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Diffusion described with quantum Langevin equation in tilted periodic potential

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ABSTRACT

In this paper, diffusion behavior of Brownian particles moving in a 1D periodic potential landscape has been theoretically investigated by using the general quantum Langevin equation. At first, in the condition of weak disorder, some anomalous diffusive behaviors have been revealed in the process. Then, two types of mean square displacement, ensemble averaged and time averaged mean square displacement, have been investigated in a long time, and the weak ergodicity breaking phenomenon has been revealed. It is shown that the general quantum Langevin equation can exhibit some novel details of the experimental diffusion process.

1. Introduction

Diffusion plays a very important role for the particle mixing, homogenization, selection and separation [1]; therefore much interest has been devoted to this topic in past decades not only experimentally but also theoretically. These investigations can also help to understand the statistical behaviors of many kinds of microscopic particles. For example, a cold atom in optical lattices [2], globular DNA in microstructures [3], enzymatic reaction cycles driving molecular motors [4] or colloidal granules in optical vortices [5,6]. The colloidal granules diffusion is a simple example of those studies and the developed methods are powerful enough to investigate the diffusion of particles in different conditions.

It has been shown that there is not only normal diffusion but also anomalous diffusion in nature. Both of them can be described with the mean squared displacement (MSD) of particles. Concentrating on the one-dimensional cases, the MSD for regular diffusion is given by Metzler and Klafter [7] $\langle x^2(t)\rangle = 2kt$, where k is the diffusion coefficient and $\langle\cdots\rangle$ can be understood either as an ensemble average over a large ensemble of trajectories or as a temporal moving average. For anomalous diffusion, the MSD has the form $\langle x^2(t)\rangle \propto k_\alpha t^\alpha$. Systems with $0 < \alpha < 1$ display subdiffusion, while values of $1 < \alpha < 2$ correspond to superdiffusion. These kinds of forms of diffusion have been observed in many experiments through tracking particles [8,9] with optical tweezers and video microscopy. It is interested that by using some complementary analysis tools to deal with the detected data, many groups found some novel features of the particle diffusion [10–13]. For example, the MSD displays some oscillation in a certain time range. Especially, it has been found that the MSD of lipid granules in *S. pombe* displays normal diffusion in short time and then a turnover to subdiffusion [14]. It in fact proves that the granule motion exhibits weak ergodicity breaking, which is interesting in understanding the mechanism of the granule motion.

Theoretically, some works have been done for explaining the novel phenomena with continuous time random walk (CTRW) and fractional Brownian motion (FBM) with overdamped approximation. The CTRW subdiffusion has not been identified until now as the stochastic mechanism; the FBM was proposed as the stochastic mechanism in some of those systems [15–17]. But the usage of the overdamped approximation is unsafe because it results in significant difference from

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the exact solution in the study of the autocorrelation function [18]. Thus, it will be interesting to investigate the problems by using other methods.

In this paper, we use the general quantum Langevin equation (GQLE) to investigate the motion of particles driven by a constant external force over a landscape consisting of a periodic potential corrugated by a small amount of spatial disorder. We shall simulate MSD by using the GQLE, and the oscillation of the MSD will be naturally shown in our data. The anomalous diffusive behavior arising from weak spatial disorder will be obtained with a more corrugated random potential. Furthermore, the ergodicity breaking will be shown in our plots. And it will also be shown that the time averaged MSD (TAMSD) strongly differs from one trajectory to another, while ensemble averaged MSD (EAMSD) obtains a convergent result in a long time.

The remaining part of this paper is organized as follows. In Section 2, we shall briefly summarize the elements of the GQLE methods and set up the technology need for the rest of the paper. In Section 3 we shall illustrate the GQLE diffusive behavior, which is somewhat different from the overdamped cases. Conclusions and further applications of diffusion law are then discussed in Section 4.

2. Dynamics of the diffusion system

Throughout this paper, we use the general quantum Langevin equation to investigate Brownian motion, which has the form [19]

$$m\ddot{x}(t) + m\int_0^t dt'\gamma(t-t')\dot{x}(t') + U'(x) = F(t). \tag{1}$$

Here, m is the mass and x is the coordinate operator of the system, and $U'(x) = dU(x)/dx$ where $U(x)$ is the potential function. The noise force operator $F(t)$ and memory kernel $\gamma(t-t')$ are given by

$$F(t) = \sum_j [\{q_j(0) - x(0)\}\kappa_j \cos\omega_j t + p_j(0)\kappa_j^{\frac{1}{2}} \sin\omega_j t], \tag{2}$$

and

$$\gamma(t-t') = \frac{1}{m}\sum_j \kappa_j \cos\omega_j(t-t'). \tag{3}$$

Here, $q_j(0)$ and $p_j(0)$ denote the initial coordinate and corresponding momentum of the j-th bath oscillator and $\kappa_j = \omega_j^2$ is the coefficient of the j-th bath oscillator coupled to the system. Eq. (1) is the well known exact quantized operator Langevin equation for which the noise properties of $F(t)$ can be derived by using a suitable initial canonical distribution of the bath coordinate and momentum operators as

$$\langle F(t)\rangle_{QS} = 0, \tag{4}$$

$$\frac{1}{2}\{\langle F(t)F(t')\rangle_{QS} + \langle F(t')F(t)\rangle_{QS}\} = \frac{1}{2}\sum_j \kappa_j\hbar\omega_j \coth\left(\frac{\hbar\omega_j}{2k_BT}\right)\cos\omega_j(t-t'), \tag{5}$$

where $\langle\cdots\rangle_{QS}$ refers to quantum statistical average [20] on the degrees of freedom and is defined as

$$\langle O\rangle_{QS} = \frac{TrO\exp(-H_{bath}/k_BT)}{Tr\exp(-H_{bath}/k_BT)} \tag{6}$$

for any operator $O(\{q_j - x\}, \{p_j\})$, where $H_{bath} = \sum_j\{(p_j^2/2) + 1/2\kappa_j(q_j - x)^2\}$. To construct the c-number Langevin equation, we firstly carry out the average to Eq. (1) as

$$m\langle\ddot{x}(t)\rangle + m\int_0^t dt'\gamma(t-t')\langle\dot{x}(t')\rangle + \langle U'(x)\rangle = \langle F(t)\rangle, \tag{7}$$

where $\langle\cdots\rangle$ denotes the quantum-mechanical average [19]. Let $f(t) = \langle F(t)\rangle$. We then have

$$f(t) = \sum_j [\{\langle q_j(0)\rangle - \langle x(0)\rangle\}\kappa_j \cos(\omega_j t) + \langle p_j(0)\rangle\kappa_j^{\frac{1}{2}} \sin(\omega_j t)]. \tag{8}$$

Thus, we can obtain the c-number equation as

$$m\langle\ddot{x}(t)\rangle + m\int_0^t dt'\gamma(t-t')\langle\dot{x}(t')\rangle + \langle U'(x)\rangle = f(t), \tag{9}$$