator for each Cartesian direction, a feature also indicated by the general structure of translation covariant quantum dynamical semigroups obtained by Holevo,²⁸ one of the few characterizations of quantum dynamical semigroups with unbounded generators.⁴⁴ In fact introducing the operators

$$\hat{a}_i = \frac{\sqrt{2}}{\lambda_M} \left(\hat{x}_i + \frac{i}{\hbar} \frac{\lambda_M^2}{4} \hat{p}_i \right),$$

where $\lambda_M = \sqrt{\hbar^2 \beta / M}$ and $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$, (51) can be also written as

$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] - \frac{D_{pp}}{\hbar^2} \frac{\lambda_M^2}{4} \sum_{i=1}^3 [\hat{a}_i^2 - \hat{a}_i^{\dagger 2}, \hat{\rho}] \\ & + \frac{D_{pp}}{\hbar^2} \lambda_M^2 \sum_{i=1}^3 \left[\hat{a}_i \hat{\rho} \hat{a}_i^\dagger - \frac{1}{2} \{ \hat{a}_i^\dagger \hat{a}_i, \hat{\rho} \} \right]. \end{aligned} \tag{60}$$

4.2. Quantum statistics

As a last application of (34) we briefly sketch the completely new results one obtains when considering the Brownian limit $\alpha \ll 1$ in the case of a free Bose or Fermi gas,^{18,19} starting from expression (38) for the dynamic structure factor which takes compactly both statistics into account. A suitable expansion of (38), despite being much more complicated than in the case of Maxwell–Boltzmann particles leads to a structurally similar result. Apart from the linear dependence on the fugacity z in the coefficients defined in (50) the dissipative part of (51) is now multiplied by an overall factor

$$\frac{1}{1-z}$$

for Bose particles and

$$\frac{1}{1+z}$$

for Fermi particles, so that one has

$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] - \frac{1}{1-z} \left\{ \frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\hat{x}_i, [\hat{x}_i, \hat{\rho}]] \right. \\ & \left. + \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\hat{p}_i, [\hat{p}_i, \hat{\rho}]] + \frac{i}{\hbar} \gamma \sum_{i=1}^3 [\hat{x}_i, \{ \hat{p}_i, \hat{\rho} \}] \right\} \end{aligned} \tag{61}$$

for the Fokker–Planck equation describing Brownian motion at quantum level in a free gas of Bose particles and

$$\begin{aligned} \frac{d\hat{\rho}}{dt} = & -\frac{i}{\hbar}[\hat{H}_0, \hat{\rho}] - \frac{1}{1+z} \left\{ \frac{D_{pp}}{\hbar^2} \sum_{i=1}^3 [\hat{x}_i, [\hat{x}_i, \hat{\rho}]] \right. \\ & \left. + \frac{D_{xx}}{\hbar^2} \sum_{i=1}^3 [\hat{p}_i, [\hat{p}_i, \hat{\rho}]] + \frac{i}{\hbar} \gamma \sum_{i=1}^3 [\hat{x}_i, \{\hat{p}_i, \hat{\rho}\}] \right\} \end{aligned} \quad (62)$$

for the corresponding dynamics in a free gas of Fermi particles. Comparing (51) and (61) or (62) one immediately sees (recalling that the fugacity is a positive number, restricted to be less than one for Bose particles) that the friction coefficient γ for Maxwell–Boltzmann particles given by the last contribution in (50) is now enhanced to

$$\frac{\gamma}{1-z}$$

in the case of Bose particles and suppressed to

$$\frac{\gamma}{1+z}$$

in the case of Fermi particles.

5. Conclusions and Outlook

In this paper we have presented some new results in the description of the subdynamics of a microsystem interacting through collisions with a macrosystem that have recently been obtained, especially in connection with quantum dissipation and the quantum description of Brownian motion. These results rely on a recent general approach to the formulation of subdynamics in a nonrelativistic field theoretical framework, where a major emphasis has been put on the choice of a suitable subset of relevant observables, whose subdynamics is to be studied on a time scale over which they are slowly varying. Particular attention is given to structural properties of the mapping giving the reduced irreversible evolution, which should satisfy complete positivity or some less stringent version of this property.

The main result presented is the master equation (34) describing the interaction of a probe particle with some macroscopic system in which the subdynamics is driven by the dynamic structure factor of the system, a two-point correlation function whose physical features are considered in Subsec. 3.1, embodying its statistical mechanics properties. Considering the long wavelength limit of this master equation the Fokker–Planck equation (51) for the description of Brownian motion is obtained, in which the quantum statistics of the fluid can be taken into account, leading to (61) and (62). These corrections due to quantum statistics to the description of quantum dissipation have been introduced for the first time and deserve further investigation, since they lead in principle to experimentally observable effects. Apart from applications in the study of quantum dissipation and decoherence of

a particle interacting with the surrounding medium (with regard to the problem of decoherence considered in this framework see also Ref. 45), these results might be used for the study of motion of test particles in degenerate quantum gases. Degenerate samples of dilute, weakly interacting Bose and Fermi atoms have in fact recently been experimentally realized,^{46,47} showing in particular the phenomenon of Bose–Einstein condensation, which is now the object of intense study (see Refs. 48 and 49 for a review). Also expressions for the dynamic structure factor, which take interactions into account and improve the result for the free case, have been recently introduced and studied.⁵⁰

A natural extension of the formalism within this approach is of course the application to many-body macroscopic systems, obtaining quantum kinetic equations for the subdynamics of suitable subsets of slowly varying observables, and will be the object of future research work.

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