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Transport properties under the influence of finite friction*

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Using the Langevin Monte Carlo method, the influence of friction on the directed motion of a Brownian particle driven by an external noise source is investigated. The results show that the existence and change of the environment friction influence the establishment and development of the steady motion of a Brownian particle derived by non-equilibrium fluctuation. The most probable correlation time, which corresponds to the maximum current, is inversely proportional to the friction coefficient. The abnormal transition of the current with different friction appears because of the coupling between the effective ratchet potential and coloured noise intensity.

Keywords: Langevin Monte Carlo, finite friction, stationary current
PACC: 0250

1. Introduction

Much attention has been paid in recent years to the directed motion of a particle driven by non-equilibrium fluctuation.[1−6] The fluctuation energy from the heat bath environment cannot cause particles to perform a directed motion, otherwise it will violate the second law of thermodynamics. When the external fluctuation exists, not only the characteristics of random motion of a Brownian particle varies but also its macroscopic average behaviour radically changes. Then, the non-thermal forces can induce the directed transport of a Brownian particle in an asymmetric periodic potential.[1−8] Although previous works have provided a basis for the explanation of the directed motion of Brownian particles, they have the limitation of using an overdamped ratchet dynamics. The ratchet dynamics supplemented by a finite inertia term is not only of experimental interest but has also exhibited interesting new theoretical aspects[9,10] in recent years. As a difference in comparison with the overdamped case, a chaotic behaviour is indeed realized in the presence of a finite inertia term.[10] Jung *et al*[11] have studied the directed motion of particles with finite inertia in the absence of noise. With finite inertia, the dynamics becomes more complex, and thus it offers a challenge for the study of the inertia ratchet mechanism in the more realistic model with noise.

In this paper, we apply the Langevin Monte Carlo approach to simulate the net current of particles by using a model with two noise sources, one coloured noise and one white noise in the framework of the inertia ratchet. The focus of this paper is to analyse the transport properties under the influence of arbitrary friction.

2. Model and simulation

Consider a particle in a one-dimensional asymmetric periodic potential $V(x) = V(x+L)$ with period L, the dynamics of which is governed by the Langevin equation

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + m\gamma\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\mathrm{d}V(x)}{\mathrm{d}x} + \Gamma(t) + \varepsilon(t). \quad (1)$$

The thermal fluctuation $\Gamma(t)$ is modelled by zero-mean Gaussian white nose with the correlation function

$$< \Gamma(t)\Gamma(s) >= \lambda^2\delta(t-s), \quad (2)$$

where the intensity $\lambda^2 = \dfrac{2\gamma k_{\mathrm{B}}T}{m}$ is proportional to temperature T of the environment, γ is the friction

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coefficient, and k_B is Boltzmann constant. The random force $\varepsilon(t)$ is a coloured noise, with

$$< \varepsilon(t) >= 0 \text{ and } < \varepsilon(t)\varepsilon(s) >= \frac{D}{\tau}\exp\left[-\frac{|t-s|}{\tau}\right], \tag{3}$$

where D denotes the coloured noise intensity and τ is the correlation time. This exponentially correlated coloured noise can be generated by a Gaussian white noise $\eta(t)$ as

$$\frac{\mathrm{d}\varepsilon(t)}{\mathrm{d}t} = -\frac{1}{\tau}\varepsilon(t) + \frac{\sqrt{2D}}{\tau}\eta(t). \tag{4}$$

For simplicity, we take mass m=1 in this paper. Equation (1) can then be put in the form

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\gamma\frac{\mathrm{d}x}{\mathrm{d}t} + f(x) + \Gamma(t) + \varepsilon(t),$$

$$f(x) = -\frac{\mathrm{d}V(x)}{\mathrm{d}x}. \tag{5}$$

The periodic potential $V(x)$ is taken to be of the form

$$V(x) = -\frac{1}{2\pi}\left[\sin(2\pi x) + \frac{1}{4}\sin(4\pi x)\right], \tag{6}$$

which is the one-dimensional asymmetric periodic potential along the x-direction as shown in Fig.1.

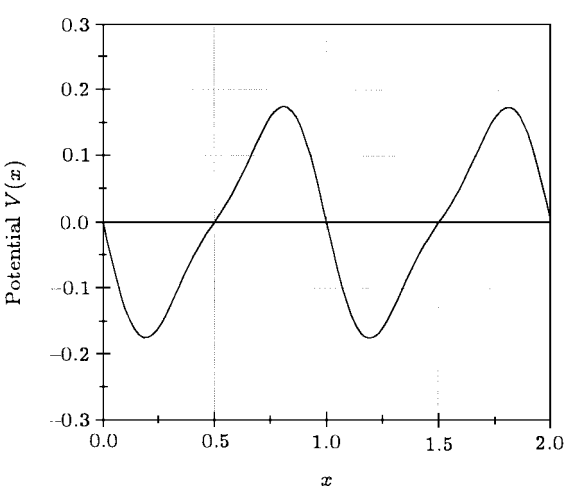


Fig.1. Asymmetric ratchet potential, L=1.0.

The Langevin equation (5) is a stochastic differential equation containing external fluctuation. It depicts the non-Markov process of a Brownian particle. An exact analytical solution of the two-dimensional Fokker–Planck equation corresponding to this equation seems impossible.[12–16] The "effective Fokker–Planck equation" is restricted to small τ up to the order of τ^2. In order to overcome these difficulties, we solve Eq.(5) directly by means of the Monte Carlo simulation method introduced in Ref.[17]. It is should be noted that all quantities which appear in Eq.(1) are dimensionless. The stationary distribution of $\varepsilon(t)$ [17] is given by

$$P(\varepsilon(0)) = \left(\frac{2\pi D}{\tau}\right)^{-1/2}\exp\left[-\frac{\tau\varepsilon^2(0)}{2D}\right]. \tag{7}$$

By using the two-step iterative method[15] and integrating Eqs.(4) and (5) formally, we obtain

$$\varepsilon(t+h) = \exp\left(-\frac{h}{\tau}\right)\varepsilon(t) + \frac{\sqrt{2D}}{\tau}\omega_0, \tag{8}$$

$$\begin{aligned} x(t+h) =& x(t) + v(t)h - \frac{1}{2}\gamma v(t)h^2 \\ &+ \frac{1}{2}f(x)h^2 + \lambda Z_1 + Z_2, \end{aligned} \tag{9}$$

$$\begin{aligned} v(t+h) =& v(t) - \gamma\left[v(t)h - \frac{1}{2}\gamma v(t)h^2\right. \\ &\left. + \frac{1}{2}f(x)h^2 + \lambda Z_1 + Z_2\right] \\ &+ f(x)h + \frac{1}{2}v(t)h^2\frac{\mathrm{d}f(x)}{\mathrm{d}x} + \lambda Z_3 + Z_4. \end{aligned} \tag{10}$$

Here h is a time step and $\alpha = \dfrac{h}{\tau}$, then

$$Z_1 = \int_t^{t+h}\mathrm{d}t'\int_t^{t'}\Gamma(s)\mathrm{d}s = \frac{h^{3/2}}{2}\left(R_1 + \frac{R_2}{\sqrt{3}}\right), \tag{11}$$

$$\begin{aligned} Z_2 =& \int_t^{t+h}\mathrm{d}t'\int_t^{t'}\varepsilon(s)\mathrm{d}s \\ =& \tau^2(\alpha + \mathrm{e}^{-\alpha} - 1)\varepsilon(t) + \frac{\sqrt{2D}}{\tau}\omega_1, \end{aligned} \tag{12}$$

$$Z_3 = \int_t^{t+h}\Gamma(t')\mathrm{d}t' = h^{1/2}R_1 \tag{13}$$

and

$$Z_4 = \int_t^{t+h}\varepsilon(t')\mathrm{d}t' = \tau(1-\mathrm{e}^{-\alpha})\varepsilon(t) + \frac{\sqrt{2D}}{\tau}\omega_2. \tag{14}$$

The variance and the cross correlation of ω_0 , ω_1 and ω_2 are readily determined from their definitions.[17] If R_1, R_2 and R_3 are three uncorrelated Gaussian variables with zero mean value and standard deviation, R_1, R_2 and R_3 can generated by the Box–Müller formulae

$$\omega_0 =< \omega_0^2 >^{1/2} R_1, \tag{15}$$

$$\omega_1 = \frac{<\omega_2\omega_0>}{<\omega_0^2>^{1/2}}R_1 + \frac{<\omega_1\omega_2><\omega_0^2> - <\omega_2\omega_0><\omega_1\omega_0>}{<\omega_0^2>^{1/2}(<\omega_1^2><\omega_0^2> - <\omega_1\omega_0>^2)^{1/2}}R_2 + \left[<\omega_2^2> - \left(\frac{<\omega_2\omega_0>}{<\omega_0^2>^{1/2}}\right)^2 - \left(\frac{<\omega_1\omega_2><\omega_0^2> - <\omega_2\omega_0><\omega_1\omega_0>}{<\omega_0^2>^{1/2}(<\omega_1^2><\omega_0^2> - <\omega_1\omega_0>^2)^{1/2}}\right)^2\right]^{1/2} R_3, \quad (16)$$

$$\omega_2 = \left(\frac{<\omega_0\omega_1>}{<\omega_0^2>^{1/2}}\right)R_1 + \left[<\omega_1^2> - \frac{<\omega_0\omega_1>^2}{<\omega_0^2>}\right]^{1/2} R_2. \quad (17)$$

3. Results and analysis

From Eq.(10), the time evolution of the Brownian particle is shown in Fig.2. In the initial time 2×10^5 particles performing random walk started from the same position (x_0=0.3). The coupling effect of the asymmetric ratchet potential and the coloured noise make the particles move simultaneously, and their velocities increase quickly. Thus an overshoot phenomenon appears in the transient process. The friction force increases with the increase of the velocity, which makes velocity of the particles approach a stationary value. Fig.2 also indicates that the average velocity of the particle eventually reaches a positive value, i.e. the particle performs the directional motion towards the right. It is observed that the stationary current and its current maximum decrease with an increase of the friction value γ. This is because the increase of γ will directly suppress the velocity v. The net current J reaches a maximum as $\gamma \to 0$, and then it decreases to zero with increasing γ. This behaviour is seen in Fig.3.

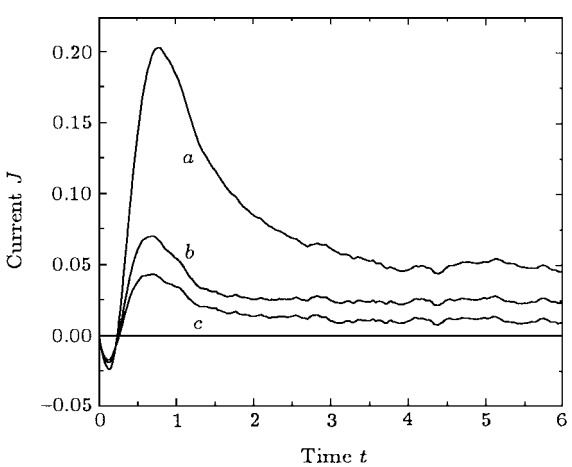


Fig.2. The current J given by Eq.(10) as a function of time t for different values of the friction coefficient γ. The parameter values are h=0.02, D=2.0, τ=0.5. Curve a γ= 0.5; curve b γ=1.2; curve c γ=7.2.

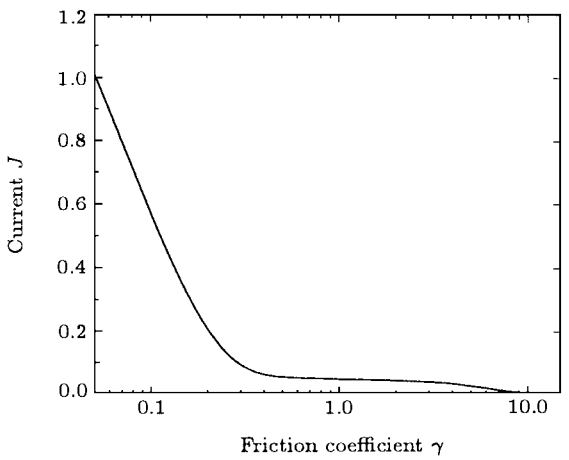


Fig.3. Simulation results for the current as a function of the friction parameter γ, with τ=0.25, h=0.02, D=3.5.

We have further studied the influence of γ on the variation of J with noise parameters such as the correlation time τ and the coloured noise intensity D. First of all, the relation of the current J and the correlation time τ is analysed. In the limit $\tau \to 0$, the induced current essentially vanishes because coloured noise $\varepsilon(t)$ tends to Gaussian white noise and two uncorrelated white noises cannot induce current. In the limit of large correlation time $\tau \to \infty$, the noise $\varepsilon(t)$ acts as a constant force which opposes the asymmetric effect of the ratchet potential;[2] consequently the current also tends to zero. We plotted the net current as a function of the correlation time τ for different values of the friction coefficient γ in Fig.4. This shows that the current increases with increasing correlation time τ, reaches a maximum, and then decreases back to zero at a large value of τ. Let us introduce a dimensionless variable $c = \frac{\tau_c}{\tau_0}$, where τ_c is a specific correlation time which corresponds to the current maximum; we call this "a most probable correlation time ". The characteristic time τ_0 is determined by the reciprocal of the friction coefficient, i.e. $\tau_0 = \gamma^{-1}$. The maximum current and the most probable correlation time τ_c decrease with the increase of γ. By comparing the four curves of A, B, C and D in Fig.4, it is found that the values of c are

approximately identical, i.e. $c = \dfrac{\tau_c}{\tau_0} = \tau_c\ \gamma \approx$constant, as seen in the inset of Fig.4, where $c = \tau\gamma$ is used as a controlled parameter.[8] The most probable correlation time is inversely proportional to the friction coefficient in the range of our study. That is to say, if the friction coefficient γ is known, the most probable correlation time τ_c can be approximately determined.

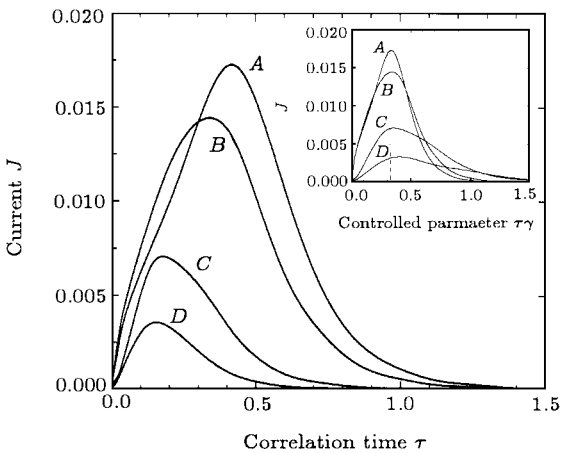


Fig.4. The probable current J versus the correlation time τ with different values of the friction coefficient γ. The insertion figure illustrates the relation of the current J and the controlled parameter $\tau\gamma$, and c values of the four curves are approximately identical: curve A γ=0.8, τ_c=0.431, c= 0.345; curve B γ=1.0, τ_c=0.4345, c=0.345; curve C γ=2.0, τ_c=0.172, c=0.350; curve D γ=3.0, τ_c=0.120, c=0.360.

The relation between the current J and the coloured noise intensity D is illustrated in Fig.5. With the increase of the friction coefficient γ, it is clear that the maximum current decreases and the entire curve moves to the right. Two curves a and b with the different friction coefficient ($\gamma_b > \gamma_a$) intersect at E. A vertical line A through point E is plotted, which divides the entire region of Fig.5 into two regions. It is noted that the current value of curve b is smaller on the left of the line A, and bigger on the right of the line A, as compared with curve a. This may be understood by analysing two effects. On the one hand, the increase of the friction causes the decrease of the velocity of the particles, which is equivalent to the increase of a barrier height $V_0 (V_0 = V_{\max} - V_{\min})$. Thus the effective barrier heights are different for the different frictions. On the other hand, there will be two threshold values for the coloured noise intensity, equal to effective max $f(x)$ and min $f(x)$. When it lies between them, the ratchet will work as we intuitively expect it to one side only. When the second threshold is exceeded, we are overdriving the ratchet that will then backslide, reducing its efficiency. It is of interest to note that the current value of curve b with larger γ_b is larger on the right of the line A, since the same intensity D lies below two thresholds for curve b while it becomes overdriven for curve a. The phenomenon is described as "an abnormal transition of the particle". These can be understood as a result of the coupling between the effective ratchet potential and the coloured noise intensity.

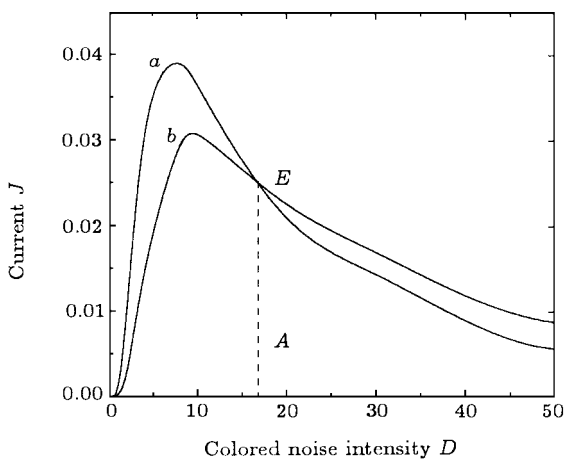


Fig.5. Simulation results for the current as a function of the coloured noise intensity D, for two different values of the friction coefficient γ. Parameter values are h=0.02, τ=0.5. Curve a γ_a=3.0; curve b γ_b=5.0.

4. Conclusions

In summary, we have studied the directed motion of particles with finite friction in the realistic model that includes two noise sources and inertia in the one-dimensional asymmetric potential. The influence of friction on the motion of Brownian particles has been investigated. We would like to point out that the appearance of friction influences transport properties of the particle, which is different from its directed motion in the overdamped case. The stationary current and its maximum will decrease with increasing friction. The most probable correlation time τ_c is inversely proportional to the friction coefficient γ. The abnormal transition of the particle appears for the large value of coloured noise intensity.

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