Helvetica Physica Acta,
Vol. 56 (1983) 797-802

0018-0238/83/010797-06$1.50+0.20/0

Quantum Brownian Motion *

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We propose a new master equation describing the irreversible process of a quantum-mechanical Brownian particle. The master equation is shown to obey the symmetry of detailed balance leading to a quantum analogue of the reciprocity relations, and the fluctuation-dissipation theorem is obtained. The relation to previous approaches is discussed.

The problem to describe damping of a quantum system arises in fields as diverse as quantum optics and nuclear physics. This question has been extensively discussed in the literature and the different approaches are presented in various review articles[1]. While some of these approaches have been applied quite successfully to irreversible quantum systems, the theory is far from having reached a status comparable to the theory of classical random processes because there are still open questions even of the principle kind.

For classical processes it is well known that the microscopic reversibility leads to a certain symmetry of the random process known as detailed balancing, and the response functions are connected with the correlation functions by the fluctuation-dissipation theorem (FDT)[2]. While these general features should certainly also be present within a quantum description, it has proven to be extremly difficult to incorporate these properties into those approaches[3] avoiding a fully microscopic treatment.

In this communication we shall consider a quantum-mechanical particle which is acted upon by a thermal bath and an outside potential. The irreversible motion of the particle will be described in terms of a master equation which is different from those put forward to date. The new master equation is distinguished by the fact that it obeys the symmetry of detailed balance leading to a quantum analogue of the reciprocity relations, and the FDT is incorporated correctly, too. Finally, the relation to previous approaches will be discussed.

A model for a damped quantum-mechanical particle can be obtained by starting from a purely dynamical model of a hea-

* Portions of this work were supported by the Swiss National Science Foundation

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vy particle of mass m coupled to a reservoir of lighter particles of mass m'. Upon eliminating the reservoir variables by means of the projection operator technique[4] one finds a closed subdynamics of the heavy particle alone. The density matrix $\rho(t)$ of the particle with momentum p and position q obeys a generalized master equation. We use an approach [4-6] different from the usual ones because our relevant density matrix is of the local-equilibrium type and not a factorizing density matrix. This allows us to avoid the assumption that the particle is not correlated with the reservoir initially. Furthermore, the generalized master equation can be shown to govern the time evolution of equilibrium correlations exactly.

When the coupling to the reservoir is of the form $q\Gamma$, where Γ is a reservoir operator, the generalized master equation can be evaluated further. Using the mass ratio , m'/m, as a small parameter, one obtains in the Markovian approximation a master equation of the form[6]

$$\rho(t) = -iL\rho(t) = -i(L_o+L_d)\rho(t) \ , \tag{1}$$

where the Liouville (super-)operator is the sum of a reversible Liouvillian

$$L_o X = (1/\hbar)[H,X] \ ; \ H = p^2/2m + V(q) \tag{2}$$

describing a particle of mass m moving in an effective potential V(q), and a dissipative Liouvillian

$$L_d X = (k_B T m / i\hbar^2) \ \left[q, \Lambda\left[q, K^{-1}X\right]\right] \tag{3}$$

describing the influence of the bath. Here

$$KX = (\beta \ \mathrm{tr}\ e^{-\beta H})^{-1} \int_o^\beta d\alpha\ e^{-\alpha H}\ X\ e^{-(\beta-\alpha)H}$$

is the Kubo transformation, $\beta = 1/k_B T$ is the inverse reservoir temperature, and

$$\Lambda X = (\beta \ \mathrm{tr}\ e^{-\beta H})^{-1} \int_o^\beta d\alpha\ \gamma(\alpha) e^{-\alpha H}\ X\ e^{-(\beta-\alpha)H}$$

is a damping operator, where $\gamma(\alpha)$ is given in terms of the correlation function of the force Γ exerted by the reservoir upon the Brownian particle

$$\gamma(\alpha) = \frac{1}{mk_B T} \int_o^\infty ds\ \langle \Gamma(s-i\hbar\alpha)\Gamma \rangle \ .$$

It can easily be shown that in the high-temperature limit the master equation (1) reduces to the standard Fokker-Planck equation for classical Brownian motion with a damping constant given by Kirkwood's formula.

Some interesting properties of the new master equation can easily be seen. Using the formula $[\rho_\beta, q] = (i\hbar/mk_B T)Kp$, where $\rho_\beta = [\mathrm{tr}\,\exp(-\beta H)]^{-1}\exp(-\beta H)$ is the equilibrium state, we find

$$<\dot{q}(t)> = (1/m) <p(t)> ,$$

$$<\dot{p}(t)> = -\left\langle\frac{\partial V(t)}{\partial q(t)}\right\rangle - \gamma <p(t)>.$$

Here

$$\gamma = \frac{1}{\beta}\int_0^\beta d\alpha \quad \gamma(\alpha)$$

is a damping constant. Thus the mean values obey the same equations that are met with classical Brownian motion. This is as it should be in view of Ehrenfest's theorem.

The symmetries of the process are easier recognized if the master equation (1) is written in the form of an Onsager-type transport equation

$$\dot{\rho}(t) = - R\mu(t) = - (V+D)\mu(t)$$

where

$$\mu(t) = k_B T K^{-1}(\rho(t) - \rho_\beta) \quad (4)$$

is a thermodynamic force operator[4] which drives the system back to the equilibrium state ρ_β, and R is a transport (super-) operator. R consists of a commutator

$$VX = -(i/\hbar)\,[\rho_\beta, X]$$

describing the reversible transport, and a double commutator

$$DX = (m/\hbar^2)\,[q, \Lambda[q, X]]$$

describing the irreversible transport.

The time-reversal transformation Π is defined by $\Pi q = q$, $\Pi p = -p$. Using $\Pi^2 = 1$ and $\Pi(i[X,Y]) = i[\Pi Y, \Pi X]$ we find[4]

$$\Pi K \Pi = K^T , \quad \Pi V \Pi = V^T , \quad \Pi D \Pi = D^T .$$

The last relations imply $\Pi R \Pi = R^T$ which is the quantal version of the reciprocity relations. Here the transpose A^T of a (super-) operator A is defined by $tr(XAY) = tr(YA^TX)$.

Next we study the linear response to an external perturbation $H_e(t)$ which acts upon the particle. The perturbation changes not only the reversible motion but the irreversible motion as well. This follows from the fact that in the presence of a time-independent perturbation the particle relaxes towards the steady state

$$\rho_s = Z^{-1}\exp\left\{-\beta(H+H_e)\right\} = \rho_\beta - \beta K H_e$$

where we have disregarded the nonlinear terms. The thermodynamic force operator (4) is therefore replaced by

$$k_B T K^{-1}\left\{\rho(t)-\rho_\beta+\beta K H_e(t)\right\} = \mu(t) + H_e(t) \quad ,$$

and we arrive at the master equation

$$\dot{\rho}(t) = -R\left\{\mu(t)+H_e(t)\right\} = - iL\rho(t) - RH_e(t). \qquad (5)$$

From (5) we obtain

$$\Delta\rho(t) = \rho(t) - \rho_\beta = -\int_{-\infty}^{t} ds\chi(t-s)H_e(s)$$

with the response operator

$$\chi(t) = \Theta(t)\exp(-iLt)R. \qquad (6)$$

Here $\Theta(t)$ is the unit step function. In particular, the response of the mean position $\langle q(t)\rangle$ to an external force $F(t)$, that is $H_e(t) = -qF(t)$, is found to be

$$\Delta\langle q(t)\rangle = \int_{-\infty}^{t} ds\ \chi_{qq}(t-s)F(s)$$

where the response functions are defined by $\chi_{XY}(t) = tr(X\chi(t)Y.)$

Besides the mean relaxation towards equilibrium, the Liouvillian L also governs the time evolution of correlations of fluctuations about equilibrium. The result is stated conveniently in terms of the canonical correlation [7]

$$C_{XY}(t) = tr(XG(t)Y)$$

where for $t>0$

$$G(t) = \exp(-iLt)K \ , \ G(-t) = G^T(t) . \tag{7}$$

The relation of $C_{XY}(t)$ to the frequently used symmetrized correlation $S_{XY}(t)$ is expressed at its clearest in terms of the associated spectral functions[7]

$$S_{XY}(\omega) = \frac{1}{2}\Omega\coth(\frac{1}{2}\Omega)C_{XY}(\omega) \tag{8}$$

where $\Omega = \hbar\omega/k_BT$. Because of $iL = k_BTRK^{-1}$, Eqs. (6) and (7) give the FDT

$$\chi(t) = -\beta\Theta(t)\dot{G}(t) .$$

Using (8) and changing to frequency space, we obtain the more familiar form

$$\coth(\frac{1}{2}\Omega)\chi''_{XY}(\omega) = (2\pi/\hbar)S_{XY}(\omega)$$

where $\chi''_{XY}(\omega) = \frac{i}{2}\{\chi_{XY}(\omega)-\chi_{YX}(\omega)\}$ is the dissipative part of the dynamic susceptibility. It is also easily established that the correlation functions satisfy the symmetry of detailed balance.

The present approach differs from most of the previous work[1] in two ways. First, the form (3) of the dissipative Liouvillian L_d is different. Second, the rules how to calculate correlation and response functions from the master equation are different. Shortcomings of the conventional theory of quantum Markov processes are discussed in detail in Ref. 8. As a consequence of general principles, the stochastic process of quantum Brownian motion has the symmetry of detailed balance, the FDT holds, and the average regression obeys Ehrenfest's theorem. The new master-equation approach meets these requirements while previous approaches violate at least one of them.

References and Notes

1. H. Haken, in "Encyclopedia of Physics" Vol.XXV/2c, (Springer, Heidelberg, 1969); M. Lax, Phys.Rev. 172, 350 (1968); F. Haake, in "Springer Tracts in Modern Physics" Vol. 66 (Springer, Heidelberg, 1973); E.B. Davies, "Quantum Theory of Open Systems" (Academic Press, London, 1976); R.W. Hasse, Rep.Progr.Phys. 41, 1027 (1978); J. Messer, Acta Phys. Austr. 50, 75 (1979)
2. We are aware of the fact that these properties are not necessarily met with far-from-equilibrium models. However, for a certain choice of parameters these models often include a case where the steady state is an equilibrium state, and then these properties have to unfold.
3. It should be pointed out that in some papers the term FDT is misleadingly used for properties which are not equivalent to those properties following from statistical mechanics.
4. H. Grabert, "Springer Tracts in Modern Physics" Vol. 95 (Springer, Heidelberg, 1982)
5. H. Grabert, Z.Phys. B49, 161 (1982)
6. A detailed derivation will be published elsewhere
7. R. Kubo, Rep.Progr.Phys. 29, 255 (1966)
8. P. Talkner, Dissertation, Stuttgart (1979)