Control of heat transport in quantum spin systems

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(Received 2 October 2008; revised manuscript received 14 November 2008; published 27 January 2009)

We study heat transport in quantum spin systems analytically and numerically. First, we demonstrate that heat current through a two-level quantum spin system can be modulated from zero to a finite value by tuning a magnetic field. Second, we show that a spin system, consisting of two dissimilar parts—one is gapped and the other is gapless—exhibits current rectification and negative differential thermal resistance. Possible experimental realizations by using molecular junctions or magnetic materials are discussed.

DOI: 10.1103/PhysRevB.79.014207 PACS number(s): 05.60.Gg, 44.10.+i, 66.10.cd, 85.75.−d

I. INTRODUCTION

When an electron moves in solids, it carries charge, spin, as well as heat. The charge degree, the basis of the modern electronics, has been fully studied over the past decades and it is still being under intensive investigation at the molecular level.[1,2] On the other hand, the spin degree of freedom, which may be utilized to carry and process information as well, has also been explored intensively in past years, which has resulted in an emerging field "spintronics."[3,4] In this context, spin (magnetization) current in insulating magnetic materials has attracted considerable attention.[5–8] However, since recent studies showed that thermal conductivity in magnetic systems can be very high,[9,10] then a natural question is to explore the heat aspect in these materials, such as the magnetothermal transport,[11–13] and especially heat control/management.

In fact, with the rapid miniaturization and increase in operational speed of microelectronic devices, a great amount of redundant heat is produced, which will in turn affect device performance. Thus heat dissipation and heat management are becoming more and more important.[14,15] Moreover, it was found recently that heat due to phonons can be used to carry and process information.[16] Therefore, the study of heat conduction is not only of fundamental important but also helpful for the design and fabrication of heat dissipator and phononic devices. Indeed, many interesting conceptual devices such as thermal rectifier (diode),[17–20] thermal transistor,[21,22] and thermal logic gate[23] have been proposed. Experimentally, a nanoscale solid-state thermal rectifier using deposited carbon nanotubes and a rectifier using quantum dot have been realized recently,[24,25] and a heat transistor—control heat current of electrons—controlled by a voltage gate has also been reported.[26] Furthermore, Segal and Nitzan[27] showed that thermal rectification can appear in a two-level system (TLS) asymmetrically coupled to phonon baths, providing the possibility to control heat at a microscopic level.

In this paper, we demonstrate that the heat part from spins can be modulated and controlled. For example, we show that heat current in a two-level system can be modulated from zero to a finite value by tuning the magnetic field, h. Near $h=0$, the two levels are almost degenerate and the system can jump easily between them; thus, heat current (proportional to h^2) is small. As h increases from zero to a finite value, heat current increases accordingly. We further consider a spin-1/2 system consists of two different segments: one is gapped and the other is gapless. We show that in such a structure thermal rectifying efficiency can be very high, up to ten times. This system also exhibits negative differential thermal resistance (NDTR), a feature which is necessary for building up a thermal transistor.

This paper is organized as follows. In Sec. II, we describe the spin model and the quantum master-equation (QME) method. Numerical results about heat modulation, rectification, and negative differential thermal resistance are presented in Sec. III. Finally, Sec. IV is devoted to a summary.

II. MODEL AND METHOD

We consider an inhomogeneous mesoscopic spin-1/2 chain whose Hamiltonian reads

$$H = \sum_{n=1}^{N} h_n \sigma_n^z - Q \sum_{n=1}^{N-1} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^z \sigma_{n+1}^z), \tag{1}$$

where N is the number of spins, the operators σ_n^x and σ_n^z are the Pauli matrices for the nth spin, Q is the coupling constant between the nearest-neighbor spins, and h_n is the magnetic-field strength (Zeeman splitting) at the nth site. Figure 1 shows a schematic representation of this model. Note that one can actually use more realistic models, e.g., the Heisenberg model [adding $\sigma_n^y \sigma_{n+1}^y$ to the second sum in Eq. (1)], but the results do not change qualitatively (see Fig. 3 for a comparison). Therefore, in the following we focus on model (1) for simplicity.

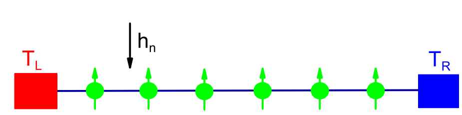

FIG. 1. (Color online) A schematic representation of the model with size $N=6$. The spin model is connected to two phonon baths held at different temperatures, T_L and T_R. An inhomogeneous field is applied to introduce an asymmetric structure.

We use the QME (Refs. 28–30) to study heat conduction in this model. Two phononic baths of different temperatures are connected to the system at the ends. By tracing out the baths within the Born-Markovian approximation, we obtain the equation of motion for the reduced density matrix of the system ($\hbar=1$),

$$\frac{d\rho}{dt} = -i[H,\rho] + \mathcal{L}_L\rho + \mathcal{L}_R\rho, \tag{2}$$

where $\mathcal{L}_L\rho$ ($\mathcal{L}_R\rho$) is a dissipative term due to the coupling with the left (right) bath. $\mathcal{L}_L\rho$ is given by $\mathcal{L}_L\rho=([X_L\rho,\sigma_1^x]+\text{H.c.})$ and $\mathcal{L}_R\rho$ can be given in a similar way. Here the operator X_L is defined through

$$\langle m|X_L|n\rangle = \lambda\varepsilon_{m,n}n_L(\varepsilon_{m,n})\langle m|\sigma_1^x|n\rangle, \tag{3}$$

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 bath. $\{|n\rangle\}$ and $\{\varepsilon_n\}$ are the eigenstates and eigenvalues of the system Hamiltonian H, respectively. λ is the coupling strength with the bath. The bath spectral function we used is an Ohmic type. The master equation [Eq. (2)] is solved by the fourth-order Runge-Kutta method. In numerical simulations, we take $\lambda=0.01$; the simulation time is chosen long enough such that the final density matrix reaches a steady state, ρ_{st}. The current operator is defined through the equation of continuity: $\partial_t H_n=i[H,H_n]=J_n-J_{n+1}$, where $H_n=(h_n\sigma_n^z+h_{n+1}\sigma_{n+1}^z)/2-Q(\sigma_n^x\sigma_{n+1}^x+\sigma_n^z\sigma_{n+1}^z)$ is the local energy density operator. In our case,

$$J_n = Qh_n(\sigma_n^y\sigma_{n+1}^x - \sigma_{n-1}^x\sigma_n^y) + 2Q^2(\sigma_{n-1}^z\sigma_n^y\sigma_{n+1}^x - \sigma_{n-1}^x\sigma_n^y\sigma_{n+1}^z). \tag{4}$$

In the steady state, $J=\text{Tr}(\rho_{\text{st}}J_n)$ is a constant over the chain (independent of n).

III. RESULTS AND DISCUSSION

First, we demonstrate the modulation of heat current by an external field in a TLS, namely, $N=1$; thus Eq. (1) becomes $H=h\sigma^z$. From the QME, we obtain heat current,

$$J = \lambda(2h)^2\frac{n_L(2h)-n_R(2h)}{1+n_L(2h)+n_R(2h)}. \tag{5}$$

Figure 2 shows heat current as a function of the field. The temperatures of the left and right baths are $T_L=T_0+0.05$ and $T_R=T_0-0.05$, respectively; T_0 is the mean temperature. In Fig. 2, we see that heat current first increases with the field and then decreases. In low fields ($h\ll T_0$), $n_{L,R}\sim T_{L,R}/h$, then $J\propto h^2$. In high fields ($h\gg T_0$), $n_{L,R}\sim e^{-2h/T_{L,R}}$, then $J\propto h^3e^{-2h/T_0}$, implying that heat current decays to zero when h is large. Therefore, in such a model we can modulate the current from zero to a finite value by gradually switching on the external field. This result is similar to those observed in one-dimensional spin-1/2 systems recently,[13] although in our case we consider just one spin.

We now consider N spins in an inhomogeneous magnetic field, namely, $h_n=1$ (as the unit of energy) if $1\le n\le N/2$ and $h_n=0$ otherwise (see Fig. 1). The temperatures of the left and right baths are $T_L=T_0(1+\Delta)$ and $T_R=T_0(1-\Delta)$, respectively, where T_0 is a mean temperature and Δ is the dimensionless temperature difference. Figure 3 shows the heat current versus temperature difference for two models: the square is for a Heisenberg model; the circle is for model (1). In both cases, we can observe very clear thermal rectification and also negative differential thermal resistance in the negative Δ region. However, for simplicity, we focus on heat conduction properties of model (1) in the following.

In Fig. 4, we show the heat current as a function of the temperature difference with the mean temperature ranging from $T_0=1$ to $T_0=5$. When the temperature is low ($T_0=1$), we observe that for $\Delta>0$ the heat current increases with Δ, while in the region $\Delta<0$ the heat current remains very small. Thus, our model exhibits thermal rectification; namely, heat flows favorably in one direction. However, when the temperature becomes high, such as $T_0=5$, the magnitude of heat current changes little as the bath temperatures are exchanged. In this case the model cannot act as a good rectifier. Never-

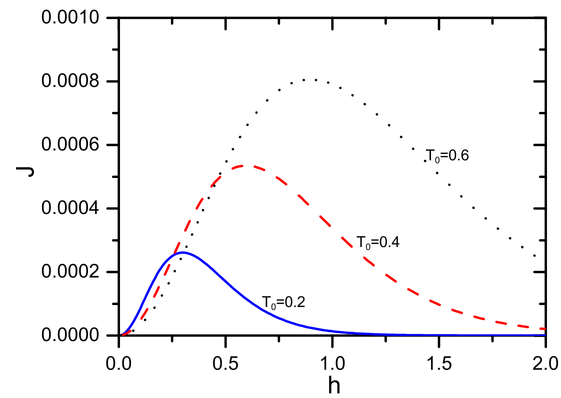

FIG. 2. (Color online) Heat current as a function of the field. The bath temperatures are $T_L=T_0+0.05$ and $T_R=T_0-0.05$. Three cases are shown: $T_0=0.2$ (solid line), $T_0=0.4$ (dashed line), and $T_0=0.6$ (dotted line).

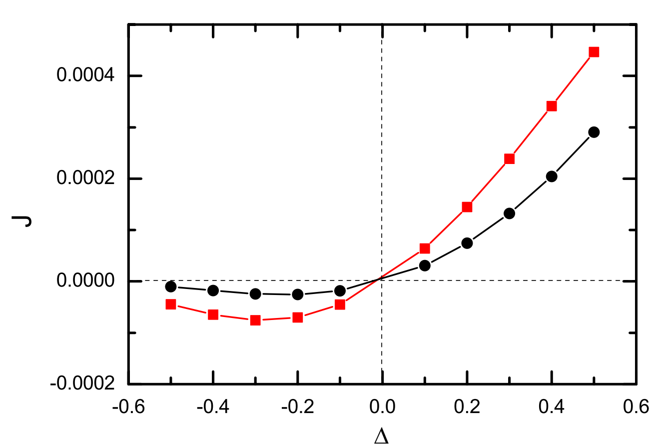

FIG. 3. (Color online) Heat current vs temperature difference. The squares show the heat current in a Heisenberg model, while the circles show the current in model (1). In both models, the bath temperatures are $T_L=T_0(1+\Delta)$ and $T_R=T_0(1-\Delta)$, where $T_0=1$ is the mean temperature. $N=6$ and $Q=0.2$. $h_n=1$ if $1\le n\le N/2$ and $h_n=0$ otherwise. The dashed lines are to guide for the eyes.

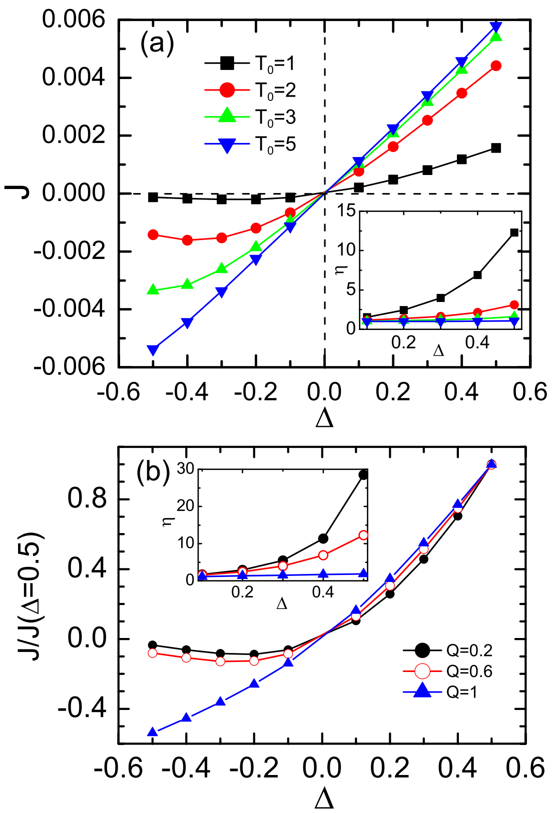

FIG. 4. (Color online) (a) Heat current vs temperature difference. The temperatures of the baths are $T_L = T_0(1+\Delta)$ and $T_R = T_0(1-\Delta)$, where T_0 is the mean temperature, ranging from $T_0=1$ to $T_0=5$. $N=6$ and $Q=0.6$. $h_n=1$ if $1 \le n \le N/2$ and $h_n=0$ otherwise. (b) Normalized heat current $[J/J(\Delta=0.5)]$ vs Δ with different couplings. Here $T_0=1$. The insets show the rectification efficiency, $\eta = |J_+/J_-|$, vs the temperature difference. The lines are guide for the eyes.

theless, in a wide range of temperature ($T_0 \lesssim 3$), this model shows thermal rectifying effect; the mechanism will be illustrated later. In Fig. 4(b), we show the heat current for a model with different couplings. We can see that the rectifying effect may sustain to large coupling constants. To quantify the rectification efficiency, we introduce the ratio, $\eta = |J_+/J_-|$, where J_+ is the current when $T_L > T_R$ and J_- is the current when the temperatures are swapped, i.e., $T_L < T_R$. In a weak-coupling case, e.g., $Q=0.2$, the efficiency may be more than 10 [see the insets of Figs. 4(a) and 4(b)]; however, as the coupling Q becomes stronger, the efficiency decreases.

To understand the rectifying effect qualitatively, we divide the system into two segments: the left in a field and the right in the absence of a field. In a quantum spin chain that is gapless at $h=0$, an external field can drive the system phase transitioned to a gapped state.[31] Indeed, we observe an energy gap of $E_g \sim 2.1$ in the left segment when $h=1$, $Q=0.1$. Therefore, if the left segment is in contact with a cold bath and the right with a hot bath, i.e., $T_L = T_c$ and $T_R = T_h$ ($T_c < T_h$), then the left segment will largely remain in the ground state, $|g_L\rangle$. This is reflected in Fig. 5(a), which shows the probability $P_L = \mathrm{Tr}(|g_L\rangle\langle g_L|\rho_{\mathrm{st}})$ (P_R) to find the left (right) segment in the ground state. Around $\Delta = -0.5$, the transition rate of the left segment between different levels is suppressed completely since $P_L = 1$, and thus the heat current vanishes [see Fig. 5(b)]. Reversely, around $\Delta = 0.5$, the left segment is in contact with a hot bath and the right with a cold one; the transition rate of the left segment between different levels becomes large, and then heat current is large. This can also explain the low rectifying efficiency when the mean temperature T_0 is increased. In this case, the transition probability of the left part between different levels may also be large; then, the magnitude of heat current changes little when the bath temperatures are exchanged, implying a low efficiency. In fact, we may observe thermal rectification provided that $T_0 \lesssim E_g$.

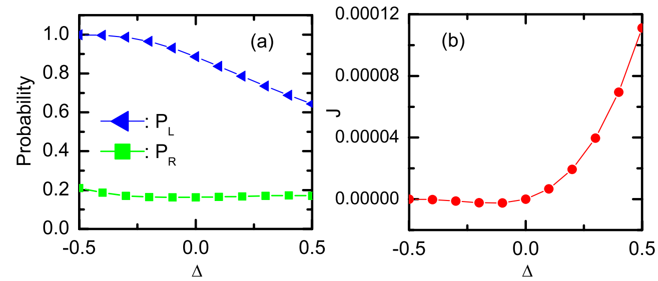

FIG. 5. (Color online) (a) The probability P_L (P_R) to find the left (right) part of the system in the ground state as a function of the temperature difference. $T_0=0.7$, $N=6$, $Q=0.1$, and $h_n=1$ if $1 \le n \le N/2$ and zero otherwise. (b) Heat current as a function of the temperature difference.

In Fig. 6, we show the heat current for a system with different sizes. In the small size case ($N=4$), we just observe thermal rectification with a low efficiency. The reason may be that the effective coupling between the left and the right parts can be strong for a small size system. As a result, the left part may be excited by the right part even though it is connected to a cold bath. However, in a larger size system, i.e., $N=6$ or $N=8$, we may observe both thermal rectification and negative differential resistance. Note also that the efficiency changes very little when $N=6$ or $N=8$, implying that the model may act as a rectifier in an even larger size case.

In fact, in Fig. 4, we can also observe NDTR in the region of $\Delta < 0$, i.e., the decrease in heat current with the increase in

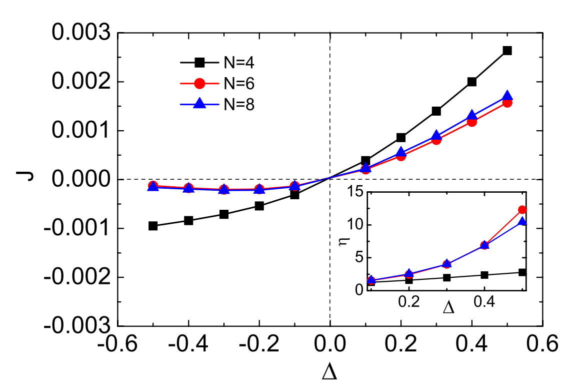

FIG. 6. (Color online) Heat current of a system with difference sizes. The bath temperatures are $T_L = T_0(1+\Delta)$ and $T_R = T_0(1-\Delta)$. $T_0=1$ and $Q=0.6$. The field is $h_n=1$ if $n \le N/2$ and $h_n=0$ otherwise. The inset shows the rectification efficiency as a function of the temperature difference.

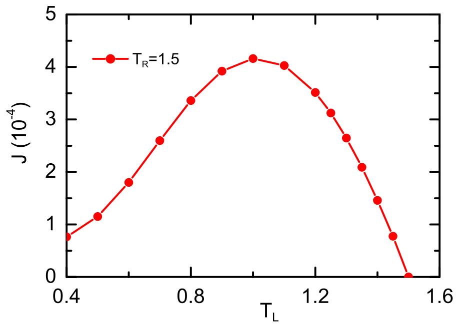

FIG. 7. (Color online) Heat current vs temperature of left heat bath, T_L, with fixed $T_R=1.5$. The other parameters are $Q=0.6$, $N=6$, $h_n=1$ if $1 \leq n \leq N/2$ and $h_n=0$ otherwise. The NTDR is clearly seen for $T_L<1.0$.

temperature difference. A clearer representation is shown in Fig. 7, where we fix the temperature of the right bath, $T_R=1.5$. We see that when the temperature of the left bath T_L is increased from 0.4 to 1.0, i.e., decreasing the temperature difference, thermal current increases. The reason is that if T_L is low, the left part is rarely excited, implying a small current; otherwise, current is large. NDTR is an important physical property that may be used to build spin-based thermal transistors.

IV. SUMMARY

We have studied the possibilities to control heat current in mesoscopic spin models. We have showed that heat current can be modulated from zero to a finite value in a two-level system by tuning the magnetic field. We have also studied thermal rectification and negative differential thermal resistance in an asymmetric model. The model consists of two parts: the left part is gapped and the right part is gapless. Such a structure is of great importance for the model to exhibit rectification and NDTR. In certain cases, we have found that the rectification efficiency, $|J_+/J_-|$, can be larger than 10. Finally, we would like to discuss the possible realizations of the model in experiment. The first is to make use of the asymmetric structure in molecular bridges that can be easily introduced. For example, we may use a molecule consisting of two (weakly) coupled nonidentical spatially separated segments; each is taken to be an anharmonic system, e.g., anharmonic vibrations or molecular librations, where at low temperatures only the lowest (two) quantum states are relevant. However, in this case, there are gaps in both segments, so the rectifying effect may be not so high. The second possible way is to use magnetic materials or molecular magnets.[32] The model may be made up of two coupled magnetic materials: one is gapped and the other is gapless. For the gapped material, one could use, for example, the spin ladder materials,[33] or introduce a magnetic field to open a gap.

ACKNOWLEDGMENTS

Y.Y. thanks Lifa Zhang for valuable discussions. The work was supported in part by an ARF Grant No. R-144-000-203-112 from the Ministry of Education, Singapore, an endowment Grant No. R-144-000-222-646 from NUS, and Grant No. B06011 from MOE of China, and NSFC.

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