Classical limit of quantum Brownian probability

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(Received 11 October 1995)

We propose a Maxwellian-type initial density matrix for a quantum particle placed in an Ohmic environment. The resulting positional Brownian variance is analytically separated into a classical contribution of Chandrasekhar, and a quantum correction term depending upon $\hbar$ and the input width.

PACS number(s): 05.40.+j

I. INTRODUCTION

Extensive literature exists on the theory of the Brownian motion, both quantum [1–3] (based on the Feynman-Vernon type influence functionals and on the master equations) as well as classical [4–6] (employing the Langevin and Focker-Planck equations). Although the quantal basis of the Langevin equation is well understood [2] yet, surprisingly, the quantum-bath model authors have not explicitly discussed so far the classical limit of their time-dependent Brownian probabilities, and indeed their formalisms have certain limitations in this context. For example, let us consider a quantum harmonic oscillator subjected to a general environment at a specified temperature, and look at the treatments of Refs. [1–3].

The reduced density matrix element $\rho_{p_0}(x_f,x_f,t)$ derived by Caldeira and Leggett [1] contains several rather complicated, unevaluated, multiple integrals. Next, the positional variance $\langle q^2\rangle_t$ at the thermal equilibrium calculated by Grabert, Schramm, and Ingold [2] is, naturally, constant in time but it cannot give information about the rich time dependence of the variances at early epochs. Lastly, since the wave packet taken by Hu, Paz, and Zhang [3] has no input momentum dependence, any additional structure with respect to the temperature cannot enter their positional spread $\sigma(t)$ even when a thermal velocity averaging is performed; and, furthermore, their quoted expression for $\sigma(t)$ has serious misprints. The aim of the present paper is to logically overcome the said limitations of the bath models, enabling us firstly to retrieve the well-known classical variances reported by Chandrasekhar [4] and secondly to identify the explicit $\hbar$ and width-dependent quantum corrections to these variances assuming for simplicity Ohmic dissipation at high temperatures.

II. THEORY

Consider a quantum oscillator of mass M and renormalized angular frequency ω_R interacting via the coefficient of friction γ with an Ohmic bath specified by temperature T and a continuous spectrum having an upper cutoff Ω. Following Caldeira and Leggett [1], the reduced density matrix diagonal element is written as

$$\rho_{p_0}(x_f,x_f,t)\propto\exp\left\{\frac{-N^2(x_f-p_0/2N)^2}{2\sigma_0^2K_1^2+\hbar C_1}\right\}, \tag{1}$$

where x_f is the position, t the time, p_0 the input momentum of an initial wave packet of width σ_0 centered at the origin, $\omega=(\omega_R^2-\gamma^2)^{1/2}$ the under-damped oscillator frequency, and

$$N=\frac{M\omega\ \exp(\gamma t)}{2\ \sin\omega t};\quad K_1=\frac{M\omega\ \cot\omega t+M\gamma}{2}, \tag{2}$$

$$C_1=\frac{\hbar}{8\sigma_0^2}+\frac{M\gamma}{\pi\ \sin^2\omega t}\int_0^\Omega d\nu\int_0^t d\tau\int_0^t ds\ \nu\ \coth\left(\frac{\hbar\nu}{2kT}\right)\sin\omega(t-\tau)\cos\nu(\tau-s)\sin\omega(t-s)\times\exp[\gamma(\tau+s)]. \tag{3}$$

This integral is left unevaluated in Ref. [1]. In order to unravel the link of Eqs. (1)–(3) with Chandrasekhar's [4] classical theory we proceed via the following steps.

Step (i). By Ehrenfest's theorem, the input wave packet is an analog of a classical particle of initial position $x_o=0$ and simultaneous momentum p_0. Hence it is logical to assume the initial distribution of p_0 to be Maxwellian corresponding to the temperature T, i.e., the initial density operator $\hat{\rho}^0$ proposed by us is

$$\hat{\rho}^0\propto\int_{-\infty}^{\infty}dp_0\exp\left(\frac{-p_0^2}{2MkT}\right)|\Psi^0\rangle\langle\Psi^0|, \tag{4}$$

where $|\Psi^0\rangle$ is the standard minimum uncertainty wave packet state [7] centered at the origin. From Eq. (1), a straightforward Gaussian integration over p_0 enables us to construct the positional quantum Brownian probability density P as

$$P(x_f,t)\propto\int_{-\infty}^{\infty}dp_0\exp\left(\frac{-p_0^2}{2Mkt}\right)\rho_{p_0}(x_f,x_f,t), \tag{5}$$

$$\propto\exp(-x_f^2/2\sigma^2), \tag{6}$$

with the exact quantum variance of the under-damped oscillator as

$$\sigma^2=\frac{MkT}{4N^2}+\frac{2\sigma_0^2K_1^2+C_1}{2N^2}, \tag{7}$$

Step (ii). Next, we use the known fact [1–3] that in the limit of the small Planck constant and high temperature, the effective action of the bath models leads directly to the

Langevin trajectories provided one replaces, inside the fluctuation-dissipation kernels,

$$\coth\left(\frac{\hbar\nu}{2kT}\right)\approx\frac{2kT}{\hbar\nu}\left\{1+\frac{1}{12}\left(\frac{\hbar\nu}{kT}\right)^2\right\};\quad \frac{\hbar\nu}{kT}\ll 1. \tag{8}$$

Going back to Eq. (3), for fixed τ and s with $\Omega\to\infty$, we readily perform the ν integration, remembering that $\int_0^\infty d\nu\,\cos\nu(\tau-s)=\pi\delta(\tau-s)$ and $\int_0^\infty d\nu\,\nu^2\cos\nu(\tau-s)=-\pi\partial^2\delta(\tau-s)/\partial\tau^2$. Next, we integrate trigonometrically over τ and s to obtain, after some rearrangement,

$$C_1=\hbar/(8\sigma_0^2)+(2\hbar\omega_R^2\sin^2\theta)^{-1}MkT\omega^2[\{1+\epsilon^2\times(1-\gamma^2/\omega^2)\}J_1+2\epsilon^2\gamma^2J_2/\omega^2]e^{2\gamma t}, \tag{9a}$$

$$\theta=\omega t;\quad \epsilon^2=(\hbar\omega/kT)^2/12, \tag{9b}$$

$$J_1=1-(1+\gamma\omega^{-1}\sin 2\theta+2\gamma^2\omega^{-2}\sin^2\theta)e^{-2\gamma t}, \tag{9c}$$

$$J_2=1-(1+\gamma\omega^{-1}\sin 2\theta-2\sin^2\theta)e^{-2\gamma t}. \tag{9d}$$

Step (iii). Next, we substitute the values of the functions N, K_1, and C_1 [cf. Eqs. (2), (9)] into Eq. (7) to arrive at the main finding of this paper, viz.

$$\sigma_{ho}^2=\sigma_{ho}^{\text{cl}^2}+\sigma_{ho}^{qu^2}, \tag{10a}$$

$$\sigma_{ho}^{\text{cl}^2}=(kT/M\omega_R^2)[1-\zeta^2e^{-2\gamma t}], \tag{10b}$$

$$\zeta=\cos\theta+\gamma\omega^{-1}\sin\theta, \tag{10c}$$

$$\sigma_{ho}^{qu^2}=\frac{kT}{M\omega^2}\left[\frac{M\omega^2}{kT}\left(\sigma_0^2\zeta^2+\frac{\hbar^2\sin^2\theta}{4M^2\omega^2\sigma_0^2}\right)e^{-2\gamma t}+\epsilon^2\left\{1-\left(1+\frac{\gamma}{\omega}\sin 2\theta-\frac{2\gamma^2}{\omega^2}\sin^2\theta\right)e^{-2\gamma t}\right\}\right], \tag{10d}$$

where the label ho stands for the harmonic oscillator. The term $\sigma_{ho}^{\text{cl}^2}$ is the classical variance and it is very satisfying to find that it coincides exactly with Langevin-equation based result given by Chandrasekhar [4] for an over-damped oscillator having parameters

$$\beta=2\gamma,\quad \beta_1=-2i\omega=(\beta^2-4\omega_R^2)^{1/2}. \tag{11}$$

Several properties of Eqs. (10) are worth mentioning for $t>0$. The term $\sigma_{ho}^{qu^2}$ represents the quantum correction to the variance arising from three causes, viz. finiteness of $\hbar$, existence of an initial spread σ_0, and the spectral density parameter ϵ of Eq. (9b). Next, Eq. (10d) shows that $\sigma_{ho}^{qu}\to\infty$ for $\sigma_0\to\infty$ which is natural because the initial wave packet is now too fuzzy. Also, $\sigma_{ho}^{qu}\to\infty$ if $\sigma_0\to 0$ which is expected [7] because the initial state, now being a position eigenstate, has infinite uncertainty in momentum. Clearly, in both these situations the probability $P(x_f,t)$ given by Eq. (6) tends to become position independent, implying that the variances deviate very significantly from the classical prediction both for $\sigma_0\to 0$ and $\sigma_0\to\infty$.

An important question now arise, viz. for what choice of the parameter σ_0 will our σ_{ho}^{qu} become negligible compared to Chandrasekhar's σ_{ho}^{cl} at all times? To answer this question, we consider the case of the *weak* damping ($\gamma\ll\omega_R$) and recall that a quantum oscillator of angular frequency ω has a ground state size of order $a_0=(\hbar/M\omega)^{1/2}$. Since the input wave packet should, semiclassically, correspond to a large oscillator quantum number, we expect its minimal width to be measured by a_0 itself, implying that

$$\sigma_0=\left(\frac{\hbar}{M\omega}\right)^{1/2}O_1;\quad \epsilon=\frac{\hbar\omega}{kT}O_1=\frac{\lambda^2}{\sigma_0^2}O_1, \tag{12}$$

where $\lambda=(\hbar^2/MkT)^{1/2}$ is the thermal de Broglie wavelength, and the symbol O_1 denotes quantities of *order* unity. Substituting the value of σ_0 into Eq. (10) we estimate

$$\sigma_{ho}^{\text{cl}^2}=(kT/M\omega_R^2)[1-O_1e^{-2\gamma t}], \tag{13a}$$

$$\sigma_{ho}^{qu^2}=(kT/M\omega_R^2)[\epsilon O_1e^{-2\gamma t}+\epsilon^2\{1-O_1e^{-2\gamma t}\}]. \tag{13b}$$

Hence classical Brownian motion of the weakly damped oscillator becomes valid at all times provided $\epsilon\ll 1$, i.e., $\lambda\ll\sigma_0$, i.e., $\hbar\omega\ll kT$ [cf. Eq. (12)].

Step (iv). Finally, let us consider a free Brownian particle labeled by the suffix fp. The corresponding quantum variance is deduced readily from Eq. (10) by taking the limit $\omega_R\to 0$, $\omega\to i\gamma$ and we obtain $\sigma_{fp}^2=\sigma_{fp}^{\text{cl}^2}+\sigma_{fp}^{qu^2}$ where

$$\sigma_{fp}^{ci^2}=(kT/2M\gamma^2)[-1+2\gamma t+e^{-2\gamma t}], \tag{14a}$$

$$\sigma_{fp}^{qu^2}=\frac{kT}{M\gamma^2}\left[\frac{M\gamma^2}{kT}\left\{\sigma_0^2+\frac{\hbar^2(1-e^{-2\gamma t})^2}{16M^2\gamma^2\sigma_0^2}\right\}+|\epsilon_{fp}|^2\{1-(2-e^{-2\gamma t})e^{-2\gamma t}\}\right] \tag{14b}$$

with $|\epsilon_{fp}|^2=(\hbar\gamma/kT)^2/12$. It is again gratifying to find that our $\sigma_{fp}^{\text{cl}^2}$ exactly coincides with Chandrasekhar's [4] classical expression in the one-dimensional case (when $\langle p_0^2\rangle=kT/M$). Also, a sufficient condition for the quantum correction to the variance to be negligible is to set

$$\sigma_0=\left(\frac{\hbar}{M\gamma}\right)^{1/2}O_1;\quad |\epsilon_{fp}|=\frac{\hbar\gamma}{kT}O_1=\frac{\lambda^2}{\sigma_0^2}O_1\ll 1. \tag{15}$$

III. CONCLUSIONS

Our formalism based on Eqs. (5)–(15) is not available in the existing literature on the quantum Brownian probabilities of either the harmonic oscillator or the free particle. Briefly speaking, we have achieved five things: (A) a Maxwellian-type initial density matrix $\hat{\rho}^0$ has been used; (B) the complicated triple integral function C_1 appearing in the work of Caldeira and Leggett [1] has been analytically evaluated; (C) from the positional quantum variance the classical contribution σ^{cl^2}, which exactly agrees with that of Chandrasekhar [4], has been extracted; (D) the quantum correction piece σ^{qu^2} depending explicitly on the input width has been identified, and (E) the conditions for the validity of the classical motion have been mentioned in terms of the ratio of the thermal de Broglie wavelength to the input width.

Before ending, we wish to point out that the quantum→classical picture of the Brownian movement cannot be successfully achieved if the initial state is prepared in any other manner different from our $\hat{\rho}^0$ in Eq. (5). Indeed, the uses of the equilibrium density matrix [2] or momentum-independent input wave packets [3] have certain limitations with regard to the time or temperature dependence of the Brownian probabilities, as mentioned above in the Introduction.

ACKNOWLEDGMENTS

V.J.M. thanks the University Grants Commission (New Delhi) and N. Chanana thanks the Council of Scientific and Industrial Research for financial support.

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