

Thermal rectification in the thermodynamic limit

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We show that an increasingly strong thermal rectification effect occurs in the thermodynamic limit in a one-dimensional, graded rotor lattice with nearest-neighboring interactions only. The underlying mechanism is related to the transition from normal to abnormal heat conduction behavior observed in the corresponding homogeneous lattices as the temperature decreases. In contrast and in addition to that by invoking long-range interactions, this finding provides a distinct scenario to make the thermal rectification effect robust.

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Thermal rectification (TR) refers to the effect whereby heat current flows across a system preferably in a certain direction rather than in the opposite direction. As the thermal counterpart of the rectification of electric current, it can be envisaged that TR may play a vital role in thermal control and management. TR is also very interesting from the viewpoint of fundamental theories. In fact, the study of this effect has a long history (see, e.g., Ref. [1] for a review) and recently it has aroused recurrent interest since the seminal work by Terraneo *et al.*, who tried to reveal the underlying mechanism based on the microscopic dynamics [2]. Encouraged by the experimental verification of TR with nanotubes [3], it is believed that, eventually, the efforts invested in studying this effect will result in novel technologies and applications [4].

So far two general, necessary conditions for TR have been identified. Above all, the system must have an asymmetric structure along the direction of the heat current. In this respect, two typical asymmetric structures have been put forward and investigated both intensively and extensively. One is the hybrid structure of sequentially coupled two or three segments different in nature [2,5–8], while another class features a mass- or geometry-graded configuration [3,9–12]. The second ingredient of TR is that the local heat transport behavior should depend on the local structure and temperature [5]. In this respect, the temperature dependence of the heat conductivity, in particular for TR in a lattice system, has been scrutinized carefully. In general, a sensitive temperature dependence of the heat conductivity is favorable. Interesting examples were proposed in Refs. [8,13], where a critical phase-transition point of the heat conductivity was exploited.

The mechanisms for fulfilling these two general conditions to obtain TR are various [14–18]. However, in spite of the progresses made, these mechanisms have not yet been satisfactorily understood, particularly in systems such as insulating crystals where the thermal energy is transported mainly

through lattice vibrations. In this situation, an outstanding puzzle is why the TR effect is observed to decay as the system size increases and eventually vanish in the thermodynamic limit [19]. To prevent the decay, graded models with long-range interactions were recently proposed based on linear-response theory [20], and its effectiveness was verified numerically in both the linear-response regime and beyond [21]. These studies have suggested the important role of long-range interactions for generating the enhanced TR effect.

In this work, we reveal a distinct mechanism that may not only prevent the decay of TR, but even make it progressively stronger in the thermodynamic limit. We adopt the rotor lattice model [22,23], where the component rotors can both vibrate and rotate with respect to their equilibrium angular positions (see Fig. 1). We show that it is possible to design a graded rotor lattice where TR increases with system size, even if the interactions act only on the nearest-neighboring rotors.

In our model, the rotors are assumed to be positioned on a one-dimensional lattice with a unity lattice constant (we use dimensionless variables throughout). For a homogeneous rotor lattice, the Hamiltonian is

$$H = \sum_i \left[\frac{1}{2} \dot{\theta}_i^2 + V(\theta_{i+1} - \theta_i) \right], \quad (1)$$

where θ_i is the angular variable of the i th rotor with respect to a given reference axis, θ_i is the corresponding conjugate variable, and $V(x)$ is a periodic potential whose conventional version is $V(x) = 1 - \cos(x)$. This model was put forward as a prototype for spin systems of statistical mechanics [22] and was found relevant in applications (e.g., its potential describes the relative rotation of nearest-neighboring polymer fragments around the axis of a macromolecule [24] and interestingly, relevant to our topic here, it has been shown recently that a strong TR effect is possible in a polyethylene nanofiber system [8]). A striking property of the rotor lattice is that its heat conduction behavior may undergo a transition [25,26]: In the low-temperature regime, the rotors only vibrate around their equilibrium positions and the heat is transported dominantly by phonons. As a result, the heat conductivity increases with

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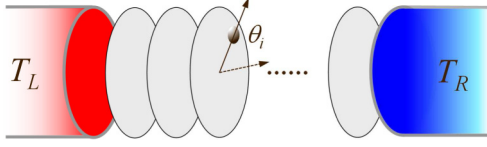


FIG. 1. Schematic plot of the rotor lattice that couples with two heat baths at its two ends. For visualization purposes, a rotor is represented by a mass point fixed on a rigid, massless disk that vibrates and rotates freely around the horizontal axis. The angular variable θ_i of the i th rotor is measured as the angle formed between the line connecting the center of the disk and the mass point and that represents the given reference direction (the dashed arrow line).

system size, showing an abnormal heat conduction behavior. But in the high-temperature regime, nonlinear modes due to rotations emerge and play a role; consequently the heat conductivity will converge to a constant as the system size increases, so that the system has a normal heat conduction behavior as described by the Fourier law.

Our motivation is to take advantage of this transition for generating enhanced TR. To this end, we first turn to a variant homogeneous rotor lattice with potential

$$V(x) = A[1 - \cos(\omega x)], \quad (2)$$

where A and ω are two parameters. To keep the maximum force $|F_{\max}|$ between any two neighboring rotors a constant, we set $\omega = 1/A$ such that $|F_{\max}| = 1$, so that A serves as the only independent parameter. First of all, we investigate how the transition temperature T^{tr} depends on the parameter A [27]. The heat conductivity is considered to characterize the system's heat conduction behavior, which is obtained numerically by following the conventional nonequilibrium simulation method. Namely, for a system of $N + 1$ rotors at a given temperature T , its two ending rotors, the zeroth and the N th, are coupled with two Langevin thermostats of temperature $T_L = T + \Delta T$ and $T_R = T - \Delta T$, respectively, whose motion equations are $\dot{\theta}_0 = -\partial V(\theta_1 - \theta_0)/\partial \theta_0 - \gamma \dot{\theta}_0 + \xi_0$ and $\dot{\theta}_N = -\partial V(\theta_N - \theta_{N-1})/\partial \theta_N - \gamma \dot{\theta}_N + \xi_N$, with ξ_0 and ξ_N being two white Gaussian noises satisfying $\langle \xi_0(t) \xi_0(t') \rangle = 2\gamma k_B T_L \delta(t - t')$ and $\langle \xi_N(t) \xi_N(t') \rangle = 2\gamma k_B T_R \delta(t - t')$. The $N - 1$ rotors in between follow their own motion equations determined by the Hamiltonian only. The system is evolved numerically from an initial condition given arbitrarily until the stationary

state is reached, then the time-averaged heat current is measured according to the definition $j = \langle j_i \rangle = \langle -[\partial V(\theta_{i+1} - \theta_i)/\partial \theta_i + \partial V(\theta_i - \theta_{i-1})/\partial \theta_i] \dot{\theta}_i / 2 \rangle$. The heat conductivity κ is thus obtained by assuming the Fourier law $j = -\kappa \nabla T$, which leads to $\kappa \approx jN/(T_L - T_R) = jN/\Delta T$. In our simulations the Boltzmann constant k_B is set to be unity throughout and, when the heat baths are involved, the coupling constant is set to $\gamma = 1$. We have also verified that when more boundary rotors are thermalized with the baths and when different values of γ are taken, the results remain the same.

The numerical results of the heat conductivity are presented in Fig. 2. We find that the transition temperature depends linearly on the parameter A , i.e., $T^{\text{tr}} \approx A/5$, which can be related to the temperature value at which the force between two neighboring rotors may reach its maximum value allowed (see below). In our simulations for Fig. 2, the temperature bias is set to $\Delta T = T/5$, which has been verified to be small enough to ensure that the system falls in the linear-response regime. Note that, in Fig. 2 and in all other figures, the errors of the data are less than 1% and the error bars are smaller than the data symbols, so error bars are omitted throughout.

At a low temperature, the rotor lattice reduces to the Fermi-Pasta-Ulam lattice [28,29] and the heat conductivity diverges in the thermodynamic limit [30]. As the temperature increases to exceed T^{tr} , localized nonlinear rotational modes [31] form and interact with the heat current to prevent its free propagation [26], bringing the system into the normal diffusive transport regime [29]. Hence as an estimation of T^{tr} , we can take advantage of the necessary condition that a rotor begins to rotate around its neighbors when the temperature is increased, which leads to that at T^{tr} , the relative angular displacement between two neighboring rotors satisfies $\omega(\theta_{i+1} - \theta_i) = \pi/2$ or, equivalently, the force between them reaches $|F_{\max}|$. Empirically, we can assume that for $T < T^{\text{tr}}$ the force between two neighboring rotors follows the Gaussian distribution and, at $T = T^{\text{tr}}$, the width of the distribution reaches $|F_{\max}|$. Then, by identifying $|F_{\max}|$ with the full width at half maximum of the force distribution, i.e., $2\sqrt{2 \ln 2} \sigma_F$ (with σ_F being the standard deviation) [32], we find that $T^{\text{tr}} \approx A/5$ over a wide range of A ($0.1 < A < 10$) that has been investigated, which agrees very well with the value of T^{tr} obtained based on the κ versus N relations (see Fig. 2). As an example, the force distribution for $A = 1$ is shown in Fig. 3.

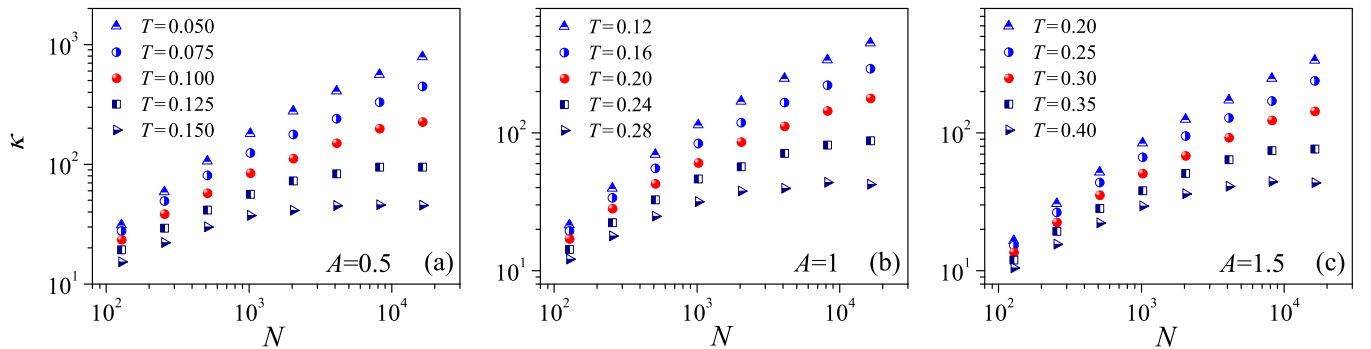


FIG. 2. The heat conductivity κ of the homogeneous rotor lattice system as a function of system size N at various temperatures for (a) $A = 0.5$, (b) $A = 1$, and (c) $A = 1.5$. It can be seen that the transition temperature $T^{\text{tr}} \approx A/5$, below which the heat conductivity tends to diverge and above which the heat conductivity tends to saturate as the system size increases.

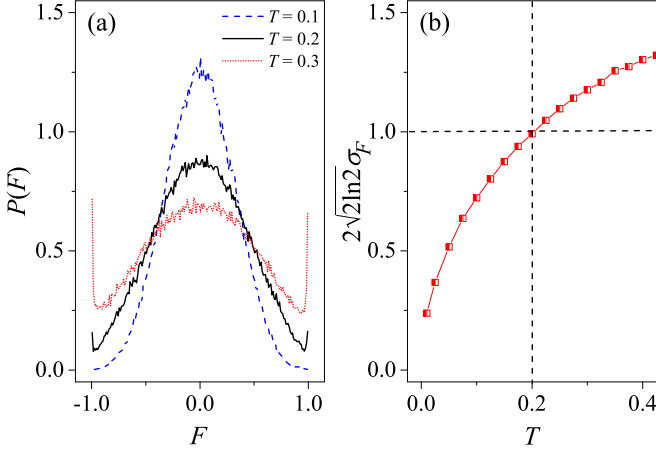


FIG. 3. (a) The distribution of the force acts on a rotor in the homogeneous rotor lattice with $A = 1$ when the system is at the equilibrium state of temperature T . (b) The full width at half maximum of the force distribution as a function of temperature. The transition temperature is estimated empirically by identifying it with $|F_{\max}| = 1$, which results in $T^{\text{tr}} \approx 0.2$ in this case for $A = 1$.

Based on the relation between T^{tr} and A , we can design a graded rotor lattice system with graded potentials, of which that between the i th and the $(i + 1)$ st rotor is

$$V_i = A_i \{1 - \cos[\omega_i(\theta_{i+1} - \theta_i)]\}, \quad (3)$$

where ω_i is fixed to be $\omega_i = 1/A_i$ and A_i changes linearly from $A_0 = A_L$ to $A_N = A_R$. Denote the transition temperature in the homogeneous system of $A = A_\alpha$ by T_α^{tr} (with $\alpha = L$ and R) and, without loss of generality, let us suppose $A_L > A_R$, so that $T_L^{\text{tr}} > T_R^{\text{tr}}$. Because the system has an asymmetric structure and the heat conduction depends on the local temperature and interactions, the TR effect is expected.

Suppose the “working” temperature range of the system is $[T_-, T_+]$, we can measure the rectification factor [1]

$$f = \frac{|\kappa_f - \kappa_r|}{\kappa_f + \kappa_r}, \quad (4)$$

where κ_f is the forward heat conductivity measured when the temperatures of the heat baths are set to be $T_L = T_+$ and $T_R = T_-$ and κ_r is the reverse one measured with the swapped heat baths, i.e., $T_L = T_-$ and $T_R = T_+$. This definition is equivalent to $f = |j_f - j_r|/(j_f + j_r)$ with j_f and j_r being the corresponding forward and backward heat current.

In the limit that interests us of large system size, a lattice can be treated as a number of sequential segments. It is partitioned in such a way that each segment is sufficiently small to justify the local equilibrium assumption, allowing the temperature and interaction gradient over it to be neglected and each segment to assume a certain local temperature and A value. On the other hand, the segments are partitioned large enough so that each one can be assigned a local transition temperature, around which the segment’s heat conduction may change drastically. It is worth noting that, the larger the system, the larger the segments, then the more abrupt this change (see Fig. 2). Hence an increasingly enhanced TR should be possible in the thermodynamic limit. This is the most intriguing property to be expected.

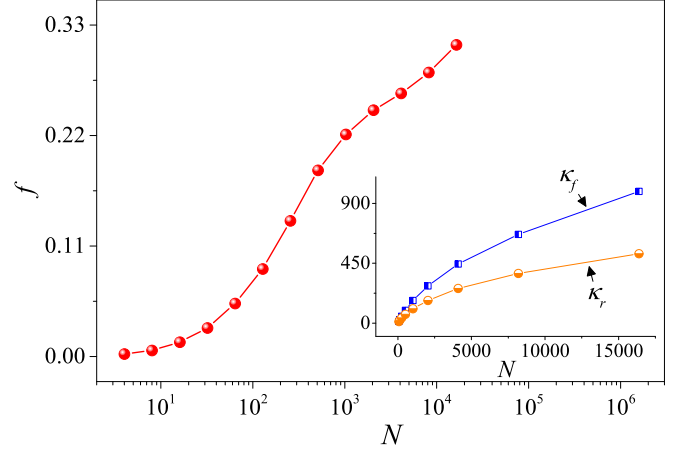


FIG. 4. The rectification factor as a function of system size in the graded rotor lattice for the case $T_L^{\text{tr}} > T_+ > T_R^{\text{tr}} > T_-$. Here $T_+ = 0.25$, $T_- = 0.05$, $A_L = 1.5$ ($T_L^{\text{tr}} \approx 0.3$), and $A_R = 0.5$ ($T_R^{\text{tr}} \approx 0.1$). The inset shows the heat conductivities evaluated with the forward and the reversed heat current, respectively.

Nevertheless, besides the system size, TR in our system also depends on the working temperature range. For example, for the case $T_L^{\text{tr}} > T_R^{\text{tr}} > T_+ > T_-$, the local temperature of any segment is below its transition temperature so both κ_f and κ_r are large. As a consequence, f should be low. Similarly, for $T_+ > T_- > T_L^{\text{tr}} > T_R^{\text{tr}}$, the local temperature of any segment is above its transition temperature, so both κ_f and κ_r are small and f should be low as well. The most interesting case is for $T_L^{\text{tr}} > T_+ > T_R^{\text{tr}} > T_-$, where for the forward current, because $T_L^{\text{tr}} > T_L > T_R^{\text{tr}} > T_R$, every segment has a temperature lower than its transition temperature, so that κ_f is large. But for the reversed current, because $T_R = T_+ > T_R^{\text{tr}}$, the segment(s) at the right end of the system is (are) above its transition temperature, so κ_r is small. As a result, the rectification effect should be remarkable. For other working temperature ranges, the TR should be in between these two limits.

The simulation results corroborate these conjectures very well. First of all, in Fig. 4 is shown the rectification as a function of system size for the optimal case $T_L^{\text{tr}} > T_+ > T_R^{\text{tr}} > T_-$. It can be seen that, indeed, the rectification increases with system size and reaches the considerably large value of $f \approx 0.3$ at the system size $N \sim 10^4$. In view of the fact that A_L and A_R are fixed so the interaction gradient actually decays linearly with the system size, TR in our model is particularly striking compared with that observed with the fixed mass gradient in oscillator lattices of long-range interactions [21]. The rectification shown in Fig. 4 is expected to increase further for $N > 10^4$, but, unfortunately, the simulations have turned out to be prohibitively expensive. In spite of this, the robust increasing trend with a roughly constant rate can be clearly recognized from the available data. In the inset of Fig. 4 are shown the forward and the reverse heat conductivity. It can be seen that the latter has not saturated yet at the largest system size $N \approx 1.6 \times 10^4$ simulated. However, to increase N further, it is expected that κ_r will saturate while κ_f keeps increasing to diverge.

The temperature profiles provide more details of the mechanism of TR in our model. As an example, those

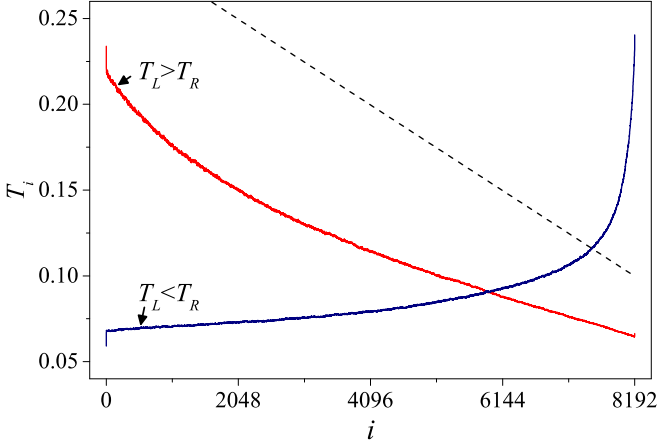


FIG. 5. The temperature profile of the graded rotor lattice for $T_- = 0.05$ and $T_+ = 0.25$ when the stationary heat current is formed with $T_L = T_+ > T_R = T_-$ (forward current, red curve) and reversely with $T_L = T_- < T_R = T_+$ (reverse current, dark blue curve). The dashed line indicates the transition temperature in a homogeneous lattice with $A = A_i$. Here $A_L = 1.5$, $A_R = 0.5$, and the system size is $N = 8192$.

corresponding to the data point next to the last one in Fig. 4 are plotted in Fig. 5. As shown, for the forward current, the local temperature is lower than the transition temperature all through the lattice, which is consistent with the strong forward current. In contrast, for the reverse current, the temperature changes mainly over the last segment, suggesting that its contribution to the thermal resistance is dominant. Therefore, it is the last segment that dominantly restricts the reverse heat current. As the system size increases, this segment grows accordingly; hence its local conductivity, and thus κ_r for the whole system, would saturate eventually.

A thorough comparison of different working temperature ranges is made in Fig. 6. That shown in Fig. 4 for $T_- = 0.05$ and $T_+ = 0.25$ is reproduced here as well. Besides it, that with $T_- = 0.05$ and $T_+ = 0.15$ also belongs to the optimal case, but with a smaller temperature bias ($T_+ - T_- = 0.1$). In this case, as expected, the rectification at a given N is smaller, but the rectification should increase further with system size. The case of $T_- = 0.05$ and $T_+ = 0.35$ corresponds to the largest temperature bias, which is why, at small N , its rectification is the strongest. However, because $T_+ > T_L^{\text{tr}}$, for the forward current, the left-most segment works at a local temperature higher than T_L^{tr} , its conductivity will saturate in the limit of large system size. Indeed, the simulation results suggest that the increasing rate decreases progressively with increasing N in the investigated range of N . For the last example case of $T_- = 0.25$ and $T_+ = 0.45$, the whole lattice is above the local transition temperature, so both the forward and reverse current are weak, which explains the decaying rectification.

Finally, note that, in the studies of Fig. 6, the temperature biases adopted are strong in the sense that $T_+ - T_-$ is comparable with the nominal temperature $T = (T_+ + T_-)/2$ of the system. As expected, for a fixed system size, the rectification factor in general decreases as the temperature bias decreases, which is also the case in our model. However, as long as

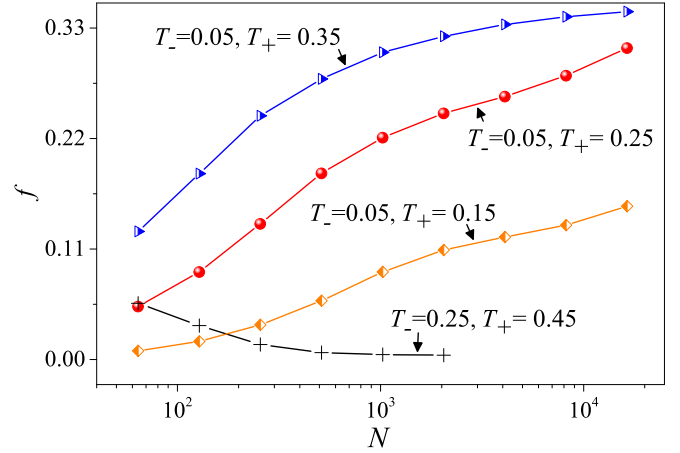


FIG. 6. Rectification factor as a function of system size in the graded rotor lattice in various working temperature ranges. Here $A_L = 1.5$ and $A_R = 0.5$.

the condition $T_L^{\text{tr}} > T_+ > T_R^{\text{tr}} > T_-$ is respected, a divergent rectification factor in the thermodynamic limit can still be predicted, just as shown by the case $T_- = 0.05$ and $T_+ = 0.15$. It suggests that a strong TR effect is in principle possible even when the temperature bias tends to zero, i.e., T_+ and T_- approach T_R^{tr} from above and below, respectively, given a large system size.

In summary, we have shown that, in the interaction-graded rotor lattice with only nearest-neighbor interactions, a progressively enhanced TR effect is possible in the thermodynamic limit. Unlike the previously proposed mechanisms, such as matching and mismatching of phonon bands in sequentially assembled lattices [2] and that of long-range-interaction-induced transport channel asymmetry [20,21], in our model TR results from the suppression of heat conduction by the local nonlinear modes stimulated at one end of the system when being coupled to the high-temperature bath. Here the local nonlinear modes are due to the relative rotational motion between the rotors; but it is interesting to note that structural rotations—e.g., that between segments of polyethylene nanofibers as a response to increasing temperature causing a morphology change from an all-trans conformation crystalline structure to a disordered structure [8]—may lead to sensitive temperature-dependent heat conduction and can be utilized to generate TR as well [8]. It suggests that other nonlinear modes, which may enhance or suppress heat conduction and meanwhile have a sensitive temperature dependence, deserve further investigation. It is also interesting to study if introducing long-range interactions may further improve TR. In this respect, it raises the question of how long-range interactions may affect the nonlinear modes and their implications on heat conduction, and the rotor lattice may serve as an ideal paradigmatic model again.

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