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Quantum Brownian Motion

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A new master equation describing the irreversible process of a quantum mechanical Brownian particle is proposed. The master equation is shown to obey the symmetry of detailed balance leading to a quantum analog of the reciprocity relations, and the fluctuation-dissipation theorem is obtained. The method is applied to the damped harmonic oscillator. The relation to previous approaches is discussed.

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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 analog of the reciprocity relations, and the FDT is incorporated correctly, too. More specific results will be obtained for the damped harmonic oscillator. 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 heavy 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[5] 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 sum of coordinates of reservoir particles multiplied by coupling constants, the generalized master equation can be evaluated further. Using the mass ratio, m'/m, as a small parameter, we find in the limit $m \gg m'$ an approximate Markovian master equation of the form

$$\dot{\rho}(t) = -iL\rho(t) = -i(L_0 + L_d)\rho(t), \qquad (1)$$

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

$$L_0 X = (1/\hbar)[H, X]; \; H = p^2/2m + V(q), \qquad (2)$$

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

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

describing the influence of the bath. Here

$$KX = (\beta \operatorname{tr} e^{-\beta H})^{-1} \int_0^\beta d\alpha\, e^{-\alpha H} X e^{-(\beta-\alpha)H}$$

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

$$\Lambda X = (\beta \operatorname{tr} e^{-\beta H})^{-1} \int_0^\beta d\alpha\, \gamma(\alpha) e^{-\alpha H} X e^{-(\beta-\alpha)H}$$

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

$$\gamma(\alpha) = (m k_B T)^{-1} \int_0^\infty ds \langle \Gamma(s - i\hbar\alpha)\Gamma \rangle .$$

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.

We are interested here chiefly in the low-temperature regime where the Brownian particle must be treated quantum mechanically. Then, the much lighter reservoir particles behave like a system close to $T=0$, and the damping operator takes the form

$$\Lambda X = \gamma S X ,$$

where $SX = \frac{1}{2}(\rho_\beta X + X\rho_\beta)$ is the symmetrized multiplication with the equilibrium state $\rho_\beta = [\operatorname{tr}\exp(-\beta H)]^{-1}\exp(-\beta H)$, while

$$\gamma = \beta^{-1}\int_0^\beta d\alpha\, \gamma(\alpha)$$

is a damping constant.

Some interesting properties of the new master equation can easily be seen. Using the formula $[\rho_\beta, q] = (i\hbar/m k_B T)Kp$, we find

$$\langle \dot{q}(t)\rangle = (1/m)\langle p(t)\rangle ,$$

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

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 more easily 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

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

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

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

describing the reversible transport and a double commutator

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

describing the irreversible transport.

The transpose A^T of a (super-) operator A is defined by $\operatorname{tr}(XAY) = \operatorname{tr}(YA^T X)$. It may easily be seen that

$$K^T = K, \; V^T = -V, \; D^T = D ,$$

so that V and D are the antisymmetric and symmetric parts of R, respectively. 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

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

The last relations imply $\Pi R \Pi = R^T$ which is the quantal version of the reciprocity relations.

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

$$\rho_s = Z^{-1}\exp[-\beta(H+H_e)] = \rho_\beta - \beta K H_e ,$$

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

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

and we arrive at the master equation

$$\dot\rho(t) = -R[\mu(t) + H_e(t)] = -iL\rho(t) - RH_e(t). \quad (5)$$

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

$$\chi(t) = \theta(t)\exp(-iLt)R. \quad (6)$$

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 $\chi_{XY}(t) = \mathrm{tr}[X\chi(t)Y]$.

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[6]

$$C_{XY}(t) = \mathrm{tr}[XG(t)Y],$$

where for $t>0$

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

The relaxation 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[6]

$$S_{XY}(\omega) = \tfrac{1}{2}\Omega\coth(\tfrac{1}{2}\Omega)C_{XY}(\omega), \quad (8)$$

where $\Omega = \hbar\omega/k_B T$. Because of $iL = k_B TRK^{-1}$, 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 familar form

$$\coth(\tfrac{1}{2}\Omega)\chi_{XY}''(\omega) = (2\pi/\hbar)S_{XY}(\omega),$$

where $\chi_{XY}''(\omega) = \frac{1}{2}i[\chi_{XY}(\omega) - \chi_{YX}(\omega)]$ is the dissipative part of the dynamic susceptibility. It is also easily established that the correlation functions satisfy the symmetry of detailed balance.

In the sequel we illustrate our results by considering a damped harmonic oscillator. Then

$$H = p^2/2m + \tfrac{1}{2}m\omega_0^2 q^2 = \hbar\omega_0(a^\dagger a + \tfrac{1}{2}), \quad (9)$$

where a and $a^\dagger$ are defined as usual, and ω_0 is an effective frequency. Now the dissipative part (3) of the Liouvillian reads

$$L_d X = (k_B T\gamma/2i\hbar\omega_0)[a + a^\dagger, S[a + a^\dagger, K^{-1}X]]. \quad (10)$$

To obtain the spectral decomposition of the Liouvillian we perform a similarity transformation

$$UX = \sum_{k,l=0}^{\infty} (k!\,l!)^{-1}(1-\exp\Omega_0)^{-k} a^{\dagger k}a^l X a^{\dagger l}a^k ,$$

where $\Omega_0 = \hbar\omega_0/k_B T$. Operating with the transformed Liouvillian ULU^{-1} upon the dyadic product $|k\rangle\langle l|$ of eigenstates $|k\rangle$, $|l\rangle$ of the Hamiltonian (9) one finds that ULU^{-1} leaves the sum of quantum numbers $N = k + l$ invariant. Hence, the eigenvalue problem $-iULU^{-1}\psi = \lambda\psi$ separates into finite-dimensional subproblems. For $N=0$ we obtain $\lambda^{(0)} = 0$ and $\psi^{(0)} = |0\rangle\langle 0|$. With use of (10) the corresponding eigenvector of $-iL$ is found to be the equilibrium density matrix $\rho_\beta = U^{-1}|0\rangle\langle 0|$.

For $N=1$ the eigenvectors of $-iULU^{-1}$ are linear combinations of $|0\rangle\langle 1|$ and $|1\rangle\langle 0|$. The eigenvalues are given by the classical expressions

$$\lambda_{1,2}^{(1)} = -\tfrac{1}{2}\gamma \pm i\omega ,$$

where $\omega^2 = \omega_0^2 - \frac{1}{4}\gamma^2$. We have assumed that $\gamma < 2\omega_0$. The $N=1$ subproblem determines the time evolution of correlation functions of p and q and the associated response functions completely. For instance, the canonical q-q correlation function is found to be

$$C_{qq}(t) = \frac{k_B T}{m\omega_0^2}\, e^{-\gamma t/2}\left(\cos\omega t + \frac{\gamma}{2\omega}\sin\omega t\right).$$

$N>1$ must only be considered if the evolution of nonlinear functions of p and q is investigated.

For $N=2$ the eigenvectors ψ^2 are linear combinations of $|2\rangle\langle 0|$, $|1\rangle\langle 1|$, and $|0\rangle\langle 2|$, and we are led to the eigenvalue problem of a 3×3 matrix. For small values of $\Omega_0 = \hbar\omega_0/k_B T$ the eigenvalues can be calculated perturbatively. Disregarding terms of the third order in Ω_0 we obtain

$$\lambda_1^{(2)} = -\gamma\left[1 + \tfrac{1}{12}(1+\gamma^2/2\omega^2)\Omega_0^2\right],\ \lambda_{2,3}^{(2)} = -\gamma\left[1 - \frac{1}{12}\frac{\omega_0^2}{\omega^2}\Omega_0^2\right] \pm 2i\omega\left[1 - \frac{1}{6}\frac{\gamma^2}{\omega^2}\left(\frac{\omega_0}{\omega} - 1\right)\Omega_0^2\right]. \quad (11)$$

These eigenvalues differ from those of the Fokker-Planck operator for the classical damped harmonic oscillator. However, for $\Omega_0 \to 0$ the correct classical eigenvalues are recovered. The eigenvalues (11) determine, e.g., the relaxation of the kinetic energy $p^2/2m$.

The damped quantum oscillator has been treated frequently by others. For a survey we refer to the articles by Haake[1] and Lax[7] and references cited therein. It should be noted that in most of the previous work an approximate Markovian description has been obtained by using the strength of the coupling to the reservoir as a small parameter. Often, the rotating wave approximation has also been used. The resulting weak-coupling master equation describes a weakly damped oscillator where $\gamma \ll \omega_0$ and $\hbar\gamma \ll k_B T$. These conditions are satisfied, e.g., for a quantum optical oscillator.

In contrast, we have carried out an adiabatic approximation using the mass ratio as a small parameter. Our master equation describes slow, possibly overdamped systems, and systems at low temperature. It can be used to study, e.g., the influence of dissipation on macroscopic quantum behavior. Finally we mention that for a weakly damped harmonic oscillator the spectral functions calculated from our master equation match those derived from the weak-coupling master equation near the resonance ($\omega \approx \omega_0$).

[1]H. Haken, *Encyclopedia of Physics* (Springer, Heidelberg, 1969), Vol. 25, Pt. 2C; F. Haake, *Springer Tracts in Modern Physics* (Springer, Heidelberg, 1973), Vol. 66; E. B. Davies, *Quantum Theory of Open Systems* (Academic, London, 1976); R. W. Hasse, Rep. Prog. Phys. 41, 1027 (1978); J. Messer, Acta Phys. Austriaca 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]For a recent review, see H. Grabert, *Springer Tracts in Modern Physics* (Springer, Heidelberg, 1982), Vol. 95.

[5]A detailed derivation will be published elsewhere.

[6]R. Kubo, Rep. Prog. Phys. 29, 255 (1966).

[7]M. Lax, Phys. Rev. 172, 350 (1968).