Molecular Motor that Never Steps Backwards

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We investigate the dynamics of a classical particle in a one-dimensional two-wave potential composed of two periodic potentials that are time independent and of the same amplitude and periodicity. One of the periodic potentials is externally driven and performs a translational motion with respect to the other. It is shown that, if one of the potentials is of the ratchet type, translation of the potential in a given direction leads to motion of the particle in the same direction, whereas translation in the opposite direction leaves the particle localized at its original location. Moreover, even if the translation is random, but still has a finite velocity, an efficient directed transport of the particle occurs.

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A particle subject to a spatially asymmetric but on large scale homogeneous potential displays a symmetric diffusive motion, since the sole violation of the $x \to -x$ symmetry is not sufficient to cause a net directional transport. As already noted more than 100 years ago by Curie [1], the additional breaking of time reversal $t \to -t$ symmetry (e.g., by dissipation) may lead to a macroscopic net velocity, so that in this case directed motion can result in the absence of any external force. Such systems, known as thermal ratchets [2], have been the subject of much activity, both theoretical [3–18] and experimental [19–25], partly motivated by possible applicability to biological motors [26–28].

In this Letter we study the classical dynamics of a particle in a one-dimensional two-wave potential. The total potential is composed of two periodic potentials that are time independent and of equal amplitudes and periodicities. One of the potentials is externally driven performing a translational motion with respect to the other. It is shown that if, in addition to the broken time reversal symmetry, the spatial symmetry is broken for one of the potentials, the relative translation can result in a twofold behavior: (i) Translation in one direction causes a deterministic motion of the particle in the same direction, whereas (ii) translation in the opposite direction leaves the particle localized at its original location. Thus, the total potential acts as a ratchet in the original sense. Moreover, an efficient directed transport occurs even if the translation is random but still has a finite velocity. The reason for the directed transport is the existence of points of irreversibility in the particle trajectory. The high rate transport stems from the fact that, if the particle once gains a distance which is an integer multiple of the potential period, this distance is preserved, different from former ratchet systems driven by random fluctuations.

We consider a simple ratchet-type potential $\Pi(x)$, which is assumed to be continuous but not necessarily differentiable. It has a periodicity b, so that $\Pi(x + b) = \Pi(x)$ $\forall\, x$, an amplitude $\Pi_0 = \max\Pi(x) = -\min\Pi(x)$, and one minimum is located at $x = 0$, i.e., $\Pi(0) = -\Pi_0$. We also assume that the potential $\Pi(x)$ has only one minimum and one maximum per period b, so that $\partial\Pi(x)/\partial x$ changes sign only twice for $x \in [0, b)$; cf. [29]. The total potential $V(x, \gamma)$ is composed of two, not necessarily identical, potentials $\Pi(x)$ and $\Pi'(x)$, i.e., $V(x, \gamma) \equiv \Pi(x) + \Pi'(x - \gamma)$, where γ defines the translation. Because of the periodicity of the potentials $\Pi(x)$, the potential $V(x, \gamma)$ is periodic in both arguments, so that $V(x, \gamma + b) = V(x, \gamma)$ $\forall\, \gamma$. In this potential landscape, the deterministic equation of motion of a particle of mass m reads as

$$m\ddot{x} + \eta\dot{x} + \frac{\partial V(x, \gamma)}{\partial x} = 0\,, \tag{1}$$

where the damping is denoted by η. It should be emphasized that, through the translation, energy is being permanently fed into the system, and that this energy has to be dissipated, i.e., $\eta > 0$. Otherwise the particle will gain energy until it decouples from the potential.

First, we restrict ourselves to the case characterized by an overdamped motion with $\eta/[(2\pi/b)\sqrt{m\Pi_0}] \gg 1$ and by a slow translation with $|\dot{\gamma}|/[2\pi\sqrt{\Pi_0/m}] \ll 1$, where $\dot{\gamma}$ is the translation velocity, and relax these restrictions towards the end. In this limit, as the translation γ is varied, the particle either (i) moves slowly remaining at the local potential minimum or (ii) if the minimum ceases to exist it jumps to the next minimum following the potential slope. The latter happens instantaneously on the time scale of the translation. In order to obtain the observables, which are the trajectory x and the average velocity $\bar{\dot{x}}$, it is therefore sufficient to study the behavior of the total potential $V(x, \gamma)$ and evaluate the positions of the minima. Below this limit is referred as "quasistatic." The initial conditions at $t = 0$ are chosen as $x = 0$ and $\gamma = 0$, so that the particle is located at a potential minimum. In what follows, we use the abbreviations $\tilde{x} \equiv x/b \bmod 1$ and $\tilde{\gamma} = \gamma/b \bmod 1$.

For simplicity, we start the discussion with a particular example for the potential $\Pi(x)$,

$$\Pi_\xi(x) \equiv \Pi_0 \begin{cases} -1 + 2\frac{\tilde{x}}{\xi} & \text{if } \tilde{x} \le \xi \\ 1 - 2\frac{\tilde{x}-\xi}{1-\xi} & \text{if } \tilde{x} > \xi \end{cases}, \tag{2}$$

which is piecewise linear, although the arguments below apply analogously for other ratchet-type potentials as well.

The parameter $\xi \in (0, 1)$ determines the asymmetry of the potential, with $\xi = 1/2$ being the symmetric case. In order to introduce only one asymmetry, we choose the translated potential $\Pi'_{\xi'}(x)$ to be symmetric, i.e., $\xi' = 1/2$. For the other potential $\Pi_\xi(x)$ we use $\xi < 1/2$ only, since the case $\xi > 1/2$ can be mapped on the case $\xi < 1/2$ by replacing the asymmetry ξ by $1 - \xi$ and the translation γ by $-\gamma$. The case $\xi = \xi' = 1/2$, where both potentials are symmetric, is excluded, since then the total potential $V_{\xi,\xi'}(x, \gamma)$ becomes piecewise flat, and the "quasistatic" treatment of Eq. (1) is no longer valid [30].

Let us first discuss a translation with a constant translation velocity $\dot{\gamma} = \text{const}$, so that $\gamma = \dot{\gamma}t$, where the velocity can be either $\dot{\gamma} < 0$ or $\dot{\gamma} > 0$. Shown in Fig. 1 is one cycle of a translation by $-b$ [$\dot{\gamma} < 0$] and b [$\dot{\gamma} > 0$] for an example with $\xi = 2/5$ and $\xi' = 1/2$. In the case $\dot{\gamma} < 0$ [the open circles in Fig. 1; the time evolves from 1(h) to 1(a)], the particle moves a distance $-b$, whereas in the case $\dot{\gamma} > 0$ [the full circles in Fig. 1, the time evolves from 1(a) to 1(h)] the particle, although moving locally, returns to its starting point. After that, the whole cycle starts over again. Hence, the particle moves either with average velocity $\overline{\dot{x}} = \dot{\gamma}$ for $\dot{\gamma} < 0$ or $\overline{\dot{x}} = 0$ for $\dot{\gamma} > 0$. For the opposite asymmetry $\xi > 1/2$, the particle remains in the vicinity of $x = 0$ for $\dot{\gamma} < 0$ and moves with average velocity $\overline{\dot{x}} = \dot{\gamma} > 0$ in the case of an opposite translation.

This behavior can be generally understood from the properties of the total potential $V(x, \gamma)$. Shown in Fig. 2 are the potential $V(x, \gamma)$ and the particle position x, for both $\dot{\gamma} < 0$ (left side) and $\dot{\gamma} > 0$ (right side), calculated for a particle located at $x = 0$ for translation $\gamma = 0$, as it follows the changes of the potential $V(x, \gamma)$. Because of the asymmetry of one of the constituting potentials, there are points of instability $\mathcal{I}$ in the $(\tilde{x}, \tilde{\gamma})$ plane, where a local minimum of the potential $V(x, \gamma)$ ceases to exist. Hence, when the minimum disappears, a particle located at such a point performs an irreversible motion jumping to the next minimum; see Figs. 1(c), 1(f), and 2. In the example considered here, this new minimum moves in the direction of the jump and a net transport occurs in the case $\dot{\gamma} < 0$, whereas in the case $\dot{\gamma} > 0$ it moves in the opposite direction and cancels the distance gained by the jump. Under our restrictions on $\Pi(x)$, in particular due to the equality of the potential amplitudes, all points $(\tilde{x}, \tilde{\gamma}) \in \mathcal{I}$ satisfy $V(x, \gamma) = 0$. Let $\mathcal{C} \equiv \{(\tilde{x}, \tilde{\gamma}) | V(x, \gamma) = 0\} \supset \mathcal{I}$ be the set of all pairs $(\tilde{x}, \tilde{\gamma})$ for which the potential $V(x, \gamma) = 0$. Since the potentials $\Pi(x)$ are continuous, the topology of $\mathcal{C}$ is such that it consists of connected points that form paths and intersections; see Fig. 2. The

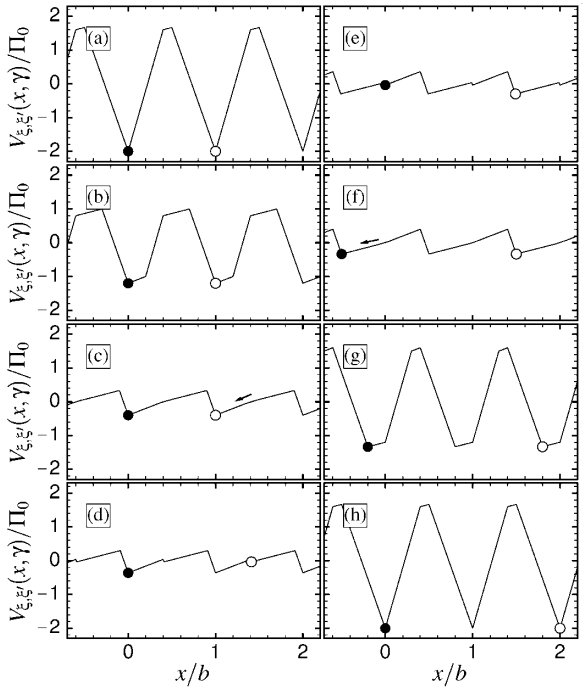

FIG. 1. Time evolution of the total potential $V_{\xi,\xi'}(x, \gamma)$ for the ratchet given by Eq. (2). In parallel, the respective positions of the particle are shown, both for $\dot{\gamma} > 0$ [full circles, the time evolves from (a) to (h)] and $\dot{\gamma} < 0$ [open circles, the time evolves in the opposite direction from (h) to (a)]. The parameters are $\xi = 2/5$ and $\xi\prime = 1/2$, and snapshots are taken at (a) $\tilde{\gamma} = 0$, (b) $\tilde{\gamma} = 1/5$, (c) $\tilde{\gamma} = 2/5$, (d) $\tilde{\gamma} = 41/100$, (e) $\tilde{\gamma} = 49/100$, (f) $\tilde{\gamma} = 1/2$, (g) $\tilde{\gamma} = 4/5$, and (h) $\tilde{\gamma} = 0$. The arrows indicate the direction of irreversible motion of the particle which occurs between snapshots (e) and (f) (full circle) and (d) and (c) (open circle).

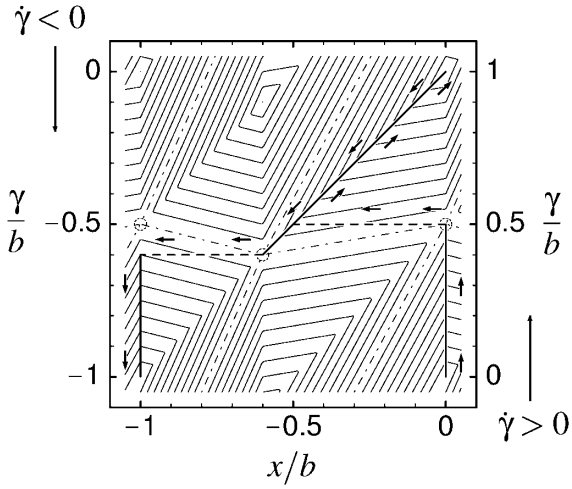

FIG. 2. Contour plot of the total potential $V_{\xi,\xi'}(x, \gamma)$ for the ratchet given by Eq. (2) with $\xi = 2/5$ and $\xi' = 1/2$; the solid equipotential lines are placed at $V_{\xi,\xi'}(x, \gamma) = \pm n\Pi_0/5$ with $1 \le n \le 10$ integer, and the dash-dotted equipotential lines indicate $V_{\xi,\xi'}(x, \gamma) = 0$. The respective trajectories of a particle starting at position $x = 0$ at translation $\gamma = 0$ are shown for both $\dot{\gamma} < 0$ (left side) and $\dot{\gamma} > 0$ (right side) with thick lines, which are solid for the part of the trajectory where the particle remains in the minimum, and dashed for the irreversible jumps. The arrows indicate the time development for $\dot{\gamma} < 0$ (downward arrows) and $\dot{\gamma} > 0$ (upward arrows). The points of irreversibility $\mathcal{I} = \{(\tilde{x}, \tilde{\gamma}) | (\tilde{x}, \tilde{\gamma}) = (0, 1/2), (2/5, 2/5)\}$ are marked by dashed circles.

intersections correspond to the points of irreversibility $\mathcal{I}$ in which a minimum of $V(x,\gamma)$ with respect to x ceases to exist. For the particular choice of the potentials $\Pi(x)$ given by Eq. (2), one obtains the two points $\mathcal{I}_{\xi,\xi'} = \{(\tilde{x},\tilde{\gamma})|(\tilde{x},\tilde{\gamma}) = (0,1-\xi'),(\xi,\xi)\}$. Within the quasistatic limit, jumps in the direction given by the potential's asymmetry occur if the particle reaches these points.

In order to decide in general if, for a given choice of potentials $\Pi(x)$, a directed transport is possible within the quasistatic limit, one has to examine the set $\mathcal{C}$ around the intersection points $\mathcal{I}$. In Fig. 3 the possible scenarios are shown, each with sketched "horizontal" and "vertical" lines corresponding to $V(x,\gamma) = 0$ around the intersection points. Concerning the question of irreversible jumps, namely, if the particle reaches the points of irreversibility as the translation is monotonously varied, one has to examine the behavior of the horizontal line, i.e., how this line is bent at the intersection point with respect to the direction of the translation. In the upper left part of Fig. 3 the horizontal line is bent downwards towards smaller values of γ and, hence, opposite to the direction of the translation $\dot{\gamma} > 0$ on both sides of the intersection point. This means that (i) the minimum in which the sketched particle is located moves towards the intersection point as γ is increased (because of the downward bending on the particle's side), and (ii) the minimum ceases to exist at the intersection point with a local slope such that the particle performs a jump leftwards to smaller values of x (because of the downward bending on the side opposite to the particle). In the lower left part of Fig. 3, the horizontal line is bent upwards on the particle's side of the intersection point, so that the minimum does *not* move towards the intersection as γ is increased, but remains always right to it at larger values of x. This behavior is independent of the bending on the side of the intersection point opposite to the particle, either upward, as shown in the figure, or downward. In the upper right part of Fig. 3, a third theoretically possible topology is shown. In this case, the particle reaches the intersection point (because of the downward bending on the particle's side), but the intersection point is *not* a point where the minimum ceases to exist (because of the upward bending on the side opposite to the particle).

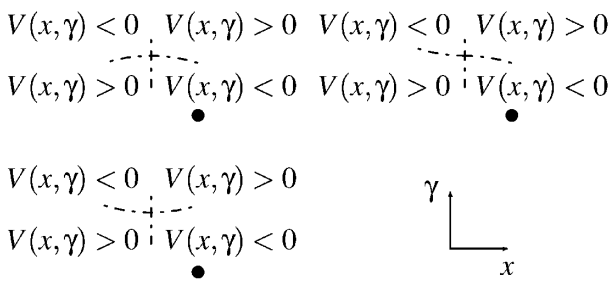

FIG. 3. Possible topologies for the set $\mathcal{C}$ around the points of irreversibility $\mathcal{I}$. The dashed lines represent $V(x,\gamma) = 0$, and the areas with $V(x,\gamma) > 0$ and $V(x,\gamma) < 0$ are indicated. The particle's position is shown as a solid circle.

However, this topology cannot occur under our restrictions on the potentials $\Pi(x)$. For the potentials $\Pi(x)$ given by Eq. (2) and for $\xi \neq 1/2$ or $\xi' \neq 1/2$, the resulting topology of $\mathcal{C}$ is always such that the points of irreversibility are reached within the quasistatic limit. Hence, depending on the asymmetry of the potentials, one observes transport for either $\dot{\gamma} < 0$ or $\dot{\gamma} > 0$, and no transport in the case of an opposite translation.

We can extend the model beyond the translation with a constant velocity, by assuming, for instance, another simple scenario with an oscillatory translation of the form $\gamma = \gamma_0 + \gamma_1 \sin(2\pi\omega t)$ with a driving frequency ω and $|\gamma_1|\omega/[2\pi\sqrt{\Pi_0/m}] \ll 1$. In this case, one finds an average velocity $\bar{\dot{x}} = \pm nb\omega$ with $n \geq 0$ integer, where the sign depends on the asymmetry of the potentials $\Pi(x)$. The actual value of n depends on the offset γ_0 and on the amplitude γ_1, since these values determine how many times the points of irreversibility $\mathcal{I}$ are reached during one cycle. For the potentials $\Pi(x)$ given by Eq. (2) with $\xi = 2/5$ and $\xi' = 1/2$, a choice of $\gamma_0 = 45b/100$ and $\gamma_1 = b/20$ results in an average velocity of $\bar{\dot{x}} = -b\omega$. This means that, in order to make the particle gain a distance b, the translation has to be varied only twice by $b/10$.

As a third possible scenario for the translation γ, we assume γ to vary randomly by following the trace of a random walker y that has locally a finite constant velocity $0 < |\dot{y}| = \text{const}$, but an average velocity $\bar{\dot{y}} = 0$. For this scenario, we relax the restriction of overdamped motion to demonstrate the validity and accuracy of the quasistatic treatment, and numerically integrate Eq. (1) with a finite damping and a finite translation velocity. However, one has to keep the restriction $|\dot{\gamma}|/[2\pi\sqrt{\Pi_0/m}] \ll 1$, since otherwise the changes in the potential due to the translation are too fast for the particle to follow, and the particle decouples from the potential. In Fig. 4 a realization of a random walker trace y and the resulting particle trajectory x for $\xi = 2/5$ and $\xi' = 1/2$ are shown. We would like to emphasize that,

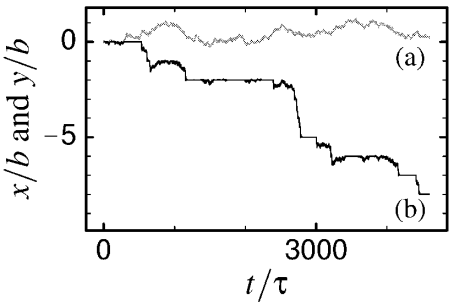

FIG. 4. Plot of a random walk trace y [(a), in grey] used as translation and the numerically obtained particle trajectory x [(b), in black] for asymmetry parameters $\xi = 2/5$ and $\xi' = 1/2$, and dissipation constant $\eta/[(2\pi/b)\sqrt{m\Pi_0}] = 0.2$. The random walker moves with velocity $|\dot{y}|/(2\pi\sqrt{\Pi_0/m}) = 0.02$ and chooses the direction anew every $t/\tau = 1$ with $\tau \equiv [(2\pi/b)\sqrt{\Pi_0/m}]^{-1}$, thus gaining a distance $|\Delta y|/b = 0.02$ during each step.

despite the relatively small damping, the numerically obtained trajectory differs from the one obtained under overdamped conditions only by small oscillations. Although the random walker, and, hence, the translation, have an average velocity $\overline{\dot{y}} = 0$, respectively, $\overline{\dot{\gamma}} = 0$, the particle's average velocity $\overline{\dot{x}}$ is nonzero. The sign of the velocity depends on the asymmetry of the potentials $\Pi(x)$; for our choice of asymmetry one finds $\overline{\dot{x}} < 0$ as expected. The transport is much more efficient than in former ratchet systems driven by random fluctuations. Here, if the particle gains a distance $d(t) \equiv |x(t)|$ equal to an integer multiple of the potential period b at a time t_n, $d(t_n) = nb$, the distance will never become smaller again, and $d(t) \geq nb$ $\forall\ t \geq t_n$. Putting this in the context of molecular motors, it means that the suggested molecular motor never executes a step backwards. These backward steps usually limit the efficiency of the motor [8].

Different realizations of the model can be thought of. One possibility is to put a small particle in a potential created by an optical tweezer such as in [20], but with two time-independent potentials added on top of each other at the same place and having a certain phase shift. Although the phase shift is changed randomly, but with a finite velocity, an efficient transport of the particle is predicted in a certain direction determined by the asymmetry of one of the potentials. Moreover, it is possible, for instance, to induce the translation of the potential through the coupling of a varying internal degree of freedom of the particle to the nontranslated potential [31]. This opens various possibilities for the construction of microscale and nanoscale devices such as pumps and motors based on the presented ratchet-type system.

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[29] Since we do not require the potential $\Pi(x)$ to be differentiable, we do not assume the derivation to have two roots $\partial\Pi(x)/\partial x = 0$, but two sign changes.
[30] If both potentials $\Pi(x)$ and $\Pi'(x)$ are spatially symmetric the total potential $V(x, \gamma)$ loses its ratchet character. Because of the unbroken spatial symmetry, either no transport occurs for both $\dot{\gamma} < 0$ and $\dot{\gamma} > 0$ or symmetric transport is observed in both directions, $\dot{x} < 0$ for $\dot{\gamma} < 0$ and $\dot{x} > 0$ for $\dot{\gamma} > 0$.
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