Quantum Dissipation versus Classical Dissipation for Generalized Brownian Motion

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We try to clarify what are the genuine quantal effects that are associated with generalized Brownian motion. All the quantal effects that are associated with the Zwanzig-Feynman-Vernon-Caldeira-Leggett model are (formally) a solution of the classical Langevin equation. Nonstochastic, genuine quantum mechanical effects are found for a model that takes into account either the disordered or the chaotic nature of some environment.　　[S0031-9007(97)02879-2]

The motion of a particle in 1D, under the influence of an environment, is commonly described in the classical literature by an appropriate generalization of Langevin equation [1–3]

$$m\ddot{x} + \eta\dot{x} = \mathcal{F}. \tag{1}$$

Here m and η are the mass of the particle and the friction coefficient, respectively. Implicit is an ensemble average over realizations of the random force $\mathcal{F}$. In the standard Langevin equation it represents stationary "noise" which is zero upon averaging, and whose autocorrelation function is

$$\langle \mathcal{F}(t)\mathcal{F}(t')\rangle = \phi(t - t'). \tag{2}$$

This phenomenological description can be derived formally from an appropriate Hamiltonian $\mathcal{H} = \mathcal{H}_0(x, p) + \mathcal{H}_{\text{env}}$, where the latter term incorporates the interaction with environmental degrees of freedom. The reduced dynamics of the system may be described by the propagator $\mathcal{K}(R, P|R_0, P_0)$ of the probability density matrix. For the sake of comparison with the classical limit, one uses the Wigner function $\rho(R, P)$ in order to represent the latter. In some cases, using Feynman-Vernon (FV) formalism [4], an exact path-integral expression for the propagator is available [3]. The FV expression is a double sum $\int\int \mathcal{D}x'\,\mathcal{D}x''$ over the path variables $x'(\tau)$ and $x''(\tau)$. It is convenient to use new path variables $R = (x' + x'')/2$ and $r = (x'' - x')$, and to transform the $\int\int \mathcal{D}R\mathcal{D}r$ integral into the form [5]

$$\mathcal{K}(R, P|R_0, P_0) = \int_{R_0, P_0}^{R,P} \mathcal{D}R\,\mathcal{K}[R], \tag{3}$$

where $\mathcal{K}[R]$ is a real functional, which is defined by the expression,

$$\mathcal{K}[R] = \int \mathcal{D}r\, e^{i(1/\hbar)(S_{\text{free}} + S_F)} e^{-(1/\hbar^2)S_N}. \tag{4}$$

The $\mathcal{D}r$ integration is unrestricted at the end points, and the free action functional is $S_{\text{free}}[R, r] = -m\int_0^t d\tau \times \ddot{R}r$. The action $S_F[R, r]$ corresponds to the friction and the action $S_N[R, r]$ corresponds to the noise. The latter are, in general, nonlocal functionals of the path variables (there may be long-time interactions between different

paths segments). Still, in practice, it is desirable to find a master equation of the form

$$\frac{\partial \rho}{\partial t} = \mathcal{L}\,\rho \tag{5}$$

that generates essentially the same dynamical behavior. Alternatively, it is desirable to find an appropriate Langevin equation of the form (1) that reproduces the reduced dynamics in phase space.

At this stage it is appropriate to gather few questions that are of conceptual significance: (a) What are the essential ingredients that define generic generalized Brownian motion (GBM)? (b) What are the necessary requirements on $\mathcal{H}_{\text{env}}$ for having generic GBM? (c) If $\mathcal{H}_{\text{bath}}$ is strongly chaotic, what is the minimal number of degrees of freedom which are required? (d) Is it possible to reproduce any generic GBM by assuming a coupling to an appropriate bath that consists of (infinitely many) oscillators? (e) Is it possible to reproduce any generic GBM by an appropriate master equation? (f) Is it possible to reproduce any generic GBM by an appropriate Langevin equation? (g) In the latter case, what is the relation between the noise and the friction, should fluctuation dissipation theorem be modified? Most frequently, questions (b) and (c) are emphasized. This Letter intends to introduce partial answers to the rest, less emphasized questions.

Classically, the answers for all the questions [(a)–(g)] are known [6,7]. Any generic $\mathcal{H}_{\text{env}}$ leads to a simple BM that is described by (1) with friction which is proportional to velocity and white noise $\phi(\tau) = 2\eta k_B T\delta(\tau)$ in consistency with the classical fluctuation-dissipation theorem. The environment should consist of at least 3 degrees of freedom with *fast* chaotic dynamics. *Fast* implies that the classical motion is characterized by a continuous spectrum with high frequency cutoff, such that the motion of the environment can be treated adiabatically with respect to the *slow* motion of the system. One can use a bath that consists of infinitely many oscillators in order to reproduce (1). Note that an oscillator bath is obviously *nongeneric* since it consists of nonchaotic degrees of freedom. Thus, the spectral distribution of the oscillators should be chosen in a *unique* way that mimics the generic spectral function and, consequently, reproduces the simple BM behavior.

We are interested in this Letter in *quantized* BM. In order to be consistent with the terminology that prevails in the literature, we shall use the notation "BM model" in a restricted sense as referring to the quantization of (1) with (2). The notation "GBM" suggests that a satisfactory model should generate *additional* physical effects. Referring to question (a), let us try to list the ingredients that should be associated with GBM: (I) fluctuations due to noise; (II) dissipation of energy due to friction effect; (III) dissipative diffusion due to competition between friction and noise; (IV) nondissipative diffusion due to "random walk" dynamics; (V) quantum localization due to quenched disorder; (VI) destruction of coherence due to dephasing. This list is intended to make a distinction between qualitatively different effects that are associated with the *reduced* dynamics, irrespective of the actual mechanism which is responsible for them.

Quantum mechanically, it would be desirable to derive first, as in the classical theory, a general description of BM, and only later to address question (d). However, this turns out to be impossible, unless uncontrollable approximations are made. Therefore we shall take the other way around. Referring to question (d), it is natural to discuss first the standard model for BM, where linear coupling to a large set of harmonic oscillators is assumed [2]. This model has been used extensively in the literature. Caldeira and Leggett (CL) and followers [3] have used it to analyze "quantum BM" that corresponds to (1) with (2). There, in the limit of high temperatures, $\phi(\tau) = 2\eta k_B T \delta(\tau)$ which coincides with the classical limit. The friction action functional is

$$S_F = -\eta \int_0^t d\tau \, \dot{R} r \,, \qquad (6)$$

and the noise functional is

$$S_N[R, r] = \frac{1}{2} \int_0^t \int_0^t d\tau_1 \, d\tau_2 \, \phi(\tau_2 - \tau_1) r(\tau) r(\tau') \,. \qquad (7)$$

In the absence of noise the $\mathcal{D}r$ integration is easily performed, leading to $\mathcal{K}[R] = \prod_\tau \delta(m\ddot{R} + \eta\dot{R})$. Furthermore, FV have observed [4] that S_N can be interpreted as arising from averaging over the realizations of the classical c-number random force $\mathcal{F}$. Thus, the reduced dynamics of the particle can be reproduced by the classical Langevin equation (1) with appropriate $\phi(\tau)$. Note, however, that $\phi(\tau)$ will depend on $\hbar$ in accordance with the fluctuation-dissipation theorem. In particular, the suppression of "normal" diffusion at low temperatures [3] can be interpreted as arising from negative noise autocorrelations [8]. Also, the relaxation of a quantal harmonic oscillator to its ground state, the dynamics of quantal parametric oscillator with dissipation, and the dynamics of the quantal kicked rotator with dissipation can be simulated by assuming the same type of noise (the latter case is analyzed in [9]). There is a somewhat more transparent way to observe that the FV-CL path-integral expression is formally identical with

its classical limit [for a given $\phi(\tau)$]. With (6) and (7), expression (4) for $\mathcal{K}[R]$ becomes invariant under the replacement $\hbar \to \lambda\hbar$. This replacement is compensated by the scaling transformation $r \to \lambda r$ of the auxiliary path variable.

The observation that quantum BM (in the restricted sense discussed above) is formally equivalent to the solution of a classical Langevin equation with colored noise is probably not new, though there is no obvious reference for it. This is probably the reason for the existence of extensive literature which utilizes rather lengthy "quantum mechanical formalism" in order to derive essentially classical results. However, there is a deeper reason for considering "quantum dissipation" as distinct from "classical dissipation" which is concerned with the extensive usage of the master equation approach. In this approach the commonly used Markovian approximation generates "nonclassical" correction. It is frequently left either unnoticed or unclarified, as in a recent publication [10], that the resultant nonclassical feature is an *artifact of the formalism* rather than of the model itself. In the Appendix this point is illustrated by considering a specific example.

The standard BM motion that is modeled by (1) with (2) is not rich enough to generate effects that are associated with the possibly disordered nature of the environment [ingredients (IV) and (V)]. In [5] we have introduced a unified model for the study of diffusion localization and dissipation (DLD). The DLD model is defined in terms of the path-integral expression (3) with

$$S_F = \eta \int_0^t d\tau \, w'\big(r(\tau)\big)\dot{R}(\tau) \qquad (8)$$

for ohmic friction. The general expression for the noise action functional is

$$\begin{aligned} S_N[x', x''] = \frac{1}{2} \int_0^t \int_0^t d\tau_1 \, d\tau_2 \, \phi(\tau_2 - \tau_1) \\ \times \big[w(x_2'' - x_1'') + w(x_2' - x_1') \\ - 2w(x_2'' - x_1') \big], \qquad (9) \end{aligned}$$

where x_i is a short notation for $x(\tau_i)$. (For white noise, see the simplified expression (13) below.) Both functionals depend on the normalized spatial-autocorrelation function $w(x - x')$ of the disordered environment. For definiteness we have assumed

$$w(x - x') = \ell^2 \exp\left[-\frac{1}{2}\left(\frac{x - x'}{\ell}\right)^2 \right]. \qquad (10)$$

The various derivations of the DLD model are discussed in [5]. Here we note its various limits: (A) In the classical limit it constitutes a formal solution of (1), where $\mathcal{F}(x, t) = -\mathcal{U}'(x, t)$ and

$$\langle \mathcal{U}(x, t)\mathcal{U}(x', t') \rangle = \phi(t - t')w(x - x') \,. \qquad (11)$$

(B) In the limit $\ell \to \infty$ it reduces to the standard BM model. (C) By dropping the friction functional S_F, one

obtains the case of the nondissipative noisy disordered environment. (D) By further taking the limit of $\phi(\tau) = $ const, one obtains the case of quenched disorder.

The *classical* DLD model is similar to the BM model for *short-time correlated noise,* such that $\phi(\tau)$ can be approximated by a delta function (white noise approximation). However, for short-time correlated noise with negative correlations $[\int_0^\infty d\tau\, \phi(\tau) \to 0]$, one cannot avoid considering the interplay with the disorder. This is the case of "superohmic" noise and also of low-temperature "ohmic noise." In the latter case $\phi(\tau) = -(C/\pi)(1/\tau^2)$ for $\tau_c < \tau$, where τ_c is a very short time scale and $C = \hbar\eta$. For BM (no disorder) the spatial spreading is $\sigma_{\text{spatial}} \sim [(C/\eta^2)(2/\pi)\ln t]^{1/2}$ with a Gaussian profile, while for the DLD model in the same circumstances [5]

$$\mathcal{K}(R|R_0) = \text{const} \times \exp\left(-\frac{|R - R_0|}{\left[4\sqrt{\frac{2}{\pi}}\left(\frac{1}{\eta^2\ell}\right)C\right]}\right). \quad (12)$$

Here $P_0 = 0$, and an integration over the final P has been performed. Note that there is a smooth crossover from the BM logarithmic "diffusion" (faint noise, dispersion on a scale less than ℓ) to the DLD frozen profile (stronger noise, dispersion on a scale larger than ℓ). The classical DLD model becomes significantly distinct from the BM model for *long-time correlated noise.* In particular, in the limit of quenched disorder, the motion of the particle is bounded. More generally, for long but finite time autocorrelations, or for higher dimensionality, the particle will execute nondissipative random walk diffusion.

The *quantal* DLD model, in contrast with the quantal BM model, does not constitute a formal solution of its corresponding Langevin equation. This leads to some *new* genuine quantal effects. Referring first to the limiting case (D) of *quenched disorder,* one may demonstrate that localization is a natural consequence of the path-integral expression [5]. One should wonder whether such an effect can be generated by a classical Langevin equation with appropriate colored noise. The frozen diffusion profile (12) is probably the best that one can achieve. However, the reduced dynamics is not the same as in the case of quantum localization, since there is a strong velocity-position correlation. Thus, it is claimed that quantal localization cannot be generated by a classical Langevin equation.

There is an additional aspect of the quantal DLD model that cannot be generated by a classical Langevin equation. *The distinction between the quantal DLD model and its classical limit persists even in the limit of high temperatures.* In order to clarify this point, one should substitute $\phi(\tau) = 2k_BT\delta(\tau)$ into (9), yielding

$$S_N[r] = 2\eta K_B T \int_0^t \left[w(0) - w(r(\tau))\right] d\tau, \quad (13)$$

and compare (8) and (13) with their classical limit, which is not by accident (6) and (7), respectively. The quantal expressions [11] differ from the classical ones for $\ell \ll |r|$.

The scaling properties of r with $\hbar$ imply that these large deviations are important for the study of interference and dephasing. Simply by inspection of the action functionals, one may draw two important observations: First, interference in the DLD model is not affected by friction, unlike the BM model. The second observation is that the dephasing factor is

$$\langle e^{i\varphi} \rangle = e^{-S_N[\ell \ll |r|]} = \exp\left[-\frac{2\eta k_BT\ell^2}{\hbar^2}t\right], \quad (14)$$

irrespective of the geometry of the interfering paths $x_a(\tau)$ and $x_b(\tau)$ which are assumed to be well separated with respect to the microscopic scale ℓ [above $r = (x_a - x_b)$]. The latter conclusion should be contrasted with the BM case, where

$$\langle e^{i\varphi} \rangle = \exp\left[-\frac{1}{2}\frac{2\eta k_BT}{\hbar^2}\int_0^t [x_a(\tau) - x_b(\tau)]^2\, d\tau\right], \quad (15)$$

which is essentially the same as the dephasing due to the interaction with extended (electromagnetic) field modes [12]. Thus, dephasing due to the interaction with disordered environment (e.g., localized impurities) is qualitatively different. Further discussion, semiclassical considerations, and specific examples will appear in [5]. In particular, it is interesting to note that, due to interference, the familiar diffusive behavior is modified by a ballistic component that decays exponentially in time as in (14).

Finally, we should refer to question (d) which is also intimately related to question (g) concerning the role of fluctuation-dissipation theorem. One should ask whether the DLD model is the "ultimate" model for the description of BM in the most generalized way (as far as generic effects are concerned). In the case of 2D generalized BM, one should also consider the effect of "geometric magnetism" [13], which is not covered by the 1D DLD model. Here we limited the discussion to 1D BM. In order to answer this question, one should consider a general nonlinear coupling to a thermal, possibly chaotic bath. In the limit of weak coupling one may demonstrate [5] that indeed the bath can be replaced by an equivalent "effective bath" that consists of harmonic oscillators, yielding the DLD model. In the opposite limit of strong coupling, and extremely adiabatic interaction, the reduced dynamics is determined by the ground state energy $E_{\text{env}}(x)$ of $\mathcal{H}_{\text{env}}$, leading to an effective "quenched" disordered potential. Such extreme adiabaticity is probably not very realistic. Gefen and Thouless [14], Wilkinson [7], and Shimshoni and Gefen [14] have emphasized the significance of Landau-Zener transitions as a mechanism for dissipation. There is a possibility that some future derivation will demonstrate that an equivalent "oscillator bath" can also be defined in this case. The existence of such a derivation is most significant, since it implies that no "new effects" (such as geometric magnetism in the case of 2D generalized BM) can be found in the context of 1D generalized BM.

Wilkinson has demonstrated that, due to the Landau-Zener mechanism, anomalous friction, which is not proportional to velocity, arises for the Gaussian orthogonal ensemble (GOE) fermion bath [7]. The BM model cannot generate such an anomalous effect due to a "memory problem" that makes it ill defined. However, one may demonstrate that the *nonohmic* DLD model can be used in order to generate this effect [5].

Appendix.—Here, we shall illustrate how an apparently nonclassical feature may arise due to the application of the Markovian approximation. To demonstrate this point in a transparent way it is best to make a reference to a related recent study [15,16] of the parametric driven harmonic quantum oscillator with ohmic dissipation. This problem has an exact solution using FV formalism [8,15]. In [16], various approximation schemes for $\mathcal{L}$ in (5) have been discussed, leading to an expression of the general form

$$\mathcal{L} = -\frac{p}{m}\,\partial_x + \frac{\eta}{m}\,\partial_p p + \cdots + D_{pp}\partial_p^2 + D_{xp}\partial_x\partial_p\,. \tag{16}$$

(The time-dependent driving term has been omitted for brevity.) The last term is the so-called "Drude correction." Because of this term, the diffusion matrix is no longer positive semidefinite. Kohler *et al.* [16] have correctly pointed out that, consequently, $\mathcal{L}$ has no equivalent Langevin representation. Because of this term, the Wigner function may become negative in some places in phase space. Note, however, that (16) is the best approximation for the actual dynamics within the framework of the master equation approach. We shall now demonstrate that the Drude correction may be derived in a very simple way from the classical Fokker-Planck equation. This derivation also sheds new light on the traditional Markovian approximation which is used within the framework of the master equation approach. Starting from (1), with a definite realization of the random force F, the Liouville equation is $\frac{\partial\rho}{\partial t} = -\nabla(\rho v)$, where $\nabla = (\partial_x,\partial_p)$ and $v = (p/m, F_{\text{total}})$ with $F_{\text{total}} = -\eta p/m - \mathcal{F}(t)$. The first two terms in (16) are immediately obtained, and the additional term due to the random force is $-\mathcal{F}(t)\partial_p\rho$. We now use the identity $\rho|_{\mathcal{F}}[x(t)|_{\mathcal{F}}, p(t)|_{\mathcal{F}}, t] = \rho|_{\mathcal{F}=0} \times [x(t)|_{\mathcal{F}=0}, p(t)|_{\mathcal{F}=0}, t]$, which holds since both sides equal $\rho(x(0), p(0), t = 0)$. One substitutes $x(t)|_{\mathcal{F}} = x(t)|_{\mathcal{F}=0} + \int_0^t G(t,\tau)\mathcal{F}(\tau)d\tau$, where G is the appropriate Green function (response kernel) of (1) with a parametric driving term that should be included. Expanding ρ with respect to $\mathcal{F}$ up to first order, and then averaging $-\mathcal{F}(t)\partial_p\rho$ over realizations of the random

force, one obtains the last two terms in (16). In particular, the Drude term is $D_{xp} = \int_0^t \phi(t-\tau)G(t,\tau)\,d\tau$. It is easy to observe that this result coincides with Eq. (85) of [16]. Evidently, in the high temperature limit (white noise), this term goes to zero. However, at the limit of zero temperature $\phi(\tau)$ constitutes a Fourier transform of $\phi(\omega) = \eta\hbar|\omega|$ in accordance with the fluctuation-dissipation theorem, leading to a diffusion matrix that is no longer positive semidefinite. Thus, we have demonstrated that the Drude correction does not imply that the exact quantum dynamics cannot be generated by an appropriate Langevin equation, rather it is an artifact of the Markovian approximation involved.

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