Transportation of Two Coupled Particles in an Asymmetric Saw-Tooth Potential *

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Based on a simple model, we theoretically show the transport behaviors of two harmonically coupled Brownian particles in an asymmetric saw-tooth potential with two slopes. The coupled particles are subject to stochastic fluctuations. It is found that when the equilibrium distance of the coupled particles is between the two slopes of the potential, the transport direction of the coupled particles will be reversed with a certain harmonic coupling strength. This current reversal can be easily understood with the near rigid approximation, where the two coupled particles can be regarded as a single particle in an effective potential. Compared with the original saw-tooth potential, the asymmetry of the effective potential could be reversed when the equilibrium distance is between the two slopes of the original potential, which results in the current reversal.

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Transport phenomena induced by asymmetric structures have attracted much interest in recent years.[1−10] They have wide applications in physics, chemistry, biology and technology, e.g., molecular motors, ion pumps and artificial devices for guiding particles.[8,9,11−23] In general, the breaking of spatial inversion symmetry coupling with an unbiased colored perturbation could induce biased transportation of Brownian particles, i.e., ratchet effects.[1,7,24−28] Two basic types of ratchet models are commonly studied: tilting ratchet, in which the Brownian particle is in a fixed periodic potential and subject to a time-periodic driving or a colored stochastic fluctuation;[1,24,29,30] pulsating ratchet, in which the Brownian particle is in a fluctuating periodic potential which is modulated by a multiplicative time-periodic or colored fluctuation.[1,31,32]

In nature, the internal interactions between objects would have influence on their transport behaviors. Two coupled particles are always used as models to study the influence of the coupling interactions on the transport behaviors.[18−20,33−50] Previous studies have shown that the transport of two coupled particles may reverse for different coupling interactions in asymmetric potential together with time-periodic driving.[36−42] Though stochastic perturbations are general in nature, for two coupled particles in tilting ratchet systems driven by stochastic perturbations the effect of the coupling interaction on their transport behaviors has not been studied systematically.

In this Letter, we consider a tilting ratchet model of two harmonically coupled particles in an asymmetric saw-tooth potential with two slopes. Both particles are subject to independent stochastic fluctuations. We show that when the length of the equilibrium distance is between the two slopes of the saw-tooth potential, current reversal occurs with certain harmonic coupling strength. The current reversal can be understood by using near rigid coupling approximation, with which the coupled particles can be regarded as a single particle in an effective potential. The asymmetry of the effective potential can be reversed from the original potential at suitable equilibrium distance, and results in the current reversal.

We consider two harmonically coupled particles in an asymmetric saw-tooth potential $V(x)$ with two slopes,

$$V(x)=\begin{cases}\frac{V_0}{L_\mathrm{u}}(x-aL), & aL\le x<aL+L_\mathrm{u},\\ \frac{V_0}{L_\mathrm{d}}(aL+L-x), & aL+L_\mathrm{u}\le x<aL+L,\end{cases} \tag{1}$$

where $a=0,\pm1,\pm2,\pm3,\ldots$, L is the spatial period of $V(x)$, V_0 is the height of the potential barrier, $L_\mathrm{u}=\frac{2}{3}L$ is the uphill slope of the saw-tooth potential, and $L_\mathrm{d}=\frac{1}{3}L$ is the downhill slope.

The motion of two coupled particles with the same mass of m in the potential $V(x)$ is governed by the following Langevin equations

$$\begin{aligned} m\ddot{x}_1(t) =& -\eta\dot{x}_1(t)-V'(x_1(t))\\ &-k(x_1-x_2-l)+\xi_1(t)+\varepsilon_1(t), \quad (2a)\\ m\ddot{x}_2(t) =& -\eta\dot{x}_2(t)-V'(x_2(t))\\ &+k(x_1-x_2-l)+\xi_2(t)+\varepsilon_2(t), \quad (2b)\end{aligned}$$

where $x_1(t)$ and $x_2(t)$ are the positions of the particles at time t, η is the friction coefficient, $k(x_1-x_2-l)$ is the harmonic coupling interaction between the two particles, in which k is the harmonic coupling strength and l is the equilibrium distance, and $\varepsilon_1(t)$ and $\varepsilon_2(t)$ are independent Gaussian white thermal noises and satisfy the fluctuation–dissipation relationship

$$\langle\varepsilon_i(t)\varepsilon_j(t')\rangle=\delta_{ij}2\eta k_\mathrm{B}T\delta(t-t'),\ i,j=1,2, \tag{3}$$

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where δ_{ij} equals 0 when $i \neq j$ and equals 1 when $i = j$, $k_{\rm B}$ is the Boltzmann constant, T is the temperature, and $\xi_1(t)$ and $\xi_2(t)$ are independent stochastic processes[4] in the form of

$$\xi_i(t') = \xi_{in} \sin(\pi t'/\tau_{in}),\ \ i,j = 1,2,\ \ n = 1,2,3,\ldots, \quad (4)$$

which means that during each time period τ_{in}, $\xi_i(t)$ is a sine function with the amplitude of ξ_{in} and the frequency of π/τ_{in}. Here $\{\tau_{1n}\}$ and $\{\tau_{2n}\}$ are two series of random numbers sampled independently from a Gaussian distribution function with the mean value of τ ($\langle\tau_{1n}\rangle = \langle\tau_{2n}\rangle = \tau$) and variance of σ_τ^2 ($\langle\tau_{1n}^2\rangle = \langle\tau_{2n}^2\rangle = \sigma_\tau^2$), τ can be treated as the auto-correlation time of $\xi_i(t)$, and $\{\xi_{1n}\}$ and $\{\xi_{2n}\}$ are sampled independently from a Gaussian distribution function with the mean value of 0 ($\langle\xi_{1n}\rangle = \langle\xi_{2n}\rangle$=0) and variance of σ_ξ^2 ($\langle\xi_{1n}^2\rangle = \langle\xi_{2n}^2\rangle = \sigma_\xi^2$).

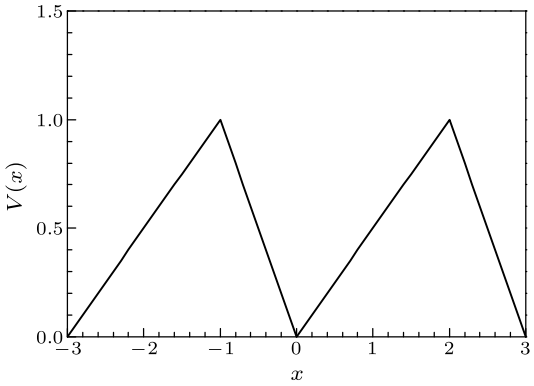

Fig. 1. An example of the asymmetric saw-tooth potential.

The average velocity $\bar{v}_i$ of each particle is defined as $\bar{v}_i = (x_i(\Delta T) - x_i(0))/\Delta T$, where ΔT represents the total runtime. We can obtain the current of the coupled system, according to the average velocity of the center of mass (CM) $\bar{v} = (\bar{v}_1 + \bar{v}_2)/2$. To simplify the calculation, we use a dimensionless unit. We set $m = 1.0$, $V_0 = 1.0$, $L = 3.0$, $k_{\rm B}T = 1$, $\eta = 0.1$ and set $\sigma_\xi^2 = 0.2$, σ_τ^2=1. Then Eqs. (1), (2a) and (2b) can be written as

$$\begin{aligned}\ddot{x}_1(t) = &-0.1\dot{x}_1(t) - V'(x_1(t)) \\ &- k(x_1 - x_2 - l) + \xi_1(t) + \varepsilon_1(t) \quad (5a)\\ \ddot{x}_2(t) = &-0.1\dot{x}_2(t) - V'(x_2(t)) \\ &+ k(x_1 - x_2 - l) + \xi_2(t) + \varepsilon_2(t) \quad (5b)\end{aligned}$$

$$V'(x) = \begin{cases} 0.5, & 3a \le x < 3a + 2, \\ -1, & 3a + 2 \le x < 3(a+1), \end{cases} \quad (6)$$

where $a = 0, \pm1, \pm2, \pm3, \ldots$.

For different values of k, l and τ, we perform the simulations with a time step of 0.0005 to calculate $\bar{v}$ over the total runtime ΔT of 100000.

Figure 2(a) shows the average velocity $\bar{v}$ of the CM as a function of the auto-correlation time τ for two independent single particles ($k = 0$). It indicates that as τ increases, $\bar{v}$ increases significantly and becomes saturated at a certain value about 0.40 when $\tau > 200$. Figure 2(b) shows $\bar{v}$ versus τ with the equilibrium distance $l = 0.5$ and the harmonic coupling strength $k = 2.0$. It shows some similarity to Fig. 2(a) that $\bar{v}$ can also become saturated at a certain value about 0.14 when $\tau > 200$. Actually, we find that for different coupling parameters k, l in our calculation, $\bar{v}$ can always become saturated at certain values when $\tau > 200$. Thus we select a certain range of τ, which is (200, 250) with the interval of 0.5, and calculate the average of $\bar{v}$ over the selected range of τ as $\langle\bar{v}\rangle$ for different k and l.

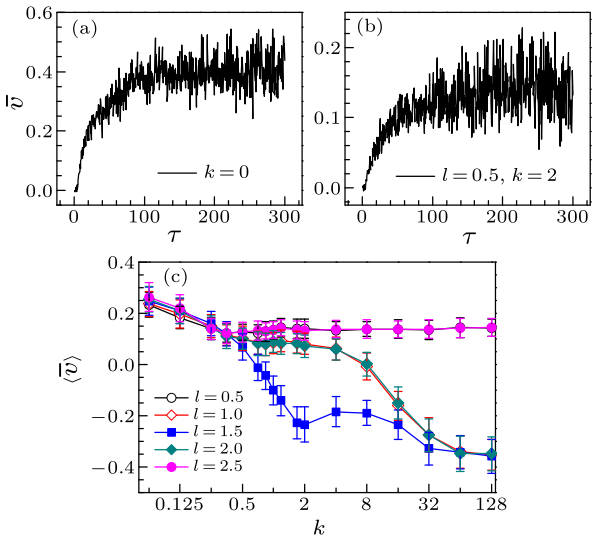

Fig. 2. (a) Average velocity $\bar{v}$ of the CM of two independent single particles experiencing the additional fluctuation $\xi_i(t)$ with the auto-correlation time τ; (b) average velocity $\bar{v}$ of the CM of two coupled particles as the function of τ, with the coupling parameters $l = 0.5$, $k = 2.0$; (c) $\langle\bar{v}\rangle$, average of $\bar{v}$ over τ (in the range of (200, 250) with the interval of 0.5), as a function of k, for $l = 0.5$, 1.0, 1.5, 2.0 and 2.5.

Figure 2(c) shows $\langle\bar{v}\rangle$ versus k for different l. Since the spatial period $L = 3.0$ and the two slopes of the saw-tooth potential $L_{\rm u} = 2.0$, $L_{\rm d} = 1.0$ as shown in Fig. 1, we select five particular values $l = 0.5$, 1.0, 1.5, 2.0 and 2.5. When k is enough small ($k < 0.3$), i.e., when the coupling interaction is weak enough, $\langle\bar{v}\rangle$ for different l decreases as k increases. As k continues to increase, functions of $\langle\bar{v}\rangle$ versus k for different l go into three classes: $\langle\bar{v}\rangle$ for $l = 0.5$ and 2.5 remain almost constant at a value about 0.14; $\langle\bar{v}\rangle$ for $l = 1.0$ and 2.0 decrease and turn from positive to negative around $k = 8$; and $\langle\bar{v}\rangle$ for $l = 1.5$ turns from positive to negative around $k = 0.7$. When k is large enough, $\langle\bar{v}\rangle$ for $l = 1.0$, 1.5 and 2.0 finally reach a value about -0.35. It is obvious that there are current reversals with certain k for $l = 1.0$, 1.5 and 2.0.

To analyze the current reversals, we consider two situations of no coupling and near rigid coupling. In the situation of no coupling, where $k = 0$, the two coupled particles turn into two independent single

particles, thus $\langle\bar{v}\rangle$ has nothing to do with l. In the situation of near rigid coupling, the equilibrium distance l keeps constant for each run. The motion of the CM can be considered as a single Brownian particle with the mass of $2m$ in an effective potential $V_{\rm eff}(x) = (V(x-L/2)+V(x+L/2))$ while undergoing combined thermal noises $(\varepsilon_1(t)+\varepsilon_2(t))$ and combined stochastic fluctuations $(\xi_1(t)+\xi_2(t))$

$$\begin{aligned} 2m\ddot{x}(t) = &-2\eta\dot{x}(t) - V'(x(t)-L/2) - V'(x(t) \\ &+ L/2) + \xi_1(t) + \xi_2(t) + \varepsilon_1(t) + \varepsilon_2(t), \quad (7) \end{aligned}$$

where x represents the position of the CM. Since both the thermal noises and the stochastic fluctuations acting on the two particles are independent and unbiased, there exists

$$\begin{aligned} &\langle(\varepsilon_1(t)+\varepsilon_2(t))(\varepsilon_1(t')+\varepsilon_2(t'))\rangle \\ &= 2\langle\varepsilon_1(t)\varepsilon_1(t')\rangle = 2\langle\varepsilon_2(t)\varepsilon_2(t')\rangle, \quad (8a) \\ &\langle(\xi_1(t)+\xi_2(t))(\xi_1(t')+\xi_2(t'))\rangle \\ &= 2\langle\xi_1(t)\xi_1(t')\rangle = 2\langle\xi_2(t)\xi_2(t')\rangle, \quad (8b) \end{aligned}$$

which indicate that $(\varepsilon_1(t)+\varepsilon_2(t))$ is still Gaussian white noise, and $(\xi_1(t)+\xi_2(t))$ is still colored stochastic fluctuation with a similar auto-correlation function to $\xi_i(t)$.

In Fig. 3, the red line shows $\langle\bar{v}\rangle$ of two independent single particles in the situation of no coupling. It shows that $\langle\bar{v}\rangle$ stays constant at a positive value about 0.40. The blue line shows $\langle\bar{v}\rangle$ of the effective single particle versus l over the range $(0.0, 3.0)$ with the interval of $\Delta l = 0.1$ in the situation of near rigid coupling. It shows that $\langle\bar{v}\rangle$ remains almost constant at a positive value about 0.14 for $l \in (0.0, 0.9] \cup [2.1, 3.0)$ and remains almost constant at a negative value about -0.36 for $l \in [1.0, 2.0]$, which is consistent with the values of $\langle\bar{v}\rangle$ for each l at the largest k in Fig. 2(c). Figure 3 shows that for $l \in [1.0, 2.0]$, the current direction in the situation of no coupling is opposite to that in the situation of near rigid coupling, which indicates that current reversal would occur with a certain k for $l \in [1.0, 2.0]$.

In the situation of near rigid coupling, the effective potential $V_{\rm eff}(x) = (V(x-L/2)+V(x+L/2))$ is different for near rigid coupled particles with different equilibrium distance l. In Fig. 4, $V_{\rm eff}(x)$ for $l = 0.5$, 2.5 are the same, which explains why $l = 0.5$ and 2.5 in Fig. 2(c) are close. Here $V_{\rm eff}(x)$ for $l = 1.0$ and 2.0 are also the same, which explains why $l = 1.0$ and 2.0 in Fig. 2(c) are close too, and $V_{\rm eff}(x)$'s for $l = 0.96$ and 2.04 are the corresponding effective potentials for the two data points with $\langle\bar{v}\rangle$ near 0 in Fig. 3. Comparing $V_{\rm eff}(x)$ for $l = 1.0$, 1.5 and 2.0 in Fig. 4 with the original saw-tooth potential $V(x)$ in Fig. 1, it is obvious that the order of the uphill slope and the downhill slope is reversed, thus the asymmetries of $V_{\rm eff}(x)$ for $l = 1.0$, 1.5 and 2.0 are reversed from the original saw-tooth potential. The reversal of the asymmetry of the potential could be the reason why there is current reversal for $l = 1.0$, 1.5 and 2.0. In addition, $V_{\rm eff}(x)$ for $l = 1.0$ and 2.0 is larger in amplitude and shorter in period than $V_{\rm eff}(x)$ for $l = 1.5$, while the ratio of the uphill slope and the downhill slope of $V_{\rm eff}(x)$ all are close to $1/2$ for $l = 1.0$, 1.5 and 2.0. This could be the reason why $\langle\bar{v}\rangle$ for $l = 1.0$, 1.5 and 2.0 are quite similar.

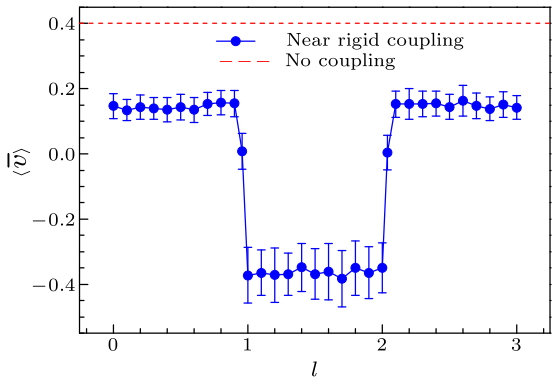

Fig. 3. Average velocity $\langle\bar{v}\rangle$ of the CM as a function of l for the situations of no coupling and near rigid coupling.

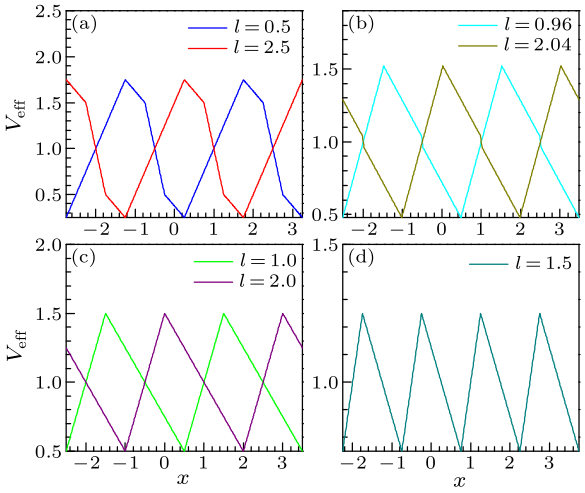

Fig. 4. The effective potential $V_{\rm eff}(x)$ for each l.

In summary, we have analyzed a tilting ratchet model of two harmonically coupled particles in an asymmetric potential and subject to independent stochastic fluctuations. It is found that when the length of the equilibrium distance is between the two slopes of the saw-tooth potential, the current reversal occurs with a certain harmonic coupling strength. This transport behavior can be understood by comparing two situations of no coupling and near rigid coupling. In the situation of no coupling, the two particles are two independent single particles in the original potential; while in the situation of near rigid coupling, the two particles can be regarded as a single particle in the effective potential. Since the effective potential is related to the equilibrium distance, its asymmetry can be reversed from the original po-

tential when the equilibrium distance is between the two slopes of the original saw-tooth potential, and the reversal of the asymmetry of the potential results in the current reversal.

Our research may be useful for understanding the mechanism of molecular motors in complex environments, since stochastic perturbations are supposed to exist there. It may also be useful for separating different kinds of coupled particles, as different kinds of coupled particles have different coupling interactions, thus they may have opposite current directions in an asymmetric periodic system with stochastic perturbations.

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