Spin transport in antiferromagnets in one and two dimensions calculated using the Kubo formula

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We study spin transport in one- and two-dimensional Heisenberg antiferromagnets. In one dimension we take spin $S=1$. The longitudinal spin conductivity is calculated using the Kubo formula. The magnetic properties of low-dimensional systems are significantly modified by strong correlations effects. The models studied here show unconventional transport behavior: the computed spin conductivity exhibits a nonzero Drude weight at finite temperatures and thus a ballistic character. We present results for the regular part of the conductivity as a function of the frequency.

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I. INTRODUCTION

Recently there has been much interest on transport phenomena in low-dimensional magnetic models. One motivation is that the study of transport is important to a better understanding of relaxation and nonequilibrium properties, especially in strongly correlated electron systems. Other motivation is the fact that power dissipation is one important limitation of electronic and spintronic devices. As pointed out by Trauzettel *et al.*,[1] in nonitinerant magnetic models, the dissipation is reduced, since magnetization transport generates much less power than charge currents. For this reason, much effort has been put in search of spin-based devices for future applications. The understanding of transport properties is also of great importance for the interpretation of dynamic properties such as nuclear magnetic relaxation (NMR) measurements.[2] Recent experimental studies[3] indicate unconventional transport and dynamic behavior in one-dimensional magnetic compounds, such as ballistic spin transport in magnetic chains with spin-1/2.

The experimental study of novel compounds demands the theoretical characterization of the conductivity in a spin model. So the first step in characterizing a system is the calculation of D in order to find out whether the system shows ballistic or dissipative behavior. In the linear-response theory, ballistic transport is defined by the existence of a finite Drude weight[4] D, which is the zero-frequency contribution to the real part of the conductivity [here the prime symbols ($'$ and $''$) denote the real and imaginary components of a complex function]

$$\sigma'(\omega) = D\delta(\omega) + \sigma^{\text{reg}}(\omega), \quad (1)$$

where we assume that $\sigma^{\text{reg}}(\omega)$ is regular at zero frequency. At $T=0$, $D=0$ is characteristic of a spin insulator and $D>0$ of a spin conductor.

Spin transport in the nearest-neighbor spin-1/2 XXZ chain

$$H = J\sum_l \left[\frac{1}{2}(S_l^+ S_{l+1}^- + S_l^- S_{l+1}^+) + \Delta S_l^z S_{l+1}^z\right] \quad (2)$$

has been the object of many studies.[1,2] In the XY limit, $\Delta=0$, the spin current commutes with the Hamiltonian, resulting in ballistic transport. For $|\Delta|<1$ (easy plane), calculations using the Bethe ansatz method[5] show that $D\neq 0$ at $T=0$. Numerical and analytical studies, at finite temperatures,[6] indicate that the spin transport is ballistic, although the spin current does not commute with H. For $\Delta>1$ (easy axis), the system has a gap and $D=0$ at $T=0$. Numerical and analytical calculations[6,7] show that D vanishes also at finite temperatures. For $\Delta=1$, there are still some controversies.[3] The numerical results are however limited to rather small size lattices and this implies limitations on the information that can be extracted on the long-time (low frequency ω) behavior of the conductivities.[4]

For the one-dimensional antiferromagnet with $S=1$, a theoretical study based on a semiclassical approach of the nonlinear sigma model[8] concluded to diffusive dynamics, while a Bethe ansatz method calculation pointed to ballistic transport.[9] Sentef *et al.*[10] analyzed spin transport in the easy-axis antiferromagnet model in two and three dimensions, but they restricted their study to $T=0$ only. Damle and Sachdev[11] treated the two-dimensional (2D) nonlinear sigma model in the gapped phase.

In this paper we will calculate the spin conductivity for the one- and two-dimensional antiferromagnet, described by the Hamiltonian

$$H = J\sum_{\langle n\cdot m\rangle} \vec{S}_n \cdot \vec{S}_m \quad (3)$$

in the framework of a modified spin-wave theory and the Kubo formalism for transport. In one dimension we take $S=1$, and in two, since the behavior does not depend on the value of the spin, we consider $S=\frac{1}{2}$.

II. SPIN TRANSPORT

While charge conductivity is studied as the current response to a time-dependent electromagnetic potential, the spin currents flow in response to a magnetic-field gradient. Following the standard procedure,[10] we will calculate the longitudinal spin conductivity. Therefore, we will add an external space- and time-dependent magnetic field $B(x,t)$ applied along the z direction to the Hamiltonian (3). This term couples to the spin system via the Zeeman energy. We have assumed a magnetic-field gradient only along the x direction and set $\hbar=k_B=1$.

From the continuity equation

$$j_{n+1} - j_n = -\frac{\partial S_n^z}{\partial t} \quad (4)$$

written for the lattice and Heisenberg's equation of motion $\dot{S}_n^z = i[H, S_n^z]$, we obtain

$$j_x(l) = \frac{iJ}{2}(S_l^+ S_{l+x}^- - S_l^- S_{l+x}^+), \quad (5)$$

where $l+x$ is the nearest-neighbor site of site l in the positive x direction. Following Ref. 10, we write the spin current response to an external field gradient as

$$\langle j(\vec{q},\omega)\rangle = \chi_{jS}(\vec{q},\omega) h(\vec{q},\omega), \quad (6)$$

where $h = g\mu_B B$ and the dynamic susceptibility is given by

$$\chi_{jS}(\vec{q},\omega) = \frac{i}{N}\int_0^\infty dt e^{i\omega t}\langle[j(\vec{q},t), S^z(-\vec{q},0)]\rangle. \quad (7)$$

From Eqs. (4), (6), and (7) we obtain

$$\langle j(\vec{q},\omega)\rangle = \frac{\langle K\rangle + \Lambda(\vec{q},\omega)}{\omega} q_x h(\vec{q},\omega), \quad (8)$$

where

$$\langle K\rangle = \frac{J}{\hbar N}\sum_n \langle S_n^+ S_{n+a}^- + S_n^- S_{n+a}^+\rangle \quad (9)$$

and

$$\Lambda(\vec{q},\omega) = \frac{i}{N}\int_0^\infty dt e^{i\omega t}\langle[j(\vec{q},t), j(-\vec{q},0)]\rangle. \quad (10)$$

For a system close to thermal equilibrium, we can write the following phenomenological expression for the spin current: $\langle \vec{j}(\vec{r},t)\rangle = \sigma \vec{\nabla} h(\vec{r},t)$, where the proportionality constant between the current and the field gradient defines the conductivity σ. A quite convenient technique to study spin transport is the Kubo formula, derived on the basis of linear-response theory. In the long-wavelength limit we arrive at the Kubo expression[12]

$$\sigma(\omega) = \frac{\langle K\rangle + \Lambda(\vec{q}=0,\omega)}{i\omega}. \quad (11)$$

Here we omit a term $(g\mu_B)^2$, which should be put back in case of comparison to experimental data. The real part of σ can be written as

$$\sigma'(\omega) = \sigma_0(\omega) + \sigma^{\text{reg}}(\omega), \quad (12)$$

where $\sigma_0(\omega) = D\delta(\omega)$, with

$$D = -\pi[\langle K\rangle + \Lambda'(\vec{q}=0,\omega\to 0)] \quad (13)$$

and

$$\sigma^{\text{reg}}(\omega) = \Lambda''(\vec{q}=0,\omega)/\omega. \quad (14)$$

The regular part, $\sigma^{\text{reg}}(\omega)$, is the continuum contribution to the conductivity. The delta function term is the contribution of thermally excited particles that propagate ballistically without any collisions with other particles. Therefore, a finite Drude weight implies ballistic transport. The dc conductivity is given by the $\omega\to 0$ limit of the regular part, $\sigma_{\text{dc}} = \sigma^{\text{reg}}(\omega \to 0)$.

As it is well known the standard spin-wave formalism is unsuitable to treat the one-dimensional antiferromagnet. However, a modified spin-wave (MSW) theory for the low-dimensional Heisenberg antiferromagnet, closely related to the Schwinger boson theory of Arovas and Auerbach,[13] was formulated by Takahashi[14] under the assumption of zero sublattice magnetization. With this constraint the number of spin waves in a one-dimensional isotropic system does not diverge as it does in the usual spin-wave treatment. This constraint is introduced in the Hamiltonian through a Lagrangian multiplier and the diagonalization of the quadratic part leads to a spin-wave energy that has a gap. Using the Dyson-Maleev transformation, we define boson operators in each sublattice according to[15]

$$S_n^+ = \sqrt{2S}a_n, \quad S_n^- = \sqrt{2S}a_n^+ \quad (15)$$

for the spin-up sublattice and by

$$S_m^+ = \sqrt{2S}b_m^+, \quad S_m^- = \sqrt{2S}b_m \quad (16)$$

for the spin-down sublattice. Taking the Fourier transform and following Refs. 14 and 15, the Bogoliubov transformation is given by

$$a_k = u_k\alpha_k + v_k\beta_k^+, \quad b_k = u_k\beta_k + v_k\alpha_k^+, \quad (17)$$

where the coefficients u_k and v_k are given by

$$u_k = \sqrt{\frac{\lambda+\omega_k}{2\omega_k}}, \quad v_k = \sqrt{\frac{\lambda-\omega_k}{2\omega_k}}, \quad (18)$$

with

$$\omega_k = \lambda\sqrt{1-\eta^2\gamma_k^2} \quad (19)$$

and $\gamma_k = \Sigma_\delta e^{i\vec{k}.\vec{\delta}}/z$, where δ are the lattice vectors to the z nearest-neighbor sites of the origin. The gap, which is the value of ω_k at $k=0$, is given by $m = \lambda\sqrt{1-\eta^2}$. The temperature dependent parameters λ and η are obtained by solving simultaneously the self-consistent equations

$$S + \frac{1}{2} = \frac{1}{N}\sum_k \frac{1}{2(1-\eta^2\gamma_k^2)^{1/2}}\coth\left[\frac{\lambda}{2T}(1-\eta^2\gamma_k^2)^{1/2}\right], \quad (20)$$

$$\frac{\eta^2\lambda}{2J} = \frac{1}{N}\sum_k \frac{\eta^2\gamma_k^2}{2(1-\eta^2\gamma_k^2)^{1/2}}\coth\left[\frac{\lambda}{2T}(1-\eta^2\gamma_k^2)^{1/2}\right]. \quad (21)$$

The temperature dependence of λ and η is discussed in Refs. 14 and 16.

From Eqs. (5), (15), and (17) the spin current $j_0 = \Sigma_l j_x(l)$ can be written as

$$j_0 = \frac{\lambda^2}{2}\sum_k \frac{\sin k_x}{\omega_k}[\eta\gamma_k(\alpha_k^+\alpha_k + \beta_k^+\beta_k) - (\alpha_k^+\beta_k^+ + \alpha_k\beta_k)]. \tag{22}$$

Our task now is to solve Eq. (10). A very convenient analytical method to treat this equation perturbatively is the Green's function theory.[17] The Green's function contains important physical information such as the ground-state energy, the energy and lifetime of excited states, and the linear response to external perturbations. In this context we start with the spin current Green's function (which is a two-particle Green's function in terms of the operators α and β) defined by

$$G_2(t) \equiv -\frac{i}{\hbar N}\langle 0|Tj(t)j(0)|0\rangle, \tag{23}$$

where T is the time-ordering operator and $|0\rangle$ the ground state.

Taking Eq. (22) into Eq. (23), using Wick's theorem, and Fourier transforming we arrive at an expression in terms of one-particle Green's functions. At low temperatures the magnon density is small and the noninteracting theory is valid.[10,11] This amounts to the replacement of the one-particle Green's function $G \to G^0$ and we obtain

$$G_2(\omega) = \frac{\lambda^4}{4}\sum_k \frac{\sin^2 k_x}{\omega_k^2}\Pi_{kk}(\omega), \tag{24}$$

where

$$\Pi_{kk}(\omega) = i\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}G^0_{\alpha\alpha}(k,\omega+\omega')G^0_{\beta\beta}(k,\omega'), \tag{25}$$

and $G^0_{\alpha\alpha}$ and $G^0_{\beta\beta}$ are the propagators for the noninteracting particles

$$G^0_{\alpha\alpha}(k,t) = -i\langle 0|T\alpha_k(t)\alpha_k^+(0)|0\rangle,$$
$$G^0_{\beta\beta}(k,t) = -i\langle 0|T\beta_k^+(t)\beta_k(0)|0\rangle \tag{26}$$

or

$$G^0_{\alpha\alpha}(k,\omega) = \frac{1}{\omega-\omega_k+i\delta}, \quad G^0_{\beta\beta}(k,\omega) = \frac{-1}{\omega+\omega_k-i\delta}. \tag{27}$$

We remark that α and β magnons carry opposite spin ($S^z = +1$ or -1).

The temperature dependent Green's function, in the Matsubara method, is obtained from the zero-temperature Green's function by replacing ω by $i\omega_n$, where $\omega_n = 2\pi nT$ and

$$\frac{1}{2\pi}\int \to iT\sum_n .$$

After performing the sum using $\sum_n (i\omega_n - x)^{-1} = (e^{x/T}-1)^{-1}/T$, a simple analytical continuation yields the frequency- and temperature-dependent Green's function.[17] The final result is

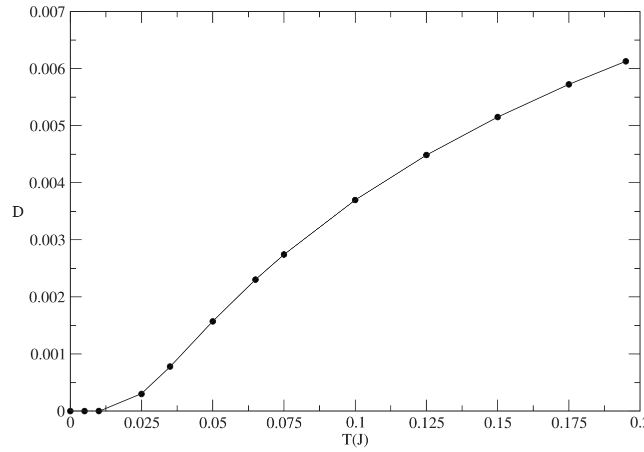

FIG. 1. Temperature dependence of the Drude weight D vs T for the one-dimensional model.

$$\Lambda(q=0,\omega) = G_2(\omega) = \frac{\lambda^4}{8}\int \frac{d^s k}{(2\pi)^s}\frac{\sin^2 k_x[1+2n(k)]}{\omega_k^2}\frac{1}{\omega - 2\omega_k}, \tag{28}$$

where $n(k) = (e^{\beta\omega_k}-1)^{-1}$ and $s=1,2$. The regular part of the conductivity is therefore given by

$$\sigma^{\text{reg}}(\omega) = \frac{\Lambda''(q=0,\omega)}{\omega} = \frac{\pi\lambda^4}{16}\int \frac{d^s k}{(2\pi)^s}\frac{[1+2n(k)]\sin^2 k_x}{\omega_k^3}\delta(\omega - 2\omega_k). \tag{29}$$

The delta function $\delta(\omega - 2\omega_k)$ accounts for two magnon excitations at energy ω_k.

III. CALCULATION OF THE DRUDE WEIGHT

To calculate D given by Eq. (13), we write Eq. (9) in the MSW formalism. After a straightforward calculation we find

$$\langle K\rangle = \frac{\lambda}{4}\sum_k \frac{\eta\gamma_k\cos k_x}{\omega_k}[1+2n(k)]. \tag{30}$$

From Eqs. (13), (28), and (30), we obtain

$$D = \frac{\eta^2\pi}{8T}\int \frac{d^s k}{(2\pi)^s}\frac{\gamma_k^2\sin^2 k_x}{\omega_k^2\sinh^2(\omega_k/2T)}. \tag{31}$$

For small values of the temperature we obtain in one dimension $D \propto \sqrt{T}\exp(-m/T)$. The behavior of D as a function of temperature, for the one- and two-dimensional models, is shown in Figs. 1 and 2. As we can see, at finite temperature the transport is ballistic characterized by a finite Drude weight. Assuming that the interactions are unimportant, the Drude peak vanishes at $T=0$ because at zero temperature there are no carriers (thermally excited spin waves) available to transmit the current. In the case of electrical conduction in three dimensions, where carriers are electrons, if $D=0$ at $T=0$, D remains zero at $T>0$, but in the model studied here, D

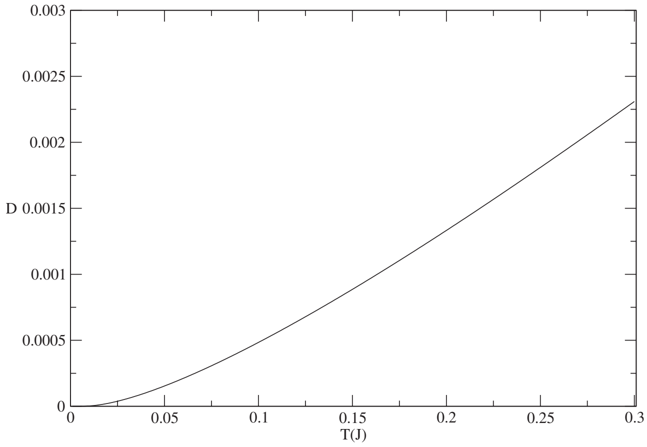

FIG. 2. Temperature dependence of the Drude weight D vs T for the two-dimensional model.

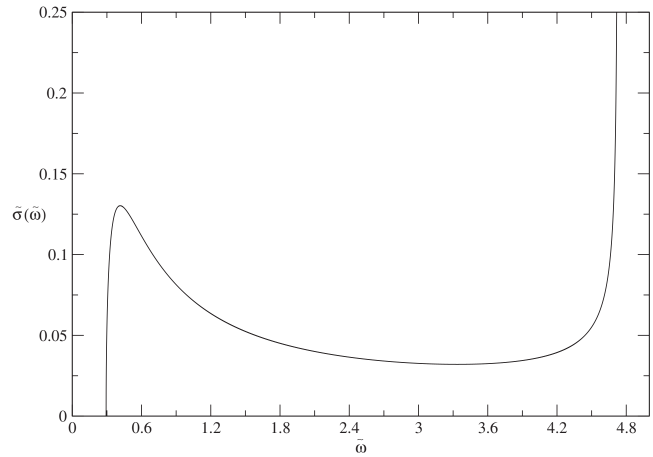

FIG. 3. Regular part of the spin conductivity $\tilde{\sigma}(\tilde{\omega})$ as a function of $\tilde{\omega}=\omega/m$ for the one-dimensional model at $T=0$.

becomes finite at finite T, turning a $T=0$ spin insulator to an ideal spin conductor. This is a characteristic of several prototype magnetic models used to describe one-dimensional (1D) materials, showing ideal transport properties (dissipationless) even at high temperature. Zotos and Prelovsek[4] pointed out that this phenomenon is the quantum analog of transport by nondecaying pulses (solitons) in 1D classical nonlinear integrable systems. Giamarchi[18] attributes this effect to the existence of (hidden) conservation laws that become impossible to relax the currents to zero. These arguments are valid in one dimension only. Up to our knowledge there is no similar explanation for the ballistic behavior in the two-dimensional model.

This behavior is in contrast to the one shown by a normal metallic system. This latter system shows a finite Drude weight at zero temperature. As the temperature rises, the zero-frequency Drude δ function broadens to a peak of width of order $1/\tau$, where τ is a characteristic scattering time.[4] In the low-dimensional antiferromagnet studied here, this broadening with temperature does not occur.

Our result for the one-dimensional model is in accordance with Konik,[9] where D is computed using a truncated form-factor expansion for the O(3) nonlinear sigma model. Probably, D decays at high T, for temperatures larger than the exchange coupling J, as a consequence of diffusive behavior. Karadamoglou and Zotos[19] calculated numerically the spin conductivity of the spin-1 antiferromagnetic chain in the high-temperature limit and found that D appeared to be equal to zero (up to numerical precision). Our calculation is not valid in this limit.

IV. REGULAR CONTRIBUTION

This is the continuum contribution to σ. In one dimension we can solve the integral (29) exactly and obtain

$$\sigma^{\text{reg}}(\omega) = \frac{\lambda^2}{16\eta^2}[1+2n(\omega/2)]\theta(|\omega|-2m)\frac{1}{\omega^2}\sqrt{\frac{\omega^2-4m^2}{4\lambda^2-\omega^2}}. \tag{32}$$

The regular part vanishes for $\omega<2m$ and diverges at the maximum two-magnons energy ($\omega=2\lambda$). This singularity will be rounded out when higher order corrections will be included. These corrections are quite complex and, we believe, will not modify significantly the results we have obtained. In Fig. 3, we show $\tilde{\sigma}(\tilde{\omega})$, where $\sigma^{\text{reg}}(\omega)=(\lambda^2m^2/16\eta^2)\tilde{\sigma}(\tilde{\omega})$, $\tilde{\omega}=\omega/m$, as a function of $\tilde{\omega}$, for the one-dimensional case, at $T=0$. In this case m is finite even at $T=0$.

In two dimensions, for small values of ω, we can use the small k limit to write $\omega_k=\sqrt{m^2+c^2k^2}$, with $c=\lambda\eta/\sqrt{2}$. The integral in Eq. (29) can then be evaluated analytically in the small ω limit. We find for the regular part of the spin conductivity in this limit

$$\sigma^{\text{reg}}(\omega) = \frac{1}{8\eta^4}[1+2n(\omega/2)]\theta(|\omega|-2m)\left(\frac{\omega^2-4m^2}{4\omega^2}\right). \tag{33}$$

In two dimensions m vanishes at $T=0$ and $\sigma^{\text{reg}}(\omega)$ is a constant, $\sigma^{\text{reg}}(\omega)=1/32$, for ω near 0. For general values of ω, Eq. (29) can be solved numerically. Qualitatively, the behavior of $\sigma^{\text{reg}}(\omega)$ is similar to the one of other 2D gapped systems.[10]

Sentef *et al.*[10] used the standard spin-wave theory to study the anisotropic 2D antiferromagnet. This theory works in the easy-axis region for any temperature, but in the isotropic limit it can be applied only at $T=0$ (the model is in the Néel phase at $T=0$ in two dimensions). On the other hand, the MSW was developed to treat the isotropic one- and two-dimensional antiferromagnets at zero and finite temperatures.

V. CONCLUSIONS

We have studied the spin conductivity of one- and two-dimensional Heisenberg antiferromagnets using the modified spin-wave approach and the Kubo formalism. The magnetization transport arises from two-magnon processes, and the models show unconventional ballistic spin transport at finite temperatures. For the 2D antiferromagnet the spin conductivity remains finite in the dc limit, at zero temperature, while for the 1D case the regular part of the conductivity is suppressed at low frequencies. As pointed out in Ref. 10, spin conductivity can be determined by measurements of magnetization currents. Possible experimental techniques were proposed in Ref. 20 and appear experimentally feasible. NMR can also be used to study spin transport. The spin dynamics of the $S=1$ one-dimensional antiferromagnet $AgVP_2S_6$ has been investigated using this technique,[21] but the experiment was performed at elevated temperatures where the behavior is diffusive. Magnetic compounds are important experimental systems for the study of low-dimensional quantum transport and new compounds certainly will be developed in the future.

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[1] B. Trauzettel, P. Simon, and D. Loss, Phys. Rev. Lett. **101**, 017202 (2008).
[2] F. H. Meisner, A. Honecker, and W. Brenig, Eur. Phys. J.: Appl. Phys. **151**, 135 (2007).
[3] K. R. Thurber, A. W. Hunt, T. Imai, and F. C. Chou, Phys. Rev. Lett. **87**, 247202 (2001).
[4] X. Zotos and P. Prelovsek, *Strong Interactions in Low Dimensions* (Kluwer, Dordrecht, 2004), Chap. 11; X. Zotos, J. Phys. Soc. Jpn. **74**, 173 (2005).
[5] F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).
[6] N. M. R. Peres, P. D. Sacramento, D. K. Campbell, and J. M. P. Carmelo, Phys. Rev. B **59**, 7382 (1999).
[7] X. Zotos and P. Prelovsek, Phys. Rev. B **53**, 983 (1996).
[8] S. Sachdev and K. Damle, Phys. Rev. Lett. **78**, 943 (1997).
[9] S. Fujimoto, J. Phys. Soc. Jpn. **68**, 2810 (1999); R. M. Konik, Phys. Rev. B **68**, 104435 (2003).
[10] M. Sentef, M. Kollar, and A. P. Kampf, Phys. Rev. B **75**, 214403 (2007).
[11] K. Damle and S. Sachdev, Phys. Rev. B **56**, 8714 (1997).
[12] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II* (Springer-Verlag, New York, 1985).
[13] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[14] M. Takahashi, Phys. Rev. B **40**, 2494 (1989).
[15] A. S. T. Pires and M. E. Gouvea, J. Magn. Magn. Mater. **241**, 315 (2002); A. F. Albuquerque, A. S. T. Pires, and M. E. Gouvêa, Phys. Rev. B **72**, 174423 (2005).
[16] J. E. Hirsch and S. Tang, Phys. Rev. B **40**, 4769 (1989); S. Tang, M. E. Lazzouni, and J. E. Hirsch, *ibid.* **40**, 5000 (1989); M. Takahashi, Phys. Rev. Lett. **58**, 168 (1987).
[17] G. D. Mahan, *Many Particles Physics* (Plenum, New York, 1990).
[18] T. Giamarchi, *Quantum Physics in One Dimension* (Clarendon, Oxford, 2004).
[19] J. Karadamoglou and X. Zotos, Phys. Rev. Lett. **93**, 177203 (2004).
[20] F. Meier and D. Loss, Phys. Rev. Lett. **90**, 167204 (2003).
[21] M. Takigawa, T. Asano, Y. Ajiro, M. Mekata, and Y. J. Uemura, Phys. Rev. Lett. **76**, 2173 (1996).