Dynamics of a dimer in a symmetric potential: Ratchet effect generated by an internal degree of freedom

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The one-dimensional dynamics of a dimer consisting of two harmonically coupled components is considered. The mutual distance between the dimer components plays the role of an internal degree of freedom. Both components are in contact with the same heat bath and are coupled to a spatially periodic, *symmetric* potential, whose amplitude is modulated periodically in time and whose coupling strength is different for the two components. In the absence of any external bias, a ratchet effect (directed transport) arises generically unless the mutual coupling of the dimer components tends to zero or infinity. In other words, the ratchet effect is generated by the internal degree of freedom. An accurate analytical approximation for the dimer's velocity and diffusion coefficient is obtained. The velocity of the system is maximized by adding an optimal amount of noise and by tuning the driving frequency to an optimal value. Furthermore, there exists an optimal coupling strength at which the velocity is the largest.

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I. INTRODUCTION

Theoretical studies of coupled Brownian particles in periodic structures are of great importance in many research areas, such as molecular motors [1], diffusion of adsorbed atoms on a surface [2,3], physics of polymers [4], ferrofluids [5], colloids [6], to name but a few. It is well-known (see [7–11] for a review) that in the absence of thermal equilibrium a so-called ratchet effect (directed transport) may arise either for a finite number of particles in asymmetric structures or for an infinite number of interacting particles (thermodynamic limit) even in symmetric potentials, namely by way of spontaneous symmetry breaking.

In the present work, we address the case of two interacting particles in a spatially symmetric, periodic potential, relevant for the diffusion of a dimer on a crystal surface and in many other physical contexts. A further motivation is that, based on the experimental studies [12], it has been suggested that the mechanism responsible for the symmetry breaking in molecular motors may be related to their own internal structure rather than their environment. That is, one can achieve symmetry breaking by making use of the internal degree of freedom—the relative distance between the dimer components—by either periodically modulating the interaction parameters of the Brownian particles [13], or by applying different forcings to different components of the dimer [14].

We note that a ratchet effect is also possible in a symmetric structure when there is no internal degree of freedom, but the heights of different potential barriers are modulated individually at different frequencies [15]. However, experimentally, such a dynamic symmetry breaking due to individual modulation of the energy barriers or dimer components may be more difficult to realize than to globally modulate the potential for all components.

In this paper, we introduce a simple model, where a transport effect occurs in a system of two interacting Brownian particles. In contrast to the numerous previous studies of such dimers e.g., in Refs. [16–24], we consider the case where the flashing potential has inversion symmetry at all times. The essential feature of our model is that different components of the system feel potentials of the same shape but different amplitudes. Experimentally, this can be realized, e.g., in the system of two dissimilar atoms, such as Si and Ge, adsorbed on a surface [2]. In what follows, we introduce the model and find an accurate analytical approximation for the velocity and diffusion coefficient. We show that the ratchet effect is caused by the internal degree of freedom in such a dimer. Furthermore, we show that the velocity of the system is maximal at an optimal coupling strength, and that it can be maximized also with respect to the noise intensity and frequency.

II. MODEL

We consider two overdamped coupled Brownian particles in symmetric synchronously flashing potentials (see Fig. 1). The equations of motion for the coordinates x_1, x_2 of the particles are

$$\eta\dot{x}_1 = -V'(x_1)f(t) - \kappa(x_1 - x_2 + l_0) + \sqrt{2\eta k_B T}\xi_1(t), \quad (1)$$

$$\eta\dot{x}_2 = -\alpha V'(x_2)f(t) + \kappa(x_1 - x_2 + l_0) + \sqrt{2\eta k_B T}\xi_2(t), \quad (2)$$

with η the viscous friction coefficient, $k_B T$ the thermal energy, and $\xi_i(t)$ independent and unbiased Gaussian noises with δ-correlation $\langle \xi_i(t)\xi_j(s)\rangle = \delta_{ij}\delta(t-s)$. The periodic potential for the first particle is a harmonic function with amplitude ΔV and spatial period L,

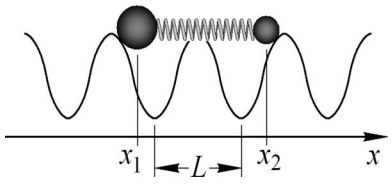

FIG. 1. Schematic representation of the model.

$$V(x) = \frac{\Delta V}{2}[1 - \cos(2\pi x/L)] \tag{3}$$

and the parameter $\alpha \neq 1$ in Eq. (2) yields the amplitude of the potential felt by the second particle, $\alpha\Delta V$. Both potentials are periodically switched on and off by a rectangular signal $f(t)=f(t+\tau)$ of periodicity $\tau=\tau_{\text{on}}+\tau_{\text{off}}$ consisting of on-phases of duration τ_{on}, such that $f(t)=1$ for $k\tau \leq t < k\tau+\tau_{\text{on}}$, and off-phases of duration τ_{off}, such that $f(t)=0$ for $k\tau+\tau_{\text{on}} \leq t < (k+1)\tau$, where $k \in \mathbb{Z}$. For simplicity, we assume the interaction between the two components to be elastic, with spring constant κ and rest length l_0.

Our goal is to evaluate the average velocity

$$v = \lim_{t\to\infty} \langle x_i(t) \rangle / t \tag{4}$$

and the diffusion coefficient

$$D = \lim_{t\to\infty} \langle [x_i(t) - \langle x_i(t) \rangle]^2 \rangle / (2t) \tag{5}$$

of the system, which are independent of the index $i=1,2$ for positive κ.

III. ORIGIN OF SYMMETRY BREAKING

As we will show below, the model [Eqs. (1) and (2)] exhibits a ratchet effect, i.e., a nonzero velocity in the absence of any external forcing. This effect in our model is caused by the internal degree of freedom. This is so because the current is zero when the internal degree of freedom is absent. This is realized in two opposite extremes of zero coupling, when the two components are independent of each other, and rigid coupling, when the dimer behaves as a single entity.

Indeed, in the uncoupled case, $\kappa=0$, each of the two particles in Eqs. (1) and (2) finds itself in the flashing sinusoidal potential, where no current is possible for symmetry reasons. On the other hand, in the opposite rigid limit, $x_2-x_1=l_0$, it is convenient to consider the equation of motion for the geometric center and the relative coordinate,

$$X = (x_1 + x_2)/2,$$

$$Y = x_2 - x_1 - l_0. \tag{6}$$

By properly adding and subtracting Eqs. (1) and (2) one readily finds that

$$\eta\dot{X} = -\frac{1}{2}\left[V'\left(X - \frac{Y+l_0}{2}\right) + \alpha V'\left(X + \frac{Y+l_0}{2}\right)\right] f(t) + \sqrt{\eta k_{\text{B}} T}\,\xi_X(t), \tag{7}$$

$$\eta\dot{Y} = -\left[\alpha V'\left(X + \frac{Y+l_0}{2}\right) - V'\left(X - \frac{Y+l_0}{2}\right)\right] f(t) - 2\kappa Y + \sqrt{4\eta k_{\text{B}} T}\,\xi_Y(t), \tag{8}$$

where $\xi_X(t)$, $\xi_Y(t)$ are again independent, unbiased, δ-correlated Gaussian noises. In the extreme case of rigid coupling, the distance between dimer components is fixed, $Y=0$, so that from Eq. (7) one concludes that the geometric center finds itself in the potential $[V(X-l_0/2)+\alpha V(X+l_0/2)]f(t)/2$. Since, according to Eq. (3), $V(x)$ is a trigonometric function containing a single wavelength, the resulting potential for X is also proportional to $\cos(2\pi X/L+\phi)$ with some phase ϕ, i.e., a spatially symmetric, periodic potential, again excluding any possibility of current in the system.

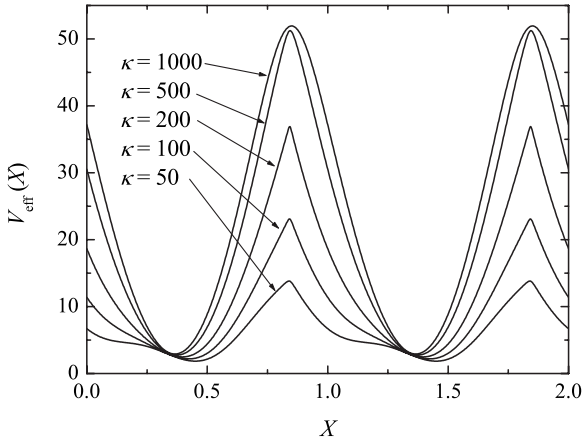

FIG. 2. Effective potential (10) for the following parameter values in Eq. (3): $V_0=100$, $L=1$, $\alpha=0.5$, $k_{\text{B}}T=1$, and five values of κ from 1000 (upper curve) to 50 (lower curve), as indicated.

In order to understand how the internal degree of freedom leads to the onset of the directed current, it is instructive to study the dynamics of the system in the asymptotic limit of large but finite stiffness κ. In this case, the dynamics of the relative coordinate Y occurs on a much faster time scale than that of the geometric center X. If the characteristic time scale of change of the geometric center is much longer than the thermalization time scale for the relative coordinate Y, one can replace the X- and Y-dependent potential energy for the geometric center with the potential averaged with respect to the fast relative coordinate. This is done with the help of the unnormalized probability distribution of the relative coordinate Y at a fixed value of X:

$$\rho(Y;X) = e^{-[\kappa Y^2/2 + V(X-Y+l_0/2) + \alpha V(X+Y+l_0/2)]/k_{\text{B}}T}. \tag{9}$$

The slow coordinate X finds itself in a mean-field potential of the free-energy type

$$V_{\text{eff}}(X) = -\frac{1}{2} k_{\text{B}} T \ln \int_{-\infty}^{\infty} dY \rho(Y;X). \tag{10}$$

Figure 2 shows this effective potential for several values of the coupling constant, κ. It is seen that at high values of κ, the effective potential indeed represents a symmetric function prohibiting spontaneous currents, while reduction of κ leads to two effects: reduction of the potential amplitude and the onset of its asymmetry, allowing for the ratchet effect in the system.

In conclusion, the main origin of the ratchet effect is an internal degree of freedom of nontrivial character, i.e., an interaction between the components of the dimer which is neither asymptotically weak nor asymptotically strong. In passing we note that for more general, symmetric potentials

than in Eq. (3), a finite effect would generically survive even in the limit of rigidly coupled dimer components, thus justifying *a posteriori* our focus on the particularly interesting special case from Eq. (3).

IV. ANALYTICAL APPROXIMATIONS

For an analytical evaluation of v and D from Eqs. (4) and (5), we assume a distinct inequality of amplitudes and deep potential wells for particle 1, i.e.,

$$\Delta V \gg k_B T, \quad \alpha \ll 1. \tag{11}$$

When the potentials are switched on, coordinate x_1 will immediately relax to the nearest minimum of the potential $V(x_1)$ almost independently of x_2. If we suitably move the origin of the x axis by integer multiples of L, we can always accomplish x_1 to be located in the interval between $-L/2$ and $L/2$, where $V(x_1)$ is minimal at $x_1=0$, thus rendering a straightforward harmonic approximation possible.

Our second assumption is that the on-phase of the driving is long enough to allow for the thermalization of the system, i.e.,

$$\tau_{\mathrm{on}} \gg \tau_{\mathrm{rel}}, \tag{12}$$

where τ_{rel} represents the characteristic relaxation time. In view of the condition (11), this quantity is essentially equal to the characteristic relaxation time of particle 2 in the potential

$$V_{\mathrm{on}}(x_2) := \alpha V(x_2) + \kappa(x_2 - l_0)^2/2, \tag{13}$$

i.e., the remaining potential after particle 1 has reached one of its local minima at an integer multiple of L.

Under the assumptions (11) and (12), the joint probability distribution in the end of the on-phase is

$$W^{\mathrm{on}}(x_1,x_2) = C^{\mathrm{on}} e^{-1/k_B T[V''(0)/2x_1^2 + \alpha V(x_2) + \kappa/2(x_1 - x_2 + l_0)^2]}, \tag{14}$$

where C^{on} is a normalization constant. This probability distribution can be transformed to the center-of-mass probability distribution by integrating out the x_i to $W^{\mathrm{on}}(X) = \int dx_1 \int dx_2 \, \delta[X-(x_1+x_2)/2] W^{\mathrm{on}}(x_1,x_2)$. The expression for the distribution $W^{\mathrm{on}}(Y)$ of the relative coordinate in the end of the on-phase is the same, but with $Y+(x_1-x_2+l_0)$ as an argument in the delta function.

In the off-phase, $f(t)=0$, the equations of motion for the geometric center, Eq. (7), and the relative coordinate, Eq. (8), describe Wiener and Ornstein-Uhlenbeck processes, respectively. Using the corresponding transition probabilities, the center-of-mass probability distribution in the end of the off-phase can be expressed as

$$W^{\mathrm{off}}(X) = C_X^{\mathrm{off}} \int dX_0 e^{-\eta(X - X_0)^2/2\tau_{\mathrm{off}} k_B T} W^{\mathrm{on}}(X_0), \tag{15}$$

C_X^{off} being a normalization constant. In the same manner, we find the distribution of the relative coordinate in the end of the off-phase,

$$W^{\mathrm{off}}(Y) = C_Y^{\mathrm{off}} \int dY_0 e^{-\kappa(Y - Y_0 e^{-2\kappa\tau_{\mathrm{off}}/\eta})^2/[2k_B T(1-e^{-4\kappa\tau_{\mathrm{off}}/\eta})]} W^{\mathrm{on}}(Y_0), \tag{16}$$

with the respective normalization constant C_Y^{off}.

At the beginning of the next on-phase, x_1 may either drop back into the same potential well where it was one period ago or fall into a neighboring well, with the respective probabilities depending on the properties of

$$W^{\mathrm{off}}(x_1) = \int dX \int dY \;\; \delta\left(x_1 - X + \frac{Y + l_0}{2}\right) W^{\mathrm{off}}(X) W^{\mathrm{off}}(Y). \tag{17}$$

This enables us to calculate the probability to find particle 1 between the kth and the $(k+1)$th maximum (i.e., within the basin of attraction of the minimum at kL) by

$$w_k = \int_{(k-1/2)L}^{(k+1/2)L} dx_1 W^{\mathrm{off}}(x_1), \tag{18}$$

resulting in the average velocity

$$v = \frac{L}{\tau} \sum_{k=-\infty}^{\infty} k w_k \tag{19}$$

and diffusion coefficient

$$D = \frac{L^2}{2\tau} \sum_{k=-\infty}^{\infty} k^2 w_k - \frac{v^2 \tau}{2}. \tag{20}$$

V. RESULTS AND DISCUSSION

In the following, we present a comparison of simulation data from the Langevin equations (1) and (2) with numerical results from our theory according to Eqs. (19) and (20). We have chosen the following constant parameter values: $\eta=L=1$, $\Delta V=100$, and $\alpha=0.05$, so that conditions (11) are guaranteed throughout. Successively, four parameters were varied: rest length, l_0, thermal energy, $k_B T$, switching frequency, ω, and coupling strength, κ. Simulation data represent averages over 15 trajectories for velocities and over 200 for diffusion coefficients, where each single trajectory covers a time span of 1.25×10^4 dimensionless time units. All simulations are performed for the duty cycle $\tau_{\mathrm{on}}/\tau = 1/2$ (i.e., $\tau_{\mathrm{on}} = \tau_{\mathrm{off}}$).

A. Dependence on dimer length l_0

The inherent mirror symmetry of the Langevin equations (1) and (2) implies that the current is an odd function of the dimer length l_0. As translational symmetry of the periodic potential $V(x)$ permits shifts by integer multiples of period L, we recognize this symmetry to be valid for all integers k according to $v(l_0) = v(kL+l_0) = -v(kL-l_0)$. This means that for all $l_0 = kL/2$ the net current must vanish, $v(kL/2)=0$.

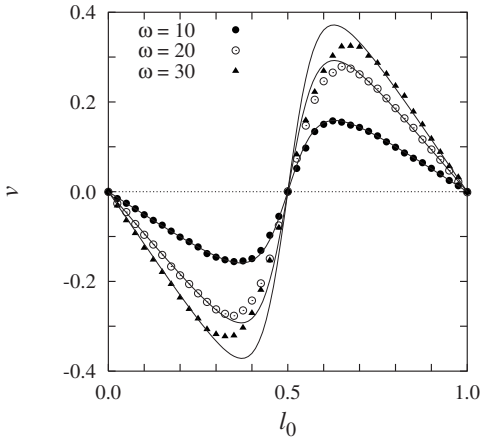

FIG. 3. Average velocity v vs rest length l_0 at three different switching frequencies $\omega=10$, 20, and 30 for $\eta=k_BT=L=1$, $\Delta V=100$, $\alpha=0.05$, and $\kappa=50$. Circles and triangles are simulation data, solid lines show the corresponding theoretical predictions. The results are uneven periodic functions with period L. Here, only one period $(0\leq l_0\leq L)$ is shown. With increasing frequency, theoretical prediction loses accuracy for l_0 around $L/2$.

Regarding the sign of the current, it depends on the character of dimer's deformation during the on-phase. If the dimer was squeezed, then after turning the potentials off, the first particle will be more likely to move to the left of its original position. Consequently, it will diffuse into the left minimum with greater probability than into the right one, and will be trapped there in the next on-phase. Since the character of the potential (13) is such that the dimer is squeezed for $kL<l_0<(k+1/2)L$, $k\in\mathbb{Z}$, the overall velocity will be negative in this case. Following an analogous line of reasoning, we conclude that the velocity will be positive for $(k+1/2)L<l_0<(k+1)L$.

Both features, current reversal and symmetry, are shown in Fig. 3 for dimer lengths l_0 within the interval from 0 to L. At low switching frequency $(\omega=2\pi/\tau=10)$, the coincidence of theory and simulation is unequivocal. Current reversal appears at l_0 equal to integer multiples of $L/2$, as explained above. In each node, the average velocity is an odd function of the dimer length. This qualitative behavior is not impaired by higher frequencies, as is also shown in this figure. For growing frequency, the exact probability distribution will increasingly deviate from the stationary Boltzmann distribution $W^{\mathrm{on}}(x_1,x_2)$ given by Eq. (14). Therefore our theoretical prediction of the average velocity exceeds the simulation data for $\omega\gtrsim 20$.

Nevertheless, even for higher frequencies, Eq. (19) very accurately predicts the behavior of the current for l_0 near all integer multiples of L. This is so, because in this case, the potential (13) felt by the second particle has a single minimum, with the relaxation time given approximately by $\tau_{\mathrm{rel}}(l_0\simeq kL)\approx\eta/[\kappa+\alpha V''(0)]$, $k\in\mathbb{Z}$. For the parameter values chosen, this relaxation time is much smaller than the duration of the on-phase, so the condition (12) is satisfied. On the other hand, for $l_0\simeq(k+1/2)L$, the potential (13) becomes bistable, so that the relaxation of the coordinate x_2 involves a slow process of thermally activated hopping over the potential barrier with a substantially longer relaxation time.

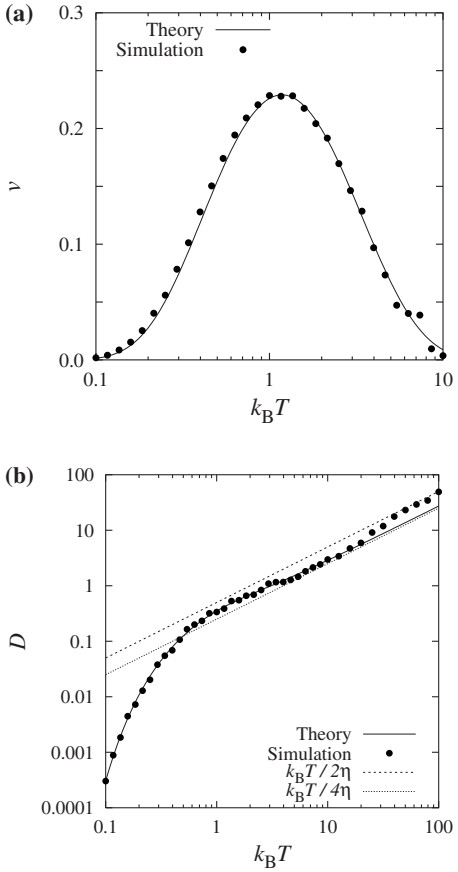

FIG. 4. (a) Average velocity v vs thermal energy k_BT for $\eta=L=1$, $\Delta V=100$, $\alpha=0.05$, $\omega=25$, $\kappa=50$, and $l_0=0.75$. Solid line: analytical expression (19); and circles: simulations. The velocity clearly shows a maximum at $k_BT\simeq 1$. (b) Diffusion coefficient D vs k_BT for the same parameter values as in (a). Solid line: analytical expression (20); and circles: simulations. At $k_BT\simeq 1$, D starts to converge toward $k_BT/4\eta$ (dashed line).

B. Temperature dependence

The temperature dependence of v reveals a good agreement of simulation and theory over two orders of magnitude of thermal energy, as does the diffusion coefficient D (Fig. 4). The v-k_BT-diagram exhibits a clear-cut maximum of the current for an optimal amount of noise in the system. On the one hand, if temperature becomes zero, there is no motion at all and the current must vanish. On the other hand, if the thermal energy exceeds all other characteristic energies of the system, the effective potential, Eq. (10), becomes insignificant and overall symmetry is restored, thus inhibiting any ratchet effect. In between, there must be a finite current (for all $l_0\neq kL/2$, $k\in\mathbb{Z}$) because at any finite value of T the distribution $W^{\mathrm{off}}(x_1)$ is nonsymmetric at $x_1=0$, leading to a nonvanishing sum in Eq. (19).

Turning to the dependence of the diffusion coefficient on the thermal energy, one can distinguish three regimes. At temperatures higher than the barrier height ΔV, the details of the flashing periodic potential become immaterial, and the diffusion coefficient asymptotically approaches the value $D_{\mathrm{free}}=k_BT/2$, corresponding to the free diffusion of the geometric center coordinate (7), see upper dashed line in Fig.

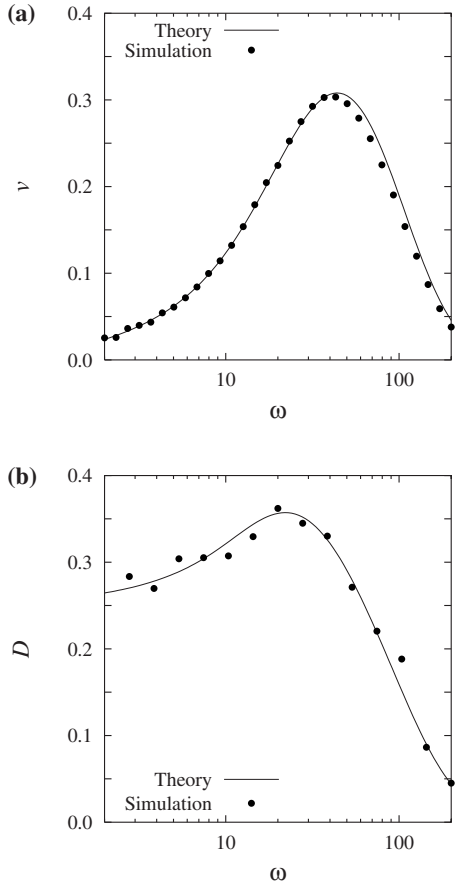

FIG. 5. (a) Average velocity v vs switching frequency ω for $\eta=k_BT=L=1$, $\Delta V=100$, $\alpha=0.05$, $\kappa=50$, and $l_0=0.7$. For $\omega \gtrsim 40$, the theoretical prediction starts to deviate slightly from simulation data. The reason for this is that τ is too short to allow for a relaxation of x_2 according to W^{on}. A resonant activationlike maximum [25] stands out at $\omega \simeq 40$. (b) Diffusion coefficient D vs ω for the same parameter values as in (a).

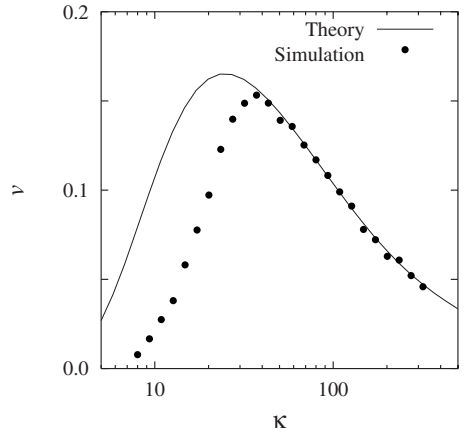

FIG. 6. Average velocity v vs elastic coupling κ for $\eta=k_BT=L=1$, $\Delta V=100$, $\alpha=0.05$, $\omega=10$, and $l_0=0.7$. For low values of κ, the assumed Boltzmann distribution $W^{\mathrm{on}}(x_1,x_2)$ cannot describe the real situation sufficiently exact, thereby predicting an exceedingly high average current. This is due to the onset of a much slower relaxation process taking effect at low κ.

4(b). At intermediate temperatures, the diffusion of the dimer is significant only during the off-phases, when the potential is switched off, with the diffusion coefficient given by $D_{\mathrm{free}}\tau_{\mathrm{on}}/\tau=k_BT/4$ for duty cycle 1/2, see the lower dashed line in Fig. 4(b). Finally, as $T\to 0$, the decline of D is much steeper than of D_{free} due to the increasing probability of x_1 returning to its starting point of the previous on-phase, corresponding to a "loss" of diffusion over a whole period.

C. Dependence on the switching frequency

Figure 5(a) shows the effect of the switching frequency $\omega=2\pi/\tau$ on the average velocity of the dimer. It exhibits the asymptotic behavior $v\to 0$ both for $\omega\to 0$ and for $\omega\to\infty$. The explanation for this is apparent: on the one hand, there will be no net probability current for extremely long times of free diffusion because $W^{\mathrm{off}}(x_1)$ gets very flat. On the other hand, $W^{\mathrm{off}}(x_1)$ will be sharply peaked for very short times of free diffusion so that $w_k \approx 0$, for $k\neq 0$, generating no net current, either. In between, there is necessarily a finite amount of probability spreading out beyond the interval from $-L/2$ to $L/2$, giving rise to a finite net current. This current shows a clear-cut maximum, too, which one would call a resonant activation in terms of escape from a metastable state [25]. The already mentioned deviation of W^{on} for high frequencies thereby leads to a slight overestimation of the maximal current.

The diffusion coefficient [Fig. 5(b)] also converges toward $D_{\mathrm{free}}=k_BT/4\eta$, which in this case is $D_{\mathrm{free}}=1/4$, but here the convergence takes place in the low-frequency limit, as it provides long times of free diffusion. In the high-frequency limit, the time of free diffusion becomes too short to allow for a finite current out of the potential minimum, so that the diffusion coefficient approaches zero as $\omega\to\infty$.

D. Dependence on elasticity κ

The line of reasoning is different when it comes to the role of the elastic coupling κ (Fig. 6). There will be an asymptotically vanishing net current for $\kappa\to 0$ and for $\kappa\to\infty$, but this is due to the decisive role of the internal degree of freedom, as explained in Sec. III. The internal degree of freedom can only exist as long as κ is finite, thus breaking symmetry and inducing a ratchet effect. Similar to the current maximization with respect to temperature and frequency, we can distinguish an optimal value of the coupling constant that leads to a maximal current. It is at this value of the coupling constant that the deformation of the dimer in the on-phase is maximal.

We shall briefly discuss the obvious inability of Eq. (19) to give any accurate quantitative prediction of the net current for small values of the elastic coupling constant. We see a pronounced spread between theory and simulation for $\kappa \lesssim 30$. For decreasing κ, the potential $V_{\mathrm{on}}(x_2)$, Eq. (13), is transformed to a multistable one-dimensional landscape consisting of two or more relative minima. The barriers separating these minima approach a height of $\alpha\Delta V$ as $\kappa\to 0$, leading to a thermalization time much larger than τ_{on}. Since $W^{\mathrm{on}}(x_1,x_2)$ relies on the equilibrium distribution, it cannot describe the actual probability distribution at the end of the

on-phase with sufficient accuracy. Consequently, the theory does not hold for low κ. For this reason, any viable theoretical prediction of the diffusion coefficient depending on the elastic coupling constant could not be made.

VI. CONCLUDING REMARKS

In this work, we have demonstrated, both analytically and by means of numerical simulations, that an internal degree of freedom can lead to the onset of the symmetry breaking and to a ratchet effect in a dimer finding itself in a flashing *symmetric* potential. The current can be maximized with respect to various system parameters describing the properties of the potential, environment, and coupling. We expect that the effect will be also observable for other asymmetry types, e.g., different values of the friction coefficient of the two particles, and inclusion of additional degrees of freedom and/or inertia should preserve the effect. Detailed studies of these intriguing possibilities will be the subject of our future research.

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