Hopping motion of interacting particles: From time-dependent interaction to directed transport

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The hopping motion of three or more pairwise interacting particles on a linear equipotential chain is investigated. It is shown that a directed transport of the particle array can be obtained by introducing time-dependent interactions such as switching the interaction strength periodically between two values. The direction and mean velocity of the motion are determined by the nature of the imposed time dependence and can, hence, be chosen dynamically. The possibility of transporting a passive cargo and some other applications are discussed.

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I. INTRODUCTION

The possibility to construct man-made machines on mesoscopic to molecular scales is fascinating and challenging for many reasons. First, such man-made molecular machines would provide a natural followup for handling and manipulating nanoscale objects such as atoms and single molecules, which have already become widespread in many areas [1]. While a few steps in this direction have already been made experimentally [2], the investigation of how to transform externally supplied energy in an efficient and controllable way into performing specific functions on the molecular scale is still in its early stages. These first realizations are nevertheless very promising and one might expect further developments to yield some yet unknown ways to control the molecular scale and to open new fields of technological applications. Man-made molecular machines might also help to shed light on the functionality of the variety of machines and motors known in biology, in particular, on the poorly understood complex energy transformations that occur in biological systems on the molecular scale. This hope is based on the fact that, in the opposite direction, biological machines and motors have stimulated physical studies leading to first experimental realizations of man-made small scale machines, for example, the so-called Brownian motors [3]. Inspired by the directed motion of biological motor proteins (see, for example, Ref. [4]), the motion of particles in ratchet potentials with spatial asymmetry under the influence of stochastic and/or periodic forces has been intensively studied. The theoretical approaches are usually either based on Newton-/Langevin-type equations of motion [5] or focus on hopping models [6]. Besides the biological motivation, one would like to understand the conditions under which directed motion of particles in these systems occur, an issue, that relates to the problem to the second law of thermodynamics [7] and to general symmetry considerations [8]. The results of the theoretical investigations have been used to produce experimentally directed transport on scales ranging from macroscopic objects down to single atoms [9]. Having the advantage of being rather simple, ratchet approaches usually share the feature that the direction and velocity of the motion are somewhat difficult to control dynamically.

Recently some alternative concepts have been proposed [10,11] that allow inherently for dynamical control of the direction and velocity of the induced motion. Within the concept developed in Ref. [10], originally formulated in continuous Newtonian dynamics, the energy is supplied by a time-dependent interparticle interaction and is then transformed via a nonlinear coupling to a deterministic directed transport, in the absence of any static spatial asymmetry in the system. In the following, a simple hopping version of the continuous model of Ref. [10] is discussed. In the case studied here, three or more particles are located on a line of equipotential sites and interact via harmonic nearest neighbor pair potentials. It is shown that within this discrete version, directed motion can be achieved with less effort, since a simple periodic drive that switches the interaction strengths between two values is sufficient to cause directed transport. As in the continuous counterpart [10], the direction and mean velocity of the motion are determined by the characteristics of the imposed time dependence and can be chosen dynamically, and the model allows for the transportation of a passive cargo.

II. MODEL

The topology of the model system under discussion is shown in Fig. 1(a). There are $N=3$ particles located along a linear chain of equipotential sites that interact via nearest neighbor pair potentials. To simplify the notation, the three particles are, henceforth, numbered 0, 1, and 2 (from left to right), whereas the two interparticle potentials or “bonds” are denoted by 0 (left) and 1 (right). The interparticle potential $V_i$ of “bond” $i$, i.e., between particles $i$ and $i+1$, is assumed to be harmonic, $V_i=V_i(0)[x_{i+1}(t)-x_i(t)]^2$, where $x_i(t)$ is the position of particle $i \in \{0,1,2\}$ at time $t$, and $V_i(0)$ denotes the interaction strength of “bond” $i \in \{0,1\}$ (length and time are measured here in units of number of sites and in units of hopping attempts per particle, respectively). The particles perform random nearest neighbor hops under the restriction of site exclusion (only one particle can occupy a given site), where the transition probability $\Gamma$ for a particle to hop to an empty site is given by $\Gamma = \text{min} \{1, \exp[-\Delta E/(k_B T)] \}$. Here, $\Delta E$ is the energy difference between the attempted and the present particle arrangement, $k_B$ denotes Boltzmann’s constant, and $T$ is the absolute
The duration of a periodic interaction is to choose the potential prefactors to realize such a time dependence. To obtain directed transport, the interparticle interaction for a given period of time, the left "bond" is "excited" before the right "bond," whereas the right "bond" is weakened after the left one, see below. It is not feasible in the nonequilibrium case focused on below. Therefore, in what follows we rely on numerical simulations of the system dynamics.

Under equilibrium conditions (particularly when the \( V_i^{\text{gs}} \) are time independent), a diffusive motion of the particle array occurs, as expected. To obtain directed transport, the interparticle potentials are taken to be time dependent. One way to realize such a time dependence is to choose the potential prefactors \( V_i^{(0)} \) to alternate between two values as shown in Fig. 1(b). Here, the value \( V_i^{(0)} \) corresponds to a ground state (gs) and the value \( V_i^{(0)} \) corresponds to an "excited" state (es) of the "bond," thus mimicking the effect of periodically "exciting" the individual "bonds," where the "excitation" causes a strengthening [as in Fig. 1(b)] or weakening of the interparticle interaction for a given period of time. In this case, the model parameters are the two values of the interaction strength \( V_i^{(0)} \) and \( V_i^{\text{es}} \), the overall frequency \( \omega \), the duration \( 0 \leq \tau \leq \omega^{-1} \) of the "excitation," and the phase shift \( \Delta t \) between the "excitation" of the two "bonds," \( -\omega^{-1/2} \leq \Delta t \leq \omega^{-1/2} \), where \( \Delta t > 0 \) means that the left "bond" is "excited" before the right "bond," whereas \( \Delta t < 0 \) indicates the opposite order.

The quantities of interest are the time-dependent center-of-mass coordinate \( x(t) = \frac{1}{3} \sum_{i=0}^{3} x_i(t) \) of the array of three particles, with \( x_i(t) = x_0(t) + x_1(t) + x_2(t) \) for a broad set of parameter values is shown in Fig. 3. The actual value of the mean velocity \( \bar{v} \) for time steps. By calculating the first moment of the latter quantity, one obtains the mean distance \( \bar{x}(t) = \frac{1}{\Delta t} \sum_{x} x P_f(x) \) after \( t \) time steps, from which the mean velocity \( \bar{v} \) is calculated as the long-time limit \( \bar{v} = \lim_{t \to \infty} \frac{\bar{x}(t)}{t} \) (in units of number of sites per hopping attempt and particle).

III. RESULTS

Let us start the discussion by looking at the probability distribution \( P_f(x) \) for some particular sets of parameter values, see Fig. 2. There are three cases shown in the figure, (i) pure diffusive motion in Fig. 2(a), which is caused by symmetrically "exciting" the "bonds" without any phase shift, \( \Delta t = 0 \), (ii) biased motion to the right in Fig. 2(b), which is caused by "exciting" (strengthening) the right "bond" after the left one, \( \Delta t > 0 \), and (iii) biased motion to the left in Fig. 2(c), which is caused by "exciting" (strengthening) the left "bond" after the right one, \( \Delta t < 0 \). An alternative view on the "excitation" is that in the case (ii) the left "bond" is weakened after the right one, whereas in the case (iii) the right "bond" is weakened after the left one, see below. It should be noted that the time dependence of the width of the probability distribution reflecting the diffusive part of the motion is approximately the same in all three cases, whereas the time dependence of the first moment of the distribution (i.e., the mean velocity \( \bar{v} \)) varies for the different values of \( \Delta t \).

The mean velocity \( \bar{v} \) for a broad set of parameter values is shown in Fig. 3. The actual value of the mean velocity \( \bar{v} \) for
Figure 3. Plot of the mean velocity $\bar{v}$ of the array of three particles vs phase $\Delta t$ for interparticle interaction strength $V_{gs}^{(0)}/(k_B T) = 1$ and $V_{es}^{(0)}/(k_B T) = 2$, overall frequency $\omega = 3/10$ and $\omega = 3/11$, and different values of the “excitation” duration $\tau$. $\tau = 1/3$ (full circle), $\tau = 2/3$ (open square), $\tau = 1$ (full triangle), $\tau = 4/3$ (open diamond), and $\tau = 5/3$ (full star). The lines are included as a guide to the eye.

Given $V_{gs}^{(0)}$ and $V_{es}^{(0)}$ depends on the value of $\Delta t$ with respect to the values of $\tau$ and $\omega$. Due to symmetry reasons one observes $\bar{v} = -\bar{v}$ when replacing $\Delta t \rightarrow -\Delta t$ for given $\omega$ and $\tau$. In the case of an array of three particles, the maximum absolute value of the mean velocity for given $\tau$ and $\omega$ is obtained for $\Delta t_{\max} = \pm \tau$ for $\tau < \omega^{-1/2}$. Since $\Delta t = \pm k/3$ corresponds to a temporally symmetric situation, as the time between the “excitations” of the two “bonds” is exactly half of the inverse overall frequency, one obtains $\bar{v} = 0$ for all values of $\tau$. This means particularly that no directed transport is observed for $\Delta t = \pm \tau$ when $\tau = \omega^{-1/2}$, so that for $\tau = \omega^{-1/2}$ the maximum velocity is obtained for $\Delta t_{\max} = \pm k/3$ instead for $\pm \tau$ (the factor of 3 accounts for the fact that the array consists of three particles), where $k$ is the smallest integer larger than $3 \omega^{-1/4}$. It should be noted that due to the discreetness of the parameters $\omega$, $\tau$, and $\Delta t$, the special case $\tau = \omega^{-1/2}/2$ exists only when $3 \omega^{-1}$ is even [see Fig. 3(a), again the factor of 3 accounts for the fact that the array consists of three particles], but is absent if $3 \omega^{-1}$ is odd [see Fig. 3(b)].

So far we have concentrated on the case in which the “excitation” strengthens the “bond,” i.e., $V_{gs}^{(0)} > V_{es}^{(0)}$. The inverse case with $V_{es}^{(0)} > V_{gs}^{(0)}$, in which the “excitation” weakens the “bond,” results similarly in directed transport, see Fig. 4. The two cases, $V_{es}^{(0)} > V_{gs}^{(0)}$ and $V_{es}^{(0)} < V_{gs}^{(0)}$, can be mapped on each other by exchanging the two values $V_{es}^{(0)} \leftrightarrow V_{gs}^{(0)}$ and by replacing $\tau \rightarrow \omega^{-1} - \tau$. Therefore, the results for $\tau > \omega^{-1/2}$ when $V_{es}^{(0)} > V_{gs}^{(0)}$ can be read off from Fig. 4, whereas when $V_{es}^{(0)} < V_{gs}^{(0)}$ the results for $\tau > \omega^{-1/2}$ can be read off from Fig. 3. Also in the case $V_{es}^{(0)} < V_{gs}^{(0)}$ one observes $\bar{v} = -\bar{v}$ when replacing $\Delta t \rightarrow -\Delta t$ for given $\omega$ and $\tau$ due to symmetry reasons. In the case of an array of three particles, the maximum absolute value of the mean velocity for given $\omega$ and $\tau < \omega^{-1/2}$ is obtained for $\Delta t_{\max} = \pm \tau$ for ratios $V_{es}^{(0)}/V_{gs}^{(0)}$ close to 1, whereas for small ratios $V_{es}^{(0)}/V_{gs}^{(0)}$ (and generally for $\tau = \omega^{-1/2}$) a better performance (although in the opposite direction) is observed for $\Delta t_{\max} = \pm k/3$, where $k$ is the smallest integer larger than $3 \tau/2$. Thus, for $V_{es}^{(0)} > V_{gs}^{(0)}$ the best performance is observed when the two “excitations” overlap for half of their duration [cf., Fig. 4], in difference to the case $V_{es}^{(0)} < V_{gs}^{(0)}$ for which the best performance is observed when the two “excitations” directly follow each other [cf., Fig. 3, with the exception $\tau = \omega^{-1/2}$ discussed above]. It is important to note that in both cases, $V_{es}^{(0)} > V_{gs}^{(0)}$ or $V_{es}^{(0)} < V_{gs}^{(0)}$, the absolute value of the mean velocity becomes larger for given $\omega$, $\tau$, and $\Delta t$, when the ratio $V_{es}^{(0)}/V_{gs}^{(0)}$ is increased (for $V_{es}^{(0)} > V_{gs}^{(0)}$), see Fig. 5, or decreased (for $V_{es}^{(0)} < V_{gs}^{(0)}$), see Fig. 6. However, the mean velocity saturates for very large [cf., Fig. 5] or very small ratios [cf., Fig. 6].

The influence of the temperature on the mean velocity is shown in Fig. 7 for both $V_{es}^{(0)} > V_{gs}^{(0)}$ and $V_{es}^{(0)} < V_{gs}^{(0)}$, where

Figure 4. Plot of the mean velocity $\bar{v}$ of the array of three particles vs phase $\Delta t$ for interparticle interaction strength $V_{gs}^{(0)}/(k_B T) = 2$ and $V_{es}^{(0)}/(k_B T) = 1$, overall frequency $\omega = 3/10$ and $\omega = 3/11$, and different values of the “excitation” duration $\tau$. $\tau = 1/3$ (full circle), $\tau = 2/3$ (open square), $\tau = 1$ (full triangle), $\tau = 4/3$ (open diamond), and $\tau = 5/3$ (full star). The lines are included as a guide to the eye.

Figure 5. Plot of the mean velocity $\bar{v}$ of the array of three particles vs interparticle interaction strength $V_{es}^{(0)}$ for interparticle interaction strength $V_{gs}^{(0)}/(k_B T) = 1$ overall frequency $\omega = 3/10$. The different symbols correspond to “excitation” duration $\tau = 1/3$ and phase $\Delta t = 1/3$ (full circles), “excitation” duration $\tau = 2/3$ and phase $\Delta t = 2/3$ (open squares), “excitation” duration $\tau = 1$ and phase $\Delta t = 1$ (full triangles), “excitation” duration $\tau = 4/3$ and phase $\Delta t = 4/3$ (open diamonds), and “excitation” duration $\tau = 5/3$ and phase $\Delta t = 5/3$ (full stars). The lines are included as a guide to the eye.
the temperature is varied by changing $V_{gs}^{(0)}$ and $V_{es}^{(0)}$ simultaneously, keeping the ratio $V_{es}^{(0)}/V_{gs}^{(0)}$ fixed. In both cases, the best performance is observed for $\min\{V_{gs}^{(0)}, V_{es}^{(0)}\} \approx k_B T$, i.e., when the thermal energy is approximately equal to the smallest barrier. The outmost particles face in order to hop away from the middle one, $V_{gs}^{(0)}$ or $V_{es}^{(0)}$. For too small or too high temperatures, $\min\{V_{gs}^{(0)}, V_{es}^{(0)}\} \ll k_B T$ or $\min\{V_{gs}^{(0)}, V_{es}^{(0)}\} \gg k_B T$, the performance drops, and the mean velocity reaches zero for both $\min\{V_{gs}^{(0)}/(k_B T), V_{es}^{(0)}/(k_B T)\} \rightarrow 0$ (high temperature limit) or $\min\{V_{gs}^{(0)}/(k_B T), V_{es}^{(0)}/(k_B T)\} \rightarrow \infty$ (low temperature limit).

Besides achieving directed transport of the particle array, the concept allows in addition for the transportation of a passive cargo, analogous to the continuous case [10]. As an example, we study the case of an array of $N=4$ particles composed of $N'=3$ particles with two active “bonds” as before and $N''=1$ particle attached by one passive “bond” at the right. Here, the rightmost “bond” is called passive as the potential prefactor is constant in time, $V_{gs}^{(0)} = V_{es}^{(0)}$, in contrast to the active “bonds” whose potential prefactors change with time as before. The center-of-mass coordinate $x(t) = [x_0(t) + x_1(t) + x_2(t) + x_3(t)]/4$ of an array being initially located at $x_0(t=0) = -1$, $x_1(t=0) = 0$, $x_2(t=0) = 1$, and $x_3(t=0) = 2$ is recorded, and the mean velocity $\bar{v}$ is obtained as for three particles and is shown in Fig. 8. (In this case the time increases in steps of 1/4 accounting for the fact that there are four particles.) It is important to note that the attachment of the cargo breaks the spatial symmetry of the particle array, i.e., the mean velocity when “pulling” the cargo is larger than the mean velocity when “pushing” the cargo. The reverse case of the cargo being attached on the left side of the active part is equivalent to replacing $\Delta t \rightarrow -\Delta t$ and $\bar{v} \rightarrow -\bar{v}$.

One observes that when a cargo is attached, there is directed transport with $\bar{v} \neq 0$ even for $\Delta t = 0$, which occurs due to the statically broken spatial symmetry. Therefore, a system consisting of one asymmetrically placed active “bond” is sufficient to observe directed transport, for example an array of $N=3$ particles that is composed of $N'=2$ particles with one active “bond” (the parameter $\Delta t$ has no meaning in this case) and $N''=1$ particle attached by one passive “bond” on the left or on the right. In this case the direction of motion is (pre)determined by the position of the active “bond,” namely, if the active bond is on the left it yields motion to the left, and vice versa.

**IV. CONCLUSIONS**

A simple hopping counterpart of a concept recently proposed [10] to achieve directed transport on mesoscopic to
molecular scales is discussed. Focusing on the case of three or more particles located on a line of equipotential sites and interacting via harmonic nearest neighbor pair potentials, it is shown that the simple periodic switching of the interaction strength between two values is sufficient to cause directed transport. As in the case of the continuous approach [10], the direction and mean velocity of the motion are determined by the characteristics of the imposed time dependence and can, hence, be chosen dynamically, and the proposed concept allows for the transportation of a passive cargo. Comparing the performance and the experimental requirements of the hopping model presented here with the continuous picture [10], it is important to note that the continuous model is studied in the absence of noise, and that the performance (such as velocity, ability of control, and predictability of the array position) drops when noise is added to the system. This should be contrasted with the observation that within the hopping model presented here, which can be viewed as a discretized version of the corresponding Langevin description in the overdamped limit, directed motion of the particle array is achieved with considerably less effort: the simple strengthening/weakening of the interparticle potential vs the more complex changing of the interparticle potential rest length. The presence of thermal noise might help to reduce the technical demand and the complexity of actual realizations, particularly, when the temperature is chosen properly.

Thus, one of the major advantages of the proposed concept is that it is very simple and should be directly feasible in actual experiments. Concerning such an experimental realization, it is important to note that the time dependence of $V_t(\tau)$ does not necessarily need to be strictly periodic as considered here for the sake of simplicity. Alternatively, one can view the time dependence of the $V_t(\tau)$ as a result of “excitations” induced externally, where the temporal order of the excitation and hence the value of $\Delta \tau$ are chosen dynamically leading to a detailed control of the induced directed motion.

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To perform the numerical simulation, the three particles are put on the sites \( x_0(t=0) = -1 \), \( x_1(t=0) = 0 \), and \( x_2(t=0) = 1 \) at \( t = 0 \). Then, in each time step \( t \), at first one of the three particles \( i \in \{0, 1, 2\} \) and one of the two directions \( \Delta x \in \{-1, 1\} \) are chosen randomly with equal probability. Second, in case there is no other particle on the site \( x_i(t-1/3) + \Delta x \), the transition of particle \( i \) from \( x_i(t-1/3) \) to \( x_i(t-1/3) + \Delta x \) is performed with probability \( \Gamma = \min\{1, \exp[-\Delta E/(k_B T)]\} \) [i.e., \( x_i(t) = x_i(t-1/3) + \Delta x \)], whereas with probability \( 1-\Gamma \) [or with probability 1 if site \( x_i(t-1/3) + \Delta x \) is already occupied] the particle remains on site \( x_i(t-1/3) \) [i.e., \( x_i(t) = x_i(t-1/3) \)]. Here, \( \Delta E \) denotes the energy difference between the attempted and the present particle arrangement. After every successful or unsuccessful attempt, the time increases by \( 1/3 \) [the factor \( 1/3 \) accounts for the fact that there are three particles, for an array of four particles, cf., Fig. 8, the time increases in steps of \( 1/4 \)], so that during one time step each particle is considered on average once for a hopping attempt. After a certain large number of time steps, the particles’ positions are obtained. The whole simulation is repeated, and an ensemble average is performed over a large number of up to \( 10^7 \) independent configurations.

It should be noted that alternatively one may realize a time-dependent interparticle interaction leading to directed transport by periodically changing the free rest lengths (analogously to the continuous case [10]), or by periodically changing the potential exponents, the latter also corresponds to an effective weakening or strengthening of the interparticle interaction.