

Quantum diffusion in a fermionic bath

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We propose a scheme for quantum Brownian motion of a particle in a fermionic bath. Based on the spin coherent-state representation of the noise operators and a canonical thermal distribution of the associated c numbers, we derive a quantum analog of generalized Langevin equation for quantum-mechanical mean position of the particle subjected to an external force field. The approach allows us to map the quantum problem on a classical setting. The quantum dispersion around the mean can be estimated order by order by a set of quantum correction equations up to a desired degree of accuracy for a given nonlinear potential. We derive a quantum diffusion equation for free particle and show that quantization, in general, enhances the mean-square displacement. Increase in temperature leads to suppression of mean-square displacement. The method is based on canonical quantization procedure and may be used for understanding diffusive transport and thermally activated processes in a fermionic bath.

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I. INTRODUCTION

The irregular movement of a particle immersed in a heat bath forms the basic paradigm of quantum Brownian motion [1]. The reservoir constitutes of a very large number of independent degrees of freedom which interact with the particle. Traditionally, the reservoir is considered to be a set of harmonic oscillators with characteristic frequencies. Although, in general, the Hamiltonian for the system-reservoir model is simple, the dynamical evolution of the system after appropriate elimination of the reservoir degrees of freedom poses serious problems for an exact solution. Depending on the issue, various approximations have been introduced to extract out the nature of underlying quantum stochastic processes that govern the dynamics of the system. In general, two distinct situations pertaining to the strength of coupling between the system and the reservoir arise. First, in the field of quantum optics and laser physics, various relaxation processes involving excited atomic states or cavity modes can be described successfully within weak-coupling approximation [1,2], in which the reservoir behaves almost like a free field. On the other hand, the treatment of back reaction of the reservoir on the system which may lead to drastic modification of the dynamics of the system is necessary in polaron theories in condensed-matter physics and Kramers' theory in chemical physics, within the framework of strong-coupling approximation [3–6]. Over the years the system-reservoir model and its variants have been extended in various directions. All these developments have been the part of a large body of literature. We refer to [1–7] for further details.

In this paper we consider a system-reservoir model where the bosonic reservoir is replaced by a fermionic one. The model is a simple generalization of a system of harmonic oscillator plus a reservoir of two-level systems, used many years ago by Sargent *et al.* [2] for description of the dynamics of a cavity mode damped by an atomic beam reservoir.

Our generalization concerns the reduced stochastic dynamics of the system under the influence of an arbitrary external potential field and governed by fermionic noise. The stochastic noise force is related to dissipation by the fluctuation-dissipation relation, which ensures that the overall system is thermodynamically closed. Since the fermions follow anti-commutation rules and have no classical analog, two distinctive features of the fermionic bath are quite imperative. First, the fluctuation-dissipation relation does not reduce to the usual classical fluctuation-dissipation relation. Second, since the temperature dependence of the fermionic bath with infinite degrees of freedom is different from that of its bosonic counterpart, one may encounter anomalous temperature dependence of the diffusive behavior of the particle. The behavior of fermionic reservoir thus makes the quantum stochastic dynamics of the particle quite conspicuous in its own way, particularly at finite temperature. Fermionic bath has attracted considerable attention over several issues. For example, Guinea *et al.* [8] examined three different fermionic Hamiltonians several years ago in connection with the phenomenon of quantum coherence in presence of dissipation. A two-level system strongly interacting with a degenerate Fermi gas has been treated to deal with spontaneous and electron-assisted tunneling [9]. Shao and Hänggi [10] investigated the dynamics of a two-level system coupled to a sea of spin- $\frac{1}{2}$ particles to show that the behavior of spin-spin bath model is similar to that of the spin-boson model at zero temperature and that increasing temperature favors coherent dynamics. Dissipative quantum systems modeled by two-level reservoir coupling have also been analyzed within the framework of the Feynman-Veron theory [11]. The effective potential generated by the system-reservoir interaction leads to “dynamical” localization [12] of the particle at low temperature and within sub-Ohmic regime. The optical conductivity and direct current resistivity have been computed [13] for charge carriers in an external electric field to demonstrate a non-Drude optical conductivity. Fermionic reservoirs are therefore useful for description of the realistic physical situations, such as magnetic relaxation [10,14] of molecular

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crystals of Mn_{12} and Fe_8 , interacting nanomagnets and a spin interacting with effectively independent spin modes or in isolated quantum dot induced by hyperfine interaction with nuclei [15], and ions in normal liquid ^3He [16]. We refer to Rosch [17] for a comprehensive review.

Our aim in this paper is to derive the quantum stochastic dynamics of a particle in contact with a fermionic bath. Based on the coherent-state representation of the fermionic noise operator and a canonical thermal distribution of the associated c numbers of the noise operators comprising the bath, we develop a scheme for quantum Brownian motion in terms of Langevin equation for quantum-mechanical mean position of the particle. The quantum dispersion around the mean can be taken into account by solving a set of correction equations developed order by order depending on the nature of the potential and memory kernel. An important offshoot of this scheme is the derivation of quantum diffusion equation for free particle in a fermionic bath. We show how the increase in temperature suppresses the mean-square displacement of the particle. The present formulation relies on canonical quantization procedure and allows us to implement the classical techniques of nonequilibrium statistical mechanics without much difficulty.

The paper is organized as follows. In Sec. II, the basic model Hamiltonian for the system and the fermionic bath and the operator Langevin equation are introduced. The spin coherent states are used for realizing c -number noise for the bath and the Langevin equation for the quantum-mechanical mean position of particle is derived. In Sec. III, an equivalent description of the quantum stochastic process is formulated in terms of probability distribution function. We have derived the quantum diffusion equation for a free particle. In Sec. IV, the quantum mean-square displacement of the particle in contact with fermionic bath is explored. The paper is concluded in Sec. V.

II. QUANTUM BROWNIAN MOTION FOR A FERMIONIC RESERVOIR

A. Model and the operator Langevin equation

We consider a particle of unit mass coupled to set of spin- $\frac{1}{2}$ fermions with characteristic frequencies ω_k . This is represented by the following Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2} + V(\hat{q}) + \hbar \sum_k \omega_k \hat{\sigma}_k^\dagger \hat{\sigma}_k + \hbar \sum_k g_k \hat{q} (\hat{\sigma}_k^\dagger + \hat{\sigma}_k), \quad (2.1)$$

where \hat{q} and \hat{p} are coordinate and momentum operators of the particle. $\hat{\sigma}_k^\dagger$ ($\hat{\sigma}_k$) is the creation (annihilation) operator for k th fermion. The potential-energy operator $V(\hat{q})$ is due to an external force field acting on the particle. g_k is the coupling constant between the k th fermion and the particle. \hat{q} and \hat{p} follow the usual commutation relation $[\hat{q}, \hat{p}] = i\hbar$. The fermions obey the anticommutation rule $\{\hat{\sigma}_k, \hat{\sigma}_k^\dagger\} = 1$ and the following algebra:

$$\begin{aligned} \hat{\sigma}_k^2 = \hat{\sigma}_k^{\dagger 2} = 0, \quad [\hat{\sigma}_k^\dagger, \hat{n}_k] = -\hat{\sigma}_k^\dagger, \quad [\hat{\sigma}_k, \hat{n}_k] \\ = \hat{\sigma}_k, \quad \text{and} \quad [\hat{\sigma}_k^\dagger, \hat{\sigma}_k] = \hat{\sigma}_{zk}, \end{aligned} \quad (2.2)$$

where the number operator for the fermions is defined as $\hat{n}_k = \hat{\sigma}_k^\dagger \hat{\sigma}_k$. Furthermore it follows from the above relations that $\hat{\sigma}_{zk} = 2\hat{n}_k - 1$.

The Heisenberg equations of motion for the particle and the fermions can be written down from Hamiltonian as follows:

$$\dot{\hat{q}} = \hat{p}, \quad (2.3)$$

$$\dot{\hat{p}} = -V'(\hat{q}) - \hbar \sum_k g_k (\hat{\sigma}_k^\dagger + \hat{\sigma}_k), \quad (2.4)$$

$$\dot{\hat{\sigma}}_k = -i\omega_k \hat{\sigma}_k + ig_k \hat{\sigma}_{zk} \hat{q}, \quad (2.5)$$

$$\dot{\hat{\sigma}}_k^\dagger = i\omega_k \hat{\sigma}_k^\dagger - ig_k \hat{\sigma}_{zk} \hat{q}, \quad (2.6)$$

$$\dot{\hat{\sigma}}_{zk} = 2ig_k (\hat{\sigma}_k - \hat{\sigma}_k^\dagger) \hat{q}. \quad (2.7)$$

The operator Langevin equation for the particle can be obtained by eliminating $\hat{\sigma}_k^\dagger$ and $\hat{\sigma}_k$ from Eq. (2.4) after formally integrating Eqs. (2.5) and (2.6) and using the results in Eq. (2.4) to yield

$$\begin{aligned} \ddot{\hat{q}} = -V'(\hat{q}) - \hbar \sum_k g_k [\hat{\sigma}_k^\dagger(0)e^{i\omega_k t} + \hat{\sigma}_k(0)e^{-i\omega_k t}] \\ - 2\hbar \sum_k g_k^2 \int_0^t dt' \hat{q}(t') \hat{\sigma}_{zk}(t') \sin \omega_k(t-t'). \end{aligned} \quad (2.8)$$

The third term of the right-hand side contains the bath operators under time integral and therefore makes it nonlinear and practically untractable for an exact approach. A simplification can, however, be made at this stage by noting the time scale of evolution of the polarization operators $\hat{\sigma}_k^\dagger$ and $\hat{\sigma}_k$ as compared to that for $\hat{\sigma}_{zk}$. Equations (2.5)–(2.7) suggest that while the polarization operators are governed by the characteristic time scale of free evolution (ω_k), the energy operators follow the slower time scale of system-bath interaction (g_k). It is therefore useful to approximate $\hat{\sigma}_{zk}(t') \sim \hat{\sigma}_{zk}(0)$ in Eq. (2.8). Furthermore, we rewrite $\hat{\sigma}_{zk}(0) = 2\hat{n}_k(0) - 1$ and note that to enable the set of fermions to act as a reservoir which is assumed to be uncorrelated from the system at $t=0$, we may set $\hat{\sigma}_{zk}(0) \approx -1$. This implies that the system starts interacting with the bath through the ground levels of most of the fermions. The underlying approximation of very weak excitation (at $t=0$) therefore entails an effective linearization of the nonlinear damping term in Eq. (2.8).

Based on these considerations, we are therefore led to the expression for the third term $2\hbar \sum_k g_k^2 \int_0^t dt' q(t') \sin \omega_k(t-t')$, which after direct integration by parts reduces Eq. (2.8) to the following form:

$$\begin{aligned} \ddot{q} + V'_{eff}(\hat{q}) = & -\hbar \sum_k g_k [\hat{S}_k(0)e^{-i\omega_k t} + \hat{S}_k^\dagger(0)e^{i\omega_k t}] \\ & - 2\hbar \int_0^t dt' \dot{q}(t') \sum_k \frac{g_k^2}{\omega_k} \cos \omega_k(t-t'), \end{aligned} \quad (2.9)$$

where we have defined

$$V_{eff}(\hat{q}) = V(\hat{q}) - \hbar \sum_k \frac{g_k^2}{\omega_k} \hat{q}^2(t), \quad (2.10)$$

$$\hat{S}_k(0) = \hat{\sigma}_k(0) + \frac{g_k}{\omega_k} \hat{q}(0), \quad (2.11)$$

$$\hat{S}_k^\dagger(0) = \hat{\sigma}_k^\dagger(0) + \frac{g_k}{\omega_k} \hat{q}(0). \quad (2.12)$$

Here Eq. (2.10) denotes the effective potential due to system-reservoir interaction which is expected to give rise to a small frequency shift. $\hat{S}_k(0)$ and $\hat{S}_k^\dagger(0)$ are the shifted bath operators. The modification of the potential arises because of the absence of any counterterm in the Hamiltonian. The counterterm of the Zwanzig form [6] is particularly well known in chemical physics literature (although there are exceptions) while this is absent in system-reservoir models in quantum optics [1] and condensed-matter physics.

We may therefore write down the operator equation for the particle in the following form:

$$\ddot{q} + \int_0^t dt' \dot{q}(t') \kappa(t-t') + V'_{eff}(\hat{q}) = \hat{f}(t). \quad (2.13)$$

Here the noise operator and the memory kernel are given by

$$\hat{f}(t) = -\hbar \sum_k g_k [\hat{S}_k(0)e^{-i\omega_k t} + \hat{S}_k^\dagger(0)e^{i\omega_k t}] = \hat{F}(t) + \hat{F}^\dagger(t) \quad (2.14)$$

and

$$\kappa(t-t') = 2\hbar \sum_k \frac{g_k^2}{\omega_k} \cos \omega_k(t-t'), \quad (2.15)$$

respectively. The noise properties of the operator $\hat{f}(t)$ can be derived by using a suitable canonical thermal distribution of bath operators at $t=0$ as follows:

$$\langle \hat{f}(t) \rangle_{qs} = 0, \quad (2.16)$$

$$\begin{aligned} & \text{Re}\{\langle \hat{F}(t)\hat{F}^\dagger(t') - \hat{F}^\dagger(t)\hat{F}(t') \rangle_{qs}\} \\ & = \hbar^2 \sum_k g_k^2 \tanh\left(\frac{\hbar\omega_k}{2KT}\right) \cos \omega_k(t-t'). \end{aligned} \quad (2.17)$$

Here $\langle \dots \rangle_{qs}$ implies quantum statistical average and is defined as

$$\langle \hat{A} \rangle_{qs} = \frac{\text{Tr} \hat{A} e^{-\hat{H}_{bath}/kT}}{\text{Tr} e^{-\hat{H}_{bath}/kT}} \quad (2.18)$$

for any bath operator \hat{A} , where $\hat{H}_{bath} = \hbar \sum_k \omega_k \hat{\sigma}_k^\dagger \hat{\sigma}_k$ at $t=0$. In defining Eq. (2.16), it is necessary to set the quantum-mechanical mean position $\langle \hat{q}(0) \rangle = 0$, without any loss of generality. This allows further simplification,

$$\langle \hat{S}_k(0) \rangle_{qs} = \langle \hat{\sigma}_k(0) \rangle_{qs}, \quad (2.19)$$

$$\langle \hat{S}_k^\dagger(0) \rangle_{qs} = \langle \hat{\sigma}_k^\dagger(0) \rangle_{qs}. \quad (2.20)$$

Equation (2.17) is the fluctuation-dissipation relation expressed in terms of noise operators appropriately ordered. The negative sign in the left-hand side of Eq. (2.17) carries the signature of anticommutation relation for fermionic bath operators in contrast to the positive sign for the corresponding bosonic case. The origin of the temperature-dependent contribution $\tanh(\frac{\hbar\omega_k}{2KT})$ can be traced to the following average:

$$\langle \hat{n}_k \rangle_{qs} = \frac{\sum_{n_k=0,1} n_k e^{-n_k \hbar\omega_k/kT}}{\sum_{n_k=0,1} e^{-n_k \hbar\omega_k/kT}} = \frac{1}{e^{\hbar\omega_k/kT} + 1} = \bar{n}_F(\omega_k) \quad (2.21)$$

and

$$\langle \hat{\sigma}_{zk}(0) \rangle_{qs} = 2\langle \hat{n}_k \rangle - 1 = -\tanh \frac{\hbar\omega_k}{2KT}. \quad (2.22)$$

Here \bar{n}_F can be identified as the Fermi-Dirac distribution function denoting the average thermal excitation number of the bath. This distribution does not contain any chemical-potential term. The absence of this term implies that our stating Hamiltonian (2.1) does not conserve fermion number. Ideally the typical system-fermionic bath model for dissipation, we have in mind, for realization of the present theoretical scheme is a single system, e.g., an ion, in a suitably designed environment of quantum dots with characteristic size distribution.

Since quantum dots are known to serve as ‘‘artificial’’ two-level atoms in several situations [18,19] and the varying system size results in a distribution of frequencies, we believe that a reservoir of two-level quantum dots can be used for studying quantum dissipation in a fermionic bath at low temperature. When the number density of dots, say, is on the order of 10^5 cm^{-3} as often found in experiments, the system experiences practically a Fermi sea with infinite degrees of freedom. The large number is an essential requirement to preclude the possibility of any recurrence and to ensure irreversibility associated with the notion of dissipation.

B. Quantum Langevin equation with c -number fermionic noise

Our object in this section is to construct a quantum Langevin equation with c -number fermionic noise. To this end, we proceed as follows. We return to Eq. (2.13) and, as a

first step, carry out its quantum-mechanical average,

$$\langle \ddot{\hat{q}} \rangle + \int_0^t dt' \langle \dot{\hat{q}}(t') \rangle \langle \hat{\kappa}(t-t') \rangle + \langle V'_{eff}(\hat{q}) \rangle = \langle \hat{f}(t) \rangle, \quad (2.23)$$

where the quantum-mechanical average is taken over the initial product separable quantum states of the particle and the fermions at $t=0$, $|\phi\rangle|\xi_1\rangle|\xi_2\rangle\cdots|\xi_N\rangle$. Here $|\phi\rangle$ denotes any arbitrary initial state of the particle and $|\xi_k\rangle$ corresponds to the initial coherent state of the k th fermion. Existence of such coherent states which are analogous to harmonic-oscillator coherent states had been proved a couple of decades ago by Radcliffe [20]. Typically for a spin- $\frac{1}{2}$ system, such a state is generated by the action of creation operator on vacuum as $|\mu\rangle = (1+|\mu|^2)^{-1/2} \exp(\mu\hat{\sigma}^\dagger)|0\rangle$, where μ is a number. Applications of the formalism of spin coherent states are well known in the context of ferromagnetic spin wave, phase transition in Dicke model of super-radiance, equilibrium statistical mechanics of radiation-matter interaction, and so on. For details we refer to [21].

The main purpose of using these spin coherent states for quantum-mechanical averaging of the bath operators is to formulate Eq. (2.23) as a classical-looking Langevin equation for quantum-mechanical mean position of the particle. We then denote the following quantum-mechanical averages as

$$\langle \hat{q}(t) \rangle = q(t), \quad (2.24)$$

$$\langle \hat{f}(t) \rangle = \eta(t), \quad (2.25)$$

where

$$\begin{aligned} \eta(t) = & -\hbar \sum_k g_k \{ \langle \hat{S}_k(0) \rangle e^{-i\omega_k t} + \langle \hat{S}_k^\dagger(0) \rangle e^{i\omega_k t} \} = \\ & -\hbar \sum_k g_k \{ \xi_k(0) e^{-i\omega_k t} + \xi_k^*(0) e^{i\omega_k t} \}. \end{aligned} \quad (2.26)$$

The last equality follows from Eqs. (2.19) and (2.20), and $\langle \hat{S}_k(0) \rangle = \langle \hat{\sigma}_k(0) \rangle = \xi_k(0)$ and $\langle \hat{S}_k^\dagger(0) \rangle = \langle \hat{\sigma}_k^\dagger(0) \rangle = \xi_k^*(0)$. Here $\xi_k(0)$ and $\xi_k^*(0)$ are the associated c numbers [note that we have set $\langle \hat{q}(0) \rangle = 0$] for the fermionic bath operators. Equation (2.23) may then be rewritten as

$$\ddot{q} + \int_0^t \dot{q}(t') \kappa(t-t') dt' + \langle V'_{eff}(\hat{q}) \rangle = \eta(t). \quad (2.27)$$

Now to realize $\eta(t)$ as an effective c -number noise, we introduce the ansatz that $\xi_k(0)$ and $\xi_k^*(0)$ are distributed according to a thermal canonical distribution of Gaussian form as follows:

$$P_k[\xi_k(0), \xi_k^*(0)] = N \exp\left[-\frac{|\xi_k(0)|^2}{2 \tanh(\hbar\omega_k/2KT)}\right], \quad (2.28)$$

where N is the normalization constant. The width of the distribution is defined by $\tanh(\hbar\omega_k/2KT)$. For any arbitrary quantum-mechanical mean value of a bath operator, $\langle \hat{A}_k \rangle$

which is a function of $\xi_k(0)$, $\xi_k^*(0)$, its statistical average can then be written down as

$$\langle \langle \hat{A}_k \rangle \rangle_s = \int \langle \hat{A}_k \rangle P_k[\xi_k(0), \xi_k^*(0)] d\xi_k(0) d\xi_k^*(0). \quad (2.29)$$

The ansatz [Eq. (2.28)] and the definition of statistical average [Eq. (2.29)] can be used to show that c -number noise $\eta(t)$ satisfies the following relations:

$$\langle \eta(t) \rangle_s = 0, \quad (2.30)$$

$$\langle \eta(t) \eta(t') \rangle_s = \hbar^2 \sum_k g_k^2 \cos \omega_k(t-t') \tanh\left(\frac{\hbar\omega_k}{2KT}\right). \quad (2.31)$$

Equations (2.30) and (2.31) imply that c -number noise $\eta(t)$ is such that it is zero centered and follow the fluctuation-dissipation relation as expressed in Eq. (2.17). Therefore, Eqs. (2.17) and (2.31) are equivalent. However, the decisive advantage of the formulation of c -number noise is that one can bypass the operator ordering prescription for deriving the noise properties of the bath. We also point out that the temperature dependence exactly like the one found here for noise correlation function was obtained for spectral function in earlier work [11–13]. This confirms the validity of the present formulation of quantum noise process for fermionic bath. The quantum Langevin equation [Eq. (2.27)] with c -number noise $\eta(t)$ as defined by Eqs. (2.30) and (2.31) is classical looking in form but quantum mechanical in its content. Therefore, the formulation allows us to implement the techniques of classical nonequilibrium statistical mechanics for various purposes. It is pertinent to digress a little bit at this point to note that for a traditional harmonic-oscillator heat bath, i.e., the bosonic reservoir, one can proceed exactly in a similar fashion and use harmonic-oscillator coherent states [22]. The canonical thermal distribution function for bosonic c -number noise corresponding to its fermionic counterpart is the Wigner thermal distribution function [23]. This has been extensively used [24–28] in several earlier occasions.

In order to quantify the properties of the thermal bath, it is convenient to introduce, as usual, a spectral density function $J(\omega)$ associated with system-bath interaction,

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{g_k^2}{\omega_k} \delta(\omega - \omega_k). \quad (2.32)$$

With the help of $J(\omega)$ one may rewrite the expression for memory kernel [Eq. (2.15)],

$$\kappa(t) = \frac{4\hbar}{\pi} \int_0^\infty d\omega J(\omega) \cos \omega t \quad (2.33)$$

and the fluctuation-dissipation relation [Eq. (2.31)]

$$\begin{aligned} \langle \eta(t) \eta(t') \rangle_s &= \text{Re} \{ \langle \hat{F}(t) \hat{F}^\dagger(t') - \hat{F}^\dagger(t) \hat{F}(t') \rangle_{qs} \} \\ &= \frac{4\hbar}{\pi} \int_0^\infty d\omega J(\omega) \frac{\hbar\omega}{2} \left(\tanh \frac{\hbar\omega}{2KT} \right) \cos \omega(t-t'). \end{aligned} \quad (2.34)$$

The relaxation induced by the bath is determined by the properties of the spectral density function. For example, a Lorentzian bath is characterized by $J(\omega) = \gamma^2 / (\gamma^2 + \omega^2)$, where γ is a constant. The Langevin equation [Eq. (2.27)] may be expressed in a more convenient form for interpretation. We add the force term $V'_{eff}(q)$ on both sides of Eq. (2.27). The resulting equation is given by

$$\ddot{q} + \int_0^t \dot{q}(t') \kappa(t-t') dt' + V'_{eff}(q) = \eta(t) + Q, \quad (2.35)$$

where

$$Q = V'_{eff}(q) - \langle V'_{eff}(\hat{q}) \rangle \quad (2.36)$$

represents the quantum correction due to the system potential. Equation (2.35) thus describes the motion of a particle (quantum-mechanical mean position) in a force field simultaneously driven by c -number quantum noise of a fermionic bath and quantum dispersion Q , characteristic of nonlinearity of the potential. Q may be expressed in a more explicit and useful form by recognizing the operator nature of the system variables \hat{q} and \hat{p} as

$$\hat{q}(t) = q(t) + \delta\hat{q}(t), \quad (2.37)$$

$$\hat{p}(t) = p(t) + \delta\hat{p}(t), \quad (2.38)$$

where $q(\equiv \langle \hat{q} \rangle)$ and $p(\equiv \langle \hat{p} \rangle)$ are quantum-mechanical mean values and $\delta\hat{q}$ and $\delta\hat{p}$ are the corresponding fluctuation operators. By construction, $\langle \delta\hat{q} \rangle = \langle \delta\hat{p} \rangle = 0$ and $[\delta\hat{q}, \delta\hat{p}] = i\hbar$. Using Eq. (2.37) in $V'_{eff}(\hat{q})$ and a Taylor-series expansion around q , we may express Q as

$$Q = - \sum_{n \geq 2} \frac{1}{n!} V_{eff}^{(n+1)}(q) \langle \delta\hat{q}^n(t) \rangle. \quad (2.39)$$

Here $V_{eff}^{(n)}(q)$ is the n th derivative of the potential $V_{eff}(q)$ with respect to q . For example, the lowest-order correction ($n=2$) is given by $Q = -\frac{1}{2} V_{eff}''(q) \langle \delta\hat{q}^2(t) \rangle$. The determination of Q to be used in quantum Langevin equation [Eq. (2.35)] therefore depends on $\langle \delta\hat{q}^2(t) \rangle$ which may be estimated by solving quantum correction equations [29,30] as discussed below and in Sec. III. We now return to quantum operator equation [Eq. (2.13)] and put Eqs. (2.37) and (2.38). Furthermore, using Eq. (2.35) in the resulting equation, we obtain

$$\begin{aligned} \delta\ddot{\hat{q}} + \int_0^\infty dt' \kappa(t-t') \delta\hat{q}(t') + V''_{eff}(q) \delta\hat{q} + \sum_{n \geq 2} \frac{1}{n!} V_{eff}^{(n+1)}(q) \\ \times [\delta\hat{q}^n(t) - \langle \delta\hat{q}^n(t) \rangle] = \delta\hat{\eta}(t), \end{aligned} \quad (2.40)$$

where $\delta\hat{\eta}(t) = \hat{f}(t) - \eta(t)$.

Equation (2.40) forms the basis for calculation of quantum-mechanical correction Q . However, this is analytically untractable for an exact solution. Depending on the

nonlinearity of the potential and memory kernel, systematic approximation schemes may be adopted. A typical case will be discussed in Sec. III.

It is thus evident that the quantum Brownian motion of a particle in a fermionic bath may be calculated, in principle, as a stochastic process by solving the Langevin equation [Eq. (2.35)] for quantum-mechanical mean values, simultaneously with quantum correction equations which describe quantum-mechanical fluctuation or dispersion around them. Before closing this section, we mention that an essential element of the present approach is to express a quantum statistical average as a sum of statistical averages over a set of functions of quantum-mechanical mean values and dispersion. To illustrate, we calculate, for example, the quantum statistical averages $\langle \hat{q} \rangle_{qs}$ and $\langle \hat{q}^2 \rangle_{qs}$. Making use of Eq. (2.37), we write

$$\langle \hat{q} \rangle_{qs} = \langle q + \delta\hat{q} \rangle_{qs} = \langle q \rangle_s + \langle \langle \delta\hat{q} \rangle \rangle_s = \langle q \rangle_s \quad (2.41)$$

and

$$\langle \hat{q}^2 \rangle_{qs} = \langle (q + \delta\hat{q})^2 \rangle_{qs} = \langle q^2 \rangle_s + \langle \delta\hat{q}^2 \rangle_{qs} = \langle q^2 \rangle_s + \langle \langle \delta\hat{q}^2 \rangle \rangle_s. \quad (2.42)$$

Thus, care must be taken to distinguish between the quantum-mechanical mean of an operator \hat{A} expressed as $\langle \hat{A} \rangle (=A)$ from the statistical average of the quantum-mechanical mean A expressed as $\langle A \rangle_s$ and from quantum statistical average of \hat{A} , denoted as $\langle \hat{A} \rangle_{qs}$.

The definition of statistical average of a quantum-mechanical mean and the usual quantum statistical average of an operator are given in Eqs. (2.18) and (2.29), respectively. Another note of caution is pertinent here. It is necessary to distinguish between the quantum-mechanical averaging, averaging by quasiclassical distribution function [1,23] like the Wigner function $W(q,p)$, and quantum statistical averaging by the present method. For example, we may note $\langle \hat{q}\hat{p} \rangle_{qs} = \langle qp \rangle_s \neq \int qp W(q,p) dq dp$ but $\langle \hat{q}\hat{p} \rangle = \int qp W(q,p) dq dp$.

The quantum nature of the dynamics manifests in two different ways. First, the fermionic reservoir is quantum mechanical in character whose noise properties are expressed through quantum fluctuation-dissipation relation. Second, the nonlinearity of the system potential gives rise to quantum correction terms.

III. QUANTUM DIFFUSION EQUATION

The Langevin equation [Eq. (2.35)] describes the stochastic dynamics of a particle with quantum-mechanical mean position q and mean momentum p , where the properties of c -number noise force $\eta(t)$ are given by Eqs. (2.30) and (2.31). An equivalent description of the stochastic process can be formulated in terms of equation of motion for probability density function $P(q,p,t)$. This probability function is distinctly different from the quasiclassical probability function of the c -number widely used for studying of quantum-classical correspondence [1,2]. In what follows we derive a quantum diffusion equation for a free particle in contact with a fermionic bath.

To begin with, we consider the particle to be free from external force field so that $V_{eff}(q)=0$. The c -number Langevin equation [Eq. (2.35)] then reduces to

$$\ddot{q}(t) + \int_0^t dt' \kappa(t-t') \dot{q}(t') = \eta(t), \quad (3.1)$$

where $\kappa(t)$ is the dissipative memory kernel given by Eq. (2.15) and $\eta(t)$ is a zero centered stationary c -number noise whose time correlation is given by Eq. (2.31).

The general formal solution of Eq. (3.1) is given by

$$q(t) = \langle q(t) \rangle_s + \int_0^t dt' H(t-t') \eta(t'), \quad (3.2)$$

where

$$\langle q(t) \rangle_s = q(0) + p(0)H(t) \quad (3.3)$$

and $q(0)$ and $p(0)$ are the initial values of the quantum-mechanical mean position and momentum of the particle, respectively. $H(t)$ is expressed as the inverse Laplace transform of

$$\tilde{H}(s) = \int_0^\infty dt e^{-st} H(t) = \frac{1}{s^2 + s\tilde{\kappa}(s)}. \quad (3.4)$$

Here $\tilde{\kappa}(s)$ is the Laplace transform of $\kappa(t)$. The time derivative of Eq. (3.2) yields

$$p(t) = \langle p(t) \rangle_s + \int_0^t dt' h(t-t') \eta(t'), \quad (3.5)$$

where

$$\langle p(t) \rangle_s = p(0)h(t) \quad (3.6)$$

and

$$h(t) = \frac{d}{dt} H(t). \quad (3.7)$$

It is easy to identify $H(t)$ and $h(t)$ as the relaxation functions. To proceed further we now make use of the symmetry property of the correlation function $\langle \eta(t) \eta(t') \rangle [\equiv C(t-t')]$ and the solutions for $q(t)$ and $p(t)$ to define the following variances:

$$\begin{aligned} \sigma_{qq}^2(t) &= \langle [q(t) - \langle q(t) \rangle_s]^2 \rangle_s \\ &= 2 \int_0^t H(t_1) dt_1 \int_0^{t_1} H(t_2) C(t_1 - t_2) dt_2, \end{aligned} \quad (3.8)$$

$$\begin{aligned} \sigma_{pp}^2(t) &= \langle [p(t) - \langle p(t) \rangle_s]^2 \rangle_s \\ &= 2 \int_0^t h(t_1) dt_1 \int_0^{t_1} h(t_2) C(t_1 - t_2) dt_2, \end{aligned} \quad (3.9)$$

and

$$\begin{aligned} \sigma_{qp}^2(t) &= \langle [q(t) - \langle q(t) \rangle_s][p(t) - \langle p(t) \rangle_s] \rangle_s = \frac{1}{2} \dot{\sigma}_{qq}^2 \\ &= \int_0^t H(t_1) dt_1 \int_0^{t_1} h(t_2) C(t_1 - t_2) dt_2. \end{aligned} \quad (3.10)$$

Assuming now the statistical distribution of c -number noise $\eta(t)$ to be Gaussian, we define the joint characteristic func-

tion in terms of standard mean values and variances (these mean and variance are not to be confused with quantum-mechanical mean of an operator and its dispersion) as follows:

$$\begin{aligned} \tilde{P}(\mu, \rho, t) &= \exp \left[i\mu \langle q \rangle_s + i\rho \langle p \rangle_s \right. \\ &\quad \left. - \frac{1}{2} \{ \sigma_{qq}^2(t) \mu^2 + 2\sigma_{qp}^2(t) \mu \rho + \sigma_{pp}^2(t) \rho^2 \} \right]. \end{aligned} \quad (3.11)$$

Using standard procedure [31], we write down below the Fokker-Planck equation obeyed by joint probability distribution function $P(q, p, t)$ which is the inverse of characteristic function $\tilde{P}(\mu, \rho, t)$. The recipe for calculation is the following: the first step is the calculation of the expressions for $\frac{1}{\tilde{P}} \frac{\partial \tilde{P}}{\partial \mu}$, $\frac{1}{\tilde{P}} \frac{\partial \tilde{P}}{\partial \rho}$ and $\frac{1}{\tilde{P}} \frac{\partial \tilde{P}}{\partial t}$ from the expression for $\tilde{P}(\mu, \rho, t)$ [Eq. (3.11)]. All these expressions contain $q(0), p(0)$ which are to be eliminated to obtain the equation for Fourier transform of Eq. (3.11),

$$\begin{aligned} \left(\frac{\partial}{\partial t} + p \frac{\partial}{\partial q} \right) P(q, p, t) &= \Lambda(t) \frac{\partial}{\partial p} P(q, p, t) + \phi(t) \frac{\partial^2}{\partial p^2} P(q, p, t) \\ &\quad + \psi(t) \frac{\partial^2}{\partial q \partial p} P(q, p, t), \end{aligned} \quad (3.12)$$

where

$$\Lambda(t) = -\frac{\dot{h}(t)}{h(t)}, \quad (3.13)$$

$$\phi(t) = \Lambda(t) \sigma_{pp}^2(t) + \frac{1}{2} \dot{\sigma}_{pp}^2(t), \quad (3.14)$$

and

$$\psi(t) = -\dot{\sigma}_{pp}^2(t) + \Lambda(t) \sigma_{qp}^2(t) + \dot{\sigma}_{qp}^2(t). \quad (3.15)$$

Equation (3.12) is the quantum analog of non-Markovian classical Fokker-Planck equation for the fermionic bath. We require that in the long-time limit the coefficients of Eq. (3.12), $\Lambda(t)$, $\phi(t)$ and $\psi(t)$, must reach steady-state values for physically allowed relaxation functions. Furthermore, the stationary solution of the Fokker-Planck equation [Eq. (3.12)] is given by

$$P_{st}(p_0) = \frac{1}{(2\pi\Delta_0)^{1/2}} \exp \left[-\frac{p_0^2}{2\Delta_0} \right], \quad (3.16)$$

where

$$\Delta_0 = \frac{\phi(\infty)}{\Lambda(\infty)}. \quad (3.17)$$

In the stationary state the system, as expected, therefore reaches a Gaussian distribution whose half-width is determined by Δ_0 . Our next task is to construct a quantum diffusion equation for the particle. Following Mazo's procedure [31] for derivation of classical diffusion equation, we set $\rho = 0$ and consider the Gaussian distribution $P_{st}(p_0)$ of initial momentum p_0 to take average over the characteristic function as follows:

$$\begin{aligned}
 \tilde{P}(\mu, t) &= \int \tilde{P}(\mu, t) P_{st}(p_0) dp_0 \\
 &= \exp\left(-\frac{1}{2}\mu^2 \sigma_{qq}^2(t) + i\mu q_0\right) \\
 &\quad \times \int \exp[i\mu p_0 H(t)] P_{st}(p_0) dp_0. \quad (3.18)
 \end{aligned}$$

Using Eq. (3.16) in Eq. (3.18) and after performing the inverse Fourier transform and proceeding as before we arrive at the following diffusion equation:

$$\frac{\partial P(q, t)}{\partial t} = D_f(t) \frac{\partial^2 P}{\partial q^2}, \quad (3.19)$$

where the quantum diffusion coefficient $D_f(t)$ for the fermionic bath is given by

$$D_f(t) = \sigma_{qp}^2(t) + \Delta_0 H(t) h(t). \quad (3.20)$$

The expression for quantum diffusion coefficient is characterized by the nature of relaxation function $H(t)$ and $h(t)$, as well as the characteristic correlation function of c -number noise for the fermionic bath through $\sigma_{qp}^2(t)$. Since the key quantity that determines the variances is the relaxation function $H(t)$, it is necessary to incorporate correct well-behaved relaxation functions to be obtained from appropriate spectral density function. For a typical choice of the Lorentzian distribution of frequency, we assume a spectral density $J(\omega)$ of the form

$$J(\omega) = \frac{\gamma^2}{\gamma^2 + \omega^2}. \quad (3.21)$$

By virtue of Eq. (3.4) the relaxation function $H(t)$ is given by

$$\begin{aligned}
 H(t) &= 1 - \left[\frac{1}{\sqrt{\gamma(\gamma-4)}} \right] \\
 &\quad \times \frac{e^{-\lambda t/2} [2\sqrt{\gamma(\gamma-4)} e^{\lambda t/2} - 2 - \lambda - e^{\sqrt{\gamma(\gamma-4)} t} (\lambda - 2)]}{2\sqrt{\gamma(\gamma-4)}}, \quad (3.22)
 \end{aligned}$$

which yields

$$h(t) = \frac{e^{-t\lambda\sqrt{\gamma/2}} (\lambda e^{t\sqrt{\gamma(\gamma-4)}} + \sqrt{\gamma-4} - \sqrt{\gamma})}{2\sqrt{\gamma-4}}, \quad (3.23)$$

where

$$\lambda = \gamma + \sqrt{\gamma(\gamma-4)}. \quad (3.24)$$

The time dependence of diffusion coefficient $D_f(t)$ owes its origin to the characteristic relaxation functions $H(t)$ and $h(t)$ and the correlation function for the Lorentzian bath. These functions govern the short-time behavior of $D_f(t)$. To illustrate, the plot of $D_f(t)$ vs time for different temperatures is shown in Fig. 1. It is apparent that while the short-time regime is characterized by a sharp increase, D_f settles down to a constant value in the asymptotic limit. An important inference of the present analysis is the temperature dependence of the steady-state diffusion coefficient D_f . This is

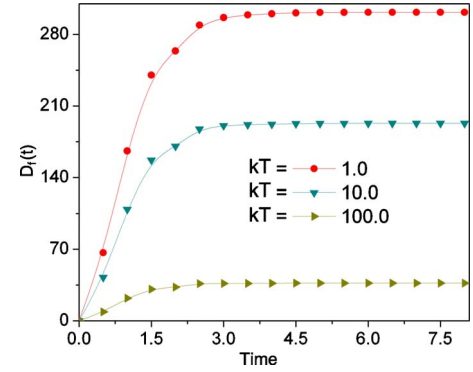


FIG. 1. (Color online) Variation of quantum diffusion coefficient vs time at different temperatures for $\gamma=4.52$ (scale arbitrary).

shown in Fig. 2. It is evident that increase of temperature impedes diffusive motion of the particle. The diffusion coefficient decreases by more than a factor of 6 between 0 and 80 K. The nature of this temperature dependence of diffusion constant for fermionic bath may be attributed to the width of thermal distribution. We note in passing that the anomalous decrease of diffusion constant with increase in temperature had been observed earlier [32] in positron diffusion in Ge-single crystal in one dimension. This is also consistent with the observation [12] that an effective system-reservoir interaction may result in dynamical localization of the particle in the sub-Ohmic regime at low temperature for a two-level reservoir. The basic difference between the behavior of the system-fermionic bath model and the standard system-boson model at finite temperature owes its origin to the restricted possibilities of thermally induced excitations of the bath degrees of freedom since only a single level of each fermion can be excited. Thus, in contrast to crossover from coherent to incoherent quantum tunneling characteristic of excitation of many levels of single degree of freedom in a bosonic reservoir, increase of temperature favors the coherent dynamics in a fermionic reservoir [10,17].

The suppression of diffusion at higher temperature as observed in the present study also points toward this coherence as a result of severe restriction on the excitations in fermionic bath degrees of freedom. This is in conformity with earlier studies [17] based on path-integral approach to quantum transport of heavy particle in fermionic bath.

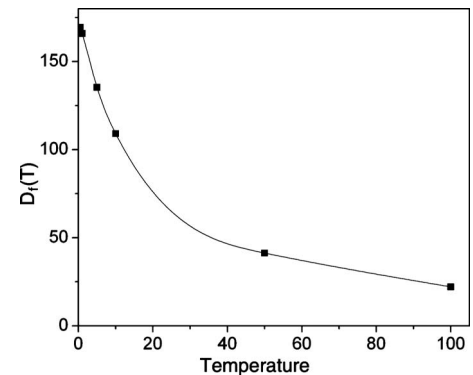


FIG. 2. Variation of steady-state diffusion coefficient as a function of temperature for $\gamma=4.52$ (scale arbitrary).

IV. QUANTUM MEAN-SQUARE DISPLACEMENT

In this section, we calculate the quantum mean-square displacement of the particle in contact with the fermionic bath. From Eq. (2.42), we have the expression

$$\langle \hat{q}^2(t) \rangle_{qs} = \langle q^2 \rangle_s + \langle \delta \hat{q}^2(t) \rangle_{qs}, \quad (4.1)$$

where $q[\equiv \langle \hat{q}(t) \rangle]$ is the quantum-mechanical mean value and $\delta \hat{q}$ is the correction operator. $\langle q^2 \rangle_s$ can be calculated as an usual statistical average of q^2 with the probability density function $P(q, t)$ as follows:

$$\langle q^2 \rangle_s = \int q^2 P(q, t) dq = 2S(t). \quad (4.2)$$

Here $P(q, t)$ is the solution of the quantum diffusion equation [Eq. (3.19)] subject to initial condition $P(q, t=0) = \delta(q)$ and is given by $P(q, t) = [1/\sqrt{4\pi S(t)}] \exp[-q^2/4S(t)]$ with $S(t) = \int_0^t dt' D_f(t')$. Now the quantum correction over the mean-square displacement $\langle \delta \hat{q}^2 \rangle_{qs}$ can be calculated for the free particle using Eq. (2.40) which assumes the following form:

$$\delta \ddot{\hat{q}} + \int_0^\infty dt' \kappa(t-t') \delta \dot{\hat{q}}(t') = \delta \hat{\eta}(t). \quad (4.3)$$

Solving Eq. (4.3) by Laplace transform leads to

$$\delta \hat{q}(t) = \delta \hat{q}(0) + H(t) \delta \hat{p}(0) + \int_0^t dt' H(t-t') \delta \hat{\eta}(t'), \quad (4.4)$$

where $H(t)$ is given by Eqs. (3.4) and (3.22). After squaring $\langle \delta \hat{q}^2(t) \rangle_{qs}$ can be written as

$$\begin{aligned} \langle \delta \hat{q}^2(t) \rangle_{qs} &= \langle \delta \hat{q}^2(0) \rangle + H^2(t) \langle \delta \hat{p}^2(0) \rangle + H(t) \langle \delta \hat{q}(0) \delta \hat{p}(0) \rangle \\ &+ \delta \hat{p}(0) \delta \hat{q}(0) + 2 \int_0^t dt' \int_0^{t'} dt'' H(t-t') H(t-t'') \\ &\times \langle \delta \hat{\eta}(t') \delta \hat{\eta}(t'') \rangle_{qs}. \end{aligned} \quad (4.5)$$

We now choose the initial conditions corresponding to minimum uncertainty state [29,30] so that $\langle \delta \hat{q}^2(0) \rangle = \frac{\hbar}{2}$, $\langle \delta \hat{p}^2(0) \rangle = \frac{\hbar}{2}$, and $\langle \delta \hat{q}(0) \delta \hat{p}(0) \rangle + \delta \hat{p}(0) \delta \hat{q}(0) = \hbar$. The double integral in Eq. (4.5) can be evaluated numerically to calcu-

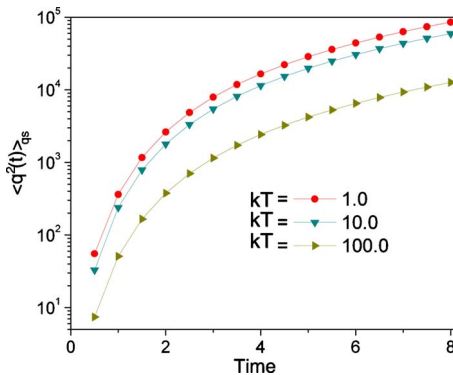


FIG. 3. (Color online) Variation of quantum mean-square displacement $\langle \hat{q}^2(t) \rangle_{qs}$ vs time at different temperatures for $\gamma=4.52$ (scale arbitrary).

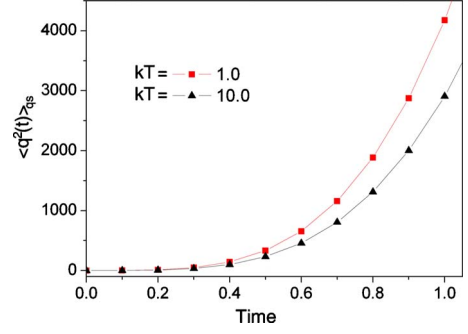


FIG. 4. (Color online) Variation of quantum mean-square displacement $\langle \hat{q}^2(t) \rangle_{qs}$ vs time in the short-time limit at different temperatures for $\gamma=4.52$ (scale arbitrary).

late $\langle \delta \hat{q}^2(t) \rangle_{qs}$. We are therefore in a position to estimate the quantum mean-square displacement $\langle \hat{q}^2(t) \rangle_{qs}$. The result as a function of time is shown in Fig. 3 at several temperatures. The detailed nature of time dependence of quantum mean-square displacement in short- and long-time limits is shown in Figs. 4 and 5, respectively. It is apparent that in the ballistic region, the rise is faster than quadratic while the mean-square displacement is superdiffusive in the asymptote regime. In order to allow ourselves a fair comparison with the “classical” result (i.e., without quantum correction term), we have compared the mean-square displacement of the particle in Fig. 6 for the classical and quantum cases at two different temperatures. The quantum nature manifestly influences the displacement, particularly, in the long-time limit. In general, one observes that quantization enhances the mean-square displacement, whereas higher temperature leads to suppression of the displacement.

V. CONCLUSIONS

The main purpose of this paper is to introduce a canonical quantization procedure for treatment of quantum Brownian motion of a particle moving in a potential field and in contact with a fermionic bath. Based on the initial coherent-state representation of the fermions and an equilibrium thermal canonical distribution of fermionic c numbers, we have derived a generalized quantum Langevin equation for quantum-

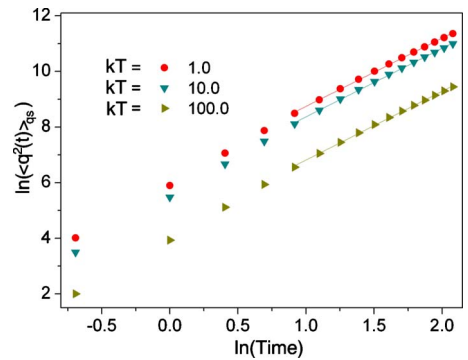


FIG. 5. (Color online) Variation of \log_e of quantum mean-square displacement vs \log_e of time in the long-time regime at different temperatures at $\gamma=4.52$ (scale arbitrary).

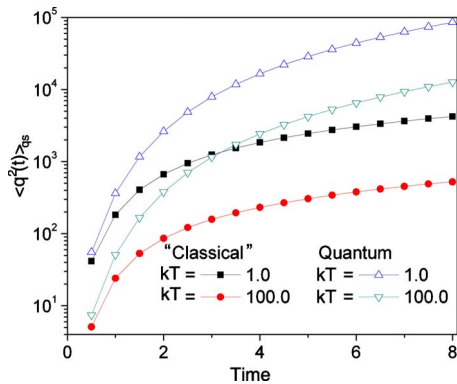


FIG. 6. (Color online) Comparative variation of mean-square displacement vs time at 1.0 and 100.0 kT at $\gamma=4.52$ for classical and quantum cases (scale arbitrary).

mechanical mean value of the position of the particle. The fermionic c numbers satisfy the essential properties of noise of the bath degrees of freedom. The main conclusions of this study are the following:

(i) Our emphasis has been to look for a natural extension of the classical theory of the Brownian motion to quantum domain. The generalized c -number Langevin equation and the diffusion equation for free particle for the fermionic bath that we derived are the quantum analogs of their classical versions. The probability distribution functions bear the true notion of probability rather than quasiprobability employed

for describing Wigner, Glauber-Sudarshan, or Q functions.

(ii) The behavior of the diffusion constant and the mean-square displacement of the particle as a function of temperature significantly differ from their classical counterparts. The generic consequence due to restricted options for thermal excitations in a fermionic bath is that the temperature favors suppression of diffusive motion, although quantization, in general, enhances mean-square displacement.

(iii) Since fermions have no classical analog, the fluctuation-dissipation relation connecting fermionic noise and dissipation does not assume the usual classical limiting form obtained for the bosonic case.

(iv) The present scheme is equipped to deal with non-Markovian features of the dynamics for a wide range of noise correlation and temperature. Since the formulation allows us to map the quantum stochastic dynamics on a classical setting, it is amenable to theoretical analysis using the methods of classical nonequilibrium statistical mechanics.

We conclude with a note that the present approach is promising for application of the c -number Langevin equation and diffusion equation for thermally activated processes and quantum transport in thermodynamically closed and open systems. A suitably designed assembly of quantum dots may serve as a good testing ground for the present theory. The method is also expected to be useful for studying of quantum-classical correspondence in stochastic processes and other related issues.

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