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Ratchet for energy transport between identical reservoirs

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A one-dimensional periodic array of elastically colliding hard points, with a noncentrosymmetric unit cell, connected at its two ends to *identical but nonthermal* energy reservoirs, is shown to carry a sustained unidirectional energy current.

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A particle subjected to fluctuating forces far from thermal equilibrium, in a medium with a vectorial asymmetry, must drift in a direction determined by the asymmetry, even if the fluctuating forces have zero mean. This idea can be seen as a consequence of the "Curie principle" [1], whatever is not ruled out by symmetries is permitted and therefore obligatory. Reviews of the many realizations of this concept of a "Brownian ratchet" and their relevance to the working of motor proteins in living cells as well as to particle separation methods can be found in Refs. [2,3]. Implementations of the ratchet idea generally involve randomly forced particles in periodic, non-centrosymmetric potentials. A nonequilibrium stationary state is maintained either by having the potential alternate between two states, or by choosing a random forcing that does not to obey a fluctuation-dissipation relation with respect to the damping.

Can these methods for particle transport without chemical-potential gradients be extended to generate *energy* currents without *temperature* gradients? We know, of course, that energy cannot flow spontaneously from one *thermal* bath to another with identical thermodynamic parameters, no matter how asymmetrical the conducting medium linking the two baths. The requirements of thermal equilibrium and, hence, of time-reversal invariance, mask the structural asymmetry of the conductor. We conjecture, therefore, that an energy current should flow through a suitably asymmetrical medium if the (identical) baths at the ends were *nonthermal*: particles emerge from collisions with the baths with velocities drawn from a distribution $P(v)$ that is not of the form $P(v) \propto v \exp[-\beta m v^2/2]$ characteristic of thermal baths (coupled with Maxwell boundary conditions).

Another motivation for the work presented in this paper is the renewed interest in heat conduction and energy propagation in momentum-conserving one-dimensional systems [4,5] with a temperature gradient imposed by connecting the two ends to heat baths at different temperatures. For a one-dimensional array of point mass particles with elastic collisions, if the masses are all equal, the system is integrable and thermal equilibrium is not achieved. Even with unequal masses, momentum conservation causes the heat conductivity to depend singularly [4] on the length L of the array, as $L^{1/3}$ [5]. The extension of these results to the nonequilibrium regime, where a nonintegrable array is connected to nonthermal baths at the ends, is clearly of fundamental interest.

We present a brief summary of our results and then discuss our studies in more detail. We study numerically the dynamics of one-dimensional arrays of particles labeled $i = 1, \ldots, L$ from left to right, with masses $\{m_i\}$ arranged in a left-right asymmetric sequence. The particles are hard points which interact only upon contact, undergoing elastic collisions. To the two ends of these arrays we attach *identical*, nonthermal reservoirs of kinetic energy: when the first or last particle collides with the reservoir beside it, it recoils with a velocity drawn from a distribution which is not of the form $P(v) \propto v \exp[-\beta m v^2/2]$. Regardless of the type of nonthermal reservoir used and the nature of the asymmetry of the array, we always find a net macroscopic energy current, confirming our conjecture above and demonstrating the robust nature of this remarkable "energy ratchet." For one class of arrays, the steady-state current J decays slowly with the system length L, roughly [6] as $1/L$, the behavior expected of a conventional heat current in response to a fixed temperature difference across a length scale L. For another, rather different class of arrays, J is found to be independent of L. In either case, it is clear that the current is not merely an edge effect present only near the nonequilibrium reservoirs. Systematics of the dependence on size, sequence, and termination can be found in Figs. 1–4.

We now present our study in more detail. We illustrate our general point with two types of arrays: (a) the "ABC" array, consisting of three species of particle A, B, and C with distinct masses $m_A < m_B < m_C$, arranged in the periodic but noncentrosymmetric sequence $\cdots ABCABCABC \cdots$, and (b) the "geometric" array, where $m_{i+1}/m_i = r =$ constant . Since the dynamics of each particle is purely ballistic between collisions, we adopt an "event-driven" approach: given the present momenta of all particles, one knows which pairs will next collide and when and, hence, the postcollision momenta and energies. If the outermost particle at either end collides with the reservoir, it is reemitted into the system with a speed v chosen from a distribution $P(v)$. More precisely, the rebound speed is first drawn from $P(v)$ and then multiplied by $1/\sqrt{2m}$, where m is the mass of the particle, so that particles recoiling from the reservoirs have the same typical kinetic energy regardless of their mass. We considered two forms for $P(v)$:

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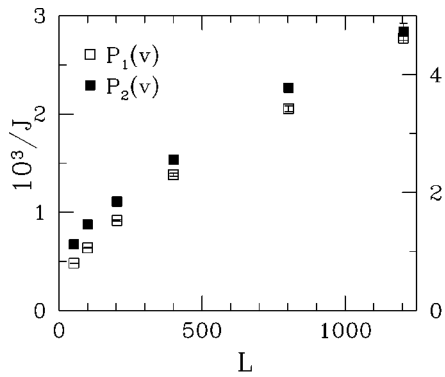

FIG. 1. Inverse current flowing from left to right in an ABC array, as a function of array length L. Note that the curve is sublinear, i.e., the current decays slightly slower than $1/L$. Particles recoil from the baths with the exponential speed distribution $P_1(v)$ of Eq. (1), or the heavy tailed distribution $P_2(v)$ of Eq. (2). The y axis for the $P_1(v)$ and $P_2(v)$ are to the left and right, respectively.

$$P_1(v) = \exp(-v) \tag{1}$$

and

$$P_2(v) \propto v/(1+v^2)^3. \tag{2}$$

Both these distributions are easily generated from the standard uniform random variable over $[0,1)$. The former is somewhat unusual, since if $P(v)$ is taken to be the distribution for particles leaking out of a large homogeneous reservoir, from phase space considerations the velocity distribution inside the reservoir must be $p(v) \sim P(v)/v$ which, for Eq. (1), is not normalizable. However, such an assumption may be too restrictive: the velocity distribution of particles in a granular flow bumping against the side walls has under certain circumstances been found [7] to be $\sim \exp(-v)$, and other nonequilibrium methods of energy injection at the walls leading to $P_1(v)$ could be conceived of.

We discuss the ABC array first, for which our studies used $m_A = 1$, $m_B = 2.5$, $m_C = 6.5$, with $P_1(v)$ [Eq. (1)], and $m_A = 1.0$, $m_B = 2.5$, $m_C = 9.0$ with $P_2(v)$ [Eq. (2)]. The mass values were selected in a rough attempt to maximize the current flowing, at least for small arrays. In both cases, lengths $L = 52,100,202,400,802,1204$ were studied, chosen so that the particle at the end of the array was always an A. For both choices of bath distribution, the steady state has a current J flowing from the left to the right of the chain and decreasing slowly with L. The current J was measured as follows: each time a particle at the end collides with the reservoir beside it, the difference between its incoming and outgoing kinetic energies give the energy transferred to the reservoir. By measuring the total energy transferred in a long time interval, the average energy transfer rate J (with dimension energy/time) can be found. Whether we use $P_1(v)$ or

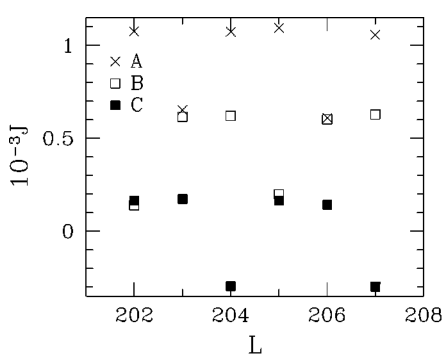

FIG. 2. Current across ABC arrays, for different chain lengths and terminating particles. The sets of points marked A, B, and C in the legend correspond, respectively, to sequences starting with A, B, and C particles. The velocity distribution at the ends is the exponential $P_1(v)$ of Eq. (1).

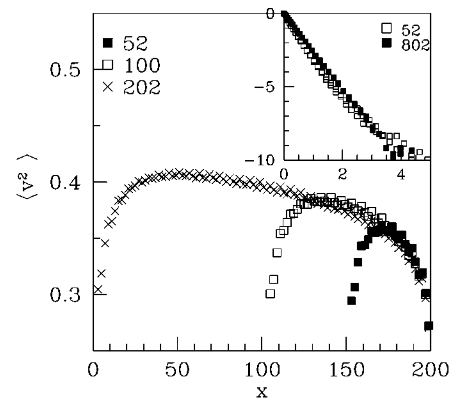

FIG. 3. Average kinetic energy of particles across chains of lengths $L = 52$, 100, 202. The right hand edges of all the chains are made to coincide, to show the approximate L independence of the right boundary region. The length of the left boundary region is also approximately independent of L. The interior region lengthens as L is increased, and the kinetic energy varies slowly here. There is a weak cycle-of-three periodicity to the kinetic energy, whose cause is not clear. The inset plots the velocity distribution, $\ln[P(v)/P(0)]$ vs v^2, for the particle beside the center. There is significant deviation from a Gaussian for $L = 52$, but not for $L = 802$.

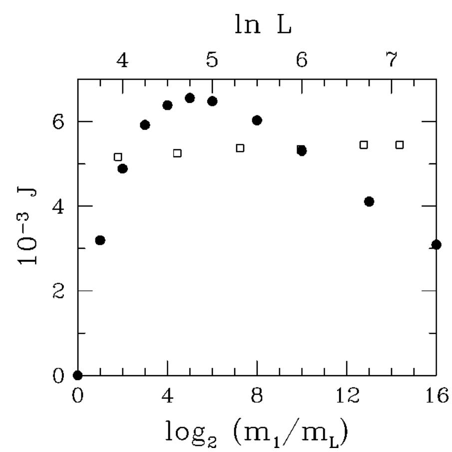

FIG. 4. Current in the "geometric" array, as a function of array length L with an end-to-end mass ratio $m_1/m_L = 5$ (open squares), and as a function of $\log_2(m_1/m_L)$ for $L = 100$ (solid circles). There is little variation seen as a function of L despite the logarithmic scale, in contrast to the pronounced maximum as a function of m_1/m_L. The error bars are less than the point sizes. The baths emit particles with the long-tailed speed distribution $P_2(v)$ of Eq. (2).

$P_2(v)$, the decay is no faster than the $1/L$ of "normal" conduction, and is clearly not an exponential decay (see Fig. 1).

Although the current decays slowly with chain length, it is sensitive to the termination of the chains. To illustrate this, we study the current J separately for arrays starting with A, B, and C, as a function of their length. For arrays of short lengths that start with A, the current is nonmonotone with a cycle-of-three periodicity. A similar periodicity is seen when the chain starts with B or with C. There is significant variation between the three cases. This is summarized in Fig. 2, where the velocity distribution used was $P_1(v)$.

The sensitivity of the current to the termination of the chains might seem surprising, in view of our earlier conclusion (Fig. 1) that the flow of current is not an end effect restricted to short chains. Our results for the length and termination dependence of the current in ABC arrays might suggest the following scenario: interparticle collisions might lead to a rapid thermalization as one proceeds from the baths into the interior of the chain, but with *different* temperatures near the two ends because of the asymmetric chain and nonequilibrium baths. If this scenario were correct, the difference between the effective temperatures near the two ends would depend on the terminations, but with the terminations specified, the energy current in a large chain would be due to the effective temperature difference, and would decay with L as slowly as for thermal conduction. We have measured the average kinetic energy across the chain for different values of L. As shown in Fig. 3, we find a rough separation into two boundary regions whose size does not vary significantly with L, and an interior (whose length increases with L) with a slowly varying average kinetic energy. However, surprisingly, the kinetic energy in the interior is higher than at the two ends, and the difference between the two ends depends on L, showing that this simple scenario is *not* valid. (The velocity distribution near the center approaches a Gaussian as L is increased.)

The existence of a nonzero energy current with athermal baths can be explained qualitatively. If one considers a chain of only two particles, when the heavy particle recoils from the bath at its end and collides with the light particle, it typically causes the light particle to rebound and itself continues to move forward. The energy it was carrying continues to move forward, although distributed between both particles. But if the light particle carries some energy from the reservoir at its end to the heavy particle, most of the energy is reflected back and returned to the reservoir it came from. Thus, we see that energy transport is more efficient in one direction compared to the other. On the other hand, the light particle has much higher typical speeds, and therefore impinges against its reservoir much more often. Thus, there is a competition between the relative inefficiency with which the light particle transmits energy to the heavy one, and its higher attempt rate. Which one of these wins depends on the parameters of the system; we have numerically verified [for baths given by $P_1(v)$] that as the mass ratio is changed, the current even changes sign. For (identical) thermal baths, the two competing effects cancel exactly.

We now turn to the second type of array we studied: the geometric array, where the ratio of the masses of any two adjacent particles is $m_i/m_{i+1}=r$, where r is independent of i. The geometric array was studied using $P_2(v)$ only. First, a fixed end-to-end mass ratio $m_1/m_L=5$ was chosen, and the chain length varied. (The mass ratio r between neighbors was therefore closer to unity for longer chains.) Chain lengths were 52, 100, 202, 400, 802, 1204. A large steady-state current flows from right to left. As the chain length increases, J asymptotes to a constant value, *independent* of L, in striking contrast to what is seen in the ABC array. Since J is (roughly) insensitive to L for fixed m_1/m_L, data was also taken with a fixed chain length of 100, the mass at the right end m_L equal to 1, and the mass at the left end varied. Not surprisingly, this yields a current that is zero when $m_1=1$, peaks as m_1 is increased, and then decays again as m_1 is increased further [8]. The peak is approximately at $m_1=32$.

These results can be justified by recalling that for a chain, where all the particles have equal mass, with thermal baths at different temperatures at the two ends, the current is L independent [9]. (There would be no current with identical baths at both ends for such a chain.) Thus for a monotonic chain, where the masses vary only gradually, one should measure the length in terms of the "scattering length" over which transport deviates appreciably from the ballistic, i.e., the length over which the mass changes by some reasonable factor. If m_L/m_1 is held fixed, the "effective length" is then independent of L. A chain with a very small effective length would look symmetric, and therefore not carry energy between identical reservoirs, while the current in a chain with a very large effective length would diminish because of repeated scattering. Although qualitative, this argument suggests that when $m_1/m_L\approx 32$ (i.e., J is maximum), the scattering length roughly equals to L (irrespective of L).

The two sets of observations on the geometric chain, taken together, lead to a surprising conclusion: if one takes a (long) monotonic chain with $m_1=4$ and $m_L=1$, and another chain with the same ratio between successive masses, with $m_1=16$ and $m_L=4$, the current in the first chain should be twice the current in the second [10], but when the two chains are connected in series (in the correct order), from Fig. 4 the current will be greater than that in either of its two components.

Several natural extensions of the work presented here suggest themselves. For example, consider the case where the baths at the ends are in identical steady states which are characterized by a parameter λ such that $\lambda=0$ corresponds to thermal equilibrium. How does the ratchet energy current depend on λ? Another intriguing issue is the effect of inelastic collisions, which are crucial if this idea is to be applied to granular matter. An analytical understanding of our results would clearly be of great interest. Most exciting would be an experimental realization, perhaps a suitably nanoengineered wire in the form of a one-dimensional array with an asymmetric unit cell, with the ends driven by cells containing identical, exothermic chemical reactions, or perhaps a row of ball bearings with particle masses varying as in our ABC or geometric arrays, driven at the ends by gas fluidization. The analysis of the latter would have to include inelasticity, but it should nonetheless display an energy current.

To summarize, our work proposes a mode of energy transport, in rough analogy to Brownian ratchets but with features quite distinct from those systems. The energy transport here requires no manipulation of the bulk of the one-dimensional medium, only a structural asymmetry. Only the two ends of the "conductor" are held in (identical) nonthermal steady states. Neither a time dependent potential nor noise that violates detailed balance is required in the bulk. Provided energy is supplied at both ends in the same nonequilibrium manner, the classical dynamics of the intervening medium extracts energy preferentially from one reservoir and sends it to the other. No violation of the second law of thermodynamics occurs: we have simply specified the properties of the nonequilibrium reservoirs without saying how they are to be maintained that way.

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[8] The velocity distribution near the center of the chain does not approach a Gaussian for any L and m_L/m_1 that we have studied, unlike for $\cdots ABC \cdots$ chains.

[9] An interparticle collision only exchanges the identity of the particles, without changing J, so the particles are effectively collisionless for computing J. Since the round trip time for a particle between the two reservoirs is $\sim L$, and there are $\sim L$ particles carrying energy between the reservoirs "in parallel," J is L independent.

[10] Scaling $m \rightarrow 4m$, $t \rightarrow 2t$, $v \rightarrow v/2$ [see discussion before Eq. (1)], $J \rightarrow J/2$ leaves the dynamics unchanged and maps the light chain to the heavy one.