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Quantum State-Dependent Diffusion and Multiplicative Noise: A Microscopic Approach

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The state-dependent diffusion, which concerns the Brownian motion of a particle in inhomogeneous media has been described phenomenologically in a number of ways. Based on a system-reservoir nonlinear coupling model we present a microscopic approach to quantum state-dependent diffusion and multiplicative noise in terms of a quantum Markovian Langevin description and an associated Fokker–Planck equation in position space in the overdamped limit. We examine the thermodynamic consistency and explore the possibility of observing a quantum current, a generic quantum effect, as a consequence of this state-dependent diffusion similar to one proposed by Büttiker [*Z. Phys. B* **68**:161 (1987)] in a classical context several years ago.

KEY WORDS: Quantum Langevin equation; quantum Smoluchowski equation; quantum multiplicative noise; state dependent diffusion; quantum ratchet.

1. INTRODUCTION

Almost three decades ago Landauer[1,2] explored the problem of characterizing nonequilibrium steady states in the transition kinetics between the two locally stable states in bistable systems. His main idea was that the relative stability of a particle diffusing in a bistable potential can be altered by an intervening hot layer which has the effect of pumping particles from a globally stable region to a metastable region. No detailed consideration of immediate neighborhood of the two states is important. In formulating the problem in terms of diffusion equation it was realized that one needs state dependence of diffusion for a correct description of the effect and more generally a careful analysis of the problem of

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diffusion in inhomogeneous media in a wider context was necessary. This was carried out by van Kampen[3] and others[4] in 1980s. An important consequence of state-dependent diffusion or noise as suggested by Büttiker[5] is the generation of current, in absence of any externally applied fields, which occurs in presence of periodic diffusion of a particle in a spatially periodic potential with same periodicity but differing in phase. This rectification of state dependent noise resulting in a directed transport and state-dependent diffusion play important role in several areas of condensed matter physics on the mesoscopic scale[6–9] and furthermore in ratchet problems[10–13] in a wider perspective.

The physics of state-dependent diffusion can be described phenomenologically in a number of ways. As reported in the literature[3,14] the diffusion term for Brownian particle may assume several forms, notably $\frac{\partial}{\partial q}D(q)\frac{\partial}{\partial q}P(q,t)$ or $\frac{\partial^2}{\partial q^2}D(q)P(q,t)$ or the other like $\frac{\partial}{\partial q}D\frac{\partial P(q,t)}{\partial q}$ supplemented by "thermal potential" or state-dependent drift term. Here $D(q)$ refers to diffusion coefficient and $P(q,t)$ is the probability distribution function for the particle. Two important points are now noteworthy. First, the phenomenological forms of diffusion coefficient being different, it is easy to realize that they do not have a common microscopic Hamiltonian origin. Thus the physics of diffusion in inhomogeneous media is somewhat model-dependent[14] and the search for a "correct" form of diffusion remains a debatable issue. Second, the diverse forms notwithstanding, the generalization of Boltzmann factor, $\exp(-V(q)/k_B T)$ (which governs the system at thermal equilibrium) for state-dependent diffusion in the steady state assumes a common structure,

$$P_{st}(q) \sim \exp[-\phi(q)] \tag{1.1}$$

with $\phi(q) = \int_0^q \frac{V'(q')}{D(q')}\, dq'$, $V(q)$ being the potential field. The steady state distribution (1.1) implies that the effective potential $\phi(q)$ is nonlocal in space. The generality in the structure of $\phi(q)$ is such that it may include the spatial variation of temperature, diffusion or drift coefficient as specific cases as considered separately by several authors.[3,5,14]. In the Langevin scheme of description, on the other hand, state-dependent diffusion has received attention under "multiplicative noise".[15–24] The microscopic origin of multiplicative noise within the framework of standard paradigm of system-reservoir Hamiltonian that includes a variety of model calculations is the nonlinear coupling between the system and bath coordinates which leads to nonlinear dissipation. A thermodynamically consistent approach in this context was put forward in early 1980s by Lindenberg and coworkers.[4] An exact Fokker–Planck equation for time and space-dependent friction was derived by Pollak *et al.*[24] several years ago. Along with these formal developments,[4,14–24] the theories of multiplicative noise have found wide applications in several areas, e.g., activated processes,[25] stochastic resonance,[26] laser and optics,[27] signal processing,[28] fluctuation-induced transport,[29,30] noise-induced transitions,[31] etc.

In this paper, we address the problem of Langevin equation with multiplicative noise and state-dependent diffusion for a thermodynamically closed system in a *quantum mechanical* context. Although the quantum-mechanical system-reservoir linear coupling model for microscopic description of additive noise and linear dissipation which are related by fluctuation–dissipation relation is well-known over many decades in several fields,[32,33] the nature of nonlinear coupling and its consequences have been explored with renewed interest only recently. For example, it has been observed that the quantum dissipation can reduce the appearance of metastable state and barrier drift in a double well potential.[34] Tanimura and co-workers[35] have extensively used nonlinear coupling in modeling elastic and inelastic relaxation mechanisms and their interplay in vibrational and Raman spectroscopy. The role of inhomogeneous dissipation in reducing quantum decay rate has also been explored very recently.[36] Based on a coherent state representation of quantum noise operator and Wigner canonical thermal distribution for harmonic bath oscillators[37] nonlinearly coupled to a system we would like to develop a microscopic approach to quantum state-dependent diffusion and quantum multiplicative noise. Specifically, our aim is:

(i) to derive a quantum Smoluchowski equation for state-dependent diffusion on the basis of a system-reservoir model and analyze the role of nonlinear coupling in state-dependence of quantum diffusion and dissipation.

(ii) to seek for a correspondence between this quantum equation and its phenomenological counterpart.

(iii) to derive a quantum generalization of Boltzmann factor for state-dependent diffusion in the steady state (1.1) and check its thermodynamic consistency.

(iv) to explore the possibility of observing a directed transport as a consequence of state dependent quantum diffusion in the spirit of Büttiker as an immediate application.

The outlay of the paper is as follows: In Section 2 we develop the scheme of quantum Brownian motion for multiplicative noise on the basis of a nonlinearly coupled system-reservoir model of Zwanzig-type form within a Markovian description. Section 3 is devoted to quantum Smoluchowski equation for state-dependent diffusion which corresponds to a specific form of a classical phenomenological equation. We derive a quantum mechanical generalization of Boltzmann factor for state-dependent diffusion. In Section 4 we carry out an application to a system with spatially periodic potential and periodic diffusion function with same periodicity but differing in phase to demonstrate a nonzero current. The paper is concluded in Section 5.

2. QUANTUM MULTIPLICATIVE NOISE

2.1. General Aspects – Langevin Equation

We consider a particle of unit mass coupled to a medium comprised of a set of harmonic oscillators with frequency ω_j. This is described by the following system-bath Hamiltonian.[34–36]

$$\hat{H} = \frac{\hat{p}^2}{2} + V(\hat{q}) + \sum_j \left[\frac{\hat{p}_j^2}{2} + \frac{1}{2}\left(\omega_j \hat{x}_j - \frac{c_j}{\omega_j} f(\hat{q}) \right)^2 \right] \tag{2.1}$$

Here $\hat{q}$ and $\hat{p}$ are the coordinate and momentum operators of the particle and the $\{\hat{x}_j, \hat{p}_j\}$ are the set of coordinate and momentum operators for the bath oscillators with unit mass. The system particle is coupled to the bath oscillators nonlinearly through the general coupling terms $\frac{c_j}{\omega_j} f(\hat{q})$. c_j is the coupling strength. The Hamiltonian Eq. (2.1) is different from Zwanzig[38] form of system-bath Hamiltonian where the coupling is linear with respect to system coordinate. The classical counterpart[4] of the form (2.1) is known for more than two decades and also the nonlinear coupling in quantum system has been studied in several contexts.[34,35] The potential $V(\hat{q})$ is due to external force field for the system particle. The coordinate and momentum operators follow the usual commutation relations $[\hat{q}, \hat{p}] = i\hbar$ and $[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$. The presence of counter term in the Hamiltonian ensures that the potential $V(\hat{q})$ felt by the particle does not get modified due to heat bath.

We now use Eq. (2.1) to obtain the following dynamical equations for the position and momentum operators:

$$\dot{\hat{q}} = \frac{\partial \hat{H}}{\partial \hat{p}} = \hat{p} \tag{2.2}$$

$$\dot{\hat{p}} = -\frac{\partial \hat{H}}{\partial \hat{q}} = -V'(\hat{q}) + f'(\hat{q}) \sum_j \frac{c_j}{\omega_j} \left(\omega_j \hat{x}_j - \frac{c_j}{\omega_j} f(\hat{q}) \right) \tag{2.3}$$

where the dot(.) indicates derivative with respect to time and the prime (′) refers to derivative with respect to $\hat{q}$.

Similarly we have the dynamical equations of motion for the bath oscillators $(j = 1, 2, 3 \ldots)$

$$\dot{\hat{x}}_j = \frac{\partial \hat{H}}{\partial \hat{p}_j} = \hat{p}_j \tag{2.4}$$

$$\dot{\hat{p}}_j = -\frac{\partial \hat{H}}{\partial \hat{x}_j} = -\omega_j^2 \hat{x}_j + c_j f(\hat{q}) \tag{2.5}$$

To eliminate the bath degrees of freedom from the equations of motion of the system we first obtain a solution for the position operator $\hat{x}_j$ by formally solving the above equations and then make use of the solution in Eq. (2.3) followed by some rearrangement. This yields the generalized operator Langevin equation for the system particle.

$$\dot{\hat{q}}(t) = \hat{p}(t) \tag{2.6}$$

$$\dot{\hat{p}}(t) = -V'(\hat{q}(t)) - f'(\hat{q}(t)) \int_0^t f'(\hat{q}(t'))\gamma(t-t')\hat{p}(t')dt' + f'(\hat{q}(t))\hat{\eta}(t) \tag{2.7}$$

where the noise operator $\hat{\eta}(t)$ and the memory kernel $\gamma(t)$ are given by

$$\hat{\eta}(t) = \sum_j \left[\left\{ \frac{\omega_j^2}{c_j} \hat{x}_j(0) - f(\hat{q}(0)) \right\} \frac{c_j^2}{\omega_j^2} \cos \omega_j t + \frac{c_j}{\omega_j} \hat{p}_j(0) \sin \omega_j t \right] \tag{2.8}$$

and

$$\gamma(t) = \sum_j \frac{c_j^2}{\omega_j^2} \cos \omega_j t \tag{2.9}$$

It is clear from the operator Langevin equation Eq. (2.7) for the system that the noise operator is multiplicative and the dissipative term is nonlinear with respect to system coordinate due to the nonlinear coupling term in the system-bath Hamiltonian. In the case of linear coupling, i.e.,

$f(\hat{q}) = \hat{q}$ the Eq. (2.7) reduces to a quantum generalized Langevin equation[32] in which the noise term is additive and the dissipative term is linear.

Since the system is thermodynamically closed, i.e., the fluctuation and the dissipation originates from the same origin, the detailed balance condition must be satisfied. The noise properties of $\hat{\eta}(t)$ can be derived by using suitable canonical thermal distribution of bath coordinates and momenta operators at $t = 0$ to obtain;

$$\langle \hat{\eta}(t) \rangle_{\mathrm{QS}} = 0 \tag{2.10}$$

$$\frac{1}{2}\langle \hat{\eta}(t)\hat{\eta}(t') + \hat{\eta}(t')\hat{\eta}(t)\rangle_{\mathrm{QS}} = \frac{1}{2}\sum_j \frac{c_j^2}{\omega_j^2}\hbar\omega_j \left(\coth\frac{\hbar\omega_j}{2k_{\mathrm{B}}T}\right) \times \cos\omega_j(t-t') \tag{2.11}$$

Here $\langle \ldots \rangle_{\mathrm{QS}}$ implies quantum statistical average on bath degrees of freedom and is defined as

$$\langle \hat{O} \rangle_{\mathrm{QS}} = \frac{Tr\hat{O}\exp(-\hat{H}_{\mathrm{bath}}/k_{\mathrm{B}}T)}{Tr\exp(-\hat{H}_{\mathrm{bath}}/k_{\mathrm{B}}T)} \tag{2.12}$$

for any bath operator $\hat{O}(\{(\omega_j^2/c_j)\hat{x}_j - f(\hat{q})\}, \{\hat{p}_j\})$, where $\hat{H}_{\mathrm{bath}} = \sum_j [(\hat{p}_j^2/2) + \frac{1}{2}(\omega_j \hat{x}_j - \frac{c_j}{\omega_j} f(\hat{q}))^2]$ at $t = 0$. By trace we mean the usual quantum statistical average. Equation (2.11) is the fluctuation–dissipation relation expressed in terms of noise operators appropriately ordered in the quantum mechanical sense.

In the Markovian limit the generalized quantum Langevin equation Eq. (2.7) reduces to the form

$$\dot{\hat{q}}(t) = \hat{p}(t) \tag{2.13a}$$

$$\dot{\hat{p}}(t) = -V'(\hat{q}(t)) - \Gamma\,[f'(\hat{q}(t))]^2\,\hat{p}(t) + f'(\hat{q}(t))\hat{\eta}(t) \tag{2.13b}$$

where Γ is dissipation constant in the Markovian limit.

To construct a c-number quantum Langevin equation we proceed[39–43] as follows. We carry out a quantum mechanical average of Eq. (2.13a) and Eq. (2.13b) to get

$$\dot{q} = p \tag{2.14}$$

$$\dot{p} = -\langle V'(\hat{q})\rangle - \Gamma\langle [f'(\hat{q})]^2 \hat{p}\rangle + \langle f'(\hat{q})\hat{\eta}(t)\rangle \tag{2.15}$$

where $q = \langle \hat{q} \rangle$ and $p = \langle \hat{p} \rangle$. The quantum mechanical average $\langle \ldots \rangle$ is taken over the initial product separable quantum states of the particle and the bath oscillators at $t = 0$, $|\phi\rangle\{|\alpha_1\rangle|\alpha_2\rangle \ldots .|\alpha_N\rangle\}$. Here $|\phi\rangle$ denotes any arbitrary initial state of the system and $|\alpha_j\rangle$ corresponds to the initial coherent state of the jth bath oscillator. $|\alpha_j\rangle$ is given by $|\alpha_j\rangle = \exp(-|\alpha_j^2|/2) \sum_{n_j=0}^{\infty} (\alpha_j^{n_j}/\sqrt{n_j!})|n_j\rangle$, α_j being expressed in terms of the mean values of the shifted coordinate and momentum of the jth oscillator, $\left\{\frac{\omega_j^2}{c_j}\langle \hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\} = \sqrt{\frac{\hbar}{2\omega_j}}(\alpha_j + \alpha_j^*)$ and $\langle \hat{p}_j(0)\rangle = \sqrt{\frac{\hbar\omega_j}{2}}(\alpha_j^* - \alpha_j)$, respectively.

Since the quantum mechanical average is taken over the initial product separable quantum states of the particle and the bath oscillators the Eqs. (2.14–2.15) can be written as:

$$\dot{q} = p \tag{2.16a}$$

$$\dot{p} = -\langle V'(\hat{q})\rangle - \Gamma\langle [f'(\hat{q})]^2 \hat{p}\rangle + \langle f'(\hat{q})\rangle \eta(t) \tag{2.16b}$$

where $\eta(t) = \langle \hat{\eta}(t)\rangle$, $\eta(t)$ is now a classical-like noise term, which, in general, is a non-zero number because of the quantum mechanical averaging and is given by

$$\eta(t) = \sum_j \left[\left\{\frac{\omega_j^2}{c_j}\langle \hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\} \frac{c_j^2}{\omega_j^2}\cos\omega_j t + \frac{c_j}{\omega_j}\langle \hat{p}_j(0)\rangle \sin\omega_j t\right] \tag{2.17}$$

To realize $\eta(t)$ as an effective c-number noise we now introduce the ansatz[37,39–43] that the momentum $\langle \hat{p}_j(0)\rangle$ and the shifted coordinates $\left\{\frac{\omega_j^2}{c_j}\langle \hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\}$ of the bath oscillators are distributed according to a canonical distribution of Gaussian form as:

$$\mathcal{P}_j\left(\left\{\frac{\omega_j^2}{c_j}\langle \hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\}, \langle \hat{p}_j(0)\rangle\right) = \mathcal{N}\exp\left\{-\frac{\left[\langle \hat{p}_j(0)\rangle^2 + \frac{c_j^2}{\omega_j^2}\left\{\frac{\omega_j^2}{c_j}\langle \hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\}^2\right]}{2\hbar\omega_j\left(\bar{n}_j(\omega_j) + \frac{1}{2}\right)}\right\} \tag{2.18}$$

so that for any quantum mechanical mean value, $\mathcal{O}_j\left(\left\{\frac{\omega_j^2}{c_j}\ \langle\hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\}, \langle\hat{p}_j(0)\rangle\right)$ of the bath operator, its statistical average $\langle\ldots\rangle_S$ is

$$\langle\mathcal{O}_j\rangle_S = \int \mathcal{O}_j \mathcal{P}_j\, d\langle\hat{p}_j(0)\rangle\, d\left\{\frac{\omega_j^2}{c_j}\langle\hat{x}_j(0)\rangle - \langle f(\hat{q}(0))\rangle\right\} \tag{2.19}$$

Here $\bar{n}_j(\omega_j)$ indicates the average thermal photon number of the jth oscillator at the temperature T and $\bar{n}_j(\omega_j) = [\exp(\frac{\hbar\omega_j}{k_B T}) - 1]^{-1}$ and $\mathcal{N}$ is the normalization constant.

The distribution $\mathcal{P}_j$ (Eq. (2.18)) and the definition of statistical average Eq. (2.19) imply that c-number noise $\eta(t)$ must satisfy

$$\langle\eta(t)\rangle_S = 0 \tag{2.20}$$

$$\langle\eta(t)\eta(t')\rangle_S = \frac{1}{2}\sum_j \frac{c_j^2}{\omega_j^2}\hbar\omega_j \left(\coth\frac{\hbar\omega_j}{2k_B T}\right)\cos\omega_j(t-t') \tag{2.21}$$

which are equivalent to (2.10) and (2.11), respectively.

In the Markovian limit the noise correlation becomes

$$\langle\eta(t)\eta(t')\rangle_S = 2D_0\delta(t-t') \tag{2.22a}$$

$$D_0 = \frac{1}{2}\Gamma\hbar\omega_0\left(\bar{n}(\omega_0) + \frac{1}{2}\right) \tag{2.22b}$$

where ω_0 is the average bath frequency and the spectral density function is considered in the Ohmic limit.

The Eqs. (2.20–2.21) imply that the c-number noise $\eta(t)$ is such that it is zero centered and satisfies the standard fluctuation–dissipation relation as expressed in Eq. (2.11). It is easy to recognize that the ansatz (2.18) is a canonical thermal Wigner distribution function for a shifted harmonic oscillator (obtained as an exact solution of Wigner equation[37] for harmonic oscillator) which always remains a positive definite function. A special advantage of using this distribution function is that it remains valid as a pure state nonsingular distribution function even at $T = 0$. At the same time the distribution of quantum mechanical mean values of the bath oscillators reduces to classical Maxwell–Boltzmann distribution in the thermal limit $\hbar\omega \ll k_B T$. Furthermore, this procedure allows us to bypass operator ordering prescription of Eq. (2.11) for deriving noise properties of the bath oscillators and to identify $\eta(t)$ as a classical looking noise with quantum mechanical content. We also mention that instead of Wigner function it is also possible to employ Glauber–Sudarshan distribution function to derive quantum fluctuation–dissipation relation.(39–43)

We now return to Eqs. (2.16a–2.16b) to add $V'(q)$, $\Gamma[f'(q)]^2 p$ and $f'(q)\eta(t)$ on the both sides of Eq. (2.16b) and rearrange it to obtain

$$\dot{q} = p \tag{2.23a}$$

$$\dot{p} = -V'(q) + Q_V - \Gamma[f'(q)]^2 p + Q_1 + f'(q)\eta(t) + Q_2 \tag{2.23b}$$

where

$$Q_V = V'(q) - \langle V'(\hat{q})\rangle \tag{2.24a}$$

$$Q_1 = \Gamma\left[[f'(q)]^2 p - \langle [f'(\hat{q})]^2 \hat{p}\rangle\right] \tag{2.24b}$$

$$Q_2 = \eta(t)\left[\langle f'(\hat{q})\rangle - f'(q)\right] \tag{2.24c}$$

Here Q_V represents quantum correction due to nonlinearity of the system potential. Q_1 and Q_2 represent quantum corrections due to nonlinearity of the system-bath coupling function. This implies that the quantum Langevin equation is governed by a c-number noise $\eta(t)$ originating from the heat bath characterized by the properties (2.20–2.21) and the quantum correction terms Q_V, Q_1 and Q_2 are characteristic of the nonlinearity of the potential and the coupling function.

Referring to the quantum nature of the system in the Heisenberg picture we now write the system operators $\hat{q}$ and $\hat{p}$ as

$$\hat{q} = q + \delta\hat{q} \tag{2.25a}$$

$$\hat{p} = p + \delta\hat{p} \tag{2.25b}$$

where $q(=\langle\hat{q}\rangle)$ and $p(=\langle\hat{p}\rangle)$ are the quantum mechanical mean values and $\delta\hat{q}$ and $\delta\hat{p}$ are the operators and they are quantum fluctuations around their respective mean values. By construction $\langle\delta\hat{q}\rangle = \langle\delta\hat{p}\rangle = 0$ and they also follow the usual commutation relation $[\delta\hat{q}, \delta\hat{p}] = i\hbar$. Using (2.25a) and (2.25b) in $V'(\hat{q})$, $[f'(\hat{q})]^2\hat{p}$ and $f'(\hat{q})$ and a Taylor series expansion in $\delta\hat{q}$ around q it is possible to express Q_V, Q_1 and Q_2 respectively as(44,45)

$$Q_V = -\sum_{n\geqslant 2} \frac{1}{n!} V^{n+1}(q)\langle\delta\hat{q}^n\rangle \tag{2.26}$$

$$Q_1 = -\Gamma\,[2\,p\,f'(q)Q_f + p\,Q_3 + 2f'(q)Q_4 + Q_5] \tag{2.27}$$

$$Q_2 = \eta(t)\,Q_f \tag{2.28}$$

where

$$Q_f = \sum_{n\geqslant 2} \frac{1}{n!} f^{n+1}(q)\langle\delta\hat{q}^n\rangle \tag{2.29}$$

$$Q_3 = \sum_{m\geqslant 1}\sum_{n\geqslant 1} \frac{1}{m!}\frac{1}{n!} f^{m+1}(q)\,f^{n+1}(q)\langle\delta\hat{q}^m\delta\hat{q}^n\rangle \tag{2.30}$$

$$Q_4 = \sum_{n\geqslant 1} \frac{1}{n!} f^{n+1}(q)\langle\delta\hat{q}^n\delta\hat{p}\rangle \tag{2.31}$$

$$Q_5 = \sum_{m\geqslant 1}\sum_{n\geqslant 1} \frac{1}{m!}\frac{1}{n!} f^{m+1}(q)\,f^{n+1}(q)\langle\delta\hat{q}^m\delta\hat{q}^n\delta\hat{p}\rangle \tag{2.32}$$

Using (2.27) and (2.28) in Eq. (2.23b) we have the c-number quantum Langevin equation in the Markovian limit

$$\dot{q} = p \tag{2.33a}$$

$$\dot{p} = -V'(q) + Q_V - \Gamma[f'(q)]^2 p - 2\Gamma\,p\,f'(q)Q_f - \Gamma\,p\,Q_3 - 2\Gamma f'(q)Q_4 \\ -\Gamma\,Q_5 + f'(q)\,\eta(t) + Q_f\,\eta(t) \tag{2.33b}$$

The quantum Langevin equation is characterized by a classical force term, V', as well as its correction Q_V. The terms containing Γ are nonlinear dissipative terms where Q_f, Q_3, Q_4 and Q_5 are due to associated quantum contribution in addition to classical nonlinear dissipative term $\Gamma[f'(q)]^2 p$. The last term in the above equation refers to a quantum multiplicative noise term in addition to the usual classical contribution $f'(q)\eta(t)$. It is therefore easy to recognize the classical limit of the above equation derived earlier by Lindenberg and Seshadri.[(4)] Furthermore, quantum dispersions due to potential and coupling terms in the Hamiltonian are entangled with nonlinearity. The quantum noise due heat bath on the other hand is expressed in terms of the fluctuation–dissipation relation.

2.2. Quantum Correction Equations

The quantum correction terms due to nonlinearity of the potential and the coupling function in Eq. (2.33b) are taken care of to all orders, in principle. In order to calculate them and the associated equations explicitly we write the system operators $\hat{q}$, $\hat{p}$ and the noise operator $\hat{\eta}$ in the Heisenberg picture as

$$\hat{q} = q + \delta\hat{q}, \tag{2.34a}$$
$$\hat{p} = p + \delta\hat{p}, \tag{2.34b}$$
$$\hat{\eta} = \eta + \delta\hat{\eta}, \tag{2.34c}$$

where $\delta\hat{\eta}$ is the fluctuation in noise around the mean value η and also $\langle\delta\hat{\eta}\rangle = 0$. We then use the above set of equations in operator Langevin equation in the Markovian limit (Eq. (2.13a) and Eq. (2.13b)) and subtract the c-number quantum Langevin equation (Eq. (2.33a) and Eq. (2.33b)) from the resultant to obtain

$$\delta\dot{\hat{q}} = \delta\hat{p} \tag{2.35}$$

$$\begin{aligned}
\delta\dot{\hat{p}} = & -V''(q)\delta\hat{q} - \sum_{n\geqslant 2}\frac{1}{n!}V^{n+1}(q)\left[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle\right] \\
& -\Gamma\left[2f'(q)f''(q)\delta\hat{q} + 2f'(q)\sum_{n\geqslant 2}\frac{1}{n!}f^{n+1}(q)\left[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle\right]\right. \\
& \left.+\sum_{m\geqslant 1}\sum_{n\geqslant 1}\frac{1}{m!}\frac{1}{n!}f^{m+1}(q)f^{n+1}(q)\left[\delta\hat{q}^m\delta\hat{q}^n - \langle\delta\hat{q}^m\delta\hat{q}^n\rangle\right]\right]p \\
& -\Gamma\left[[f'(q)]^2\delta\hat{p} + 2f'(q)\sum_{n\geqslant 1}\frac{1}{n!}f^{n+1}(q)\left[\delta\hat{q}^n\delta\hat{p} - \langle\delta\hat{q}^n\delta\hat{p}\rangle\right]\right. \\
& \left.+\sum_{m\geqslant 1}\sum_{n\geqslant 1}\frac{1}{m!}\frac{1}{n!}f^{m+1}(q)f^{n+1}(q)\left[\delta\hat{q}^m\delta\hat{q}^n\delta\hat{p} - \langle\delta\hat{q}^m\delta\hat{q}^n\delta\hat{p}\rangle\right]\right] \\
& +\eta(t)\left[f''(q)\delta\hat{q} + \sum_{n\geqslant 2}\frac{1}{n!}f^{n+1}(q)[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle]\right] \\
& +\delta\hat{\eta}\left[f'(q) + \sum_{n\geqslant 1}\frac{1}{n!}f^{n+1}(q)\delta\hat{q}^n\right]
\end{aligned} \tag{2.36}$$

We now carry out quantum mechanical average of Eq. (2.36) over initial product separable bath states $\Pi_{j=1}^{\infty}\{|\alpha_j(0)\rangle\}$ to get rid of $\delta\hat{\eta}$ term. With this the correction equations result in,

$$\delta\dot{\hat{q}} = \delta\hat{p} \tag{2.37a}$$

$$\begin{aligned}
\delta\dot{\hat{p}} = & -V''(q)\delta\hat{q} - \sum_{n\geqslant 2}\frac{1}{n!}V^{n+1}(q)\left[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle\right] \\
& -\Gamma\left[2f'(q)f''(q)\delta\hat{q} + 2f'(q)\sum_{n\geqslant 2}\frac{1}{n!}f^{n+1}(q)\left[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle\right]\right. \\
& \left. + \sum_{m\geqslant 1}\sum_{n\geqslant 1}\frac{1}{m!}\frac{1}{n!}f^{m+1}(q)f^{n+1}(q)\left[\delta\hat{q}^m\delta\hat{q}^n - \langle\delta\hat{q}^m\delta\hat{q}^n\rangle\right]\right]p \\
& -\Gamma\left[[f'(q)]^2\delta\hat{p} + 2f'(q)\sum_{n\geqslant 1}\frac{1}{n!}f^{n+1}(q)\left[\delta\hat{q}^n\delta\hat{p} - \langle\delta\hat{q}^n\delta\hat{p}\rangle\right]\right. \\
& \left. + \sum_{m\geqslant 1}\sum_{n\geqslant 1}\frac{1}{m!}\frac{1}{n!}f^{m+1}(q)f^{n+1}(q)\left[\delta\hat{q}^m\delta\hat{q}^n\delta\hat{p} - \langle\delta\hat{q}^m\delta\hat{q}^n\delta\hat{p}\rangle\right]\right] \\
& +\eta(t)\left[f''(q)\delta\hat{q} + \sum_{n\geqslant 2}\frac{1}{n!}f^{n+1}(q)[\delta\hat{q}^n - \langle\delta\hat{q}^n\rangle]\right]
\end{aligned} \tag{2.37b}$$

The operator equations (2.37a and 2.37b) are the basis of calculation of quantum correction terms Q_V, Q_f, Q_3, Q_4 and Q_5 to an arbitrary order. More specifically, we are to set up the equations for $\langle\delta\hat{q}^2\rangle$, $\langle\delta\hat{q}\delta\hat{p} + \delta\hat{p}\delta\hat{q}\rangle$, $\langle\delta\hat{p}^2\rangle$ in the second order and similarly for third order and so on. They are, in general, coupled and the infinite set of hierarchy of equations must be truncated after the desired order for practical purpose. The procedure is exactly similar to what had been done earlier in the case of additive noise.[(39–43)] Thus upto third order we may construct the following set of equations from Eq. (2.37a and 2.37a);

$$\frac{d}{dt}\langle\delta\hat{q}^2\rangle = \langle\delta\hat{q}\delta\hat{p} + \delta\hat{p}\delta\hat{q}\rangle \tag{2.38a}$$

$$\begin{aligned}
\frac{d}{dt}\langle\delta\hat{q}\delta\hat{p} + \delta\hat{p}\delta\hat{q}\rangle = & -2\chi(q,p)\langle\delta\hat{q}^2\rangle + 2\langle\delta\hat{q}^2\rangle - \Gamma[f'(q)]^2\langle\delta\hat{q}\delta\hat{p} + \delta\hat{p}\delta\hat{q}\rangle \\
& -\zeta(q,p)\langle\delta\hat{q}^3\rangle - 2\Gamma f'(q)f''(q)\langle\delta\hat{q}^2\delta\hat{p} + \delta\hat{p}\delta\hat{q}^2\rangle
\end{aligned} \tag{2.38b}$$

$$\frac{d}{dt}\langle\delta\hat{p}^2\rangle = -2\Gamma[f'(q)]^2\langle\delta\hat{p}^2\rangle - \chi(q,p)\langle\delta\hat{q}\delta\hat{p}+\delta\hat{p}\delta\hat{q}\rangle - \frac{1}{2}\zeta(q,p)\langle\delta\hat{q}^2\delta\hat{p}+\delta\hat{p}\delta\hat{q}^2\rangle - 2\Gamma f'(q)f''(q)\langle\delta\hat{q}\delta\hat{p}^2+\delta\hat{p}^2\delta\hat{q}\rangle \quad (2.38c)$$

$$\frac{d}{dt}\langle\delta\hat{q}^3\rangle = \frac{3}{2}\langle\delta\hat{q}^2\delta\hat{p}+\delta\hat{p}\delta\hat{q}^2\rangle \quad (2.38d)$$

$$\frac{d}{dt}\langle\delta\hat{p}^3\rangle = -3\Gamma[f'(q)]^2\langle\delta\hat{p}^3\rangle - \frac{3}{2}\chi(q,p)\langle\delta\hat{q}\delta\hat{p}^2+\delta\hat{p}^2\delta\hat{q}\rangle \quad (2.38e)$$

$$\frac{d}{dt}\langle\delta\hat{q}^2\delta\hat{p}+\delta\hat{p}\delta\hat{q}^2\rangle = -2\chi(q,p)\langle\delta\hat{q}^3\rangle + 2\langle\delta\hat{q}\delta\hat{p}^2+\delta\hat{p}^2\delta\hat{q}\rangle - \Gamma[f'(q)]^2\langle\delta\hat{q}^2\delta\hat{p}+\delta\hat{p}\delta\hat{q}^2\rangle \quad (2.38f)$$

$$\frac{d}{dt}\langle\delta\hat{q}\delta\hat{p}^2+\delta\hat{p}^2\delta\hat{q}\rangle = 2\langle\delta\hat{p}^3\rangle - 4\chi(q,p)\langle\delta\hat{q}^2\delta\hat{p}+\delta\hat{p}\delta\hat{q}^2\rangle - 2\Gamma[f'(q)]^2\langle\delta\hat{q}\delta\hat{p}^2+\delta\hat{p}^2\delta\hat{q}\rangle \quad (2.38g)$$

where

$$\chi(q,p) = V''(q) + 2\Gamma\, p\, f'(q)f''(q) - \eta(t)f''(q) \quad (2.38h)$$

$$\zeta(q,p) = V'''(q) + 2\Gamma\, p\, f'(q)f'''(q) + 2\Gamma p[f''(q)]^2 - \eta(t)f'''(q) \quad (2.38i)$$

2.3. Calculation of Quantum Statistical Averages

Summarizing the discussions of the last two sections 2.1 and 2.2 we now see that the quantum Langevin dynamics can be calculated for a stochastic process by solving the coupled Eqs. (2.33a, 2.33b) and (2.38a–2.38g) for quantum mechanical mean values simultaneously with quantum correction equations which describe quantum dispersion around these mean values. In principle, the equations for quantum corrections constitute an infinite set of hierarchy which must be truncated after a desired order, in practice, to make the system of equations closed. Care must be taken to distinguish three averages, the quantum mechanical mean $\langle\hat{O}\rangle(= O)$, statistical average over quantum mechanical mean $\langle O\rangle_S$ and the usual quantum statistical average $\langle\hat{O}\rangle_{QS}$ as discussed in Section 2.1. To illustrate the relation among them let us calculate, for example, the quantum statistical averages $\langle\hat{q}\rangle_{QS}$, $\langle\hat{q}^2\rangle_{QS}$ and $\langle\hat{q}^2\hat{p}\rangle_{QS}$. By (2.34a) and (2.34b) we write

$$\hat{q} = q + \delta\hat{q}$$
$$\langle\hat{q}\rangle_{QS} = \langle q + \delta\hat{q}\rangle_{QS} \tag{2.39}$$
$$= \langle q\rangle_S + \langle\langle\delta\hat{q}\rangle\rangle_S = \langle q\rangle_S \tag{2.40}$$

Again

$$\langle\hat{q}^2\rangle_{QS} = \langle(q + \delta\hat{q})^2\rangle_{QS}$$
$$= \langle q^2\rangle_S + \langle\langle\delta\hat{q}^2\rangle\rangle_S \tag{2.41}$$

In the case of harmonic potential and linear coupling, $\langle\delta\hat{q}^2\rangle$ is independent of q or p so that one may simplify (2.41) further as

$$\langle\hat{q}^2\rangle_{QS} = \langle q^2\rangle_S + \langle\delta\hat{q}^2\rangle \tag{2.42}$$

In ref. 41 the explicit exact expressions for $\langle\hat{q}^2\rangle_{QS}$ and $\langle\hat{p}^2\rangle_{QS}$ have been derived for harmonic oscillator in linear system-bath coupling and they are found to be in exact agreement with those of Grabert *et al.*[46] For anharmonic potential, however, one must have to use (2.41) to carry out further the statistical average over $\langle\delta\hat{q}^2\rangle$ *i.e* $\langle\langle\delta\hat{q}^2\rangle\rangle_S$, since $\langle\delta\hat{q}^2\rangle$ is a function of stochastic variables q and p according to quantum correction equations. Furthermore, we consider $\langle\hat{q}^2\hat{p}\rangle_{QS}$

$$\langle\hat{q}^2\hat{p}\rangle_{QS} = \langle(q + \delta\hat{q})^2(p + \delta\hat{p})\rangle_{QS}$$
$$= \langle q^2 p\rangle_S + \langle p\,\langle\delta\hat{q}^2\rangle\rangle_S + \langle\langle\delta\hat{q}^2\,\delta\hat{p}\rangle\rangle_S + 2\,\langle q\,\langle\delta\hat{q}\,\delta\hat{p}\rangle\rangle_S \tag{2.43}$$

The essential element of the present approach is thus expressing the quantum statistical average as the sum of statistical averages of set of functions of quantum mechanical mean values and dispersions. Langevin dynamics being coupled to quantum correction equations, the quantum mechanical mean values as well as the dispersions are computed simultaneously for each realization of the stochastic "path". A statistical average implies the averaging over many such "paths" (typically three to five thousands) similar to what is done to calculate statistical averaging by solving classical Langevin equation. Before leaving this section we mention a few pertinent points.

First, the distinction between the ensemble averaging by the present procedure and by the standard approach using Wigner function is now clear. From Eq. (2.43) we note that, for example,

$$\langle\hat{q}^2\hat{p}\rangle_{QS} = \int q^2 p\,W(q, p) \neq \langle q^2 p\rangle_S \tag{2.44}$$

where $W(q, p)$ is the Wigner function for the system. (This is not be confused with the Wigner function we introduced in Eq. (2.18) for the bath oscillators).

Second, our formulation of the Langevin equation coupled to quantum correction equations belongs to quantum stochastic process driven by c-number noise, which is classical-like in form. Its numerical solutions can be obtained[41,42] in the same way as one proceeds in a classical theory.

Third, quantum nature of the dynamics appears in two different ways. The heat bath is quantum mechanical in character whose noise properties are expressed through quantum fluctuation–dissipation relation. The nonlinearity of the system potential and coupling, on the other hand, give rise to quantum correction terms. Thus the classical Langevin equation can be easily recovered (i) in the limit $\hbar\omega \ll k_B T$ to be applied in the Eq. (2.21) so that one obtains the classical fluctuation–dissipation relation and (ii) if the quantum dispersion terms vanish.

3. THE OVERDAMPED LIMIT AND THE STATIONARY DISTRIBUTION

3.1. The Langevin Equation with Multiplicative Noise Under Strong Friction

In the case of large dissipation, one eliminates the fast variables adiabatically to get a simpler description of the system which is valid in a much slower time scale. This adiabatic elimination of fast variables is basically a zeroth order approximation. In this zeroth order approximation the number of system variables get reduced. When the Brownian particles move in a bath with constant large dissipation this adiabatic elimination of fast variables leads to the correct description of the system. This wellknown approximation, known as Smoluchowski approximation, results in correct equilibrium distribution. However, in presence of hydrodynamic interaction, i.e., when the fluctuation is position/state dependent or equivalently when the noise is multiplicative with respect to system variables the conventional adiabatic reduction of fast variables does not give the correct description of the system. Several years ago Sancho *et al.*[16] had proposed an alternative approach to get a correct Langevin equation in the case multiplicative noise system. Based on the Langevin equation they carried out a systematic expansion of the relevant variables in powers of Γ^{-1} neglecting terms smaller than $O(\Gamma^{-1})$. Then by ordinary Stratonovich interpretation it is possible to obtain the correct Langevin equation corresponding to a Fokker–Planck equation in position space. This description leads to the correct stationary probability distribution of the system with position dependent friction.

In order to get the quantum Langevin equation in the overdamped limit we follow this procedure. In what follows we discard the quantum correction terms Q_4 and Q_5 from Eq. (2.33b) since they involve quantum dispersions $\delta\hat{p}$ and therefore decays exponentially in the large damping limit. In this limit these transient correction terms do not affect the dynamics of the position which varies in a much slower time scale. So the quantum Langevin equation Eq. (2.33a) and Eq. (2.33b) can be written as, respectively,

$$\dot{q} = p \tag{3.1}$$

$$\dot{p} = -V'(q) + Q_V - \Gamma\, h(q) p + g(q)\, \eta(t) \tag{3.2}$$

where

$$h(q) = [f'(q)]^2 + 2f'(q) Q_f + Q_3 \tag{3.3}$$

$$g(q) = f'(q) + Q_f \tag{3.4}$$

The method of Sancho *et al.*[16] is followed further to obtain the Fokker–Planck equation in position space corresponding Langevin equation Eq. (3.2)

$$\frac{\partial P(q,t)}{\partial t} = \frac{\partial}{\partial q}\left[\frac{V'(q) - Q_V}{\Gamma\, h(q)}\right] P(q,t) + D_0 \frac{\partial}{\partial q}\left[\frac{1}{\Gamma\, (h(q))^2}\, g'(q) g(q)\right] P(q,t) + D_0 \frac{\partial}{\partial q}\left[\frac{g(q)}{\Gamma\, h(q)}\, \frac{\partial}{\partial q}\, \frac{g(q)}{\Gamma\, h(q)}\right] P(q,t) \tag{3.5}$$

In the ordinary Stratonovich description the Langevin equation corresponding to the Fokker–Planck Eq. (3.5) is given by

$$\dot{q} = -\frac{V'(q) - Q_V}{\Gamma\, h(q)} - D_0 \frac{g'(q) g(q)}{\Gamma\, (h(q))^2} + \frac{g(q)}{\Gamma\, h(q)}\, \eta(t) \tag{3.6}$$

Equation (3.6) is c-number quantum Langevin equation for multiplicative noise with position dependent friction in the overdamped limit (i.e., corrected upto $O(1/\Gamma)$).

In the classical limit, i.e., $\hbar\omega_0 \ll k_B T$, $h(q) = [f'(q)]^2$, $g(q) = f'(q)$, $Q_V = 0$ and $D_0 = \Gamma\, k_B T$ so the c-number quantum Langevin equation reduces to

$$\dot{q} = \frac{1}{\Gamma\, [f'(q)]^2}\left[-V'(q) - \Gamma\, k_B T\, \frac{f''(q)}{f'(q)} + f'(q)\, \eta(t)\right] \tag{3.7}$$

which is exactly the form derived by Sancho *et al.*[16]

Our next task is to establish the quantum corrections in the overdamped limit. To this end we return to Equation (2.37b), neglect the $\delta\dot{\hat{p}}$ term and keep the leading order correction equation (since in the overdamped limit higher order quantum contributions are small) to obtain

$$\frac{d}{dt}\delta\hat{q} = \frac{1}{\Gamma[f'(q)]^2}\Big[-V''(q)\,\delta\hat{q} - 2\Gamma\, p\, f'(q) f''(q)\delta\hat{q} + \eta(t) f''(q)\delta\hat{q}\Big] + O(\delta\hat{q}^2) \tag{3.8}$$

From Eq. (3.8) it is easy to calculate the equations of motion for quantum correction in the lowest order as

$$\frac{d}{dt}\langle\delta\hat{q}^2\rangle = \frac{2}{\Gamma[f'(q)]^2}\Big[-V''(q)\langle\delta\hat{q}^2\rangle - 2\,\Gamma\, p\, f'(q) f''(q)\langle\delta\hat{q}^2\rangle + \eta(t) f''(q)\langle\delta\hat{q}^2\rangle\Big] \tag{3.9}$$

A simplified expression for the leading order quantum correction term $\langle\delta\hat{q}^2\rangle$ can be estimated by neglecting the higher order coupling terms in the square bracket in Eq. (3.9) and rewriting it as $d\langle\delta\hat{q}^2\rangle = \frac{2}{\Gamma[f'(q)]^2} V''(q)\langle\delta\hat{q}^2\rangle\, dt$. The overdamped deterministic classical motion on the other hand gives $dq = -\frac{V'(q)}{\Gamma[f'(q)]^2}\,dt$. These together yield after integration

$$\langle\delta\hat{q}^2\rangle = \Delta_q[V'(q)]^2 \tag{3.10}$$

where $\Delta_q = \frac{\langle\delta\hat{q}^2\rangle_0}{[V'(q_0)]^2}$ and q_0 refers to initial position.

3.2. The Stationary Solution of Fokker–Planck Equation in Overdamped Limit

The Fokker–Planck equation Eq. (3.5) in the overdamped limit can be rewritten in a more compact form as

$$\frac{\partial P(q,t)}{\partial t} = \frac{\partial}{\partial q}\frac{1}{\Gamma h(q)}\left[V'(q) - Q_V + \frac{D_0}{\Gamma}\frac{\partial}{\partial q}\frac{g(q)^2}{h(q)}\right]P(q,t) \tag{3.11}$$

Equation (3.11) is the quantum Smoluchowski equation for multiplicative noise (damping is corrected upto $O(1/\Gamma)$). To capture the essential content of state-dependent diffusion we now proceed as follows. Under the stationary condition

$$\frac{\partial P(q,t)}{\partial t}=0 \tag{3.12}$$

Eq. (3.11) reduces to

$$\frac{D_0}{\Gamma}\frac{d}{dq}\left[\frac{g(q)^2}{h(q)}P_{\rm st}(q)\right]+V'(q)-Q_V=0 \tag{3.13}$$

After integration of Eq. (3.13) we have the stationary probability distribution in the overdamped limit as

$$P_{\rm st}(q)=N\frac{1}{[g(q)^2/h(q)]}\exp\left[-\int_0^q\frac{V'_{\rm quan}(q')}{D(q')}dq'\right] \tag{3.14}$$

with

$$D(q)=\hbar\omega_0\left(\bar{n}(\omega_0)+\frac{1}{2}\right)\left[g(q)^2/h(q)\right]$$

and

$$V'_{\rm quan}=V'(q)-Q_V$$

and N is the normalization constant. In the classical limit we have $g(q)^2/h(q)=1$, $Q_V=0$ and $\hbar\omega_0(\bar{n}(\omega_0)+\frac{1}{2})=k_{\rm B}T$; the stationary probability distribution function (3.14) reduces to classical equilibrium Boltzmann distribution $P^{\rm c}_{\rm st}=N\exp[-V(q)/k_{\rm B}T]$. Therefore, the stationary distribution (3.14) is essentially a quantum generalization of Boltzmann factor for state-dependent diffusion. This diffusion arises where the inhomogeneity is due to quantum corrections entangled with nonlinearity of the system-bath coupling. The state-dependent diffusion is wellknown in several classical contexts as pointed out earlier notably in Landauer Blowtorch effect,[1,2] where localized heating in a region along the reaction coordinate lying between the lower energy minimum and barrier top can raise the relative population of the higher minimum above what is allowed by Boltzmann factor. The example also includes noise-induced transport processes due to phase difference between periodic modulation of drift and modulation of diffusion as suggested by Büttiker.[5] It is however worth-noting that the inhomogeneity of $D(q)$ as implied in Eq. (3.14) is reminiscent of some sort of quantum nonlocal effect. A number of points are pertinent here. First, in realizing inhomogeneity through $D(q)$ we have taken care of quantum corrections to all orders. Second, the state-dependence is essentially due to nonlinear coupling mechanism in Hamiltonian (2.1) and is therefore model dependent and because of c-number nature of our treatment it corresponds to one of the classical forms of the phenomenological state-dependent diffusion term. This correspondence makes classical-quantum correspondence more clear. It is also worthnoting that the model-dependent nature of escape rate in classical Blow-torch effect had been discussed recently.[14] Third, for harmonic potential and linear coupling $f(q)=q$, we have $Q_V=0$ and $g(q)^2/h(q)=1$ and the probability distribution function reduces to well-known Wigner distribution for harmonic oscillator $V(q)$ as $P_{\rm st}^{\rm h}(q)=N\exp[-V(q)/\hbar\omega_0(\bar{n}(\omega_0)+\frac{1}{2})]$. Fourth, although model-dependent the inhomogeneous nature of the quantum diffusion must be thermodynamically consistent. To this end we examine in the next section the equilibrium condition as well as typical nonzero current situation (due to symmetry breaking under special condition) for a periodic potential and periodic derivative of coupling function. By thermodynamic consistency we imply that in absence of any external field, no directional component should remain after appropriate averaging over ensemble or over the period of space or time.

4. APPLICATION: A PERIODIC POTENTIAL

4.1. Solution Under Periodic Boundary Condition – Thermodynamic Consistency

In the overdamped limit the stationary current from Eq. (3.11) can be represented as,

$$J=-\frac{1}{\Gamma h(q)}\left[V'(q)-Q_V+\frac{D_0}{\Gamma}\frac{d}{dq}\left(\frac{g(q)^2}{h(q)}\right)\right]P_{\rm st}(q) \tag{4.1}$$

Integrating the Eq. (4.1) we have the expression of stationary probability distribution in terms of stationary current as,

$$P_{\rm st}(q)=\frac{e^{-\phi(q)}}{[g(q)^2/h(q)]}\left[\frac{g(0)^2}{h(0)}P_{\rm st}(0)-J\frac{\Gamma^2}{D_0}\int_0^q h(q')e^{\phi(q')}dq'\right] \tag{4.2}$$

where

$$\phi(q) = \frac{\Gamma}{D_0} \int_0^q \frac{V'(q') - Q_V}{[g(q')^2/h(q')]} dq' \tag{4.3}$$

We now consider a symmetric periodic potential with periodicity 2π, i.e., $V(q) = V(q+2\pi)$ and periodic derivative of coupling function with the same periodicity as that of the potential, i.e., $f'(q) = f'(q+2\pi)$.

Since the potential is periodic, Q_V is also a periodic function because $Q_V = V(q) - \langle V(\hat{q})\rangle$. Similarly Q_f is also periodic because $Q_f = \langle f'(\hat{q})\rangle - f'(q)$, and also $Q_3 + 2f'(q)Q_f$ is also periodic since $Q_3 + 2f'(q)Q_f = \langle [f'(\hat{q})]^2\rangle - [f'(q)]^2$. So from Eqs. (3.3) and (3.4) it is clear that $h(q)$ and $g(q)$ are also periodic functions of q with periodicity 2π. This will be made more explicit when we consider a specific example in the next section.

Now applying the periodic boundary condition on $P_{\rm st}(q)$, i.e., $P_{\rm st}(q) = P_{\rm st}(q+2\pi)$ we have from Eq. (4.2)

$$\frac{g(0)^2}{h(0)} P_{\rm st}(0) = J \frac{\Gamma^2}{D_0} \left[1 - e^{\phi(2\pi)}\right]^{-1} \int_0^{2\pi} h(q)\, e^{\phi(q)} dq \tag{4.4}$$

By applying the normalization condition on stationary probability distribution which is given by

$$\int_0^{2\pi} P_{\rm st}(q)\, dq = 1 \tag{4.5}$$

we obtain from Eq. (4.2)

$$\int_0^{2\pi} \frac{e^{-\phi(q)}}{[g(q)^2/h(q)]} \left[\frac{g(0)^2}{h(0)} P_{\rm st}(0) - J \frac{\Gamma^2}{D_0} \int_0^q h(q')\, e^{\phi(q')} dq'\right] dq = 1 \tag{4.6}$$

Elimination of $\frac{g(0)^2}{h(0)} P_{\rm st}(0)$ from (4.4) and (4.6) yields the expression of stationary current after some rearrangement

$$\begin{aligned} J = \frac{D_0}{\Gamma^2} \Bigg\{ \left\{1 - e^{\phi(2\pi)}\right\} \Bigg/ & \\ \Bigg\{ \int_0^{2\pi} \frac{h(q)}{g(q)^2} e^{-\phi(q)} dq \int_0^{2\pi} h(q')\, e^{\phi(q')} dq' & \\ - [1 - e^{\phi(2\pi)}] \int_0^{2\pi} \frac{h(q)}{g(q)^2} e^{-\phi(q)} \int_0^q h(q')\, e^{\phi(q')} dq' dq \Bigg\} \Bigg\} & \end{aligned} \tag{4.7}$$

From the condition of periodicity of potential and different quantum correction terms it is clear that for the periodic potential and the periodic derivative of coupling function with same periodicity $\frac{V'(q)}{[g(q)^2/h(q)]}$ and $\frac{Q_V(q)}{[g(q)^2/h(q)]}$ are both periodic with same periodicity. This makes effective potential $\phi(q)$ equal to zero;

$$\phi(2\pi) = \frac{\Gamma}{D_0} \int_0^{2\pi} \frac{V'(q) - Q_V}{[g(q)^2/h(q)]} \, dq = 0 \tag{4.8}$$

Therefore, the numerator of the expression for current (4.7) reduces to zero. We thus conclude that there is no occurrence of current for a periodic potential and periodic derivative of coupling with same periodicity. At the macroscopic level this confirms that there is no generation of perpetual motion of second kind, i.e., no violation of second law of thermodynamics. Therefore, the thermodynamic consistency based on symmetry considerations ensures the validity of the present formalism and of the overdamped quantum multiplicative Langevin equation.

4.2. Phase Induced Current

Bütikker[5] in 1987 had shown that in case of space-dependent friction in the overdamped limit a classical particle under a symmetric sinusoidal potential field and also in presence of a sinusoidally modulated space-dependent diffusion with same periodicity experiences a net drift force resulting in generation of current. This current is basically due to the phase difference between the symmetric periodic potential and the space-dependent diffusion. The current does vanish when the phase difference is either zero or integral multiple of π. van Kampen[3] in a later work also ended up with similar kind of conclusion for a system with space-dependent temperature under the overdamped condition. The result of van Kampen is a re-examination of the earlier observation due to Landauer.[1,2]

We now explore, in the spirit of Büttiker but in the present quantum-mechanical context a system with a symmetric periodic potential, i.e., $V(q) = V(-q)$, and a periodic derivative of coupling function with same periodicity but with a phase difference between them leading to a net directed motion or current. This is because of the fact that the phase bias gives a tilt to the effective potential $\phi(q)$, (if $\phi(q)$ is plotted as a function of q), which makes the transition between left to right and right to left unequal. The phase difference therefore breaks the detailed balance of the system. We show that when the phase difference is zero or integral multiple of π the quantum current vanishes.

We proceed with a sinusoidal symmetric potential of the form

$$V(q) = V_0\,[1 + \cos(q + \theta)] \tag{4.9}$$

where V_0 can be taken as the barrier height and θ is phase factor which can be controlled externally.

The derivative of the chosen coupling function, $f(q) = (q + \alpha \sin q)$, is

$$f'(q) = 1 + \alpha \cos q \tag{4.10}$$

where α is a modulation parameter.

Given the form of potential $V(q)$ and coupling function $f(q)$ we obtain from Eq. (3.10) the second order quantum correction in the over-damped limit as

$$\langle \delta\hat{q}^2 \rangle = -\,\Delta_q\, V_0^2 \sin^2(q + \theta) \tag{4.11}$$

Therefore, the correction to the potential in the leading order from Eq. (2.26) is given by

$$Q_V = -\frac{1}{2}\,\Delta_q\, V_0^3 \sin^3(q + \theta) \tag{4.12}$$

The quantum corrections Q_f and Q_3 in the same order can be estimated using Eqs. (2.29) and (2.30):

$$Q_f = -\frac{1}{2}\,\Delta_q\,\alpha\, V_0^2 \cos q\, \sin^2(q + \theta) \tag{4.13}$$

$$Q_3 = \Delta_q\,\alpha^2\, V_0^2 \sin^2 q\, \sin^2(q + \theta) \tag{4.14}$$

Furthermore, from Eqs. (3.3) and (3.4) we calculate $h(q)$ and $g(q)$, respectively, using Eqs. (4.10), (4.13) and (4.14) to obtain

$$h(q) = (1 + \alpha \cos q)^2 - \Delta_q\,\alpha\, V_0^2 \cos q\, \sin^2(q + \theta)\,(1 + \alpha \cos q) + \Delta_q\,\alpha^2\, V_0^2 \sin^2 q\, \sin^2(q + \theta) \tag{4.15}$$

$$g(q) = 1 + \alpha \cos q - \frac{1}{2}\,\Delta_q\,\alpha\, V_0^2 \cos q\, \sin^2(q + \theta) \tag{4.16}$$

With these preliminaries we now calculate the current given by Eq. (4.7) explicitly using (4.9), (4.12), (4.15) and (4.16). A key quantity for this analysis is $\phi(q)$ [(4.3)] which involves the phase θ. In units of $\hbar = k_B = 1$ we set the parameter values $\langle \delta \hat{q}^2 \rangle_0 = 1/2$, minimum uncertainty value, $\Delta_q = 0.5$, $V_0 = 1.0$, $\omega_0 = 1.0$, $\alpha = 1.0$, $T = 1.0$ and $\Gamma = 1.0$. The variation of current J as a function of phase θ is exhibited in Fig. 1. It is interesting to observe that for $\theta \neq 0, n\pi$ where $n = \pm 1, \pm 2 \ldots$, phase induces a current which is a periodic function of the phase difference between modulations of potential and diffusion. The origin of the current can be traced to the inhomogeneous diffusion of a quantum particle in contrast to classical one proposed by Büttiker. That this current depends on the amplitude of modulation α of the diffusion is shown in Fig. 2 for $\theta = 3.6$, $V_0 = 1.0$, $\omega_0 = 1.0$ for several values of $k_B T$. For $\alpha = 0$, the current vanishes and we have only linear coupling and the phase bias has no relevance in such situation. We observe for a fixed temperature a sharp increase in current beyond a moderate value of α and that for an optimum temperature the current is maximum for a given strength of modulation. Figure 3 illustrates the variation of current (J) as a function of temperature for the phase $\theta = 3.6$ and for several values of strength of modulation of diffusion α for $V_0 = 1.0$, $\omega_0 = 1.0$. One observes that even at $T = 0$, the vacuum field of the heat bath induces a finite current. As the temperature increases the current decreases after an initial increase and reaching a maximum.

We thus observe that nonlinear system-bath coupling may give rise to state-dependent noise and diffusion in a quantum system. For a periodic potential and for a periodic derivative of coupling function, with same

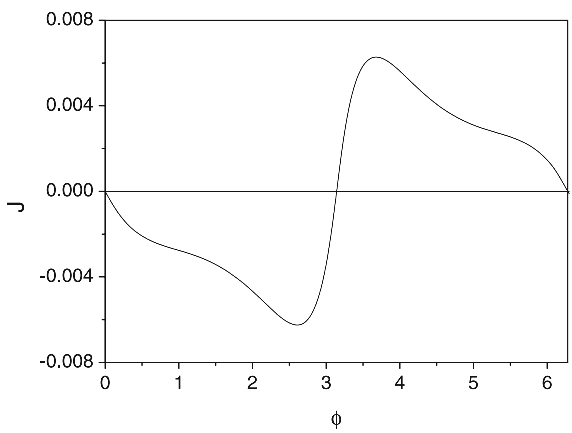

Fig. 1. Variation of current J as a function of phase θ between 0 and 2π for $T = 1.0$, $\omega_0 = 1.0$, $\alpha = 1.0$, $V_0 = 1.0$ and $\Gamma = 1.0$ (units arbitrary).

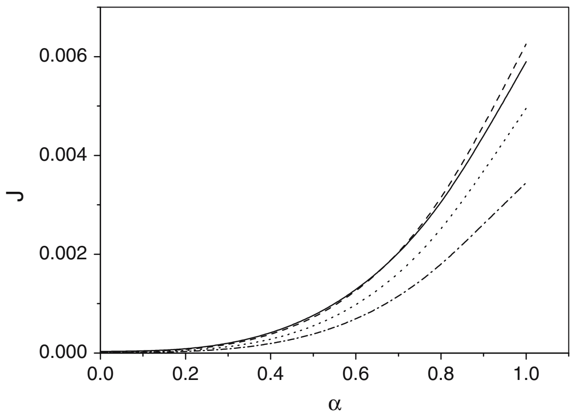

Fig. 2. Plot of current J vs. strength of modulation α for $\theta = 3.6$, $V_0 = 1.0$, $\omega_0 = 1.0$ and for $T = 0.1$ (dashed-dotted line); $T = 0.5$ (dotted line); $T = 1.0$ (dashed line); $T = 3.0$ (solid line) (units arbitrary).

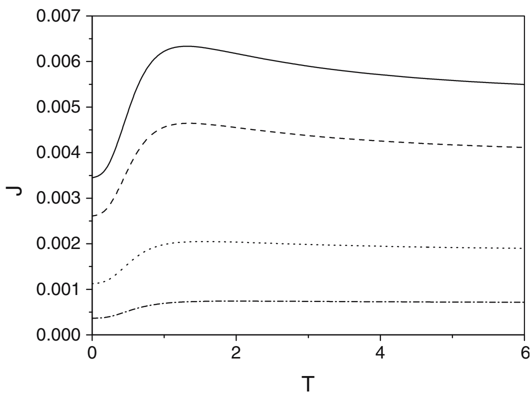

Fig. 3. Variation of current J as a function of temperature T for $\theta = 3.6$, $V_0 = 1.0$, $\omega_0 = 1.0$ and for strength of modulation $\alpha = 0.5$ (dashed-dotted line); $\alpha = 0.7$ (dotted line); $\alpha = 0.9$ (dashed line); $\alpha = 1.0$ (solid line) (units arbitrary).

periodicity, the state-dependent noise may lead to symmetry breaking in presence of a phase bias. This generates a directional flow which vanishes in absence of the bias and can be optimized by application of suitable strength of modulation and temperature.

5. CONCLUSION

In this paper, we have developed a theory of diffusion of a quantum particle in inhomogeneous media. The approach is based on the system-reservoir model with a nonlinear coupling. We derive the quantum Langevin equation with a multiplicative noise and a nonlinear dissipation in the Markovian limit, which is coupled to a set of quantum correction equations developed order by order. A systematic expansion of the relevant variable in powers of inverse of the dissipation constant and use of large friction limit lead to a quantum Smoluchowski equation for state-dependent diffusion. It is apparent that the state dependence owes its origin to nonlinear coupling between the system and bath degrees of freedom and the corresponding generalization of Boltzmann factor for the steady state has been shown to be thermodynamically consistent. We have applied the formalism to the problem of diffusion of a quantum particle in a periodic potential where the derivative of coupling function is periodic with same periodicity. We have shown that a phase difference between these two spatially periodic modulations may give rise to a directed quantum current. This current vanishes in the classical limit and is a consequence of state-dependent diffusion where nonlocality in the effective potential is essentially a quantum effect.

The Brownian motion of a quantum particle in inhomogeneous media is an active area of contemporary research in stochastic energetics. We hope that our formalism of quantum Langevin equation with multiplicative noise and the associated Smoluchowski equation for state-dependent diffusion as a description of the stochastic processes may be useful for other similar issues, particularly for calculations of quantum decay rate of metastable state, energy dissipation and so on. The extension of the theory to non-Markovian and weak friction regime is also worth-pursuing. We hope to address these issues elsewhere.

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