Thermal Diode: Rectification of Heat Flux

Baowen Li,[1] Lei Wang,[2] and Giulio Casati[3,4,1]

[1]*Department of Physics, National University of Singapore, Singapore 117542, Republic of Singapore*
[2]*Temasek Laboratories, National University of Singapore, Singapore 119260, Republic of Singapore*
[3]*International Center for Nonlinear and Complex Systems, Universita' degli studi dell'Insubria, Como, Italy*
[4]*Istituto Nazionale di Fisica della Materia, Unita' di Como, Italy*
and Istituto Nazionale di Fisica Nucleare, sezione di Milano, Milano, Italy

By coupling two nonlinear one dimensional lattices, we demonstrate a thermal diode model that works in a wide range of system parameters. We provide numerical and analytical evidence for the underlying mechanism which allows heat flux in one direction while the system acts like an insulator when the temperature gradient is reversed. The possible experimental realization in nanoscale systems is briefly discussed.

The understanding of the underlying dynamical mechanisms which determines the macroscopic laws of heat conduction is a long standing task of nonequilibrium statistical mechanics [1]. Recent years have witnessed some important progress in this direction even though a satisfactory understanding is, so far, unavailable. For example, it has been surmised that for a one dimensional lattice, momentum conservation leads, in general, to anomalous heat conduction [2], with heat conductivity κ which diverges with the system size L as $L^{2/5}$ [3]. If the transverse motion is considered, then $\kappa \sim L^{1/3}$ [4]. A connection between the anomalous conductivity and anomalous diffusion has been also established [5]. Moreover, after two decades of debates, it is now clear that exponential local instability is not a necessary condition for the validity of Fourier law [6].

A better understanding of the mechanism of heat conduction may also lead to potentially interesting applications based on the possibility to control the heat flow. Indeed, recently, a model for a thermal rectifier has been proposed [7] in which the rectifying effect is obtained by acting on the parameters which control the nonlinearity of the lattice. Although this model is far away from a realistic implementation, nevertheless, it opens the possibility to propose thermal devices which may have practical relevance.

In this Letter we demonstrate, via computer simulations, the possibility to build a thermal diode by coupling two nonlinear lattices. Indeed, our model allows the heat flow from one end to the other, but it inhibits the flow in the opposite direction. The model works in a wide range of system parameters, and the underlying microscopic mechanism is different from the one in Ref. [7] even though it is based on the same general idea. In the present case the ratio of the heat currents in the two opposite directions is 100 times larger than that in model [7] and it is, therefore, sufficiently large to encourage experimental work.

Our system consists of two segments of nonlinear lattices coupled together by a harmonic spring with constant strength k_{int}. Each segment is described by the Hamiltonian

$$H = \sum \frac{p_i^2}{2m} + \frac{1}{2}k(x_i - x_{i+1} - a)^2 - \frac{V}{(2\pi)^2}\cos 2\pi x_i. \quad (1)$$

In fact, Eq. (1) is the Hamiltonian of the Frenkel-Kontorova (FK) model which is known to have normal heat conduction [8].

For simplicity we set the mass of the particles and the lattice constant $m = a = 1$. Thus the adjustable parameters are k_{L}, k_{int}, k_{R}, V_{L}, V_{R}, T_{L}, and T_{R}, where the letters L and R indicate the left and right segment and $T_{\text{L,R}}$ is the temperature of the left-right heat bath. In order to reduce the number of adjustable parameters, we set $V_{\text{R}} = \lambda V_{\text{L}}$, $k_{\text{R}} = \lambda k_{\text{L}}$, $T_{\text{L}} = T_0(1 + \Delta)$, $T_{\text{R}} = T_0(1 - \Delta)$, and, unless otherwise stated, we fix $V_{\text{L}} = 5$, $k_{\text{L}} = 1$ so that the adjustable parameters are reduced to four $(\Delta, \lambda, k_{\text{int}}, T_0)$. Notice that when $\Delta > 0$, the left bath is at higher temperature and vice versa when $\Delta < 0$.

In our numerical simulations we use fixed boundary conditions and the N particle chain is coupled, at the two ends, with heat baths at temperatures T_{L} and T_{R} respectively. We use Langevin heat baths and we have checked that our results do not depend on the particular heat bath realization (e.g., Nosé-Hoover heat baths). We then integrate the differential equations of motion by using the fifth-order Runge-Kutta algorithm as described in [9]. We compute the temperature profile inside the system, i.e., the local temperature at site n defined as $T_n = m\langle \dot{x}_n{}^2 \rangle$, where $\langle \, \rangle$ stands for temporal average, and the local heat flux $J_n = k\langle \dot{x}_n(x_n - x_{n-1}) \rangle$ [1]. The simulations are performed long enough to allow the system to reach a nonequilibrium steady state where the local heat flux is constant along the chain.
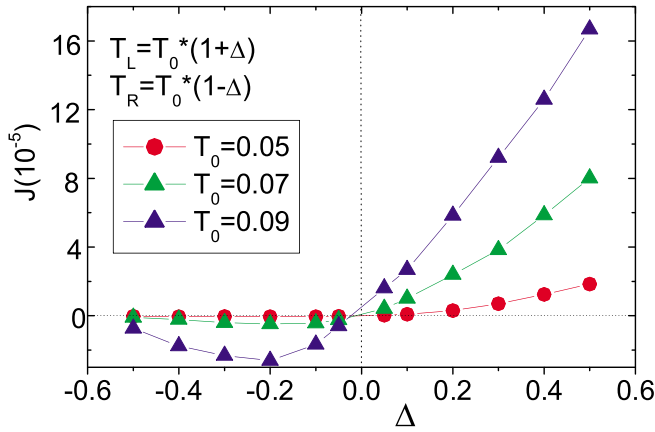
FIG. 1 (color online). Heat current J versus the dimensionless temperature difference Δ for different values of T_0. Here the total number of particles $N = 100$, $k_{int} = 0.05$, $\lambda = 0.2$. The lines are drawn to guide the eye.

In Fig. 1 we plot the heat current J versus Δ for different temperatures T_0. It is clearly seen that when $\Delta > 0$ the heat current increases with Δ, while in the region $\Delta < 0$ the heat current is almost zero, i.e., the system behaves as a thermal insulator. The results in Fig. 1 show that our model has the rectifying effect in a wide range of temperatures. The rectifying efficiency depends on temperature as well as on other parameters as described below:

k_{int} *effect*. The interface elastic constant k_{int} is a very important parameter as it plays the role of coupling left and right lattices. By adjusting this parameter one can control the heat flow. Indeed, once the parameters of the two lattices are fixed, then the smaller the coupling, the smaller is the heat current through the system.

In order to describe quantitatively the rectifier efficiency we introduce the ratio $|J_+/J_-|$ where J_+ is the heat current (from left to right) when the bath at higher temperature T_+ is at the left end of the chain and J_- is the heat current (from right to left) when the left end of the chain is in contact with the bath at lower temperature T_-.

Figure 2(a) shows that, by varying k_{int}, the rectifier efficiency $|J_+/J_-|$ changes from about 2 times at $k_{int} = 0.5$ to more than 100 times for $k_{int} \leq 0.01$. More importantly, this figure shows that the rectifying effect is very significant in a wide range of k_{int}. In the inset of this figure we show $|J_\pm|$ versus k_{int} for a system of eight particles. It is seen that, for small k_{int}, numerical data follow the dependence $J_\pm \propto k_{int}^2$ over almost 2 orders of magnitude. Therefore the ratio $|J_+| / |J_-|$ is a constant independent of k_{int}.

Figure 2(b) shows the temperature profile for different k_{int}. There exists a large temperature jump at the interface and this jump is much larger when the high temperature bath is at the right end. In this case there is very small temperature gradient inside each lattice and, as a consequence, the heat current is almost vanishing.
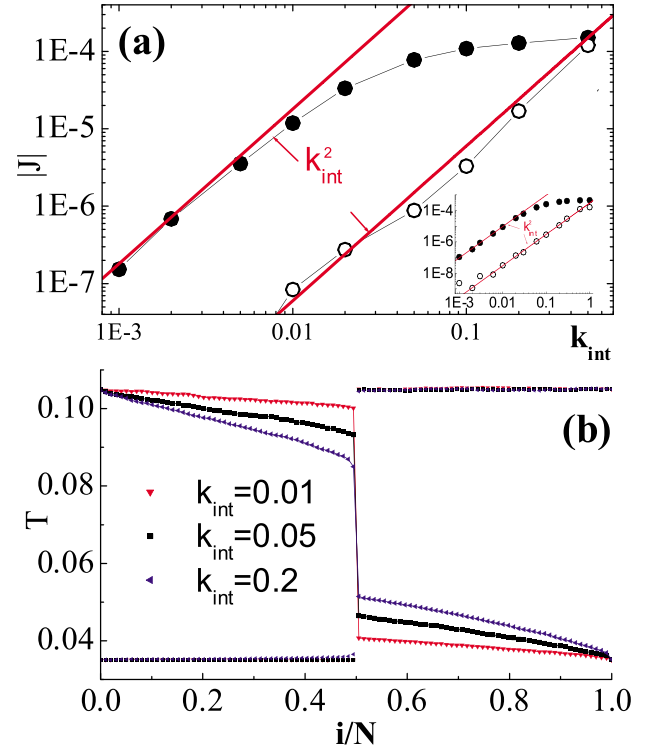

FIG. 2 (color online). (a) Heat current $|J_\pm|$ versus the interface elastic constant k_{int} for $N = 100$, $\lambda = 0.2$, $T_+ = 0.105$, $T_- = 0.035$. The solid circles are the current J_+ while empty circles are the current J_-. Inset in (a) is $|J_\pm|$ versus k_{int} for a system of eight particles. The solid lines in the figure and in the inset have slope equal two. (b) The temperature profile for $k_{int} = 0.01, 0.05, 0.2$ for the same parameters of (a).

Effect of the lattice parameter λ. As it is known [8], in the FK model the elastic constant and the strength of the on-site potential can be scaled to a single parameter. Therefore, it is sufficient to study the properties of the system (1) as a function of the single parameter λ.

In Fig. 3, we show the current $J_\pm$ versus λ for two different interface constants: $k_{int} = 0.05$ and $k_{int} = 0.2$. This figure clearly show that in a wide range of parameters our model has a quite good rectifying efficiency, i.e., $|J_+/J_-| \sim 100$.

Rectifying mechanism. To understand the underlying rectifying mechanism, let us start from the energy spectrum of the interface particles. Figure 4 shows the phonon spectra of the left and right interface particles at different temperature when the two lattices are decoupled ($k_{int} = 0$).

The match/mismatch of the energy spectra of the two interface particles controls the heat current. It is clearly seen from Fig. 4 that, if the left end is in contact with the high temperature bath T_L, and the right end with the low temperature bath T_R ($< T_L$), then the phonon spectra of the two particles at interface overlap in a large range of frequencies, thus the heat current can easily go through the system from the left end to the right end. However, if
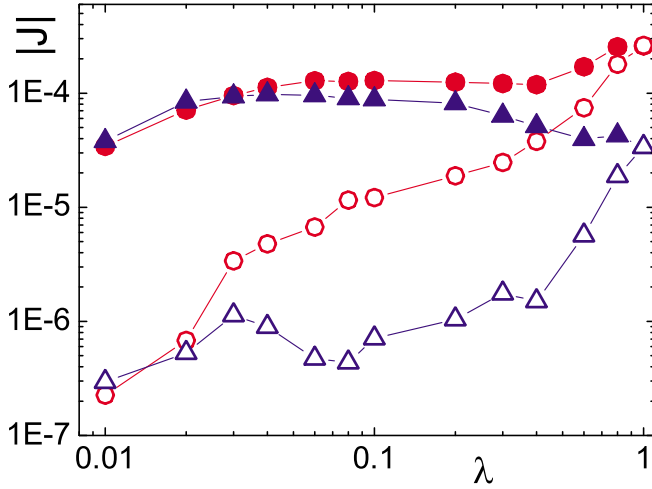
FIG. 3 (color online). Heat current versus λ for $k_{int} = 0.2$ (circles), and $k_{int} = 0.05$ (triangles). The solid symbols refer to $T_L = T_+$, $T_R = T_-$, while empty symbols refer to $T_L = T_-$, $T_R = T_+$. Here $T_+ = 0.105$, $T_- = 0.035$ and $N = 100$.

the left end is at lower temperature T_L and the right end is at higher temperature T_R ($> T_L$), then the phonon spectrum of the right interface particle is mainly in the low frequency part, while the left interface particle is in the high frequency part. Then there is almost no overlap in phonon frequency; the heat current can hardly go through from right to left, and the system behaves as an insulator. Why the left and right particles at the interface have so different phonon spectra? This can be understood from the following analysis in different temperature regimes.

(1) *Low temperature limit.* At low temperature, the particle is confined in the valley of the on-site potential. By linearizing the equation of motion one can easily obtain the frequency band [7]:

$$\sqrt{V} < \omega < \sqrt{V + 4k}. \qquad (2)$$

For the case of Fig. 4 with $T = 0.01$ (left) and $T = 0.002$ (right), this corresponds to $0.36 < \omega/2\pi < 0.48$ for the left particle and to $0.16 < \omega/2\pi < 0.21$ for the right particle.

As the temperature is increased, the interparticle potential $kx^2/2$ becomes more and more important until a critical value $T_{cr} \approx V/(2\pi)^2$ is reached (we take the Boltzman constant equal unity), when the kinetic energy is large enough to overcome the on-site potential barrier. At this point low frequency appears and this happens at the critical temperatures $T_{cr} = 0.13$ for $V = 5$ (left), and $T_{cr} = 0.025$ for $V = 1$ (right). This is in quite good agreement with the data of Fig. 4.

(2) *High temperature limit.* In the high temperature limit the on-site potential can be neglected, the system is close to 2 coupled harmonic chains, and the phonon band is [10]
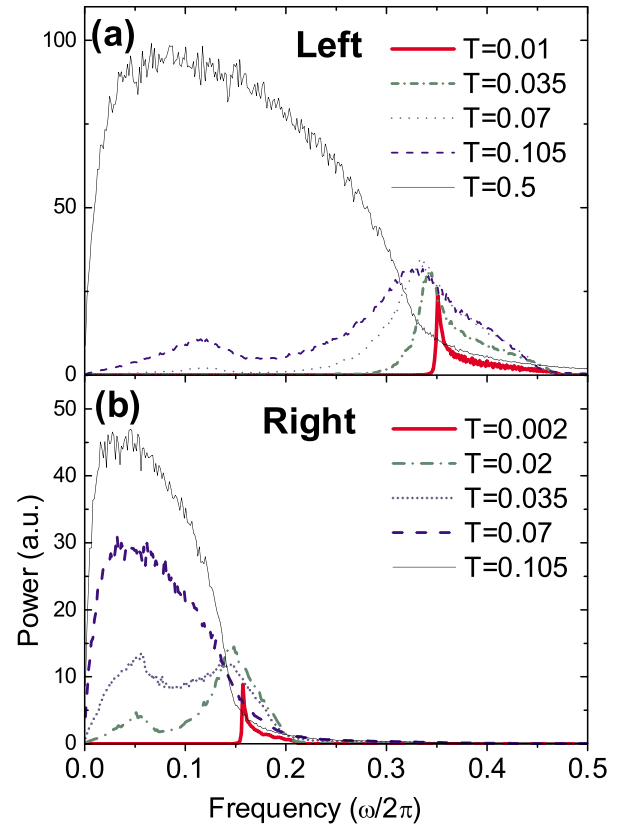

FIG. 4 (color online). Spectra of the two particles at the interface for different temperatures at $k_{int} = 0$. (a) Particle at the left side of the interface. (b) Particle at the right side of the interface. Here $\lambda = 0.2$, $N = 100$.

$$0 < \omega < 2\sqrt{k}, \qquad (3)$$

which gives $0 < \omega/2\pi < 0.32$ for the left particle and $0 < \omega/2\pi < 0.14$ for the right particle, again in good agreement with Fig. 4.

In fact, in order to optimize the rectifying effect, one should avoid the overlapping of the phonon bands in the low temperature limit [Eq. (2)] and that in the high temperature limit [Eq. (3)] for each segment of the system. According to the above estimates, one should have $V > 4k$, which is satisfied for the case of Fig. 4.

The analysis presented here allows also to understand why in Fig. 1 there is a region of negative conductivity for $T_0 = 0.09$ and $-0.5 < \Delta < -0.2$. Indeed in this interval it is seen that by increasing the temperature difference between the two heat baths, the current decreases! As explained above, the reason for such unusual behavior is due to the fact that by decreasing the temperature of the left bath, the phonon spectra of the two interface particles separate one from the other.

It is worth pointing out that it is the temperature dependence of the phonon band that makes the rectifying effect possible. This dependence is due to the nonlinearity of the potential and, therefore, it should be possible to
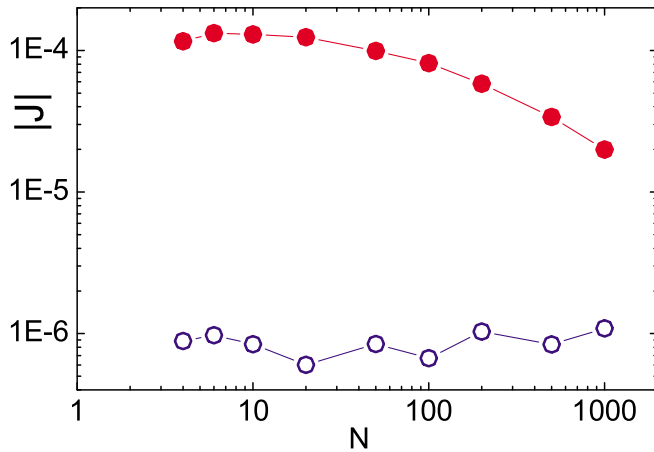
FIG. 5 (color online).   The finite size effect of the rectifying efficiency. Here we plot $|J_+|$ (solid circles) and $|J_-|$ (empty circles) versus N. Parameters are $\lambda = 0.2$, $k_{int} = 0.05$, $T_+ = 0.105$, and $T_- = 0.035$.

observe the rectifying effect in any nonlinear lattice. The difference between different choices of the on-site potential is quantitative rather than qualitative. For example, we have observed the rectifying effect in the ϕ^4 model wherein the on-site potential is $kx^2/2 + \beta x^4/4$, but the rectifying efficiency is not as significant as it is in the FK model. The main reason for the very large rectifying efficiency in the FK model is the finite height of the on-site potential.

Finite size effect. The results shown above are for a system with total number of particles $N = 100$. Since the rectifying mechanism in our model is due to the coupling between two dissimilar lattices it is reasonable to expect that the number of nonlinear oscillators will definitely affect the rectifying efficiency. This is shown in Fig. 5 where we plot $|J_+|$ and $|J_-|$ versus the system size N with $T_+ = 0.105$, and $T_- = 0.035$.

The decrease of the rectifying efficiency by increasing N (Fig. 5) and k_{int} (Fig. 2) can be understood in the following way: If we denote by R the sum of thermal resistances of the two segments, then the total resistance of the system is $R_\pm = R + R_{int}^\pm$, where $R_{int}^\pm$ is interface resistance when $\Delta > 0$ and $\Delta < 0$, respectively. As $J_\pm = (T_L - T_R)/R_\pm$, the rectifying efficiency is $|J_+/J_-| \approx (R + R_{int}^-)/(R + R_{int}^+)$. Notice that R increases with N while $R_{int}^\pm$ are N independent, they decrease with increasing k_{int}, and R_{int}^+ is much smaller than R_{int}^-. It is therefore clear that the efficiency decreases with increasing k_{int} (Fig. 2) at fixed N and by increasing N at fixed k_{int} (Fig. 5).

For the data of Fig. 5 we have $R_{int}^- \gg R$ and, therefore, J_- is a small constant that is almost independent of N, while $J_+ \sim 1/N$. As N is increased over a critical value N_c where $|J_+| \approx |J_-|$, the rectifying effect vanishes. For the case of Fig. 5 this happens at $N_c \sim 10^5$. However, we should point out that the value of N_c depends on k_{int} and by decreasing k_{int} we may increase N_c.

Finally, we would like to discuss the possibility of an experimental realization of our diode model. In our calculations, we take dimensionless units. For a typical atom, the dimensionless temperature T_0 used in this paper is related to the real temperature T^r by $T^r \sim 10^2 - 10^3 T_0$ [8]. Therefore, $T_0 \sim 1°$ is of the order of room temperature. If we consider the lattice distance of 1 Å, then a lattice of 100 particles is about 10 nanometers long, which is of a size scale that can be fabricated in today's laboratory. Another problem for real experiments is that the on-site potential is due to the interaction with a substrate. In our numerical simulations, we neglect the heat current in the substrate. This may affect the rectifying efficiency of the diode. Therefore, one needs to choose a substrate with substantially low thermal conductivity.

In summary, we have devised a thermal diode by using two coupled nonlinear lattices. Our model exhibits a very significant rectifying effect in a very wide range of system parameters. The underlying mechanism has been discussed as well as a possible realization of the model in a nanoscale system.

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