Thermal diode from two-dimensional asymmetrical Ising lattices

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Two-dimensional asymmetrical Ising models consisting of two weakly coupled dissimilar segments, coupled to heat baths with different temperatures at the two ends, are studied by Monte Carlo simulations. The heat rectifying effect, namely asymmetric heat conduction, is clearly observed. The underlying mechanisms are the different temperature dependencies of thermal conductivity κ at two dissimilar segments and the match (mismatch) of flipping frequencies of the interface spins.

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I. INTRODUCTION

Research on thermal transport and thermal management in nanoscale systems has attracted rapidly growing interest recently. In practical terms it sheds lights on developing microscopic thermal devices that control heat flow just like electronic devices, e.g., diodes and transistors, do for electric current. The most fundamental thermal device is the thermal diode, which provides a one-way traffic road for heat flow, namely, it allows heat flow in one direction but forbids heat flow in the opposite direction. The earliest efforts for this can be traced back to nearly a century ago, when the thermal rectifying effect was first observed in a copper–cuprous oxide interface in the 1930s [1], followed by extensive studies of heat flow across such material interfaces, often involving steel and aluminium [2]. Without a well accepted explanation for this novel physical phenomenon, these early studies were stalled for several decades, until in the year 2002 Terraneo *et al.* proposed a simple three-segment nonlinear lattice model to study possible mechanisms [3]. The rectifying efficiency was increased by two or three orders of magnitude by Li *et al.* [4] by using two-segment lattices thereafter, which makes experimental realization practical. Just two years later, a nanoscale solid state thermal rectifier was demonstrated experimentally with asymmetrically deposited nanotubes [5] and with two segments of cobalt oxide [6]. This topic has been picking up momentum and is becoming hot again [7]. Thermal rectification has been found not only in many toy models [8] but also in many nanostructures [9]. More importantly, more advanced functional thermal devices such as thermal transistors [10], thermal logic gates [11], thermal memory [12], and heat pumps [13] were successfully proposed. The door to "phononics," a new physical dimension to information processing in addition to electronics and photonics, has been opened [7].

II. SIMULATION ALGORITHMS

In this paper, we present the thermal rectifying effect in the simplest spin lattice model, the Ising model. Most of the conventional simulation algorithms apply on adaptations of the well known Metropolis algorithm [14], which is based on the notion of detailed balance that describes equilibrium for a system. It generates a sequence of configurations via a Markovian process such that the probability of encountering any given configuration is proportional to its Boltzmann factor $e^{-E/T}$, where E is the energy of that configuration and T is the temperature. Starting from a configuration with energy E_A, one can make a possible change in the configuration (e.g., flip a randomly chosen spin) to obtain a new configuration with energy E_B. Accept the change if $E_B < E_A$, otherwise accept it with probability $p = e^{-(E_B-E_A)/T}$. The Metropolis algorithm works well in high-temperature cases. However, it performs badly near the Curie point where correlation length (correlations between spins) and correlation time (correlations between successive Monte Carlo configurations) both diverge in an infinite system, because the updates are local; that is, only one spin at a time is updated. In order to solve this problem, a novel algorithm, the Swendsen-Wang (SW) cluster algorithm, which provides much higher efficiency, was presented in 1987 [15]. In this algorithm, clusters of spins are created by introducing bonds between neighboring spins with certain probabilities, and then updated by choosing a random new spin value for each cluster and assigning it to all the spins in the same cluster. Another cluster algorithm was proposed by Wolff [16] in 1989. In this algorithm, a spin is chosen at random and a single cluster constructed around it, using the same bond probabilities as for the SW algorithm. All the spins in this cluster are then flipped, i.e., changed to a random new spin different from the old one.

Metropolis and all its adaptations are applicable only to equilibrium state, while heat conduction is a typical nonequilibrium phenomenon. In order to study the nonequilibrium state, dynamics of the model must be established and a virtual momentum (or its corresponding kinetic energy) conjugate to the spin is usually necessary. A practical applicable algorithm was presented by Creutz in 1983 [17]. A "demon" with a value of kinetic energy moves randomly and exchanges energy with spin that it visits by flipping it. The total potential energy is statistically conserved. However, the dynamics is not relevant to any real dynamics of the physical system. Creutz presented later, in 1986, the Creutz cellular automaton (CCA), a deterministic dynamics for the 2D Ising model, in which each

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site is issued kinetic energy and a checkerboard update scheme is applied [18]. Another algorithm is the so-called Q2R [19], in which a spin flips if and only if exactly half of its neighbors are up. A checkerboard update scheme is also applied. Q2R preserves the total energy. CCA and Q2R were applied to studied heat conduction in the 2D Ising model by Saito *et al.* in 1999 [20]. The thermal conductivity was calculated near the Curie point with the Kubo formula and the results show, unlike in some previous works suggesting that thermal conductivity vanishes at the Curie point T_C [21], no singularity for thermal conductivity at T_C. Another algorithm which is called the KS move, introduced by Kadanoff and Swift [22], considers a diagonal with two opposite spins and flips them simultaneously if this operation preserves the energy. The KS move preserves both total energy and total spin. Because Q2R does not work well at low temperature, the RQ2R algorithm, i.e., adjusting the checkerboard update scheme of Q2R to random order, and the KQ algorithm, which is a combination of Q2R and the KS move, are used to study heat flow in the 2D Ising model [23]. It was found that KQ performs much better than RQ2R. Later, under the same dynamics, a steady state with coexisting phases transversal to the heat flow was observed [24].

In order to make a thermal diode, spatial symmetry must be broken, and thus we must use an inhomogeneous system. In general, however, Q2R, KS, and their extended algorithms are only applicable to homogeneous systems. Therefore the update algorithm we shall apply is a modified CCA algorithm. Since there are no intrinsic or physical reasons for the checkerboard update scheme [23] and it may sometimes cause unphysical effects, we apply a random update scheme. The rule is as follows: (1) The kinetic energy of each spin is initially set to a random value according to a reasonable temperature. (2) A spin is randomly chosen. (3) If the resulting change of the potential energy upon flip of this spin can be absorbed by its kinetic energy, then the spin is flipped and the kinetic energy is changed accordingly so as to conserve the total energy. If, however, its kinetic energy is not enough to absorb the potential energy change, then nothing is changed. In each time step, (2) and (3) are performed the total number of spin times; i.e., each spin is updated averagely once.

Since energy transport is ballistic in the one-dimensional Ising lattice under Q2R dynamics [20] (although an early work reported Fourier's law under 26R dynamics [25]), it is not suitable to build a thermal diode. We thus study two-dimensional cylindrical Ising models in $N_X \times N_Y$ rectangular lattices. Each spin is labeled by $s_{i,j}$ where $i \in [1, N_X]$ and $j \in [1, N_Y]$. The spin variable $s_{i,j}$ equals 1 or -1. The potential energy of the system is as follows:

$$H = -\sum_{i,j}\left(Q^X_{i,j} s_{i,j} s_{i+1,j} + Q^Y_{i,j} s_{i,j} s_{i,j+1}\right) - \sum_{i,j} H_{i,j} s_{i,j}. \quad (1)$$

$Q^X_{i,j}$ denotes the coupling between site (i,j) and its right neighbor while $Q^X_{i,j}$ denotes the coupling between site (i,j) and its lower neighbor. $H_{i,j}$ denotes the external field applied to the site (i,j). In this paper we study nonexternal field cases only; thus $H_{i,j} = 0, \forall i,j$. Periodic and open boundary conditions are applied in the Y and X directions, respectively. Two heat baths with temperature T_1 and T_2 are in contact with the left and right boundaries. As introduced in [17], the values of the kinetic energy should be distributed exponentially with the Boltzmann weight corresponding to temperature T: $P(E_k) = \frac{1}{T} e^{-(E_k/T)}$. Thus the heat baths are simulated as follows: in each time step, the kinetic energy of a spin in contact with a heat bath with temperature T is refreshed according to this exponential distribution. We have set the Boltzmann constant to unit.

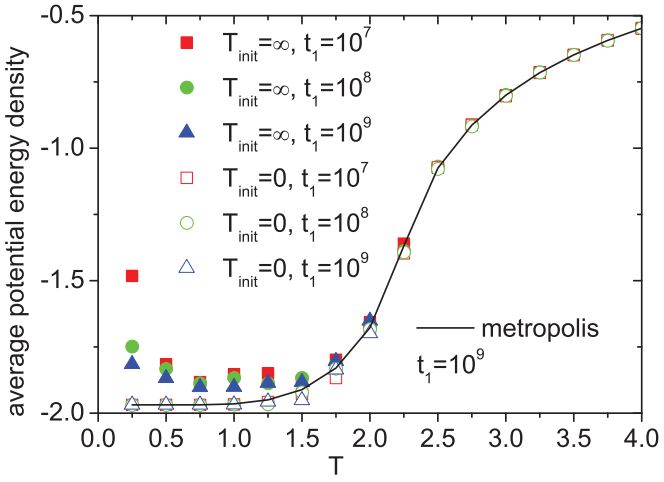

FIG. 1. (Color online) Comparison between Metropolis algorithm and present algorithm for equilibrium. The agreement is very good for $T > 2$. In the case of $T < 2$ the transient process becomes very long. When $T_{\text{init}} = 0$ [i.e., all spins are all up (down) at beginning] the agreement is still good. Even in the $T_{\text{init}} = \infty$ cases (i.e., all spins are set completely randomly) the performance of the present algorithm is still much better than the RQ2R algorithm shown in Ref. [23], Fig. 5. And as the average time length increases the agreement becomes better and better.

In the case in which the temperatures of the two heat baths equal each other, i.e., $T_1 = T_2 = T$, the system should reduce to an equilibrium one, and thus outputs from this algorithm should be equivalent to those from the standard Metropolis algorithm, which has been proven correct theoretically. We first check it by simulating a 32×32 homogeneous lattice ($Q_{i,j} = Q = 1, \forall i,j$). The comparison is presented in Fig. 1. In order to show the independence of initial conditions, two different kinds of initial conditions, i.e., initial temperature T_{init} equals 0 (initial spins are all the same) and ∞ (spins are initially chosen completely randomly), are both applied. The averages were taken over t_1 time steps, after $t_2 = t_1/2$ steps transient. We see that for $T > 2$ the agreement is always very good. Only in infinite initial temperature cases at very low T can distinct discrepancy be seen. However, this discrepancy decreases as t_1 and t_2 increase. It is only a transient effect due to the "bad" initial condition. Even in these cases the overall performance of this algorithm is much better than that of RQ2R (see Ref. [23], Fig. 5).

In nonequilibrium cases, temperature is no longer a constant throughout the whole system. The local temperature should be defined. Under this algorithm, the local temperature can be naturally defined, like in a Hamiltonian system, by local kinetic energy density [20]. However, since in this algorithm kinetic energy can be changed only by integer times of a fixed value, which may be different at the boundary or interface, the fluctuation induced by the initial condition is quite large and

hard to remove. We thus define the local temperature according to the local potential energy density E_p. For a homogeneous system in equilibrium, E_p as a function of temperature reads [26]

$$E_p = -Q\mathrm{ctanh}(2Q/T)\left(1 \pm \frac{2}{\pi}\sqrt{1-k^2}K(k)\right), \quad (2)$$

where

$$k = \frac{2\sinh(2Q/T)}{\cosh^2(2Q/T)},$$

and $K(k)$ is the complete elliptic integral of the first kind. The $+(-)$ sign holds below (above) the Curie point, which equals 2.27 for this lattice with $Q = 1$. We thus reasonably define the potential energy temperature by the inverse function of Eq. (2). In fact Eq. (2) is exact only in an infinitely large lattice. The exact solution in a finite lattice was studied in [27]. The correction therefrom is quite small and thus we do not consider it here. The definition performs reasonably, only except for the boundary spins, whose neighbors are not identical.

In order to further validate this algorithm, we apply it to nonequilibrium cases, i.e., $T_L = 6$, $T_R = 4$. Simulations are performed for lattices with fixed width N_Y and various length N_X ranging from 32 to 1024 (see Fig. 2). Reasonable local temperature profiles that display good scaling are clearly observed. Since the temperature definition does not apply to the boundary spins, data for them are not plotted. The heat current density J is found to be inversely proportional to lattice length N_X; i.e., heat conduction in this model obeys Fourier's law. The validity of this algorithm is thus further confirmed.

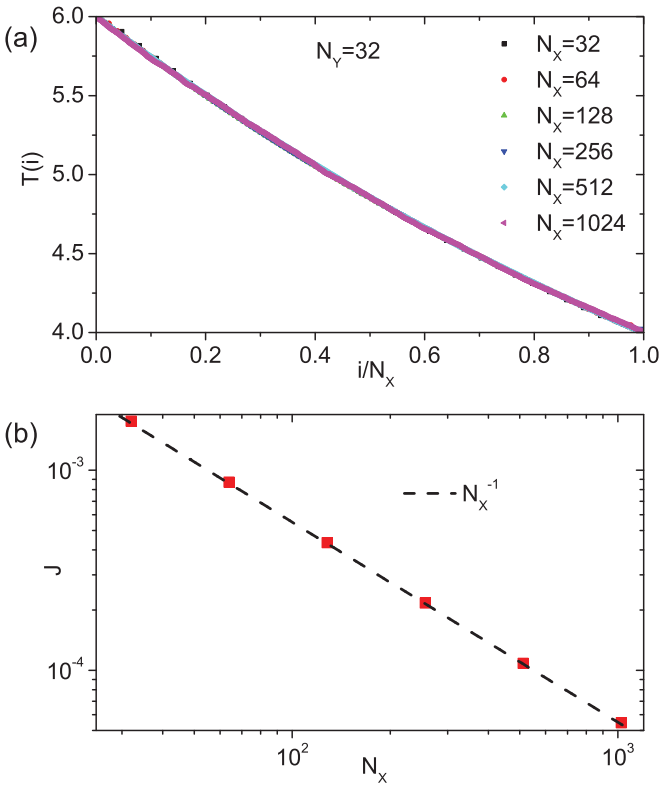

FIG. 2. (Color online) Heat conduction in homogeneous lattices with fixed lattice width N_Y and various lattice length N_X. $T_L = 6$, $T_R = 4$. (a) Temperature profiles [see Eq. (2) for definition]. Symbols for different N_X well overlap with each other. (b) Heat current density J versus lattice length N_X. Data fit N_X^{-1} very well, which indicates Fourier's law in such a system.

III. THERMAL DIODE MODEL

After confirming the validity of this algorithm, we turn to apply it to a cylindrical rectangular Ising lattice that consists of two weakly coupled dissimilar segments. Parameters are set to

$$Q_i^X = \begin{cases} Q_L, & i \in [1, N_L - 1], \\ Q_{\mathrm{int}}, & i = N_L, \\ Q_R, & i \in [N_L + 1, N_X - 1], \end{cases}$$
$$Q_i^Y = \begin{cases} Q_L, & i \in [1, N_L], \\ Q_R, & i \in [N_L + 1, N_X]. \end{cases} \quad (3)$$

In short there is an interface between $N_L - 1$ and N_L columns. All the couplings left of the interface equal $Q_L = 2$, right of the interface equal $Q_R = 1$, and at the interface equal $Q_{\mathrm{int}} = 0.2$. Hereafter we set the left and right segments with equal length, thus $N_L = N_X/2$.

In order to present the asymmetrical heat conduction properties of the system, we set the temperatures of the two heat baths to $T_L = T_0(1 + \Delta)$ and $T_R = T_0(1 - \Delta)$, where T_0 is the average temperature of the two heat bath and Δ is the relative temperature drop from left to right. Positive Δ means $T_L > T_R$ and vice versa. We plot the heat current density J versus Δ for three different values of T_0 in Fig. 3. If the heat conduction of the lattice is symmetric then the heat current density J should have the same absolute value for positive and negative Δ. However, it can be clearly seen that

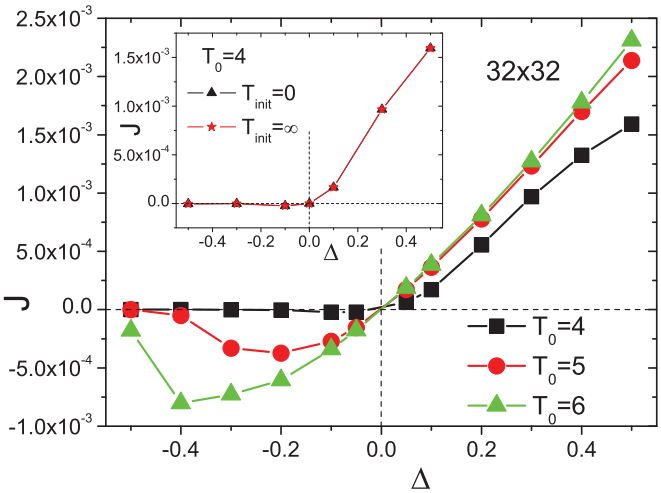

FIG. 3. (Color online) Asymmetric heat conduction in the cylindrical rectangular Ising lattice consists of two weakly coupled dissimilar segments. $Q_L = 2$, $Q_R = 1$, $Q_{\mathrm{int}} = 0.2$, $N_X = N_Y = 32$, $N_L = 16$. Different symbols correspond to different T_0 from 4 to 6. $T_L = T_0(1 + \Delta)$ and $T_R = T_0(1 - \Delta)$. Not only a very strong thermal diode effect is observed, but also negative differential thermal resistance (NDTR), which is the key for many useful thermal devices, is clearly seen for $T_0 = 5$ and 6. Inset: $T_0 = 4$, different initial temperatures $T_{\mathrm{init}} = 0$ and $T_{\mathrm{init}} = \infty$ result in the same heat current density J.

when $\Delta > 0$, J increases with Δ more or less proportionally, while in the case $\Delta < 0$, it increases quite slowly. For $T_0 = 4$, $J_- = J(\Delta = -0.5)$ is several orders of magnitude smaller than $J_+ = J(\Delta = 0.5)$, which means the system behaves as a thermal insulator for negative temperature drop while a good thermal conductor for positive temperature drop. The rectifying ratio $r \equiv \frac{|J_+|}{|J_-|}$ is thus quite exciting. Similarly to the case of the thermal diode from the Frenkel-Kontorova (FK) model [4], negative differential thermal resistance (NDTR), namely, the larger the temperature drop, the smaller the heat current, is observed for $T_0 = 5$ and 6 at the large negative Δ region. Since NDTR is the key for many useful thermal devices from thermal transistors to thermal memory [10–12], this system might have wide applications and be worth extensive studies. Due to the long transient effect we do not study even lower T_0; however, it is reasonably expected and easily confirmed that the rectifying ratio can be even greater for lower T_0. In the inset of Fig. 3 we have presented that the results referred to above do not depend on the initial conditions, e.g., $T_{\text{init}} = 0$ or ∞.

The underlying mechanism of the thermal rectifying effect can be understood with the different temperature dependence of thermal conductivity κ at two dissimilar segments. κ changes remarkably near the Curie temperature T_C [20]. The temperature profiles [defined as in Eq. (2)] for $T_0 = 5$ and $\Delta = \pm 0.5$ are shown in Figs. 4(c) and 4(d). In this system, because the temperature definitions are not applicable not only to the boundary spins but also to the interface spins, data for them are not plotted. In this system the Curie temperatures of left and right segments are different. They are 4.54 and 2.27, respectively. At a typical situation, $T_0 = 5$ and $\Delta = 0.5$, the temperatures of both segments are beyond their Curie temperatures, thus making heat conduction high. However, for the same $T_0 = 5$ but $\Delta = -0.5$, the left segment is under its Curie temperature and thus its heat conduction is quite low. Correspondingly we see the typical snapshots of the system in Figs. 4(a) and 4(b). In (a) the spins are distributed quite evenly, while in (b) a big cluster dominates the whole left segment. Almost all spins are aligned, which causes a very high heat resistance. On the other hand, as the flipping frequencies of the spins left and right of the interface match, heat easily flows through; otherwise things become quite difficult. In the former case we found that the flipping frequencies of the spins left and right of the interface are 0.55 and 0.53, respectively, while in the latter case, they are 0.2 and 0.8, respectively. Correspondingly we see in Figs. 4(c) and 4(d) that the temperature jumps at the interface are similar. However, notice the heat flow in the latter case is only about 10^{-3} of that in the former case; its interface thermal resistance is about 10^3 times higher. The above two facts make the significant thermal diode effect possible.

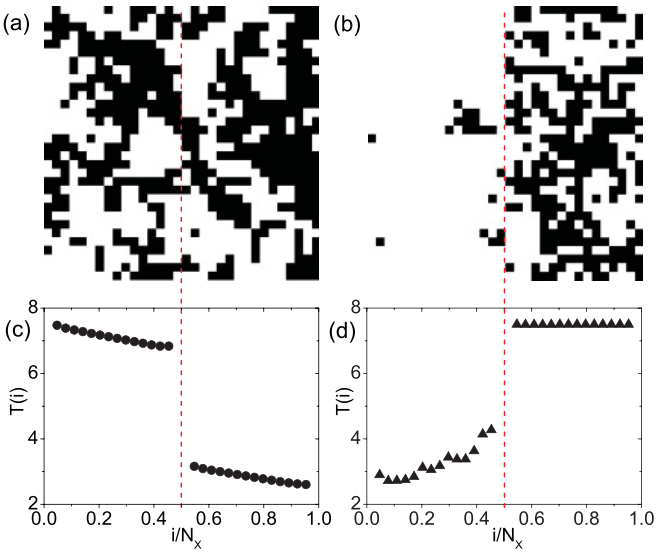

FIG. 4. (Color online) Snapshots [(a) and (b)] and temperature profiles [(c) and (d)] of the lattice, $T_0 = 5$. White and black squares indicate up and down spins, respectively. Vertical red lines indicate the position of interface. Left column: $\Delta = 0.5$, right column: $\Delta = -0.5$. In the two cases heat flow is about 2×10^{-3} and 4×10^{-6}, respectively.

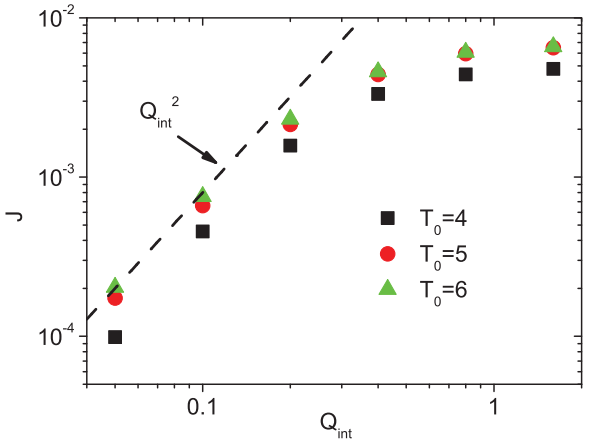

FIG. 5. (Color online) Heat current density J versus the interface coupling strength Q_{int} for $T_0 = 4$, 5, and 6. $\Delta = 0.5$. System parameters are all the same as those in Fig. 3. In all cases J follows Q_{int}^2 in the low Q_{int} limit quite well.

In such a two-segment lattice, interface coupling connects the left and the right. Its strength controls the heat current passing through and thus plays an important role. In order to present this we have also studied the heat current dependence on the interface coupling strength Q_{int}. As expected, heat current decreases as Q_{int} decreases. In the low coupling limit, the heat current decays as the square of the interface coupling strength, Q_{int}^2 (see Fig. 5). This square law has been widely observed in thermal transport through a weak link by phonons [28]. Finding it in this spin system might indicate its universality in more general cases.

IV. CONCLUSIONS

In summary, we have introduced a random update scheme to the existing CCA algorithm. We first apply the revised algorithm to a two-dimensional homogeneous Ising lattice. We find that in equilibrium states the outputs of this algorithm are consistent with that of the standard Metropolis method and that the discrepancies vanish as the simulation time increases. In nonequilibrium states, reasonable local temperature profiles are well established and Fourier's law is confirmed, which is also consistent with existing algorithms. We then apply this

algorithm to an asymmetric Ising lattice which consists of two weakly coupled dissimilar segments. As two heat baths at different temperatures are coupled to this lattice, we find that the value of heat current flows through this lattice can be quite different when the two heat baths are swapped. Namely, a strong thermal rectifying effect is observed. This effect can be attributed to different Curie points of the two segments which cause different temperature dependencies of heat conduction and the match (mismatch) of the flipping frequencies of the spins at the interface. Since the Ising model is a quite typical and popular spin model and those mechanisms can also be easily achieved in other methods, e.g., an asymmetric external magnetic field, we expect that similar phenomena can be observed in other, more realistic models, e.g., the Heisenberg model, and also be experimentally realized in true spin systems. Nowadays theoretical models for various thermal devices from thermal diodes to thermal memory have been successfully proposed, while on the other hand experimental realizations of those devices progress quite slowly. This work may provide an alternative physical mechanism to build those thermal devices and thus shed light on the road to phononics.

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