Dissipative Systems and Objective Description: Quantum Brownian Motion as an Example

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ABSTRACT

A structure of generator of a quantum dynamical semigroup for the dynamics of a test particle interacting through collisions with the environment is considered, which has been obtained from a microphysical model. The related master-equation is shown to go over to a Fokker-Planck equation for the description of Brownian motion at quantum level in the long wavelength limit. The structure of this Fokker-Planck equation is expressed in this paper in terms of superoperators, giving explicit expressions for the coefficient of diffusion in momentum in correspondence with two cases of interest for the interaction potential. This Fokker-Planck equation gives an example of a physically motivated generator of quantum dynamical semigroup, which serves as a starting point for the theory of measurement continuous in time, allowing for the introduction of trajectories in quantum mechanics. This theory had in fact already been applied to the problem of Brownian motion referring to similar phenomenological structures obtained only on the basis of mathematical requirements.

1 INTRODUCTION

Despite its age the issue about the relationship between quantum and classical world, perhaps most deeply stressed at the very beginning of quantum mechanics by Niels Bohr, cannot be considered settled and still gives rise to a lively debate, as confirmed for example by a book recently published on the subject [1], tackling it from the point of view of decoherence. This very word has in fact recently become very popular for the description of phenomena connected to the transition from quantum to classical regime. While the interest in the phenomenon of decoherence was previously mainly connected to foundational issues, it is now mostly related to applications in quantum computing. The extremely short time scales associated to the phenomenon of decoherence, even in few-body systems, are in fact one of the key problems to solve in order to leave the possibility open of realizing in the future practically useful quantum computers [2].

The term decoherence is used to denote the transition to dynamics other than unitary even for few- or one-body systems, the effective non-unitary subdynamics for these systems arising from the impossibility to completely isolate them from the rest of the laboratory, at least on sufficiently long time scales. As a result one cannot expect that the physics of the microscopic system can be correctly described by a unitary, reversible evolution driven by a suitable self-adjoint Hamiltonian. Thus a simple picture in terms of a Schrödinger equation fails, the correspondence principle is no longer useful in order to envisage the generator of the dynamics, and one is compelled to resort to a more general formalism. In this connection the studies on the foundations of quantum mechanics, in particular on quantum structures [3] and on quantum measurement theory [4], have led to important results, indicating possible new sceneries for quantum dynamics and especially putting into evidence mathematical structures and properties relevant for the quantum realm. More specifically a more modern formulation of quantum mechanics has by now emerged [5], where the notions of effect (first introduced by Ludwig [6]), coexistent observable, POV-measure, operation and instrument allow for a better formulation of irreversible dynamics and measurement processes. Based...
on these concepts a formulation of continuous measurement theory in quantum mechanics has been given, mainly developed by Davies [7], the Milan group [8] and Holevo [9] (for an extensive review see [5]). This theory relies on the introduction of the generator of a quantum dynamical semigroup [10] for the dynamics of the observed microscopic system, to which an operation-valued stochastic process can be associated. It is then possible to introduce well-defined functional probability densities in the space of time trajectories of certain observables of the system, thus recovering, in this highly non trivial way, elements of objective description, the very notion of trajectory being a classical one (see [11] for a compact review on the subject and [12] for a related approach to the problem of objectivity in quantum mechanics). The observables for which trajectories can be introduced depend on the very structure of the quantum dynamical semigroup giving the irreversible time evolution, the operators appearing in it and determining the irreversible part of the dynamics also indicating the possible measuring decompositions of the mapping giving the time evolution.

The general structure of bounded generators of quantum dynamical semigroups, also satisfying the property of complete positivity [13, 14], has been fully characterized by Lindblad [15], while in the unbounded case only a few results are available [16]. It is therefore of interest to obtain physical examples of generators of quantum dynamical semigroups, especially in the case in which the generator is unbounded. In the following we will recall a result recently obtained in this framework for the description of the motion of a test particle in a quantum fluid [17, 18, 19, 20], giving a new formulation in terms of superoperators and further calculating the diffusion coefficient for interaction potentials of physical interest. The considered generator of quantum dynamical semigroups, obtained through a microphysical derivation based on a scattering theory approach, falls within a class known as quantum Brownian motion [21]. This class of models has already been considered within the framework of continuous measurement theory [22], leading to a description in terms of trajectories for the expectation values of the operators position and momentum of the particle. The starting point for [22] was the phenomenological structure of generator of quantum Brownian motion proposed by Lindblad [23, 24] on the basis of his general result on completely positive quantum dynamical semigroups and physical requirements on the dynamics originated from a classical analogy. The result presented here gives a physically motivated particular expression for the coefficients, determined in terms of microphysical quantities, and for the selection of contributions appearing in the structure of the generator.

2 MASTER EQUATION FOR A TEST PARTICLE IN A QUANTUM GAS IN TERMS OF THE DYNAMIC STRUCTURE FACTOR

Let us consider the following problem of non-equilibrium statistical mechanics: a test particle interacts through collisions with a fluid. This model is known as Rayleigh gas [25] and on a suitable time scale, much longer than the typical relaxation time of the macroscopic fluid, one expects a Markovian dynamics described in terms of a master-equation. In the quantum case an expression has recently been proposed for the generator of such a dynamics, which is in particular the generator of a completely positive quantum dynamical semigroup [20]. The master-equation takes the following form

\[
\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\varrho}] + \mathcal{L}[\hat{\varrho}],
\]

where \(\hat{\varrho}\) is the statistical operator associated to the test particle of mass \(M\), \(\hat{H}_0\) the free Hamiltonian \(\hat{p}^2/2M\) and the mapping giving the dissipative part of the time evolution has
the following Lindblad structure

\[ \mathcal{L}[-] = \frac{2\pi}{\hbar} (2\pi\hbar)^3 n \int_{\mathbb{R}^3} d^3 q \left| \tilde{U}(q) \right|^2 \left[ \tilde{U}(q) \sqrt{S(q, \tilde{p}) \cdot \sqrt{S(q, \tilde{p}) \tilde{U}^\dagger(q)}} - \frac{1}{2} \{S(q, \tilde{p}), \cdot \} \right]. \] (2.2)

The unitary operators \( \tilde{U}(q) \) are given by \( e^{\frac{i}{\hbar} q \cdot \tilde{x}} \), while the function \( \tilde{U}(q) \) is the Fourier transform with respect to the transferred momentum \( q \) of the T-matrix describing the collisions between test particle and fluid, supposed to depend only on the modulus of the momentum transfer and in a negligible way on energy. The function \( S(q, p) \) appearing operator-valued in (2.2) is a positive two-point correlation function known in the physical community as dynamic structure factor \([26, 27]\), and it is usually expressed as a function of momentum and energy transfer, \( q \) and \( E \). It is defined by

\[ S(q, E) \equiv S(q, p) = \frac{1}{2\pi \hbar} \int_{\mathbb{R}} dt \int_{\mathbb{R}^3} d^3 x e^{\frac{i}{\hbar} [E(q, p)t - q \cdot x]} \frac{1}{N} \int_{\mathbb{R}^3} d^3 y \langle N(y) N(y + x, t) \rangle, \] (2.3)

with

\[ E(q, p) \equiv E = \frac{(p + q)^2}{2M} - \frac{p^2}{2M} = \frac{q^2}{2M} + \frac{p \cdot q}{M} \]

thus being the Fourier transform of the two-point time dependent density correlation function of the fluid, calculated with respect to the statistical operator describing the fluid at equilibrium. The dynamic structure factor is always positive since it is proportional to the energy dependent scattering cross-section of a microscopic probe off a macroscopic sample \([28]\), and it gives the spectrum of spontaneous fluctuations of the macroscopic sample.

In particular the dynamic structure factor can be exactly calculated in the case of a free quantum gas, thus obtaining close expressions for Bose-Einstein and Fermi-Dirac statistics, which both go over to Maxwell-Boltzmann statistics in the limit of low density. Denoting by \( S_{\text{BE}}(q, p) \) the dynamic structure factor for a free gas of particles of mass \( m \) obeying Bose-Einstein statistics one has \([20]\)

\[ S_{\text{BE}}(q, p) = \frac{1}{(2\pi \hbar)^3} \frac{2\pi m^2}{n \beta q} \frac{1}{1 - \exp \left[ \frac{\beta}{2m} (2\sigma(q, p)q - q^2) \right]} \times \log \left[ 1 - \left\{ 1 - \exp \left[ \frac{\beta}{2m} (2\sigma(q, p)q - q^2) \right]\right\} \right] \frac{\exp \left[ -\frac{\beta}{2m} \sigma^2(q, p) \right]}{1 - \exp \left[ -\frac{\beta}{2m} \sigma(q, p) - q^2 \right]}, \] (2.4)

with \( \beta = 1/\kappa T \) the inverse of the temperature, \( n \) the particle density, \( z \) the fugacity of the gas, which is a number positive and less than one for Bose-Einstein particles \([29]\), and

\[ \sigma(q, p) = \frac{1}{2q} \left[ q^2 + 2mE(q, p) \right]. \]

Similarly for Fermi-Dirac statistics

\[ S_{\text{FD}}(q, p) = \frac{1}{(2\pi \hbar)^3} \frac{2\pi m^2}{n \beta q} \frac{1}{1 - \exp \left[ \frac{\beta}{2m} (2\sigma(q, p)q - q^2) \right]} \times \log \left[ 1 + \left\{ 1 - \exp \left[ \frac{\beta}{2m} (2\sigma(q, p)q - q^2) \right]\right\} \right] \frac{\exp \left[ -\frac{\beta}{2m} \sigma^2(q, p) \right]}{1 + \exp \left[ -\frac{\beta}{2m} \sigma(q, p) - q^2 \right]}, \] (2.5)

so that the difference only lies in a suitable change of signs and in the range of the fugacity \( z \) which is positive without further restrictions for Fermi-Dirac particles \([29]\). Both (2.4) and (2.3) in the limit of low density, corresponding to \( z \) much smaller than one, lead in a
straightforward way to the expression for a gas of Maxwell-Boltzmann particles, as can be seen expanding the logarithm:

\[ S_{MB}(\mathbf{q}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z \exp \left[ -\frac{\beta}{2m} \sigma^2(\mathbf{q}, \mathbf{p}) \right], \tag{2.6} \]

where the fugacity is now given by the explicit expression

\[ z = n \left( \frac{2\pi\hbar^2\beta}{m} \right)^{3/2}. \]

A case of particular interest in which to apply (2.1) is the description at quantum level of Brownian motion, that is the case in which the mass \( M \) of the test particle is much bigger than the mass \( m \) of the gas particles. One therefore needs expressions for the dynamic structure factor in the Brownian limit in which the ratio \( \alpha = m/M \) is much smaller than one. To do this one writes the argument of the exponentials in (2.4), (2.5) and (2.6) as a polynomial in \( \alpha \), keeping only the contributions in the lowest order. Concentrating on the simplest case of a gas of Maxwell-Boltzmann particles, writing \( \sigma^2 \) as a polynomial in \( \alpha \)

\[ \sigma^2(\mathbf{q}, \mathbf{p}) = \frac{q^2}{4} + \frac{1}{2} \alpha |q^2 + 2\mathbf{p} \cdot \mathbf{q}| + \frac{1}{4} \frac{\alpha^2}{q^2} |q^2 + 2\mathbf{p} \cdot \mathbf{q}|^2, \]

and keeping terms up to first order one has

\[ S_{MB}^\infty(\mathbf{q}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} z e^{-\frac{\alpha}{8m}\frac{q^2}{2} - \frac{\alpha}{2m} \frac{q^2 + q^2}{M}}, \tag{2.7} \]

where the index \( \infty \) denotes the Brownian limit \( \alpha \ll 1 \). Eq. (2.1) now becomes

\[
\frac{d\hat{\varnothing}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\varnothing}] + \frac{2\pi}{\hbar} (2\pi\hbar)^3 n \int_{\mathbb{R}^3} d^3q |\tilde{\varnothing}(q)|^2 \\
\times \left[ \hat{U}^\dagger(q) \sqrt{S_{MB}^\infty(q, \hat{\varnothing})} \hat{\varnothing} \sqrt{S_{MB}^\infty(q, \hat{\varnothing})} \hat{U}(q) - \frac{1}{2} \left\{ S_{MB}^\infty(q, \hat{\varnothing}), \hat{\varnothing} \right\} \right] \tag{2.8}
\]

and in view of (2.7), introducing the operators

\[ V(q, \hat{p}, \hat{x}) = e^{\frac{i}{\hbar} q \hat{x}} e^{-\frac{\beta}{4m} q \hat{p}} \]

(2.8) takes the more manifest Lindblad structure

\[
\frac{d\hat{\varnothing}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\varnothing}] + z \frac{4\pi^2 m^2}{\beta \hbar} \int_{\mathbb{R}^3} d^3q \frac{|\tilde{\varnothing}(q)|^2}{q} e^{-\frac{\beta}{8m}(1+2\alpha)q^2} \\
\times \left[ V(q, \hat{p}, \hat{x}) \hat{\varnothing} V^\dagger(q, \hat{p}, \hat{x}) - \frac{1}{2} \left\{ V^\dagger(q, \hat{p}, \hat{x}) V(q, \hat{p}, \hat{x}), \hat{\varnothing} \right\} \right] \\
= -\frac{i}{\hbar} [\hat{H}_0, \hat{\varnothing}] + z \frac{4\pi^2 m^2}{\beta \hbar} \int_{\mathbb{R}^3} d^3q \frac{|\tilde{\varnothing}(q)|^2}{q} e^{-\frac{\beta}{8m}(1+2\alpha)q^2} \\
\times \left[ e^{\frac{i}{\hbar} q \hat{x}} e^{-\frac{\beta}{4m} q \hat{p}} \hat{\varnothing} e^{-\frac{\beta}{4m} q \hat{p}} e^{\frac{i}{\hbar} q \hat{x}} - \frac{1}{2} \left\{ e^{-\frac{\beta}{4m} q \hat{p}}, \hat{\varnothing} \right\} \right]. \tag{2.9}
\]

The action of the operators position and momentum of the microsystem \( \hat{x} \) and \( \hat{p} \) is best seen introducing the following superoperators

\[
\mathcal{L}_- [\cdot] = \frac{i}{\hbar} [\hat{A}, \cdot]_- = \frac{i}{\hbar} [\hat{A}, \cdot] \\
\mathcal{L}_+ [\cdot] = \frac{1}{\hbar} [\hat{A}, \cdot]_+ = \frac{1}{\hbar} [\hat{A}, \cdot], \tag{2.10}
\]
which will also prove useful for future expansions. In terms of (2.10) eq. (2.9) takes the remarkably simple structure
\[
\frac{d\hat{\theta}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\theta}] + \frac{4\pi^2 m^2}{\beta h} \int \mathbb{R}^3 d^3q \frac{\tilde{f}(q)}{q} e^{-\frac{\nu}{\beta m} (1+2\alpha)q^2} \times \left[ \exp (L_{q,i}^-) \exp (L_{q,j}^+) \hat{\theta} \right] - \frac{1}{2} \left\{ \exp \left( \frac{2\kappa}{h} \hat{q} \cdot \hat{p} \right), \hat{\theta} \right\}
\] (2.11)
with \( \kappa = -\frac{\beta h}{4M} \). The master-equation (2.3) gives a physical realization of a general structure of generators of translation-covariant quantum dynamical semigroups recently introduced by Holevo [30]. In fact (2.9) and more generally (2.1) are invariant under spatial translations in the sense that
\[
\mathcal{L}[U_n[\hat{w}]] = U_n[\mathcal{L}[\hat{w}]],
\] (2.12)
with \( \hat{w} \) a statistical operator and \( U_n[j] = e^{-\frac{\pi a^2}{\hbar} \cdot j} e^{+\frac{\pi a^2}{\hbar} \cdot \hat{p}} \). In particular, provided the macroscopic system is in a \( \beta \)-KMS state [31], thus implying the detailed balance condition for the dynamic structure factor [32], a stationary solution of (2.1) is given by
\[
\hat{w}_0(\hat{p}) = e^{\frac{-\beta^2}{2M}}.
\] (2.13)
Further formal properties of (2.1) are discussed in [20, 33].

3 FOKKER-PLANCK EQUATION FOR THE DESCRIPTION OF QUANTUM DISSIPATION

Given the master-equation (2.11) one is naturally led to the question, whether some small parameter having a definite physical meaning exists, allowing for a Kramers-Moyal expansion leading from the master-equation to a Fokker-Planck equation [14]. This is in fact the case for the momentum transfer \( \mathbf{q} \), small \( \mathbf{q} \) corresponding through the physical meaning of the dynamic structure factor to the long wavelength part of the density fluctuations’ spectrum of the macroscopic system with which the Brownian particle is interacting. In the limit of small momentum transfer, keeping terms at most second order as typical in Fokker-Planck equations [35], the operator part of (2.11) becomes
\[
\left[ \exp (L_{q,i}^-) \exp (L_{q,j}^+) \hat{\theta} \right] \approx \left[ \exp \left( \frac{2\kappa}{h} \mathbf{q} \cdot \hat{p} \right), \hat{\theta} \right] \approx L_{q,i}^- \hat{\theta} + \frac{1}{2} L_{q,i}^{-2} \hat{\theta} + L_{q,j}^+ \hat{\theta} + \frac{1}{2} L_{q,j}^{+2} \hat{\theta} + L_{q,i}^- L_{q,j}^+ \hat{\theta} - L_{q,j}^+ L_{q,i}^- \hat{\theta} - L_{q,j}^{-2} \hat{\theta} - L_{q,i}^{-2} \hat{\theta}
\]
\[
= \sum_{i=1}^{3} q_i L_{q,i}^- \hat{\theta} + \frac{1}{2} \sum_{i,j=1}^{3} q_i q_j \left\{ L_{q,i}^- L_{q,j}^+ \hat{\theta} + L_{q,j}^- L_{q,i}^+ \hat{\theta} + L_{q,j}^{-2} \hat{\theta} + L_{q,i}^{-2} \hat{\theta} \right\}.
\]
Integrating over \( \mathbf{q} \) only terms bilinear in the momentum transfer with \( i = j \) survive, and exploiting further the isotropy of the gas implying \( q_i^2 = \frac{1}{3} q^2 \) one obtains
\[
\frac{d\hat{\theta}}{dt} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\theta}] + \frac{2\pi^2 m^2}{\beta h} \int \mathbb{R}^3 d^3q \frac{|\tilde{f}(q)|}{q} e^{-\frac{\nu}{\beta m} (1+2\alpha)q^2} \times \sum_{i=1}^{3} \left\{ L_{q,i}^{-2} \hat{\theta} + L_{q,i}^{-2} \hat{\theta} + L_{q,i}^{+2} \hat{\theta} \right\}.
\] (3.1)

We now want to evaluate the overall coefficient for some cases of physical interest. Before this we note that the linear dependence on the fugacity \( z \) in (3.1) is a result typical of a gas
of Maxwell-Boltzmann particles. Keeping effects due to quantum statistics into account \[36\] the factor \( z \) has to be replaced by a function \( \zeta(z) \) defined in the following way

\[
\zeta(z) = \begin{cases} 
  z & \text{Maxwell – Boltzmann} \\
  z/(1 - z) & \text{Bose} \\
  z/(1 + z) & \text{Fermi}
\end{cases}
\]

so that we will generally consider the coefficient

\[
D_{pp} = \zeta(z) \frac{2}{3} \frac{\pi^2 m^2}{\beta \hbar} \int_{\mathbb{R}^3} d^3 q |\tilde{t}(q)|^2 q e^{-\frac{\beta q^2}{2m}}.
\]

(3.2)

We will give two examples. We consider first the case of a short range potential characterized by a strength \( v_0 \) and a typical range \( r_0 \), according to

\[
t(x) = v_0 e^{-|x|^2/r_0^2}.
\]

(3.3)

The Fourier transform of (3.3) is given by

\[
\tilde{t}(q) = \int_{\mathbb{R}^3} d^3 x \frac{e^{i q x}}{(2\pi \hbar)^3} t(x) = \frac{\pi^{3/2}}{(2\pi \hbar)^3} v_0 r_0^3 e^{-\frac{q^2 r_0^2}{4\hbar^2}}
\]

and the coefficient \( D_{pp} \) becomes accordingly

\[
D_{pp} = \zeta(z) \frac{1}{48} v_0^2 m \frac{\nu^3}{\hbar (1 + \nu)^2}
\]

with \( \nu \) a characteristic constant given by the square ratio between potential range and thermal wavelength \( \lambda_T = \sqrt{2\pi \beta \hbar^2/m} \) of the particles of the gas

\[
\nu = 8\pi \frac{r_0^2}{\lambda_T^2}.
\]

(3.4)

As a second example we consider the case in which the range of the potential shrinks to zero, so that the collisions are described by an effective T-matrix of the form

\[
t(x) = \frac{2\pi \hbar^2}{M} a_0 \delta^3(x),
\]

(3.5)

where \( a_0 \) is a characteristic scattering length. The Fourier transform of (3.3) is

\[
\tilde{t}(q) = \frac{1}{4\pi^2} \frac{a_0}{\hbar M}
\]

and as a consequence

\[
D_{pp} = \zeta(z) \frac{32}{3} \frac{m}{\hbar^2 \alpha^2} \frac{a_0^2}{\lambda_T^2}.
\]

As it can be seen, given some exact expression or some phenomenological Ansatz for the T-matrix describing the collisions, one obtains a definite expression for the coefficient \( D_{pp} \), which as we shall see is connected to diffusion in momentum, depending on the physical parameters of interest.

To make the comparison with the literature easier \( (3.1) \) using \( (2.10) \) can be also written

\[
\frac{d\hat{\theta}}{dt} = - \frac{i}{\hbar} [\hat{H}_0, \hat{\theta}] - D_{pp} \sum_{i=1}^{3} \left\{ \frac{1}{\hbar^2} [\hat{x}_i, [\hat{x}_i, \hat{\theta}]] + \frac{\kappa^2}{\hbar^2} [\hat{p}_i, [\hat{p}_i, \hat{\theta}]] - \frac{i}{\hbar^2} 2\kappa [\hat{x}_i, \{\hat{p}_i, \hat{\theta}\}] \right\}.
\]

(3.6)
The Fokker-Planck equation (3.6) gives an example of unbounded generator of a completely positive quantum dynamical semigroup and corresponds to a particular physical realization of the diffusive continuous component of the general structure of translation-covariant quantum dynamical semigroup characterized by Holevo [30]. In fact (3.6) is invariant under translations according to (2.12), moreover an operator of the form (2.13) is still a stationary solution due to the particular ratio between the friction coefficient and the coefficient of diffusion in momentum [37], as discussed in the following. To draw a connection with the classical description of Brownian motion the last three terms of (3.6) can be recognized as being due to diffusion in momentum, diffusion in position and friction respectively [38]. In fact exploiting the correspondence principle the commutator with the position operator corresponds to a derivative with respect to momentum, the commutator with the momentum operator corresponds to a derivative with respect to position and the anti-commutator with the momentum operator corresponds to a linear multiplication by momentum with a factor two, as can also be most directly seen in terms of the Wigner function [39, 40]. In particular the ratio between the coefficient responsible for diffusion in momentum and the coefficient responsible for friction is given by $M/\beta$ as in the classical Kramers’ equation for Brownian motion in phase space [41, 34], thus granting the expected stationary solution (2.13).

Eq. (3.6) is a particular realization, obtained on the basis of a microphysical model, of the general phenomenological expression for quantum Brownian motion considered in [22] as a starting point for the application of the theory of measurement continuous in time. It does provide a physically motivated structure of generator of quantum dynamical semigroup allowing for the introduction of an objective description in terms of trajectories in the sense clarified in [11].

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