Transport of overdamped Brownian particles in a two-dimensional tube: Nonadiabatic regime

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Transport of overdamped Brownian particles in a two-dimensional asymmetric tube is investigated in the presence of nonadiabatic periodic driving forces. By using Brownian dynamics simulations we can find that the phenomena in nonadiabatic regime differ from that in adiabatic case. The direction of the current can be reversed by tuning the driving frequency. Remarkably, the current as a function of the driving amplitude exhibits several local maxima at finite driving frequency.

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I. INTRODUCTION

Rectification of noise leading to unidirectional motion in ratchet systems has been an active field of research over the last decade [1]. This comes from the desire to understand molecular motors [2], nanoscale friction [3], surface smoothing [4], coupled Josephson junctions [5], optical ratchets and directed motion of laser-cooled atoms [6], and mass separation and trapping schemes at the microscale [7]. In these systems possessing spatial or dynamical symmetry breaking, Brownian motion combined with unbiased external input signals, deterministic and random alike, can assist directed motion of particles at submicron scales.

Several models have been proposed to explain this transport mechanism under various nonequilibrium situations. Typical examples are rocking ratchets [8], flashing ratchets [9], diffusion ratchets [10], correlation ratchets [11]. The ratchet setup demands three key ingredients [12] which are (a) nonlinearity: it is necessary since the system will produce a zero men out put from zero-mean input in a linear system. (b) Asymmetry (spatial and/or temporal): it can violate the left/right symmetry of the response. (c) Fluctuating input zero-mean force: it should break thermodynamical equilibrium, which forbids appearance of a directed transport due to the Second Law of Thermodynamics.

Most studies have revolved around the energy barrier. The nature of the barrier depends on which thermodynamic potential (internal energy or Helmholtz free energy) varies when passing from one well to the other, and its presence plays an important role in the dynamics of the system. Whereas energy barriers are more frequent in problems of solid-state physics (metals and semiconductors, coupled Josephson junction, and photon crystal). However, in some cases, such as soft condensed-matter and biological systems, the entropy barriers should be considered. Brownian particles, when moving in a confined geometry, instead of diffusing freely in the host liquid phase, undergo a constrained motion, where their kinetic behavior could exhibit peculiar behavior. This feature of constrained motion is ubiquitous in ion channels, nanopores, zeolites, and generally for processes occurring at subcellular level [13]. Entropic barriers may appear when coarsening the description of a complex system in order to simplify its dynamics. Reguera and Rubi [14] used the mesoscopic nonequilibrium thermodynamics theory to derive the general kinetic equation of the motor system and analyzed in detail the case of diffusion in a domain of irregular geometry in which the presence of the boundaries induces an entropy barrier when approaching the dynamics by a coarsening of the description. In their recent work [15] they studied the current and the diffusion of a Brownian particle moving in a symmetric channel with a biased external force. They found that temperature dictates the strength of the entropic potential, and thus an increase in temperature leads to a reduction of the current. In our previous work [16], we found that the asymmetry of the tube can induce a net current in the absence of any net macroscopic forces or in the presence of the unbiased forces in the adiabatic case. The present work is extended to the study of transport to the nonadiabatic regime. We emphasize on finding how the finite driving frequency affects the transport.

II. MODEL AND METHODS

In this paper, we study a ratchetlike periodic tube driven by a thermal noise and a periodic driving force. Since most of the molecular transport occurs in the overdamped regime, we can safely neglect initial effects. So, its overdamped dynamics can be described by the following Langevin equations written in a dimensionless form [15,16],

$$\eta\frac{dx}{dt} = A_0 \sin(\omega t) + \sqrt{\eta k_B T}\xi_x(t), \tag{1}$$

$$\eta\frac{dy}{dt} = \sqrt{\eta k_B T}\xi_y(t), \tag{2}$$

where x, y, are the three-dimensional (3D) coordinates, η is the friction coefficient of the particle, k_B is the Boltzmann constant, T is the absolute temperature, and $\xi_{x,y}(t)$ is the Gaussian white noise with zero mean and correlation function: $\langle\xi_i(t)\xi_j(t')\rangle=2\delta_{i,j}\delta(t-t')$ for $i,j=x,y$. $\langle\cdots\rangle$ denotes an ensemble average over the distribution of noise. $\delta(t)$ is the Dirac delta function. A_0 and ω are the amplitude and frequency of the external driving force, respectively. Imposing reflecting boundary conditions in the transverse direction ensures the confinement of the dynamics within the tube, while periodic boundary conditions are enforced along the longitudinal direction for the reasons noted above. The shape of the tube is described by its half width (Fig. 1)

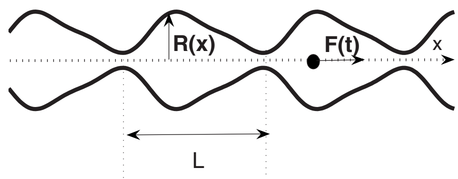

FIG. 1. Schematic of a tube with periodicity L. The shape is described by the half width of the tube $R(x)$ $=a[\sin(\frac{2\pi x}{L})+\frac{\Delta}{4}\sin(\frac{4\pi x}{L})]+b$. Δ is the asymmetric parameter of the tube shape. $F(t)=A_0\sin(\omega t)$ is an external driving force.

$$R(x)=a\left[\sin\left(\frac{2\pi x}{L}\right)+\frac{\Delta}{4}\sin\left(\frac{4\pi x}{L}\right)\right]+b, \tag{3}$$

where a is the parameter that controls the slope of the tube, Δ the asymmetry parameter of the tube shape. b is the parameter that determine the half width at the bottleneck.

If $F(t)$ changes very slowly with respect to t, namely, its period is longer than any other time scale of the system, there exists a quasisteady state. In adiabatic limit and $|R'(x)|\ll 1$, by following the method in [14,15], we can obtain the current

$$j[F(t)]=\frac{k_BT\left[1-\exp\left(-\frac{F(t)L}{k_BT}\right)\right]}{\int_0^L\int_0^L dxdy\frac{R(x)}{R(x+y)}\exp\left[\frac{-F(t)y}{k_BT}\right][1+R'(x+y)^2]^{\alpha}}, \tag{4}$$

where $\alpha=1/3$ and the prime stands for the derivative with respect to the space variable x. So the average current [15,16] is

$$J=\frac{1}{\tau}\int_0^{\tau}j(F(t))dt=\frac{1}{2}[j(A_0)+j(-A_0)], \tag{5}$$

and the average velocity $v=JL$.

Our model can be analytically studied in the adiabatic limit [15]. However, in present work we are interested in the intermediate frequency and strong amplitude of driving force. In this case, no general valid analytical expressions are possible. Therefore, we use Brownian dynamic simulations performed within the stochastic Euler-algorithm by integration of the dimensionless Langevin Eqs. (1) and (2). For the numerical simulations the single integration steps read [17]

$$x(t+\Delta t)=x(t)+A_0\sin(\omega t)\Delta t+\sqrt{2k_BT\Delta t}R_1, \tag{6}$$

$$y(t+\Delta t)=y(t)+\sqrt{2k_BT\Delta t}R_2, \tag{7}$$

where R_1, R_2 are two Gaussian distributed random numbers with unit variance. Δt is the integration step time. If the new desired position is not allowed in the sense that it is lying outside the channel then the boundary conditions have to be considered, i.e., the particle returns to its previous position. For the numerical simulations, we have considered more than 1×10^4 realizations to improve accuracy and minimize statistical errors. In order to provide the requested accuracy of the system dynamics time step was chosen to be smaller than 10^{-4}. The average particle velocity along the x direction,

$$v=\langle\dot{x}\rangle=\lim_{t\to\infty}\frac{\langle x(t)\rangle}{t}. \tag{8}$$

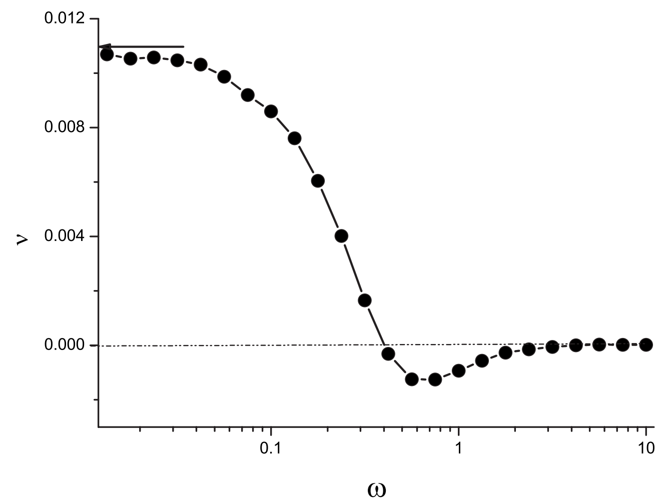

FIG. 2. The mean velocity v as a function of driving frequency ω at $a=1/2\pi$, $b=1.2/2\pi$, $A_0=0.5$, $\Delta=1.0$, $T=0.3$, and $L=2\pi$. The arrow marks the mean velocity calculated in the adiabatic limit.

III. NUMERICAL RESULTS AND DISCUSSION

Our emphasis is on finding the asymptotic mean velocity which is defined as the average of the velocity over the time and thermal fluctuations. In the nonadiabatic regime, we cannot obtain the similar expression for the current to that in adiabatic limit [Eq. (5)], therefore, we carried out extensive numerical simulations. For simplicity we set $\eta=1$ and $k_B=1$ throughout the work.

Figure 2 shows the mean velocity v as a function of the driving frequency ω. The only resource driving particle current across the tube is the nonequilibrium, external driving force $F(t)$, which generates positive and negative driving force in first and second half of the driving period. In the adiabatic limit $\omega\to 0$, the external force can be expressed by two opposite static forces A_0 and $-A_0$, yielding the mean current $J=\frac{1}{2}[j(-A_0)+j(A_0)]$. In this case it is easier for the particles moving toward the slanted side than toward the steeper side, so the current is positive. On increasing the frequency ω, due to higher frequency the Brownian particles do not get enough time to cross the slanted entropic barrier (the right side) which is at a larger distances from the minima. Since the distance from a entropic minima to the basin of attraction of next minima is less than from the steeper side (the left side) than from the slanted side (the right side, hence in one period the particles get enough time to climb the entropic barrier from the steeper side than from the slanted side, resulting in a negative current. When the

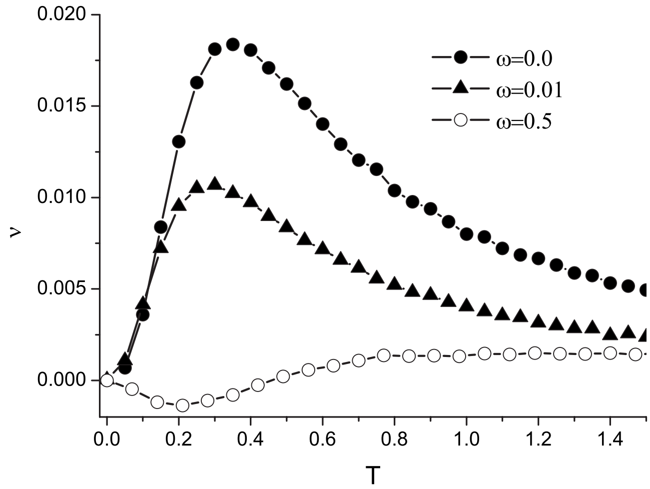

FIG. 3. The mean velocity ν as a function of the temperature T for different values of driving frequency ω at $a=1/2\pi$, $b=1.2/2\pi$, $A_0=0.5$, $\Delta=1.0$, and $L=2\pi$.

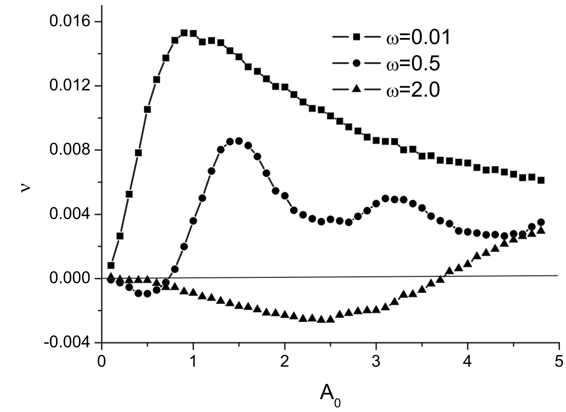

FIG. 4. The mean velocity ν as a function of driving amplitude A_0 for different values of driving frequency ω at $a=1/2\pi$, $b=1.2/2\pi$, $T=0.3$, $\Delta=1.0$, and $L=2\pi$.

external driving force changes very fast $\omega\to\infty$, the particle will experience a time averaged constant force $F=\int_0^{\frac{2\pi}{\omega}}F(t)dt=0$, so the current tends to zero. At the adiabatic limit the values of ν from Eq. (5) agree well with the numerical results. Interestingly, at some intermediate value ω, the current crosses zero and subsequently reverses its direction. There exists a valley in velocity-frequency curve. This peculiar reversal is due to different strength and symmetry of relaxation processes. The symmetry of relaxation processes changes with the system parameters, so the current may changes its direction when the parameters are changed.

In Fig. 3, the mean velocity ν is plotted for several driving frequency ω as a function of the temperature T. The adiabatic limit $\omega=0$ drawn as dotted line is readily evaluated from Eq. (5). In the determined limit $T\to 0$, the particle cannot reach the 2D area and the effect of the asymmetry of the tube disappears and there is no current. We must point out that in the determined limit no currents occur even for very large amplitude driving forces which is different from that in rocking potential ratchets [18–20]. In the potential case, the current will occur in the determined limit for large amplitude driving forces. When the temperature is very high, the influence of the external driving forces becomes negligible, so the current will also go to zero. In the adiabatic limit, the current is always positive for $\Delta>0$. However, the current will change its direction on increasing T for finite-frequency driving force ($\omega=0.5$). In this case, at low temperature the particles get enough time to climb the entropic barrier from the left side and do not get enough time climb the entropic barrier from the right side, so the current is negative. On increasing the temperature, the particles get kicks of larger intensity and hence they easily cross the right side, resulting in positive current. On further increasing the temperature, the effect of the external driving force disappears, so the current tends to zero.

Figure 4 shows the mean velocity ν versus the driving amplitude A_0 for different values of ω. It is found that the current will tend to zero for very small and large amplitude driving force. This can be understood upon noting that the driving force can be negligible for small amplitude driving forces and the effect of the asymmetry of the tube will disappear for large amplitude driving forces. In the adiabatic limit, the mean velocity will be always positive for $\Delta>0$. However, these phenomena will change drastically for nonadiabatic case. The current reversal will occur when the amplitude of the driving force is increased. Remarkably, one finds several extrema in velocity-amplitude characteristics which is similar to that in periodically rocked thermal ratchet [18–20]. This is due to the mutual interplay between noise and finite-frequency driving forces.

IV. CONCLUDING REMARKS

In this study, we have studied the transport properties of overdamped Brownian particles moving in an asymmetric periodic tube. The model can be analytically studied in the adiabatic limit and numerically in the nonadiabatic regime. We focus on finding how the finite driving frequency affects the transport of the overdamped particles. The phenomena in nonadiabatic regime are different from those in adiabatic limit. From Brownian dynamics simulations, we observe several novel and complex features arising due to the mutual interplay between the thermal noise and the finite-frequency driving force. The directed transport is determined by two factors: the thermal noise induced the particles escape from the well and the external force induced relaxation processes inside the tube. It is found that at some intermediate value of the driving frequency the current crosses zero and subsequently reverse its direction. Therefore, one can control the direction of the current by suitably tailoring the frequency of the driving force. In addition one finds several extrema in the current-amplitude characteristic.

Though the model presented does not pretend to be a realistic model for a real system, the results we have presented have a wide application in many processes, such as catalysis, osmosis, and particle separation, and on the noise-induced transport in periodic potential landscapes that lack reflection symmetry such as ratchet systems. It is very important to understand the novel properties of these confined geometries, zeolites, biological channels, nanoporous materials, and microfluidic devices, as well as the transport behavior of species in these systems.

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