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Enhanced Transport of Overdamped Particles in a Disordered Biased Periodic Potential

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Abstract

This paper considers the diffusive properties of Brownian motion driven by an Ornstein-Uhlenbeck (OU) colored noise in a biased periodic potential corrugated by spatial disorders in the form of zero-mean random correlated potential. Through Langevin Monte-Carlo simulation, a giant enhancement diffusion is observed in a range of bias forces. Then, theoretical analysis based on the trajectory of a particle in the random correlated potential (RCP) is performed to investigate the transport phenomenon of particles. The effective diffusion coefficient is measured by the envelope width of the spatial distribution of the particle, and it becomes wider due to the emergence of the RCP. This is because the roughness of the potential causes a large proportion of the test particles to be locked or trapped. Furthermore, the positive-correlation characteristics of the OU noise are considered, and the optimal value of the effective diffusion coefficient is discussed.

Keywords

Diffusion, Enhancement Phenomenon, the Random Correlated Potential, Roughness

1. Introduction

The dynamics of Brownian particles in a biased periodic potential is a basic non-equilibrium model of statistical physics. It describes a surprising range of physical situations, including the Josephson junctions [1], diffusion of atoms and molecules on the crystal surface [2], superionic conductors [3], and cold atoms dwelling in optical lattices [4] [5]. This model is simple but has a rich phenomenology as a nonlinear stochastic system [6]. Diffusion of a particle driven by white noise in the one-dimensional or two-dimensional biased periodic potential has been investigated in [7] [8] [9] [10], where the effective diffusion coefficient is greatly enhanced and even quantitatively larger than that in the case of free diffusion. The above results can be explained by a simple two-state theory, *i.e.*, test particles exit a locked state or a running state and transfer between each other. However, some disorders should be imposed on such periodic potential to study more realistic reactions such as the protein folding, where the potential surface may have a hierarchical structure [11]-[16].

In recent decades, the random correlated potential (RCP), which is formed of wells and hills and whose location and magnitude are random quantities, attracts much attention [17]. It has been applied to various disordered media [18]-[24], especially the motion of colloidal particles in both experimental observation and numerical simulation [25]. The asymptotical behavior of a force-free particle in the RCP is sub-diffusion at a low temperature. This is caused by a reduction of the kinetic energy related to both friction and the RCP [26]. Meanwhile, it has been pointed out that a nail effect induced by the roughness in a metastable potential leads to an opposite-Arrhenius decrease in the rate with the increase of rough intensity [27]. However, not all occurrences of RCP are harmful. Recent studies [26] [28] on the diffusion have indicated that roughness can help to separate the spatial probability peaks at many disordered barriers when the external tilted force approaches the critical value. So, the diffusion is enhanced, and the value of the effective diffusion coefficient is more pronounced than the peak value of the biased periodic potential. Moreover, this behavior has been observed experimentally when tracking the motion of colloidal spheres through a periodic potential [29].

During the last few years, significant progress has been made in understanding diffusion in nonlinear systems driven by colored noise. This problem is critical not only because of its immediate relevance to numerous particular systems but also because the white-noise approximation is an idealization [30] [31]. The Ornstein-Uhlenbeck (OU) colored noise has been widely investigated and discussed. Especially, the correlation underlying the OU noise is exponential and non-negative [32], which implies that the noise stays in one direction and the direction of the following ones will likely remain consistent with it. In addition, the study [33] has demonstrated an enhancement for the effective diffusion coefficient (D_{eff}) of a particle driven by the OU noise in a one-dimensional and two-dimensional periodic potential.

All these studies present interesting viewpoints and inspire our work. The diffusion of a particle driven by the OU colored noise in the biased and disordered periodic potential might be related to the more complex and realistic processes. This paper aims to explore whether an enhancement phenomenon of a particle driven by the OU noise will appear. Meanwhile, it is important to determine the contributions of the RCP superimposed on the potential to the diffusion process.

The rest of this paper is organized as follows. In Section II, the dynamical equations to describe the over-damped particle driven by the OU noise and detailed characterization of the RCP are presented. Then, a numerical study for the motion of a particle embedded in a biased disordered potential under a biasing external force is presented in Section III. Next, the roles of the parameters of RCP and the noise are studied. Finally, in Section V, some comments and conclusions are given.

2. The Model

This paper considers the motion of overdamped independent Brownian particles evolving in a quenched random potential $U(x)$ and subject to a constant external force *F*. In a one-dimensional scenario, each particle obeys the Langevin equation:

$$\gamma \frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\mathrm{d}U(x)}{\mathrm{d}x} + F + \varepsilon(t), \tag{1}$$

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = -\frac{1}{\tau}\varepsilon + \frac{\sqrt{2D}}{\tau}\xi(t), \tag{2}$$

where x is the reaction coordinate, t is the time, γ is the friction coefficient, F is the applied external force, D represents the intensity of noise; the Gaussian white noise $\xi(t)$ obeys $\langle \xi(t) \rangle = 0$, and $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$; the angular brackets denote statistical averages.

The OU colored noise $\varepsilon(t)$ has a positive correlation function: $\langle \varepsilon(t)\varepsilon(t') \rangle = D/\tau^{-1}\exp\left(-|t-t'|/\tau\right)$, where τ is the correlated time of the OU noise. The OU colored noise will be reduced into the white noise when $\tau \to 0$, and the fluctuation vanishes if $\tau \to \infty$. **Figure 1** presents the stochastic trajectories of the OU colored noise under various correlated time. It can be seen that the OU noise exhibits a positive-correlation characteristic, which means that the particle needs more time to reach the stationary position, especially when the correlated time becomes longer.

The potential $U(x)$ consists of a fixed part and a spatially random part, *i.e.*,

$$U(x) = U_f(x) + U_r(x), \tag{3}$$

where the RCP U_r is characterized by its statistics properties. Its mean $\langle U_r(x) \rangle$ is set to zero, and its correlation function given by

$$\begin{aligned} &\langle U_r(x)U_r(x') \rangle = g_0 \exp\left(\frac{-|x-x'|^2}{2\lambda^2}\right), \\ &g_0 = \frac{\varepsilon}{\sqrt{2\pi}\lambda}, \end{aligned} \tag{4}$$

where the angular brackets indicate a spatial average. The characteristic length λ and the effective intensity ε are two basic parameters characterizing the RCP [26] [34]. The RCP can be generated by the method of discrete Fast Fourier Transform (FFT).

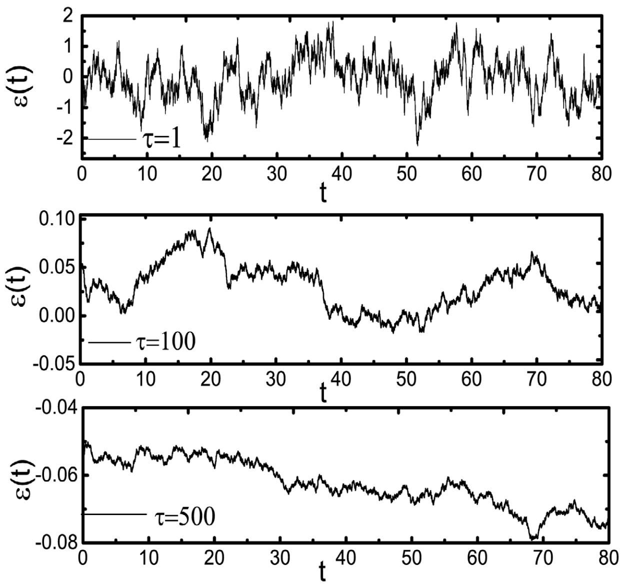

Figure 1. Typical trajectories for the OU noise under various correlated time. The correlated time is $\tau = 1$ (top panel), $\tau = 100$ (middle panel), and $\tau = 500$ (bottom panel), respectively. The parameters used is $D = 0.5$.

The perturbation $U_r(x)$ will be eliminated if $U(x)$ is spatially averaged, and only the smooth background remains. The average of total potential $\langle U(x) \rangle$ over the realization of $U_f(x)$ is set as an periodic potential

$$U_f(x) = -U_0 \cos\left(\frac{2\pi x}{L}\right), \tag{5}$$

where U_0 represents the amplitude strength of the periodic potential, and L represents the spatial period. **Figure 2** shows the realization of the RCP $U_r(x)$ and the background potential $U_f(x)$. It can be seen that there are many barriers in the RCP profile, and the number of barriers increases when the scaled correlation length λ decreases. In contrast, the increase of the intensity g_0 results in deeper wells of the RCP.

3. The Giant Diffusion in Rough Titled Periodic Potential

In our study, the quantity of central interest will be the effective diffusion coefficient. Previous works have shown that it can be expressed as $D_{eff} = \lim_{t\to\infty} \Delta x^2(t)/(2t)$, where $\Delta x^2(t) = \langle x^2(t) \rangle - \langle x(t) \rangle^2$ is the mean square displacement (MSD), and the bracket denotes the average over trajectories [8]. The approach of double-averaging over statistic ensemble and test particles is adopted to calculate the coordinate variance when the RCP is added [27]. The Time-dependent MSD is determined numerically by

$$\langle \Delta x^2(t) \rangle = \frac{1}{K} \sum_{j=1}^{K} \langle \Delta x_i^2(t) \rangle_j, \tag{6}$$

$$\langle \Delta x_i^2(t) \rangle_j = \frac{1}{N} \sum_{i=1}^{N} \left[\langle x_i^2(t) \rangle - \langle x_i(t) \rangle^2 \right]_j, \tag{7}$$

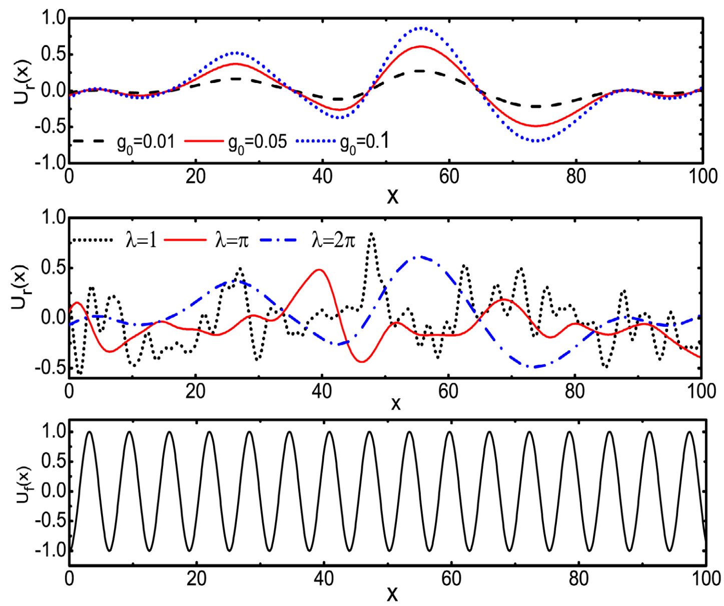

Figure 2. The realization of the RCP $U_r(x)$ and the background potential $U_f(x)$. The parameters used are $g_0 = 0.01$, 0.05, and 0.1 at fixed $\lambda = 2\pi$ (top panel); $\lambda = 1$, π, and 2π at fixed $g_0 = 0.1$ (middle panel); $U_0 = 1$ and $L = 2\pi$ (bottom panel).

where $\langle \Delta x_i^2(t) \rangle_j$ is the MSD of the *i*-th test particle for the *j*-th rough titled periodic potential at time *t*. The present Monte Carlo simulations involves the time step $\Delta t = 5 \times 10^{-3}$, total integration time $N_t = 3 \times 10^4$, and test particles $N = 10^4$. Besides, the particles are initially located at $x(0) = 0$ for all simulations, and the number of the RCP $K = 100$ is considered to perform double statistical averages.

This part first presents the results under the influence of the external biasing force. In Figure 3, the D_{eff} as a function of the tilted force F for different g_0 is depicted. Meanwhile, the diffusion behavior of the particle driven by the white noise corresponding to the case of $\tau \to 0$ is shown. The test particles cannot be trapped in well and diffuse freely when the periodic potential is tilted with its local minima disappearing; the motion of the particle is locked only when the tilted force is small. However, a particle experiences diffusion for a medium tilted force *F*, and it exhibits two spatial motion modes: the compact running state and the locked behind state. These two modes coexist and transform, leading to an increase in the effective coefficient of the diffusion. Furthermore, due to the positive correlation characteristic of the OU noise, the diffusion is enhanced, as demonstrated in the subgraph of Figure 3(a). The correlation effect of the noise is beneficial to biased diffusion.

This paper pays more attention to the influence of the roughness of the potential, especially the intensity g_0 that affects the depth of the small potential wells in periodic potential directly. It can be seen from Figure 3 that D_{eff} increases as the value of g_0 increases. The distinct potential wells will become deeper due to the emergence of the RCP, which results in a large proportion of the test particles

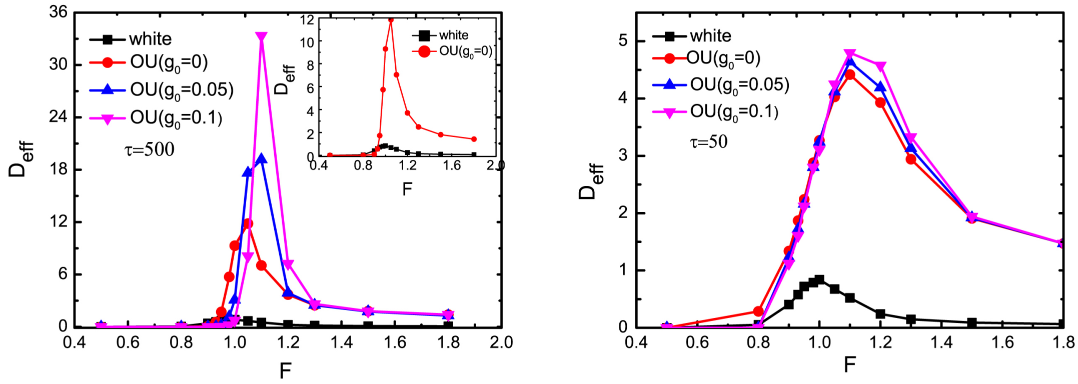

Figure 3. The effective diffusion coefficient D_{eff} as a function of F for different roughness g_0 with the correlated time of the OU noise. The applied parameters are $\lambda = 2\pi$ and $D = 1.0$.

being trapped or locked. This phenomenon is especially pronounced near the critical tilted force F_c, where the value $F_c = 1.0$.

In view of this phenomenon, this paper presents the variation of the diffusion coefficient with the intensity g_0 under different external force values in Figure 4. For a small F, the value of D_{eff} decreases as the intensity g_0 increases. Due to the introduction of the RCP, the test particles are almost trapped in a distinct potential well. The locked state does not disappear in the absence of the RCP until the tilted force reaches the critical value. However, due to the existence of RCP, the local minima still exist, and the probability peaks are distributed at the potential barriers even if the external force is greater than the critical value F_c. The number of particles in locked state increases and the particles in the running state also coexist at this time. Thus a giant diffusion appears near the critical force, especially when the value of g_0 increases. The diffusion is also enhanced as the intensity g_0 increase for a larger F comparing with the case when F is small. Similarly, the probability of a particle locked in local minima of the potential increases when g_0 is large. However, due to the large tilting force, the number of the local minima in the potential will decrease, which leads to a reduction of the D_{eff} comparing with the case when F is near the critical value. Moreover, the occurrence of the RCP is not always harmful, which can be a promotion for the movement of particles under the right conditions.

Note that this paper takes two different types of correlated time as examples in Figure 3 and Figure 4. The correlated time τ of the noise also affects the value of the diffusion coefficient. In this regard, this paper conducts a further in-depth study, and the results are illustrated in Figure 5. It can be seen that the effective diffusion coefficient D_{eff} does not depend monotonically on the correlated time τ, and there exists an optimal τ that makes the effective diffusion coefficient maximum. In addition, the value of D_{eff} induced by the OU colored noise in the rough potential with a finite τ is larger than that in the tilted periodic potential $g_0 = 0$ under the condition of $F = F_c = 1.0$. When the value of τ is small, the correlation of the noise is weak. As the correlated time increases, the constant

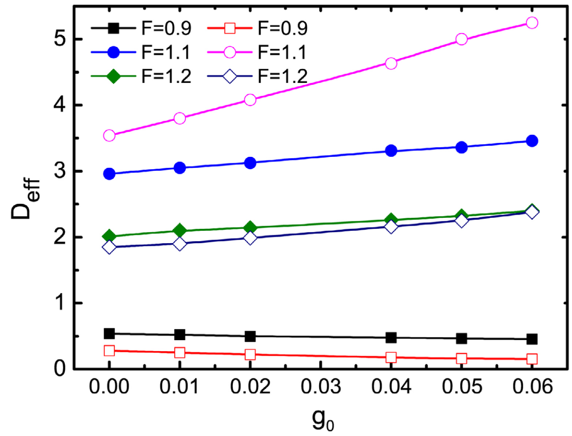

Figure 4. The D_{eff} as a function of g_0 for different correlated time τ, where the solid and open symbols correspond to $\tau = 50$ and $\tau = 100$ respectively. The parameters used are $\lambda = 2\pi$ and $D = 0.5$.

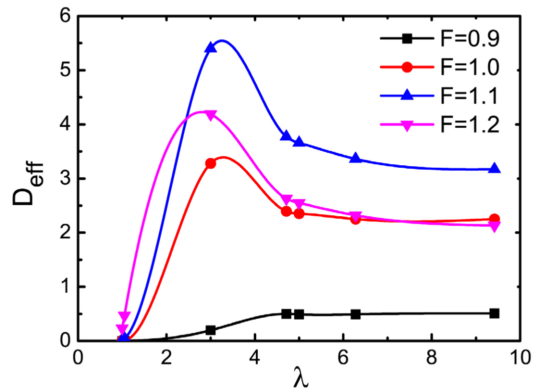

Figure 5. The D_{eff} as a function of τ for different values of roughness g_0 and external force F. The parameters used are $\lambda = 2\pi$ and $D = 1.0$.

driving force increases the kinetic energy of the particle, and thus the particle can move and transfer into the running state. At this time, the envelope width of the spatial distribution of the particle can measures the size of D_{eff}. However, the width of this spatial distribution will shrink when the value of τ is large. For example, $F = 1.0$, $g_0 = 0.05$, and this is because the probability of a particle in the locked state increases. If the value of τ is large enough, all particles will be locked in the located state, and the diffusion coefficient decays to zero.

The correlation length λ, as an important parameter in RCP, also affects the diffusion behavior of the particle. The calculations show that D_{eff} is a non-monotonic function of λ, as shown by **Figure 6**. From the discussions above, it can be seen that the roughness of the potential helps to separate the peaks of the spatial distribution of the particle around the disordered barrier. Meanwhile, the value of λ directly determines the number of small potential wells. When the value of λ is small, the number increases, causing many particles to be trapped in a small barrier and a locked state. Therefore, the phenomenon of diffusion is not obvious at this time. By contrast, when the value of λ is large, the number of

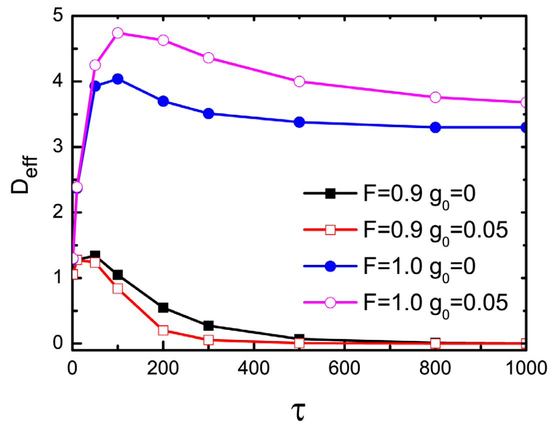

Figure 6. The effective diffusion coefficient D_{eff} as a function of λ for different values of the external force F. The applied parameters are $\lambda = 2\pi$ and $D = 1.0$.

small potential wells will become smaller, as shown by **Figure 5**. In this case, the RCP has little effect on the diffusion of the particles. The coexistence of the locked state and the running state is beneficial to the biased diffusion when λ takes the proper value.

4. Summary

This work explores the diffusive properties of overdamped Brownian motion driven by an Ornstein-Uhlenbeck noise in a biased periodic potential corrugated by the spatial disorder. As for the influence of the roughness of the potential, the rough potential is not conducive to directional transport. However, an enhancement for the effective diffusion coefficient of a particle can be observed when the tilted force is close to the critical value. Particularly, this enhancement is sensitive to the two parameters of the RCP: the correlation length λ and the intensity g_0. The number of the local minima may increase as the roughness decreases. Also, the distinct potential wells become deeper with a larger value of g_0. These all cause a large proportion of the test particles to be trapped or locked, and the whole distribution of the particle forms a wider envelope width. At this time, the effective diffusion coefficient D_{eff} is enhanced. Furthermore, D_{eff} varies non-monotonically with correlated time τ. The probability of a particle in a locked state increases under the effect of the OU noise, which exhibits a positive correlation. Therefore, the diffusion can be enhanced under the co-modulation of these parameters, and even the appearance of non-monotonicity depends on a certain parameter.

Thus, the introduction of roughness can be used to promote the movement of particles under the right conditions. Our results provide a better understanding of the complex transport phenomenon of particles in a rough potential, which may provide useful information for some realistic but complicated problems.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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