Reversible ratchets as Brownian particles in an adiabatically changing periodic potential

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The existence of transport of Brownian particles in a one-dimensional periodic potential which changes adiabatically is proven. The net fraction of particles crossing a given point toward a given direction during an adiabatic process can be expressed as a contour integral of a nonexact differential in the space of parameters of the potential. Since the work done to change the potential is an exact differential in the space of parameters, cycles can be designed where transport of particles is induced without any energy consumption. These cycles can be called *reversible ratchets*, and a concrete example is described. The repercussions of these results on equilibrium thermodynamics are discussed. [S1063-651X(98)01406-8]

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Magnasco has drawn the attention of the scientific community to a simple phenomenon, namely, that an asymmetric potential, perturbed by external fluctuations or periodic external forces, can induce a transport of Brownian particles [1]. Since this seminal work, there have been a number of papers proposing modifications and new models [2–11], designing experiments where the transport can be effectively observed [12,13], and calculating general properties and new features of these models — such us flows [3–5,7–11], escape rates [14], and reversing currents [4,7,11,15]. There are also sparse but significant precedents pointing out that nonequilibrium fluctuations can induce a flow of Brownian particles [16,17]. All these models are generically called *ratchets*, since they are somehow inspired by the discussion in Ref. [16] of a ratchet working as a thermal engine (originally proposed by Smoluchowski [18]).

Two types of ratchets can be distinguished: *changing force ratchets* or *rocked ratchets*, where the external fluctuations or external periodic forces are additive [1,3–5,7,14]; and *flashing ratchets*, where a periodic potential is modulated either by a signal periodic in time or by nonthermal fluctuations [2,3,10–13,15]. It is worth mentioning that the latter seem to be more relevant both for biological applications [3] and for segregation experiments [2,12]. In this paper, I will focus only on flashing ratchets, i.e., Brownian particles in a periodic potential changing in time.

These systems belong to the realm of nonequilibrium thermodynamics or statistical mechanics. It is believed that the two basic ingredients for noise-induced transport are nonequilibrium and anisotropic potentials. In equilibrium, detailed balance ensures a null local current all over the system [19]; thus the first requirement seems to be unavoidable. The second one stems from simple symmetry considerations.

However, in this paper I show that adiabatically moving a one-dimensional periodic potential can induce transport of Brownian particles. Moreover, it is possible to design a potential, periodic in space and time, where transport of Brownian particles can be induced without any energy consumption. These types of systems can be called *reversible ratchets*, and an explicit example is discussed below.

The existence of reversible ratchets is of extreme importance for designing Brownian motors with high efficiency. Feynman [16] calculated under very simple assumptions the efficiency of a ratchet, finding that it is equal to Carnot efficiency in the quasistatic limit. However, we have revealed the inconsistency of this arguments by proving the intrinsic irreversibility of the system under consideration [20]. Most of the ratchets proposed in the literature are also intrinsically irreversible (see discussion below), and their efficiency turns out to be very low, whereas reversible ratchets posses a comparatively high efficiency [21].

I consider Brownian overdamped particles moving in the interval $x\in[0,1]$ under the action of a periodic potential $V(x,\mathbf{R})$, which depends on a set of parameters collected in a vector $\mathbf{R}$. If these parameters change in time as $\mathbf{R}(t)$ where $t\in[0,T]$, the probability density $\rho(x,t)$ obeys the Smoluchowski equation

$$\partial_t\rho(x,t)=\partial_x[V'(x;\mathbf{R}(t))+\partial_x]\rho(x,t)=-\partial_x\mathcal{J}_{\mathbf{R}(t)}\rho(x,t), \tag{1}$$

where $\mathcal{J}_{\mathbf{R}}=-V'(x;\mathbf{R})-\partial_x$ is the *current operator*, and the prime indicates derivative with respect to x. I have taken units of time, length, and energy such that the diffusion coefficient and the temperature times the Boltzmann constant are equal to 1.

My aim is to calculate the net fraction of particles crossing $x=0$ to the right or *integrated flow* of particles along the process, which is defined by $\phi=\phi(0)$, with

$$\phi(x)\equiv\int_0^T dt\ \mathcal{J}_{\mathbf{R}(t)}\rho(x,t). \tag{2}$$

This quantity can be obtained analytically when the potential is adiabatically changed. Notice first that the solution of Eq. (1), in the adiabatic limit, is given by the equilibrium Gibbs state:

$$\rho(x,t)\simeq\rho(x;\mathbf{R}(t))\equiv\frac{e^{-V(x;\mathbf{R}(t))}}{Z(\mathbf{R}(t))}, \tag{3}$$

with $Z(\mathbf{R})=\int_0^1 e^{-V(x;\mathbf{R})}$. This state has zero current everywhere, i.e., $\mathcal{J}_{\mathbf{R}(t)}\rho(x;\mathbf{R}(t))=0$. Consequently, the total fraction of particles crossing $x=0$ to the right should be zero in the adiabatic limit. However, it can be shown that this is not the case. To start, I will prove the following lemma.

Lemma. Consider a Brownian particle in equilibrium with respect to a potential $V_0(x)$ at time $t=0$. If the potential is suddenly changed to $V_1(x)$, then the net fraction of particles crossing one of the boundaries of the system to the right, during the relaxation to the new equilibrium state, is given by

$$\phi=\int_0^1 dx\int_0^x dx'\,\frac{e^{V_1(x)}}{\int_0^1 dx'' e^{V_1(x'')}}[\rho_1(x')-\rho_0(x')], \quad (4)$$

where $\rho_i(x)=e^{-V_i(x)}/Z_i$ is the Gibbs state corresponding to potential $V_i(x)$.

The proof is as follows. Let us define the function

$$\varphi(x)=\int_0^\infty dt[\rho(x,t)-\rho_1(x)]. \quad (5)$$

If $\mathcal{J}_1$ is the current operator corresponding to potential $V_1(x)$, the integrated flow of particles through a point x in the interval can be written as $\phi(x)=\mathcal{J}_1\varphi(x)$, since $\mathcal{J}_1\rho_1(x)=0$. Applying the operator $-\partial_x\mathcal{J}_1$ to Eq. (5), one has

$$-\partial_x\mathcal{J}_1\varphi(x)=\int_0^\infty dt\,\frac{\partial\rho(x,t)}{\partial t}=\rho_1(x)-\rho_0(x). \quad (6)$$

$\varphi(x)$ can be determined by solving this second-order differential equation with periodic boundary conditions, $\varphi(0)=\varphi(1)$, and imposing that the integral of $\varphi(x)$ along the interval vanishes. These conditions are easily derived form the definition of $\varphi(x)$ [Eq. (5)]. Finally, once $\varphi(x)$ is obtained, one finds Eq. (4) by setting $x=0$ in $\phi(x)=\mathcal{J}_1\varphi(x)$.

Let us now consider the following setup for an adiabatic change of the potential $V(x;\mathbf{R}(t))$, occurring from $t=0$ to $t=T$ ($T\to\infty$). The parameter vector $\mathbf{R}$ changes by jumps $\Delta\mathbf{R}$. After each jump, the system is allowed to relax before the next jump takes place. Therefore, the system should relax for a time much longer than its relaxation time in any of the potentials $V(x;\mathbf{R})$. This adiabatic limit is achieved if $T\to\infty$ and $\Delta\mathbf{R}\to 0$ with $T/N_{\text{steps}}\to\infty$, N_{steps} being the number of steps taken to complete the whole process. Using the above lemma, it is not hard to prove the following theorem.

Theorem: The total fraction of particles crossing $x=0$ to the right, during the complete process in the adiabatic limit described above, is given by the contour integral

$$\phi=\int_{\mathbf{R}(0)}^{\mathbf{R}(T)} d\mathbf{R}\cdot\int_0^1 dx\int_0^x dx'\,\rho_+(x;\mathbf{R})\nabla_{\mathbf{R}}\rho_-(x';\mathbf{R}), \quad (7)$$

where

$$\rho_\pm(x;\mathbf{R})=\frac{e^{\pm V(x;\mathbf{R})}}{Z_\pm(\mathbf{R})}, \quad Z_\pm(\mathbf{R})=\int_0^1 dx e^{\pm V(x;\mathbf{R})}.$$

This is the main result of this paper. It tells us that, even in the adiabatic limit, the net fraction of particles ϕ crossing one of the boundaries of the system in a given direction can be different from zero. Moreover, it indicates that this fraction of crossing particles in an infinitesimal process

$$\delta\phi=\int_0^1 dx\int_0^x dx'\,\rho_+(x;\mathbf{R})\,\delta\rho_-(x';\mathbf{R}) \quad (8)$$

is not an exact differential. Consequently, it is possible to have transport of particles in a cyclic process, $\mathbf{R}(0)=\mathbf{R}(T)$, in the adiabatic limit.

To stress the singularity of this result and to prove the existence of reversible ratchets, let us repeat the same arguments for the energy introduced in the system by changing the potential. If one has a Brownian particle in equilibrium with $V_0(x)$ and suddenly changes the potential to $V_1(x)$, the energy introduced is equal to

$$E_{in}=\int_0^1 dx\rho_0(x)[V_1(x)-V_0(x)]. \quad (9)$$

Part of this energy can be dissipated to the thermal bath in the relaxation from $\rho_0(x)$ to $\rho_1(x)$. The input energy along the whole adiabatic process described above is given by the contour integral

$$E_{in}=\int_{\mathbf{R}(0)}^{\mathbf{R}(T)} d\mathbf{R}\cdot\int_0^1 dx[\nabla_{\mathbf{R}}V(x;\mathbf{R})]\rho(x;\mathbf{R})$$
$$=-\int_{\mathbf{R}(0)}^{\mathbf{R}(T)} d\mathbf{R}\cdot\nabla_{\mathbf{R}}\ln Z(\mathbf{R}). \quad (10)$$

This expression has a simple interpretation in the context of equilibrium statistical mechanics: $\nabla_{\mathbf{R}}\ln Z(\mathbf{R})$ is a generalized pressure which, when multiplied by $-d\mathbf{R}$, gives us the work done *on* the system. Remarkably, this work is an exact differential in the $\mathbf{R}$ space. Hence the total work done on the system along an isothermal cycle is always zero. Since the fraction of crossing particles $\delta\phi$ is not an exact differential, we can have transport without any energy consumption, i.e., a reversible ratchet.

Still, one could be suspicious about Eq. (7). What is wrong with the adiabatic solution given by Eq. (3) and the argument discussed right below this equation? How can a system present a net transport of particles if, *at any time*, it is globally in thermal equilibrium and every local current vanishes? An alternative and more general proof of Eq. (7) helps to clarify these questions.

Let us find the correction of the adiabatic solution (3) up to first order on $\dot{\mathbf{R}}(t)$:

$$\rho(x,t)\simeq\rho(x;\mathbf{R}(t))+\dot{\mathbf{R}}(t)\cdot\vec{\varphi}(x;\mathbf{R}(t)). \quad (11)$$

Inserting Eq. (11) into the Fokker-Planck equation (1) and neglecting $\partial_t[\dot{\mathbf{R}}(t)\cdot\vec{\varphi}]$, one finds

$$\nabla_{\mathbf{R}}\rho(x;\mathbf{R}(t))=-\partial_x\mathcal{J}_{\mathbf{R}(t)}\vec{\varphi}(x;\mathbf{R}(t)). \quad (12)$$

Solving this equation with periodic boundary conditions $\vec{\varphi}(0)=\vec{\varphi}(1)$, and imposing that the integral of each component of $\vec{\varphi}(x)$ along the interval $x\in[0,1]$ vanishes (exactly as in the proof of the lemma), the correction $\vec{\varphi}$ can be found. Finally, the fraction of particles crossing x to the right during the process is [see Eq. (2)]

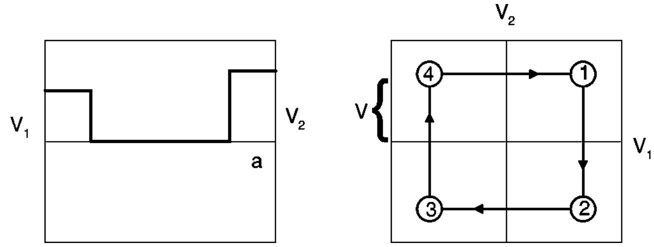

FIG. 1. Graphical representation of the reversible ratchet described in the text: the potential depends on two parameters, V_1 and V_2, which are the height of two barriers or wells (left), and they adiabatically change along the path depicted on the right (V being the half side of the square).

$$\phi(x)=\int_{\mathbf{R}(0)}^{\mathbf{R}(T)} d\mathbf{R}\cdot \mathcal{J}_{\mathbf{R}}\vec{\varphi}(x;\mathbf{R}), \tag{13}$$

which, using the solution of Eq. (12) and setting $x=0$, reproduces Eq. (7). We see that the correction $\dot{\mathbf{R}}(t)\cdot\vec{\varphi}$, although vanishing in the adiabatic limit, gives a nonzero fraction of particles ϕ crossing $x=0$ during the interval $[0,T]$. This proof resembles the derivation of the well-known *Berry's phase* [22] in quantum mechanics.

Before going on with a concrete example, I would like to stress an important property of Eq. (7). From this equation, it follows that no transport of particles occurs if one slowly modulates a potential or, more generally, if one slowly switches between two potentials $V_A(x)$ and $V_B(x)$ in the following way: $V(x,t)=r(t)V_A(x)+[1-r(t)]V_B(x)$, with $r(t)\in[0,1]$ periodic in time. This particular case is, remarkably, the only one which has been significantly studied to date [2,3,10–13,15], and it turns out that the efficiency of these flashing ratchets, when considered as engines, has been found to be very low [21] (see, however, Ref. [19]).

In order to have a reversible ratchet, the cycle must be a process along a loop. A first and rather trivial example consists of a well or a barrier around a point $x=a$ within the interval $[0,1]$. If the parameter a is moved from 0 to 1, due to the periodic boundary conditions, we have a cycle with ϕ different from zero. This example has been studied before by Landauer and Büttiker in the context of reversible computation [23]. The application of Eq. (7) reproduces their expression for the current [Eq. (6.8) in Ref. [23]]. However, in this model we are actually pushing the particles in a given direction, and, therefore, it cannot be considered as a genuine ratchet.

We can obtain a less trivial system if the potential depends on two parameters and these parameters change adiabatically along a loop. As an example of such a reversible ratchet, I consider the potential of Fig. 1, which depends on two parameters V_1 and V_2. If these parameters are changed following the path described in the same figure, then a transport of particles is induced towards the positive x direction. In Fig. 2, I plot the shape of the potential at the four points of Fig. 1. The way this ratchet works is apparent from this figure, and one can see that a transport of particles to the right is always induced. In Fig. 3, the net fraction of particles ϕ crossing the boundaries of the interval to the right in a period, calculated with Eq. (7), has been plotted as a function of the width a of the barriers or wells of the potential. For infinite large barrier and wells ($V\to\infty$), the fraction ϕ is equal to one for any value of a between 0 and $\frac{1}{2}$, as is evident from Fig. 2: at step 2, the particle is within the well with probability one, as it is at steps 3 and 4; then it must cross $x=0$ with probability one when moving from 3 to 4 and it can never jump back.

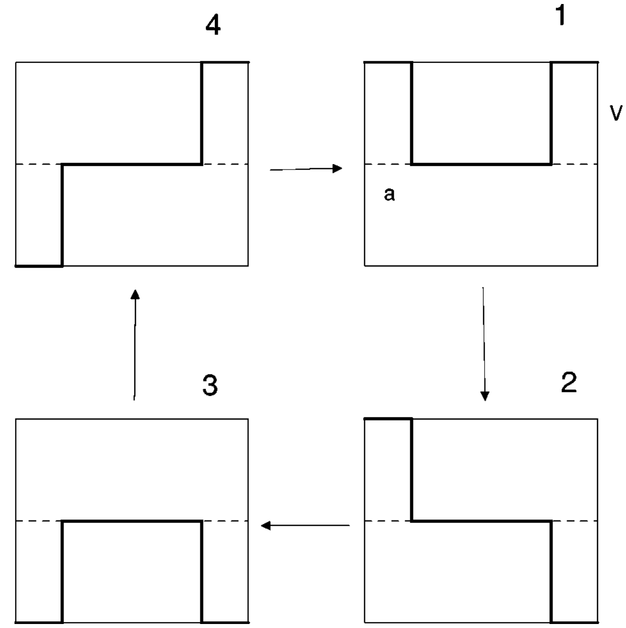

FIG. 2. Shape of the potential at the numbered steps of the adiabatic process plotted in Fig. 1.

In summary, the existence of reversible ratchets has been proven. Moreover, I have presented a thermodynamic differential given by Eq. (8), which is not exact in the space of parameters $\mathbf{R}$ of the potential. This is a nontrivial result in the field of equilibrium thermodynamics, and it opens the possibility of developing a complete thermodynamics of periodic potentials, including adiabatic changes of temperature, chemical potential, and other thermodynamic functions.

There is a corollary of the theorem, which is important for Brownian motors or noise-induced transport. From the above results, it is clear that, in order to have transport, the change of the potential must be driven, not only slowly, but also in a given direction. Therefore, if this change is driven by a noise, i.e., if $\mathbf{R}$ fluctuates along a given path in the parameter space, we cannot have adiabatic transport unless the noise were biased toward a given direction. If, for instance, $\mathbf{R}$ is

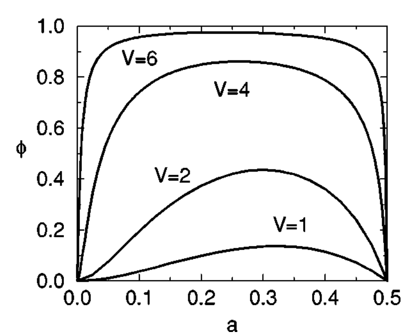

FIG. 3. Net fraction of particles ϕ crossing $x=0$ to the right, calculated using Eq. (7), as a function of the width a of barriers or wells, for different values of the maximum height V.

driven by a chemical coordinate, this bias can be supplied by reactants with concentrations far from equilibrium (fuel), as pointed out by Magnasco [6] in a different but related context.

The above considerations are only valid in the adiabatic limit, and Eq. (7) cannot be applied to irreversible processes. The discovery of flashing ratchets by Prost *et al.* [2] and Astumian and Bier [3] can now be interpreted in a different way: they found a path in the **R** space which induces a current in a given direction *no matter how it moves along the path*, if it does so irreversibly. However, this is not strange in thermodynamics. For instance, the change of entropy is always positive for an irreversible process, no matter what the direction of the process. Nevertheless, as mentioned above, these irreversible ratchets have a low efficiency, i.e., the induced transport is very energy consuming [21].

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