Ballistic magnetothermal transport in a Heisenberg spin chain at low temperatures

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We study ballistic thermal transport in Heisenberg spin chain with nearest-neighbor ferromagnetic interactions at low temperatures. Explicit expressions for transmission coefficients are derived for thermal transport in a periodic spin chain of arbitrary junction length by a spin-wave model. Our analytical results agree very well with the ones from nonequilibrium Green's function method. Our study shows that the transmission coefficient oscillates with the frequency of thermal wave. Moreover, the thermal transmission shows strong dependence on the intrachain coupling, the length of the spin chain, and the external magnetic field. The results demonstrate the possibility of manipulating spin-wave propagation and magnetothermal conductance in the spin-chain junction by adjusting the intrachain coupling and/or the external magnetic field.

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I. INTRODUCTION

Thermal transport properties of low-dimensional systems have gained much attention recently.¹ Intensive studies in low-dimensional systems have made some important progress not only in understanding the underlying physical mechanism but also in controlling of heat. In particular, several conceptual thermal devices have been proposed such as thermal rectifiers or diodes,² thermal transistors,³ thermal logical gates,⁴ thermal memory,⁵ and some molecular level thermal machines.^{6,7} Much work has also been done to the quantum transport in nanostructures.⁸

Low-dimensional systems, especially one-dimensional (1D) materials, offer the possibility to study quantum effects that are masked in three-dimensional systems. In recent years, many interesting experiments on thermal transport in 1D spin chains $^{9-12}$ are performed, where the 1D-spin-chain compound materials give us nice physical realizations of 1D toy model systems. From these experiments, it is possible to control heat transport in spin systems by a magnetic field. There are also theoretical studies about thermal transport in 1D spin chains, some of which show anomalous transport due to the integrability,^{13–16} such as the anisotropic Heisenberg S=1/2 model, the *t*-V model, and the XY spin chain. The properties of energy transport through the chains differ for different anisotropies of the intrachain spin interactions. In all spin systems, the mean-free path of itinerant spin excitations increases as temperature decreases. Therefore in the low-temperature limit, the thermal transport in spin chain can be regarded as ballistic.

The phononic transmission coefficients in quasi-onedimensional atomic models can be calculated by transfermatrix method.^{17–20} However, if there are evanescent modes with large $|\lambda|$ (λ is an eigenvalue of the transfer matrix), the evaluation of the transfer matrix can be numerically rather unstable, particularly when the system size becomes large. Alternatively, nonequilibrium Green's function (NEGF) is an efficient method to calculate the transmission coefficient. Unfortunately, both of these two methods cannot give an analytical expression easily. In this paper we give an explicit analytical expression of transmission coefficient through a spin-wave model from a wave scattering picture. Here we study magnetothermal transport in an isotropic Heisenberg spin junction coupled to two semi-infinite spin chains in equilibrium at different temperatures. By Holstein-Primakoff²¹ transformation we map the spin operators to spinless boson operators and consider only the harmonic terms of Hamiltonian in the low-temperature limit, which is discussed in Sec. II. The analytical solution from the spin-wave model is shown in Sec. III; we get the explicit formula for transmission coefficient. In Sec. IV, we introduce the nonequilibrium Green's function method and use it to study thermal transport. The results and discussion are given in Sec. V. A short summary is presented in Sec. VI.

II. MODEL

The Heisenberg spin chain consists of three parts: two semi-infinite leads and a junction region (see Fig. 1). The two leads are in equilibrium at different temperatures T_L and T_R . We apply different external magnetic fields to the three parts along z direction. So the Hamiltonian of this system is given by

$$\hat{H} = -\sum_{i} J_{i}(\hat{S}_{i} \cdot \hat{S}_{i+1}) - \sum_{i} h_{i}S_{i}^{z},$$
(1)

where J_i is the interaction between spin site *i* and *i*+1 and h_i is the magnetic field applied to spin site *i*. Using Holstein-Primakoff transformation,²¹

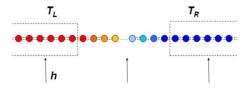


FIG. 1. (Color online) The system is an infinite Heisenberg spin chain, which consists of two semi-infinite leads with an arbitrary junction region. The two leads are in equilibrium at different temperatures T_L and T_R . We can apply different magnetic fields to the three parts.

it is easy to map spin operators to spinless boson operators a^+, a . In the low-temperature limit, $\langle a^+a \rangle \ll 2S$, we obtain the following Hamiltonian by neglecting the terms containing products of four or more operators:

$$H = E_0 + \sum_{i,j} a_i^+ K_{ij} a_j,$$
 (3)

where $E_0 = -\sum_i (J_i S^2 + h_i S)$, and $K_{ii} = (J_{i-1} + J_i)S + h_i$ and $K_{i,i+1} = K_{i+1,i} = -J_i S$, where *S*, which can be any integer and half-odd-integer, is the maximum value of spin. We choose S = 1, without loss of generality.

III. ANALYTICAL SOLUTION FROM THE SPIN-WAVE MODEL

Because only harmonic terms are contained in the Hamiltonian, we can assume a spin-wave solution transmitting from the left lead to the right lead through the junction region. We consider the two leads as uniform spin chains of intrachain spin coupling J_L in a magnetic field h_L . The junction has an alternating coupling, J_1 and J_2 , in a field h. The unit cell of the junction part contains two spin sites. We assume an incident wave as $\lambda_1^j e^{-i\omega t}$. When it arrives at the center part, it partially will be reflected and partially will be transmitted. The reflected wave is $r\lambda_1^{-j}e^{-i\omega t}$ and the transmission wave can be written as

$$\varphi_{j=2m+1} = u\lambda_2^{j-1}e^{-i\omega t},\tag{4}$$

$$\varphi_{j=2m} = v \lambda_2^{j-1} e^{-i\omega t}.$$
 (5)

The coefficients r, u, and v are obtained from the continuity condition at the interface. The transmission wave will be reflected and transmitted by the right end of the junction; the amplitudes of reflection wave are ur_{u1} and vr_{v1} for the odd site and even one, respectively. The transmission wave from the right end is

$$\varphi_j = u\lambda_2^L t_1 \lambda_1^j e^{-i\omega t}, \tag{6}$$

where L=N-1, N is the number of sites in the junction part. The reflection wave will be reflected (r_{u2} of amplitude) at the left end again and then reflected again. Finally the total wave function transmitted from the junction is a superposition of multiple reflections and transmissions,

$$\varphi_j = u\lambda_2^L (1 + r_{u1}r_{u2}\lambda_2^{2L} + (r_{u1}r_{u2}\lambda_2^{2L})^2 + \cdots)t_1\lambda_1^j e^{-i\omega t}.$$
 (7)

From the time dependent Schrödinger equation,

$$i\frac{\partial}{\partial t}\Psi = H\Psi, \quad \Psi = (\varphi_j),$$
 (8)

where we set $\hbar = 1$ for simplicity; we can get the dispersion relations for the leads $\lambda_1 = e^{iq_1}$ and for the junction $\lambda_2 = e^{iq_2}$ as

$$\omega - (2J_L + h_L) = -J_L \left(\frac{1}{\lambda_1} + \lambda_1\right),\tag{9}$$

$$[\omega - (J_1 + J_2 + h)]^2 = J_1^2 + J_2^2 + J_1 J_2 \left(\frac{1}{\lambda_2^2} + \lambda_2^2\right).$$
(10)

Which root of the equations should we use? By adding a small imaginary part to ω , that is, replacing it by $\omega + i\eta$, then none of the eigenvalues λ will have modulus exactly 1. Considering η as a small perturbation, we find for the traveling waves²²

$$|\lambda| = 1 - \eta \frac{a}{v}, \quad \eta \to 0^+. \tag{11}$$

That is, the forward moving waves with group velocity v > 0 have $|\lambda| < 1$. In the formulas below, we take the root with $|\lambda| < 1$. The energy band for our model $(J_1 < J_2)$ is

$$([h,h+2J_1] \cup [h+2J_2,h+2(J_1+J_2)]) \cap [h_L,h_L+4J_L].$$
(12)

Finally, we obtain the transmission coefficient (for N odd) as

$$\widetilde{T}(\omega) = \left| \frac{ut_1 \lambda_2^L}{1 - r_{u1} r_{u2} \lambda_2^{2L}} \right|^2.$$
(13)

Here,

$$\alpha = -\frac{\omega - (J_1 + J_2 + h)}{J_1 \lambda_2 + J_2 / \lambda_2} = -\frac{J_1 / \lambda_2 + J_2 \lambda_2}{\omega - (J_1 + J_2 + h)}, \quad (14)$$

$$u = \frac{J_L(1 - \lambda_1^2)}{J_L - J_2 - \lambda_1 J_L + \alpha J_2 / \lambda_2}, \quad v = u\alpha,$$
(15)

$$r_{u1} = -\frac{\omega - (J_L + J_2 + h) + \alpha J_2 / \lambda_2 + J_L \lambda_1}{\omega - (J_L + J_2 + h) + J_2 \lambda_2 / \alpha + J_L \lambda_1},$$
 (16)

$$r_{u2} = -\frac{\omega - (J_L + J_1 + h) + J_1 / (\alpha \lambda_2) + J_L \lambda_1}{\omega - (J_L + J_1 + h) + J_1 \lambda_2 \alpha + J_L \lambda_1},$$
 (17)

$$r_{v1} = r_{u1}/\alpha, \quad r_{v2} = r_{u2}\alpha,$$
 (18)

$$t_1 = \lambda_1 (1 + r_{u1}), \quad t_2 = \lambda_1 (1 + r_{u2}). \tag{19}$$

If the number of the sites is even, that is, the length of the chain is odd, the transmission can be written as

$$\widetilde{T}(\omega) = \left| \frac{u\lambda_2^L t_1'}{1 - r_{u1}' r_{u2} \lambda_2^{2L}} \right|^2,$$
(20)

$$r'_{u1} = \alpha^2 r_{u2}, \quad t'_1 = \alpha t_2.$$
 (21)

If $J_1=J_2$, all the formulas are reduced to those of the uniform spin chain. Although we only discuss the period-two spin chain, it is easy to derive similar formulas of transmission coefficient for any other arbitrary periodic junction by this method.

For a ballistic transport, the thermal current can be written as a Landauer-type expression,

$$\langle I \rangle = \frac{1}{2\pi} \int_0^\infty \omega [f_L(\omega) - f_R(\omega)] \widetilde{T}(\omega) d\omega.$$
 (22)

The conductance is

$$\sigma = \frac{1}{2\pi} \int_0^\infty d\omega \omega \widetilde{T}(\omega) \frac{\partial f(\omega)}{\partial T}.$$
 (23)

IV. NONEQUILIBRIUM GREEN'S-FUNCTION METHOD

From the discussion in Sec. II, we can write the Hamiltonian, by neglecting the ground-state energy E_0 , as follows:

$$H = \sum H_{\alpha} + \left(\sum_{lm} \left(a_{l}^{L+} V_{lm}^{LC} a_{m}^{C} + a_{m}^{C+} V_{ml}^{CL} a_{l}^{L}\right) + \text{H.c.}\right), \quad (24)$$

where $H_{\alpha} = \sum_{lm} a_l^{\alpha+} K_{lm}^{\alpha} a_m^{\alpha}$, with $\alpha = L, C, R$, where L, C, R denote left lead, center part, and right lead, respectively. The Hamiltonian matrix of the full linear system is

$$H = \begin{pmatrix} K_L & V_{LC} & 0 \\ V_{CL} & K_C & V_{CR} \\ 0 & V_{RC} & K_R \end{pmatrix}.$$
 (25)

We use nonequilibrium Green's function method⁸ to study the thermal transport in the spin chain. First we define the retarded Green's function as

$$G^{r}(t,t') = -i\theta(t-t')\langle [a(t),a^{+}(t')]\rangle.$$
(26)

In nonequilibrium steady states, Green's function is timetranslationally invariant and so it depends only on the difference in time. The Fourier transform of $G^r(t-t')=G^r(t,t')$ is defined as

$$G^{r}[\omega] = \int_{-\infty}^{+\infty} G^{r}(t) e^{i\omega t} dt.$$
 (27)

We also need the advanced Green's function,

$$G^{a}(t,t') = i\theta(t'-t)\langle [a(t),a^{+}(t')]\rangle, \qquad (28)$$

the "greater than" Green's function,

$$G^{>}(t,t') = -i\langle a(t)a^{+}(t')\rangle, \qquad (29)$$

and the "less than" Green's function,

$$G^{<}(t,t') = -i\langle a^{+}(t')a(t)\rangle.$$
(30)

Without interaction, the free Green's functions for three parts in equilibrium can be written as

$$[(\omega + i\eta) - K_{\alpha}]g_{\alpha}^{r}(\omega) = I, \quad \alpha = L, C, R,$$
$$g_{\alpha}^{a}(\omega) = g_{\alpha}^{r}(\omega)^{\dagger}.$$
(31)

There is an additional equation relating g^r and $g^<$,

$$g^{<}(\omega) = f(\omega)[g^{r}(\omega) - g^{a}(\omega)], \qquad (32)$$

where $f(\omega) = \langle a^+ a \rangle = [e^{\omega/T} - 1]^{-1}$ is the Bose-Einstein distribution function at temperature *T*; we have set the Boltzmann constant $k_B = 1$.

The energy current flow from the left lead to the central region is

$$I_L = -\langle \dot{H}_L \rangle, \tag{33}$$

which can be expressed by Green's function as

$$I_{L} = \lim_{t' \to t^{-}} \operatorname{Tr}\{V_{CL}K_{L}G_{LC}^{>}(t,t') - G_{CL}^{>}(t,t')K_{L}V_{LC}\}.$$
 (34)

In frequency domain, the current expression can be written as

$$I_L = -\int_{-\infty}^{\infty} \operatorname{Tr} \{ G_{CL}^{>}(\omega) K_L V_{LC} - V_{CL} K_L G_{LC}^{>}(\omega) \} \frac{d\omega}{2\pi}.$$
 (35)

Because of the following relations,

$$K_{\alpha}g_{\alpha}^{>,<} = g_{\alpha}^{>,<}K_{\alpha} = \omega g_{\alpha}^{>,<}, \qquad (36)$$

$$G_{CC} = g_C + g_C \Sigma G_{CC}, \qquad (37)$$

$$\Sigma = \Sigma_L + \Sigma_R, \quad \Sigma_\alpha = V_{C\alpha} g_\alpha V_{\alpha C}, \tag{38}$$

$$G_{CL} = G_{CC} V_{CL} g_L, \quad G_{LC} = g_L V_{LC} G_{CC}, \tag{39}$$

the current $\langle I \rangle = \frac{1}{2} (\langle I_L \rangle - \langle I_R \rangle)$ can be reduced to Landauertype expression [Eq. (22)], where the transmission coefficient is

$$\widetilde{T}(\omega) = \operatorname{Tr}\{G_{CC}^{r}\Gamma_{R}G_{CC}^{a}\Gamma_{L}\}.$$
(40)

The Γ_{α} functions are given by $\Gamma_{\alpha} = i(\Sigma_{\alpha}^{r} - \Sigma_{\alpha}^{a})$.

For the 1D spin junction coupled to two semi-infinite leads, which are uniform spin chains of intrachain interaction J_L in a magnetic field h_L , the transmission coefficient can be written as

$$\widetilde{T}(\omega) = 4J_L^4 [\operatorname{Im}(g_{00}^r)]^2 |G_{N-1,0}|^2, \qquad (41)$$

where $g_{00}^r = -\lambda_1/J_L$, λ_1 is given by Eq. (9), Green's function G_{CC}^r is abbreviated as G, and

$$G_{N-1,0} = (\omega - K_C - \Sigma)_{N-1,0}^{-1} = \frac{(-1)^{N-1} \prod_i J_i}{\det(\omega - K_C - \Sigma)}.$$
 (42)

For N=3, we can get $G_{2,0}=\frac{J_1J_2}{abc-aJ_2^2-cJ_1^2}$, where $a=\omega-J_L-J_1$ $-h-J_L^2g_0^r$, $b=\omega-J_1-J_2-h$, and $c=\omega-J_L-J_2-h-J_L^2g_0^r$. For general N, it is difficult to get an explicit formula.

V. RESULTS AND DISCUSSIONS

In our calculations, we take $k_B=1$ and $\hbar=1$. The unit of coupling J is 1 meV, the unit of magnetic field is 17.5 T, the unit of temperature is 11.6 K, and the unit of conductance is 3.86×10^{-2} nW/K.

If the whole system is uniform, i.e., the magnetic fields applied to the three parts—two leads and the junction—are the same, the transmission coefficient $\tilde{T}(\omega)$ is always 1 in the whole domain [h,h+4J]. However, if the magnetic fields in three parts are different, e.g., h > 0 in the junction and h_L

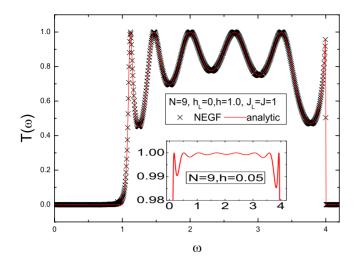


FIG. 2. (Color online) The transmission coefficient of the uniform spin chain with coupling J=1. We apply a magnetic field to the junction. The transmission $\tilde{T}(\omega)$ shifts along the frequency axis with magnetic field and oscillates with frequency in the range of [1,4]. The number of sites in the junction part is N=9, with magnetic field h=1. The scattered crosses and solid line correspond to the results from NEGF and the spin-wave model, respectively. The inset shows the case with a weak magnetic field, h=0.05. The numbers of peaks is N-1.

=0 in the two leads, the transmission coefficient oscillates with frequency ω in the domain [h, 4J], where the whole system has the same intrachain coupling J. If the magnetic field is weak, the oscillation region is very near to 1, and the number of peaks $[T(\omega)=1]$ is equal to N-1. With the strengthening of magnetic field in the junction, the transmission $T(\omega)$ shifts along the axis of frequency ω , the oscillation range extends to the domain [0,1], and some peaks will be cut off because of the shift of the curve. The numerical results come from NEGF are exactly the same with analytical solution from the spin-wave model, which is shown in Fig. 2. All the phenomena are still the same when the size of the spin chain is very large. However, for small size spin chain, the transmission at the forbidden band is not zero because of quantum tunneling effect, which can be given from both of the two methods and the results are exactly consistent. The shift and oscillation of transmission coefficient are due to interference of the spin-wave transmission through the junction.

If the intrachain spin coupling of junction is different from that of leads, the transmission coefficient oscillates also with the frequency. In Fig. 3, we show that the transmission coefficient for the junction with periodic coupling, $J_1=1$, $J_2=0.5$, and the leads with J=1, oscillates with frequency in the energy bands [0,1] and [2,3] which is consistent with Eq. (12). From this figure, it can be further concluded that our analytical results from the spin-wave model are exact. The numerical results from NEGF method are consistent with this analytical approach.

When an external magnetic field h=1 is applied to the junction part, the transmission coefficient shifts to $[1,2]\cup[3,4]$, and the oscillation shape changes, which is shown in Fig. 4. The shapes of oscillation are different for

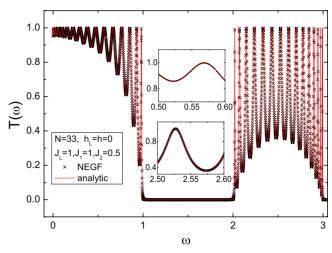


FIG. 3. (Color online) The transmission coefficient of the junction part with periodic coupling $J_1=1$ and $J_2=0.5$. There is no magnetic field applied to the spin chain. The transmission oscillates in the bands of [0,1] and [2,3], which is consistent with Eq. (12). Here, the number of sites in the junction part is N=33. The crosses and solid line curve correspond to the results from NEGF and spin-wave model, respectively. The inset shows the fine curves in the range of $\omega \in [0.5, 0.6]$ and [2.5,2.6]. The results from two methods are consistent with each other.

odd-site and even-site junctions. For the even-site junction, the spin chain is symmetric along the chain direction, while it is asymmetric for odd-site case. Therefore, the reflection in two ends of the junction for asymmetric chain is different, which causes the difference of the transmission compared with symmetric case.

From the above results, we know that the periodicity of the junction can give rise to gaps in the transmission. Can we

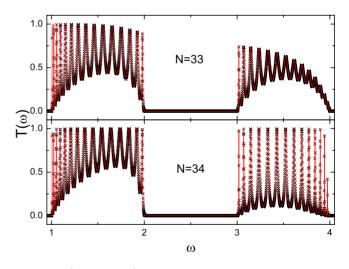


FIG. 4. (Color online) The transmission coefficient of the periodic intrachain coupling junction in an external magnetic field h=1. Here, the coupling of leads J_L =1 and J_1 =1, J_2 =0.5 for the junction. The upper and lower panel are for N=33 and N=34, respectively. The results of the spin-wave method (solid line curve) [for N=33 and N=34, we use Eq. (13) and Eq. (20), respectively] are identical with the numerical results from NEGF (the scattered crosses).

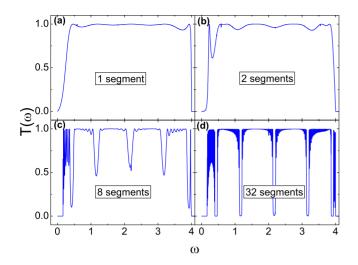


FIG. 5. (Color online) The transmission coefficient for junctions connected in series. Here, every segment has five sites and all segments in a magnetic field of h=0.2 are connected by a spin with no magnetic field. (a), (b), (c), and (d) correspond to 1, 2, 8, and 32 segments, respectively. For 32 or more segments, there are obvious five gaps (forbidden bands), i.e., six transmitted bands, which is due to the period of magnetic field along the chain; here the period is equal to 6 (five sites with magnetic field plus one spin with no magnetic field).

merely apply magnetic field periodically to the junction to induce gaps in the transmission, while the whole system has the same coupling J=1, so that we can choose the frequency to transmit from the junction? It is possible because the transmission oscillates with frequency when the junction is subjected to a magnetic field. If we connect many junctions in series, then the range of oscillation extends and may give gaps in transmission. In Fig. 5, at first we let the heat transfer through a five-site junction in a magnetic field h=0.2, then the transmission oscillates a little near 1; if we connect two junctions together by a site without magnetic field, that is, N=11, h(i=1-5;7-11)=0.2, and h(6)=0, the oscillation will be extended. The gaps are shown evidently when 32 or more segments are connected in series by the sites without magnetic field. For a fixed size junction, if we apply magnetic field periodically, there are p-1 gaps (p is the period of magnetic field along the junction) in the transmission, which are shown in Fig. 6. Therefore, we can choose the frequencies to transmit through the junction by adjusting the periodicity of the intrachain coupling or the magnetic field.

We can calculate the thermal conductance from transmission coefficient. In Fig. 7, we show the thermal conductance versus system size, temperature, and magnetic field for uniform and periodic spin chain. It is shown that the conductance is independent of the system size because of ballistic transport while the oscillation of transmission coefficient changes with the system size. The conductance increases to a constant with the increase in temperature, which is consistent with all other ballistic cases. From Fig. 7(b), we see that the conductance decreases to zero as the intensity of magnetic field is increased. These results indicate that the transmission coefficient will shift along the axis of frequency, which cuts off the contribution of low frequency to the thermal current;

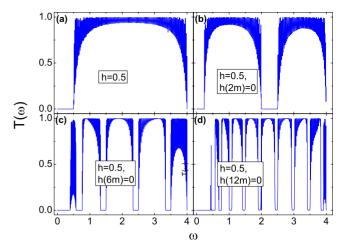


FIG. 6. (Color online) The transmission coefficient for a fixed junction in different periods of magnetic field. The total number of sites is N=191. The magnetic field is applied to the junction as $h(p \times m)=0, m=1,2,3,...$, others=0.5, and p is the period of magnetic field along the junction. (a), (b), (c), and (d) correspond to uniform, p=2, p=6, and p=12 magnetic fields, respectively. It is shown that there are p-1 gaps for different cases.

therefore the thermal current decreases. Because the thermal wave of low frequency contributes most to the heat flux, the thermal conductance decreases quickly with the increase in the intensity of magnetic field. Although the transmission has a big difference for uniform and periodic chains, the thermal conductance has the similar behavior merely with a difference of magnitude.

VI. CONCLUSION

In this paper, we have studied the ballistic magnetothermal transport in a Heisenberg spin chain at low temperatures. We have obtained explicitly an analytical expression for the transmission coefficient through a spin-wave model from a wave scattering picture. The analytical results have been verified by the nonequilibrium Green's function method. We

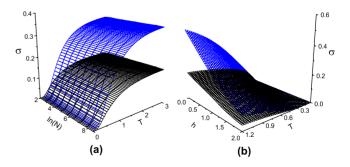


FIG. 7. (Color online) (a) The thermal conductance, σ , versus system size, N, and temperature T. σ increases with temperature to a constant whereas it keeps invariant with system size, where magnetic field is h=0.5. (b) The thermal conductance σ versus magnetic field, h, and temperature. It shows that the conductance decreases to zero with strengthening magnetic field at different temperatures. The upper blue surface and lower black surface correspond to uniform (J=1) and periodic $(J_1=1, J_2=0.5)$ spin chains, respectively.

have found that the transmission coefficient oscillates with the frequency because of interference of the transmission waves; furthermore, the thermal transmission coefficient shows strong dependence not only on the intrachain coupling and length of the spin chain but also on the external magnetic field. There are gaps in the transmission and the number of gaps is equal to p-1, where p is the period of intrachain coupling or the external transverse magnetic field applied to the junction; i.e., the number of transmitted bands is equal to the value of periods. Therefore, it is easy to choose special frequencies to transmit through the spin-chain junction by adjusting its intrachain coupling or the external magnetic field and the heat current in the junction can be switched off with the magnetic field strengthening. The thermal conductance of Heisenberg spin chain at low temperature tends to a constant with the increasing temperature, decreases to zero with intensity of the magnetic field, while it has no dependence on the system size.

Our analytical spin-wave model solution can be applied to the ballistic magnetothermal transport in an arbitrary periodic spin chain. The properties of the magnetothermal transport found in this paper provide the possibility to manipulate magnetothermal conductance and the propagation of spin waves in the Heisenberg spin chain, which may have potential applications in thermal control and designing of filter and waveguide for spin waves.

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