

## On High-Temperature Markovian Equation for Quantum Brownian Motion.

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**Abstract.** - It is shown that a systematic Markovian approximation yields a given new term to the known master equation, ensuring conservation of positivity for arbitrary initial conditions and for all times.

There is a rather long history of searches for the quantum analogue of the classical Brownian motion. For a given model of particle-reservoir interaction, several independent calculations [1-4] have yielded the following master equation (ME) for the statistical operator  $\rho$  of the Brownian particle, in the high-temperature ( $T$ ) limit:

$$\dot{\rho} = -\frac{i}{\hbar}[H_R, \rho] - \frac{i}{\hbar}\gamma[x, \{p, \rho\}] - \frac{1}{2}\gamma\lambda_{dB}^{-2}[x, [x, \rho]], \quad (1)$$

where  $x, p$  are the canonical coordinate and momentum, respectively,  $\gamma$  is proportional to the friction coefficient. The operator  $H_R$  stands for the (renormalized) Hamiltonian.  $\lambda_{dB}$  denotes the thermal de Broglie wavelength of the Brownian particle of mass  $M$ :

$$\lambda_{dB} = \hbar/\sqrt{4MkT}. \quad (2)$$

The ME (1) is dedicated to high-temperature applications. Nevertheless, it turns out [5, 6] that there are further restrictions on applicability. The coherent length (or lengths) pertaining to the state  $\rho$  must always be greater than the thermal de Broglie wavelength (2), otherwise the ME (1) tends to violate the positivity of  $\rho$ . For example, the ME (1) cannot be applied to wave packets (nor to any superposition or mixture of wave packets) of widths less than  $\lambda_{dB}$ .

The violation of positivity does not occur for MEs of the Lindblad class [7]. To turn the ME

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(1) into the Lindblad form it is most easy to append a further double commutator to its r.h.s.:

$$\dot{\rho} = -\frac{i}{\hbar}[H_R, \rho] - \frac{i}{\hbar}\gamma[x, \{p, \rho\}] - \frac{1}{2}\gamma\lambda_{dB}^{-2}[x, [x, \rho]] - \frac{1}{2}\kappa\gamma\lambda_{dB}^2\hbar^{-2}[p, [p, \rho]]. \quad (3)$$

This equation belongs to the Lindblad class provided the numeric constant  $\kappa$  satisfies the condition  $\kappa > 1$ .

There is an apparent discrepancy between our ME (3) on the one hand, and several exact calculations [1-4,8] on the other, suggesting the lack of  $[p, [p, \cdot]]$  term in the exact evolution equations. In the Markovian approximation, the usual time-coarse-graining will, however, induce a  $[p, [p, \cdot]]$  term even if it were absent in the exact fine-grained equations.

Simply to illustrate such a mechanism heuristically, we show that a particular coarse-graining of the ME (1) would lead to the ME (3). Consider the ME (1) in interaction picture. Then the double commutator reads  $[x(t), [x(t), \cdot]]$ . Replace time  $t$  by  $t + \tau$ , where  $\tau$  is a random variable of zero mean and of variance  $\approx \hbar/kT$ ; then insert  $x(t + \tau) = x(t) + p(t)\tau/M$  and take the average over the random  $\tau$ . Finally one obtains  $[x(t), [x(t), \cdot]]$  plus  $\approx (\hbar/kT)^2$  times  $[p(t), [p(t), \cdot]]$ , in accordance with the ME (3).

We are going to show that the heuristically introduced new term of the ME (3) can be, in fact, derived from the Markovian approximation of the exact evolution equation. For concreteness, we follow the calculations of ref.[1]. In coordinate representation, the evolution equation of the statistical operator  $\rho$  takes the general form

$$\dot{\rho}(x, y, t) = \int J(x, y, t; x', y', 0)\rho(x', y', 0)dx'dy'. \quad (4)$$

For the concrete dynamical model, the so-called superpropagator  $J$  is expressed by the following double-functional integral over paths  $x(\tau)$ ,  $y(\tau)$ :

$$J(x, y, t; x', y', 0) = \int \int Dx Dy \exp \left[ \frac{i}{\hbar} \left\{ S_R[x] - S_R[y] - M\gamma \int_0^t (x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x}) d\tau + i\Phi[x, y] \right\} \right], \quad (5)$$

where  $S_R$  is the (renormalized) classical action.

This form already contains the Markovian approximation! The dissipation integrand  $(x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x})$  is the result of time-coarse-graining. The original memory kernel—the retarded Green's function of the reservoir—has been replaced by  $M\gamma\delta'(\tau - s)$ . This replacement can be justified if the cut-off frequency  $\Omega$  of the reservoir is much larger than the (renormalized) characteristic frequency  $\omega_R$  of the particle dynamics [1]. Note that this assumption has nothing to do with the temperature  $T$ .

The fluctuation functional  $\Phi[x, y]$  in eq. (5) has the following exact form:

$$\Phi[x, y] = \frac{2M\gamma}{\pi} \int_0^\Omega \text{ctgh} \frac{\hbar\nu}{2kT} \int_0^t \int_0^\tau [x(\tau) - y(\tau)] \cos \nu(\tau - s)[x(s) - y(s)] ds d\tau d\nu. \quad (6)$$

Here one makes two assumptions. The first is the Markovian assumption  $\Omega \gg \omega_R$  already applied to the dissipation term. The second one assumes high temperature:  $kT \gg \hbar\Omega$ . Under

these conditions, we obtain the following expansion of the fluctuation functional:

$$\Phi[x, y] = \frac{2kT\gamma M}{\hbar} \int_0^t [x(\tau) - y(\tau)]^2 d\tau + \frac{\hbar\gamma}{6kTM} \int_0^t [\dot{x}(\tau) - \dot{y}(\tau)]^2 d\tau + \dots, \quad (7)$$

where the ellipse concerns terms containing higher-order time derivatives of the coordinates  $x$  and  $y$ , with coefficients of higher power of  $1/T$ . (The form (7) was achieved [6] by the Taylor expansion of  $\text{ctgh}(\hbar\nu/2kT)$ , followed by partial integrations over  $t$  and  $\tau$ . To order  $1/T$ , two further terms proportional to  $\hbar\Omega/kT$  have been ignored due to the high-temperature limit  $kT \gg \hbar\Omega$ .)

If one [1] only retains the first term on the r.h.s. of eq. (7), the ME (1) follows from eqs. (4) and (5). As was mentioned earlier, this ME is of limited validity because it does not belong to the Lindblad class. One tends, nevertheless, to believe that there is a natural hierarchy of systematic Markovian approximations yielding MEs of Lindblad class. In the lowest order one neglects all time derivatives of the coordinates  $x, y$  in expressions (5) and (7). This choice would lead to the oversimplified Lindblad ME

$$\dot{\rho} = -\frac{i}{\hbar}[H_R, \rho] - \frac{1}{2}\gamma\lambda_{\text{dB}}^2[x, [x, \rho]], \quad (8)$$

which describes fluctuation of coordinate without incorporating dissipation. In the next order of approximation one considers velocities  $\dot{x}, \dot{y}$ , too, in the expression of  $J$  but one still ignores accelerations (actually the ellipse on the r.h.s. of eq. (7)). The corresponding ME takes the wanted form (3) with  $\kappa = 4/3$ . This equation, first derived in ref. [6], is the simplest systematic Markovian approximation taking dissipation into account. It belongs to the Lindblad class ensuring consistency, *e.g.* conservation of positivity of the statistical operator for all initial conditions and for all times.

Finally we note that every Lindblad ME associates pure-state quantum stochastic equations [9-11]. Examples given in ref. [12, 13] suggest that quantum Ito equations offer a unique tool to investigate the phase space behaviour and classical limit of the quantum Brownian motion.

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