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Nonlinear and nonadiabatic phenomena in Brownian motors

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The term "Brownian motor" or "thermal ratchet" appeared in the literature due to attempts of theoretical physics to describe some phenomena in biological systems [1,2]. One can determine a Brownian motor as a nanoparticle which can move directionally under the nonequilibrium fluctuations of its characteristics. Such a fluctuations can be caused by chemical reactions occurring on a particle or due to various external processes [3]. There are three important requirements for the directed-motion generation: nonequilibrium fluctuations, energy pumping to the system induced by them, and the asymmetry of the potential profile. It is of importance that Brownian motor operation is a typical nonlinear process.

A fluctuation-induced transport of Brownian particles is widely discussed in the literature and is described by models (generically called ratchets) of various levels of complexity. A so called flashing ratchet operates through the fluctuations of the spatially asymmetric periodic potential profile [4]. In our work we consider deterministic temporal fluctuations of the potential energy.

An essential step in understanding the mechanism of influence of space–time variations of the potential energy on the characteristics of directed motion was the adiabatic motor (reversible ratchet) introduced by Parrondo [5]. This motor operates without any energy consumptions, provided that it performs no effective work. A striking property of this motor is that the system is at thermodynamic equilibrium with a zero instantaneous particle flux at every time, while the flux averaged over the period τ of the adiabatically slow variation of the potential energy is nonzero. Necessary condition of the operation of this motor is that the slow variation of the potential energy should be specified by more than one function of time.

At the same time, the adiabaticity of the process, i.e., the absence of heat transfer between the system and the environment, may be realized also for an instantaneous change in the potential profile (so called adiabatically fast process). In this case, for the existence of the nonzero flux, it is sufficient that the potential energy $V(x, \sigma(t))$ periodic in the coordinate space is specified by a single function of the time $\sigma(t)$ having at least one jump over its period τ in the limit $\tau \to \infty$. The significant difference of this motor from the adiabatic one is the presence of heat exchange occurring after the jump of the potential energy.

A typical example of a Brownian motor with a stepwise change in the potential energy is a dichotomic process characterized for a deterministic case by the function $\sigma(t)$ having two jumps over its period τ and two regions with constant values between them. However, the assumption of the instantaneous change is an idealization never present in nature. In reality, there is always a transient process with the duration τ_0 characterizing the rate of the variation of the potential energy (i.e., there is always nonadiabaticity of the process). The smallness of the parameter τ_0 is established by its comparison with the characteristic time parameter of the system; such a parameter for the Brownian motor with a smooth potential profile is a characteristic diffusion time of a particle $\tau_D = L^2/D$ over the potential period L (D is the diffusion coefficient).

In work presented here, we demonstrate how to calculate corrections to the flux and velocity if the potential profile does not change instantaneously. Such a nonadiabatic corrections are determined by the characteristic features of the potential profile and are important both from applied and from fundamental points of view.

For this purpose, we use the formalism of Brownian dynamics described by the Smoluchowski equation for the distribution function $\rho\,(x,t)$. The average velocity of a Brownian particle with potential energy periodic in space and time can be determined through the fraction of particles $\Phi(x)$ crossing the point x during the time τ. For the steady periodic processes (with $\rho\,(x,\tau) = \rho\,(x,0)$) and $\sigma(\tau) = \sigma(0)$), the function $\Phi(x)$ is independent of x, and the quantity $\Phi(0)$, i.e., the fraction of particles crossing the point $x = 0$, certainly determines the average flux $\langle J\rangle_\tau \equiv \tau^{-1}\Phi(0)$ and average velocity $L\,\langle J\rangle_\tau$.

We have obtained $\Phi(0)$ as a sum of adiabatic contribution $\Delta\Phi^{ab}_{\text{ad}}$ coinciding with the Parrondo's result [5] and nonadiabatic correction $\Delta\Phi^{ab}_{\text{nonad}}$ for the system with sharp change of the potential energy plotted in Fig.1 (line $M_1M_2M_4$) [6]:

$$
\begin{aligned}
&\Delta\Phi^{ab} = \Delta\Phi^{ab}_{\text{ad}} + \Delta\Phi^{ab}_{\text{nonad}}\,,\\
&\Delta\Phi^{ab}_{\text{ad}} = \int_0^L dx\rho_+(x,b)\int_0^x dy\,[\rho_-(y,b)-\rho_-(y,a)]\,,\\
&\Delta\Phi^{ab}_{\text{nonad}} = -\tfrac{1}{2}\beta^3D^2\int_0^L dx\rho_+(x,b)\rho_-(x,a)\,[V'(x,a)+V'(x,b)]\times\\
&\qquad\times\int_0^{\tau_0} dt\,[V'(x,b)-V'(x,\sigma(t))]\int_0^t dt'\,[V'(x,\sigma(t'))-V'(x,a)]\,,\\
&\rho_\pm(x,\sigma) = \exp\left[\pm\beta V(x,\sigma)\right]\Big/\int_0^L dx\exp\left[\pm\beta V(x,\sigma)\right]
\end{aligned}
\tag{1}
$$

($\beta = (k_BT)^{-1}$, k_B is the Boltzmann constant and T is the absolute temperature). Here we assumed that the system at the time $t = 0$, when $\sigma(0) = a$, is in the equilibrium state with the distribution function $\rho_-\,(x,a)$; after the sharp change from $V(x,a)$ to $V(x,b)$ in the short range

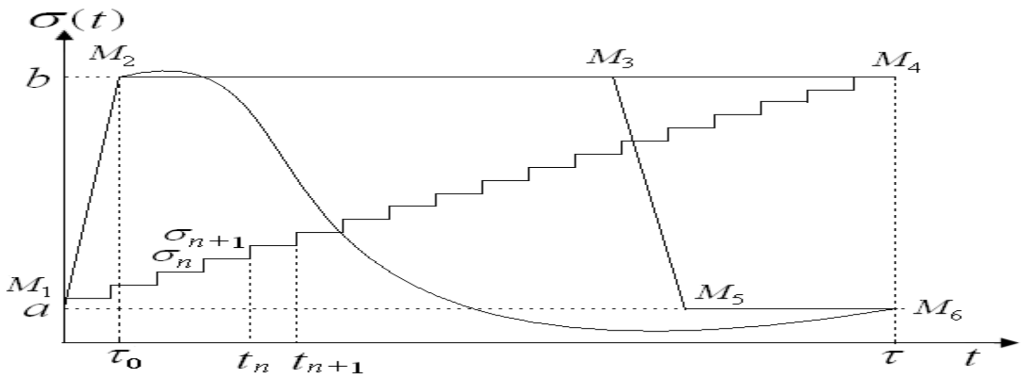

FIG. 1.

$\tau_0 < t < \tau$, which is described by the function $\sigma(t)$, the potential energy stays equal to $V(x, b)$ in the range $\tau_0 < t < \tau$. For $\tau >> \tau_D$, the system has the time to relax to a new state with the new potential profile corresponding to the equilibrium distribution function $\rho_-(x, b)$.

These equations allowed us to write average flux (in the low-frequency limit $\tau^{-1} \to 0$) for a deterministic dichotomic process with two transient states (line $M_1M_2M_3M_5M_6$ in Fig.1), $\langle J\rangle_\tau^{\text{dikh}} = \tau^{-1}\left(\Delta\Phi^{ab} + \Delta\Phi^{ba}\right)$, and to analyze the cycle process, which includes regions (a, b) with the sharp and (b, a) with the smooth variations of the potential energy (line $M_1M_2M_6$ in Fig. 1). It is shown that for antisymmetric potential profiles, the average flux in the last case is equal to half the contribution from the dichotomic process in which two transient states are identical. Thus, the Brownian motors with the potential energy periodic in the coordinate space specifying by a single function of the time $\sigma(t)$ operate only at the cost of step. The smooth region of the potential does not matter.

We have also obtained the explicit expressions for the adiabatic contribution and nonadiabatic correction for the saw-tooth antisymmetric potential profile (see Fig.2a) [6] which lead to the following conclusions: (i) the nonadiabatic correction reduces the absolute value of the flux; (ii) for the extremely asymmetric potential profile ($l \to 0$ or $l \to L$) the adiabatic flux is

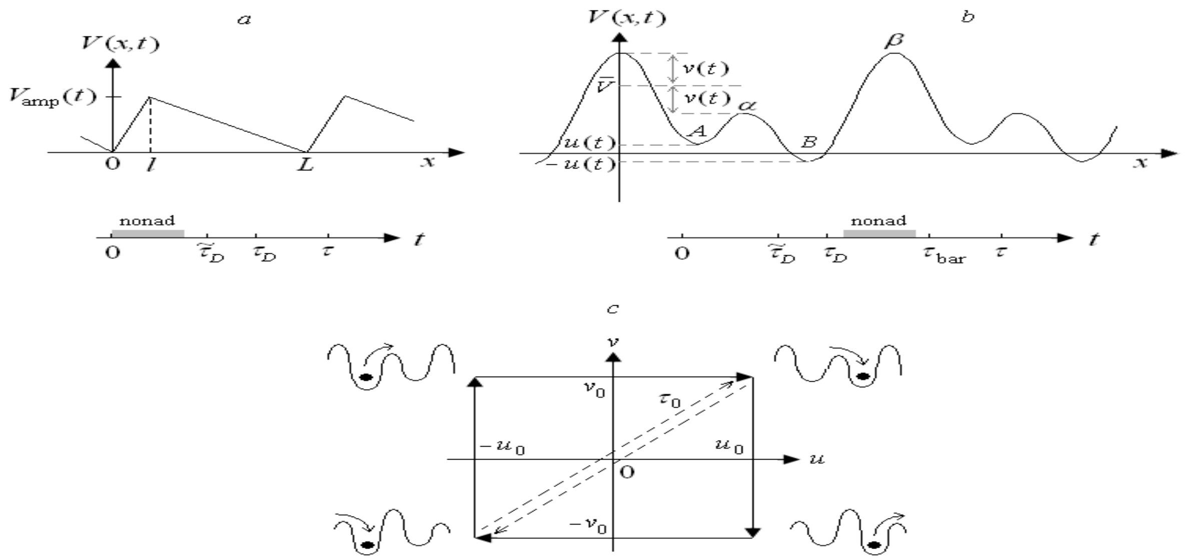

FIG. 2.

maximal and has a finite value, while the nonadiabatic correction diverges. The latter means a new characteristic time of the system $\tilde{\tau}_D \equiv l(L-l)/D$ which is less than τ_D is occurred and it determines the time interval $\tau_0 << \tilde{\tau}_D$ in which the nonadiabatic correction $\Delta\Phi^{ab}_{\text{nonad}}$ is valid. For $\tilde{\tau}_D < \tau_0 << \tau$, we are beyond the framework of the adiabatic approximation. In this case, the average flux is proportional to τ^{-2} [7].

The singularity of the potential profile can induce both small and large renormalized time parameters. For example, if the spatial period of the potential profile includes several narrow high barriers ($V_{\text{bar}} >> k_B T$, V_{bar} is the barrier height), and the profile variations are slow (e.i., $\tau >> \tau_D$), then the time is sufficient for the local thermodynamic equilibrium to be established in every well separated by the barriers and the directed motion becomes of a hopping type. Under these conditions, the system can be described in the kinetic approach, which deals with the time dependencies of the probabilities of the occupation of potential wells and with the transfer rates between the wells. In the framework of kinetic approach a new long characteristic time of the system such as $\tau_{\text{bar}} \sim \tau_D \exp \beta V_{\text{bar}}$ appears in addition to short times such as $\tilde{\tau}_D$.

The new time parameter τ_{bar} sets the time necessary for a Brownian particle to overcome the barrier.

We use very popular in literature model [8] with the potential profile with two wells and two barriers (as it shown in Fig.2b). The potential well minima and the barrier maxima are described by the functions of time $u(t)$ and $v(t)$, which are measured in units of k_BT. If functions $u\,(t)$ and $v\,(t)$ are changed following the rectangular path with vertices $\pm u_0$, $\pm v_0$ (see Fig.2c), then the flux is equal to $\langle J\rangle_\tau^{\text{ad}} = \tau^{-1}\tanh v_0 \tanh u_0$ and requires no energy. This is an adiabatic motor. It is interesting that the same flux may be created also by a dichotomic process, when the functions $u(t)$ and $v(t)$ change synchronously and instantaneously from certain values $-u_0$, $-v_0$ to u_0, v_0, respectively, and from u_0, v_0 back to $-u_0$, $-v_0$, respectively. The flux in this case requires an energy income $4k_BT\tau^{-1}u_0\tanh u_0$ per unit time [8].

In the adiabatic limit ($\tau >> \tau_{\text{bar}}$), the nonadiabatic correction to the average flux corresponding to the linear (for simplicity) variation of the functions $u(t)$ and $v(t)$ during a short time interval τ_0 is given by the expression [6]

$$\langle J\rangle_\tau^{\text{nonad}} = -\frac{u_0\sinh 2v_0 - v_0\sinh 2u_0}{(v_0^2-u_0^2)\cosh v_0\cosh u_0}\frac{w\tau_0}{\tau} \tag{2}$$

($w = w_0\exp(-\bar{V}) \sim \tau_{\text{bar}}^{-1}$; w_0 is the pre-exponential factor, which depends on the diffusion coefficient and the curvature of the potential profile at the maxima and minima.)

The significant difference of the nonadiabatic correction in the kinetic approach given by this Eq. appropriate for $\tau_D << \tau_0 << \tau_{\text{bar}}$ from the corrections given by Eq. (1) and appropriate for $\tau_0 << \tilde{\tau}_D < \tau_D$ is that the former and latter corrections are linear and quadratic in τ_0, respectively. This difference is due to the fact that at the time scale of kinetic description τ_0 is enough to establish the equilibrium distribution in the smooth potential regions. Thus, we have new time scale and new hierarchy of the characteristic times of the system and new region in which the calculated nonadiabatic corrections are valid: $\tau_D << \tau_0 << \tau_{\text{bar}}$. τ_{bar} will stand as τ_D.

In conclusion, we note that adiabatically slow and adiabatically fast variations of the potential profile initiate the transport of Brownian particles in quite a similar way, although there are certain significant differences. The same flux can be induced in both processes. The main difference of adiabatically slow process from adiabatically fast one is that at least a two-parameter time dependence of the potential energy is required to initiate the directed motion in the former, while a one-parameter dependence is sufficient for the latter processes. It is also important that the realization of the adiabatically fast process is quite simple. The dichotomic process is an example. At the same time, this process is always an idealization of the real situation, when the transition between two states occurs during a nonzero time τ_0. That is why it is important to take into account the variation of the average velocity of a Brownian particle induced by the nonadiabaticity of the process. It is always exists in reality and depends on transient process durations and characteristic system times. The nonadiabatic corrections also dominate in limiting the high motion rectification coefficients for the high-efficiency motor operation mode [6]. Thus, the study of the nonadiabatic nonlinear effects gives a possibility to determine the hierarchy of the characteristic times of the system generated by the peculiarities of the potential profile.

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