Reversal of thermal rectification in quantum systems

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We study thermal transport in anisotropic Heisenberg spin chains using the quantum master equation. It is found that thermal rectification changes sign when the external homogeneous magnetic field is varied. This reversal also occurs when the magnetic field becomes inhomogeneous. Moreover, we can tune the reversal of rectification by temperatures of the heat baths, the anisotropy, and size of the spin chains.

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Considerable progress has been made both theoretically and experimentally on thermal transport in microscale and nanoscale in last decade.[1] It has been found that similar to electrons, the heat due to phonons can be used to carry and process information.[2] In particular, several conceptual thermal devices have been proposed, such as thermal rectifiers,[3] thermal transistors,[4] thermal logical gates,[5] thermal memory,[6] some molecular level thermal machines,[7,8] and thermal ratchet.[9] Much work has also been done in quantum heat transport of nanostructures[10] and spin systems[11–22] where the magnetic field is another degree of freedom to control heat flow. Indeed, it is demonstrated that thermal rectification and negative-differential thermal resistance are observable in quantum spin chain by applying a nonuniform magnetic field.[23]

In this Brief Report, we would like to concentrate on the thermal rectification in a quantum spin model. Our primary interest is to understand how far we can control the heat flow by tuning the system parameters such as magnetic field, system size, configurations of the system, etc. In particular, we would like to see whether the reversal of thermal rectification, which has been observed in classical system,[24] can happen in such a quantum system.

We consider a Heisenberg spin-1/2 chain, whose Hamiltonian reads

$$H = -\sum_{i=1}^{N-1} (J_x\sigma_i^x\sigma_{i+1}^x + J_y\sigma_i^y\sigma_{i+1}^y + J_z\sigma_i^z\sigma_{i+1}^z) - \sum_{i=1}^{N} h_i\sigma_i^z, \quad (1)$$

where N is the number of spins, the operators σ_i^x, σ_i^y, and σ_i^z are the Pauli matrices for the ith spin, J_x, J_y, and J_z are the coupling constants between the nearest-neighbor spins, and h_i is the magnetic field strength at the ith site. We set $J_x=J(1+\gamma), J_y=J(1-\gamma), J_z=J$ to consider the anisotropy in x-y plane, where γ is the anisotropy parameter, and $J=1$, without loss of generality. Figure 1 shows a schematic representation of this model.

The total Hamiltonian including two baths is

$$H_{tot} = H + H_B + H_I. \quad (2)$$

Here H_B is the Hamiltonian of the heat baths $H_B=\Sigma_{K=L,R}H_B^K$ and $H_B^K=\Sigma_{j\in K}\omega_j b_j^+ b_j$, where b_j^+ and b_j are phonon creation and annihilation operators with the mode ω_j; H_I is the interaction between the spin chain and phonon heat baths, $H_I=\Sigma_{K=L,R}X_K\otimes Y_K$, where $X_L=\sigma_1^x$, $X_R=\sigma_N^x$, and Y_K is bath operator $Y_K=\Sigma_{j\in K}(c_j b_j^+ + c_j^* b_j)$.

We use the quantum master equation method (Refs. 23 and 25–27) to study heat conduction in this model. By tracing out the baths within the Born-Markovian approximation, we obtain the equation of motion for the reduced density matrix of the system ($\hbar=1$)

$$\frac{d}{dt}\rho = -i[H,\rho] + \mathcal{L}_L\rho + \mathcal{L}_R\rho, \quad (3)$$

where $\mathcal{L}_L\rho$ and $\mathcal{L}_R\rho$ are the dissipative terms due to the coupling with the left and right heat bath. $\mathcal{L}_L\rho$ is given by $\mathcal{L}_L\rho=[\mathcal{X}_L\rho,X_L]$+H.c. and $\mathcal{L}_R\rho$ can be given in the similar way. Here the operator $\mathcal{X}_L$ can be written as

$$\langle m|\mathcal{X}_L|n\rangle = \lambda_L\varepsilon_{m,n}N_L(\varepsilon_{m,n})\langle m|X_L|n\rangle, \quad (4)$$

where $\varepsilon_{m,n}\equiv\varepsilon_m-\varepsilon_n$ and $N_L(\varepsilon_{m,n})=(e^{\varepsilon_{m,n}/T_L}-1)^{-1}$ is the Bose distribution ($k_B=1$) with T_L being the temperature of left heat bath. $|n\rangle$ and ε_n are the eigenstates and eigenvalues of the spin-chain system. The bath spectrum function we used is of an Ohmic type. Assuming that the temperature is high enough to make dephasing fast,[27] we can solve the resulting kinetic equations of the state probabilities numerically. The evolution time is chosen long enough such that the final density matrix reaches a steady state ρ_{st}, that is, $\dot{\rho}_{nn}=0$. In the steady state, $\Sigma_n\varepsilon_n\dot{\rho}_{nn}=J_L+J_R=0$, then we can get the heat current as $J=J_L=-J_R$, if $T_L>T_R$. To quantify the rectification efficiency, we define rectification R as: $R=(J_+-J_-)/\max\{J_+,J_-\}$, where the forward heat flux J_+ is the heat current (from left to right) when the bath at higher

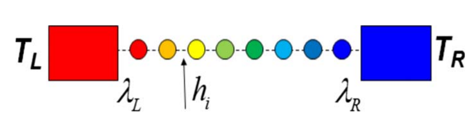

FIG. 1. (Color online) A schematic representation of the model with size $N=8$. The spin chain is connected to two phonon baths with coupling λ_L and λ_R. The phonon baths are at different temperature T_L and T_R. A magnetic field is applied to the spin chain.

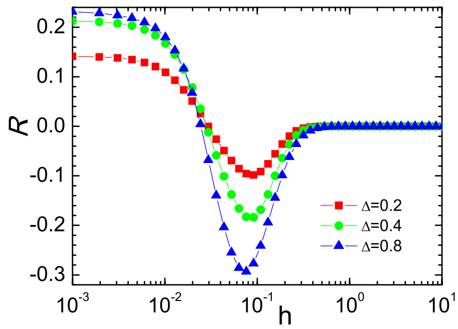

FIG. 2. (Color online) Rectification as a function of the magnetic field in a chain of size $N=6$. The temperature of the heat bath are $T_+=T_0(1+\Delta)$ and $T_-=T_0(1-\Delta)$, where $T_0=0.1$ is the mean temperature. The coupling between the spin chain and heat bath are $\lambda_L=0.16$ and $\lambda_R=0.04$, anisotropy parameter $\gamma=0.1$. The square, circle, and triangular correspond to $\Delta=0.2$, 0.4, and 0.8, respectively.

temperature T_+ is connected to the left end of the chain and the backward flux 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_-.

The quantum spin chain is a nonlinear system; if we introduce asymmetry to the system then it may show the rectification effect. We connect the spin chain to the two heat baths by different couplings $\lambda_L=0.16$ and $\lambda_R=0.04$. As is shown in Fig. 2, when the applied magnetic field increases,

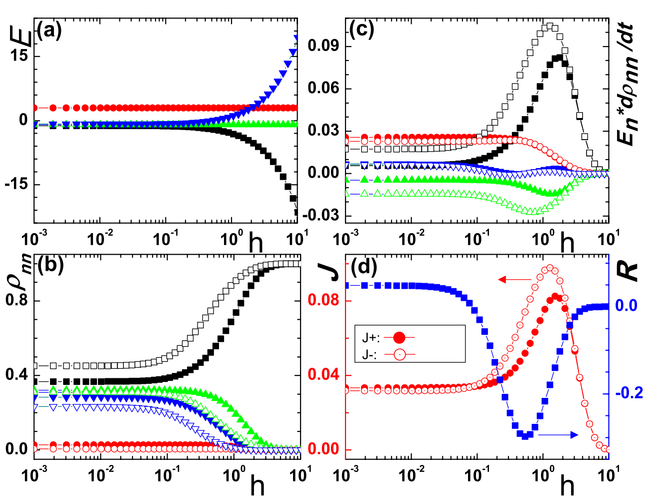

FIG. 3. (Color online) Analysis of the reversal of rectification in a two-spin system. Parameters: $T_0=1.0$, $\Delta=0.8$, $\lambda_L=0.16$, $\lambda_R=0.04$, and $\gamma=0.1$. (a) The eigenvalues E_n vs magnetic field h. (b) The density ρ_{nn} (probability of each eigenstate) vs h. (c) The product of E_n and the derivative of ρ_{nn} from high-temperature heat bath, which is the contribution to heat flux from each eigenstate. In (a), (b), and (c), the square, circle, up triangle, and down triangle correspond to eigenstates 1, 2, 3, and 4, respectively. In (b) and (c), the solid and hollow symbols correspond to forward and backward thermal transport, respectively. (d) The heat fluxes J_+ and J_- vs magnetic field h (left scale). The square curve shows rectification effect R vs magnetic field h (right scale).

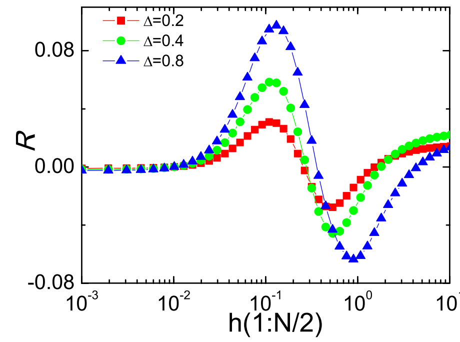

FIG. 4. (Color online) The rectification R vs nonuniform magnetic field. The chain size is $N=6$, $h(1:N/2)$ is the magnetic field applied to site 1 to $N/2$, and others are zero, that is, $h(N/2+1:N)=0$. Here $\gamma=0$, $T_0=0.1$, and $\lambda_L=\lambda_R=0.1$. The square, circle and triangular correspond to $\Delta=0.2$, 0.4, and 0.8, respectively.

the rectification changes sign. This phenomenon is not observed in electronic counterpart. From Fig. 2, we can see that rectification R can be positive, zero, or negative, depending on the magnetic field h. The behavior of R remains similar for different Δ, the temperature difference of the baths.

The mechanism of thermal rectification reversal can be understood from a two-spin system which has four eigenstates, whose contribution to heat transport can be seen clearly in Fig. 3. Figure 3(a) shows the eigenvalues E_n vs magnetic field h, where two eigenvalues do not change with the magnetic field. Figure 3(b) shows the steady density ρ_{nn} as a function of magnetic field. From this figure, we find that when the magnetic field is weak, the ground state and the excited states have some probability to be occupied (the ground state has the largest probability). If the magnetic field increases, the probability of the ground state becomes larger; after a certain value, the probability of ground state is close to one while others are zero. The heat current from the contribution of each eigenstate is shown in Fig. 3(c). When the magnetic field is weak, each state contributes to the heat flux either positively or negatively. We find that the contribution from ground state in the backward thermal transport is larger than the forward case. But the contributions from other excited states have negative effect; therefore the total effect is the forward heat flux larger than the backward flux, that is, the rectification is positive. When the magnetic field increases over a certain value, the ground state will dominate the heat transport, and the contribution from other states decrease. At the time the total heat flux will have the similar behavior with the contribution of ground state: the backward flux is larger than the forward one; both of them increase first and decrease to zero at last, when the system will stay in the ground state. Therefore, the rectification changes from positive to negative, then from negative to zero at last, which can be seen in Fig. 3(d). In short, the heat flux from the contribution of ground state is larger when the more weakly coupled reservoir is hotter, that is, the backward one is larger than the forward one; however for the flux from excited states, the forward one is larger than the backward one. The

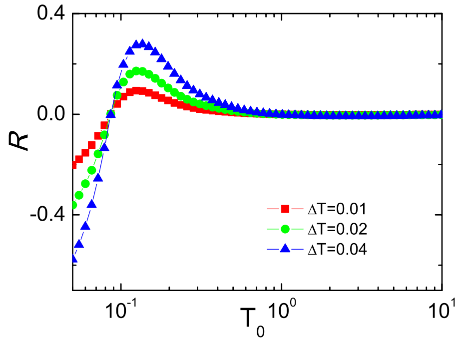

FIG. 5. (Color online) Rectification as a function of mean temperature T_0. The size of spin chain is $N=6$. The temperature of the heat bath are $T_+=T_0+\Delta T$ and $T_-=T_0-\Delta T$. Here, $\lambda_L=0.16$, $\lambda_R=0.04$, $\gamma=0.1$, and $h=0.01$. The square, circle, and triangular correspond to $\Delta T=0.01$, 0.02, and 0.04, respectively.

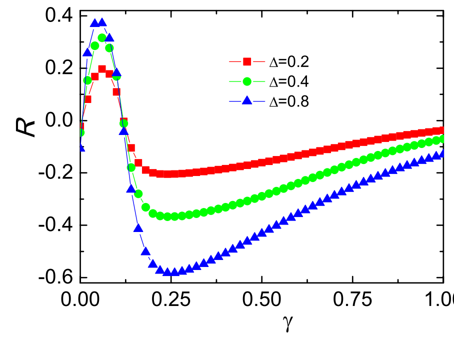

FIG. 7. (Color online) The rectification changes with anisotropy in the spin chain. The chain size is $N=6$. The square, circle, and triangular correspond to $\Delta=0.2$, 0.4, and 0.8, respectively. Here the parameters are: $T_+=0.18$, $T_-=0.02$, $\lambda_L=0.16$, $\lambda_R=0.04$, and $h=0.01$.

rectification is determined by the competition of the contributions to heat flux from the ground state and the excited states.

Applying a nonuniform magnetic field to the spin chain is another possible way to introduce asymmetry to the system and the system can also exhibit rectification. Figure 4 demonstrates this phenomenon in such a system. The rectification is zero when the magnetic field is zero because of no asymmetry in the system. When a weak magnetic field is applied to the left half part of the spin chain, the rectification becomes positive. When magnetic field increases, the energy difference increases for the left part, which enlarges the rectification. If the field increases further then the rectification reverses. For different temperature difference, the rectification has similar effect but different magnitude.

From the above discussions, we find that the rectification can change sign with the applied magnetic field. Indeed, an increase in mean temperature can also induce reversal of rectification. Figure 5 shows that the rectification as a function of mean temperature T_0. Here we keep the temperature difference fixed and increase the mean temperature of the heat baths; the rectification changes sign from negative to positive. When the temperature is very low, the ground state dominates the thermal transport, the backward flux is larger than the forward one; if we raise the temperature, more excited states will contribute to the heat flux and gradually control the thermal transport, when the rectification changes to positive. For different temperature difference, the rectification changes sign at almost the same mean temperature.

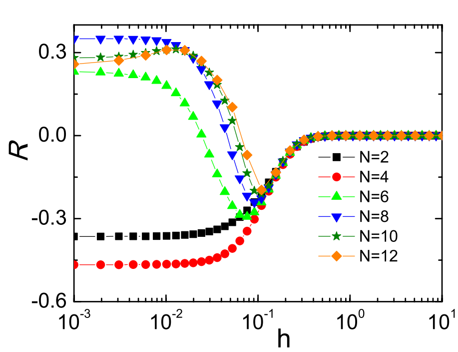

FIG. 6. (Color online) The rectification changes with magnetic field for the spin chain with different sizes. The curves of square, circle, and up triangle, and down triangle, star, and diamond correspond to $N=2$, 4, 6, 8, 10, and 12, respectively. Here the parameters are: $T_+=0.18$, $T_-=0.02$, $\lambda_L=0.16$, $\lambda_R=0.04$, and $\gamma=0.1$.

Rectification can change sign with the external parameter, such as magnetic field and the temperatures of the heat baths. In our study, we find that thermal rectification can reverse with the properties of the spin chain itself, such as the size and the anisotropy of the spin chain. Figure 6 shows the rectification changes with the magnetic field for different size cases. The rectification effect behaves differently for different size. In Fig. 6, there is no reversal of rectification for small size cases $N=2$ and $N=4$; but for larger size cases $N=6$, 8, 10, and 12, it shows reversal of rectification. Figure 7 shows the rectification reverses with the anisotropy of the spin chain. In the weak anisotropy range, the rectification coefficient is positive but it changes to negative when the anisotropy is strong. During the changing of anisotropy, the forward total flux is larger than the backward one at first, and then reverses, although the heat contribution from ground state in the backward transport is always larger than that in the forward one.

In conclusion, we have studied thermal rectification in quantum spin-chain systems by using quantum master equations. It has been shown that rectification can change sign when the magnetic field, temperature, the anisotropy, and the system size change. Although the reversal of rectification is complicated parameter-dependent, it is believed to be a universal phenomenon for the thermal transport in one-dimensional systems.

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