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Low-temperature spin transport in a $S = 1$ one-dimensional antiferromagnet

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Abstract
We study spin transport in the insulating antiferromagnet with $S = 1$ in one dimension. The spin conductivity is calculated, at zero temperature, using a modified spin wave theory and the Kubo formalism, within the ladder approximation. Two-magnon processes provide the dominant contribution to the spin conductivity. At finite temperature, free magnons are activated, and turn the system into a perfect spin conductor, i.e., the spin conductivity has a Drude form with infinite scattering time.

1. Introduction

As is well known, the low-temperature properties of the one-dimensional quantum antiferromagnet (1DAF) depend on the spin value S [1]. For integer spin values, the model exhibits a non-magnetic singlet ground state well separated from the first excited triplet state by an energy gap m, whereas the excitation spectrum is expected to be gapless for half-integer spin values. The integer spin case has been studied mainly using the mapping to the one-dimensional quantum O(3) non-linear sigma model (NLSM) [2]. The NLSM is a highly nontrivial field theory and it is often approximated using other models.

The standard spin wave formalism is unsuitable for treating the 1DAF due to the divergence of quantum fluctuations. However, a modified spin wave theory (MSW) for the low-dimensional Heisenberg antiferromagnet, closely related to the Schwinger boson formalism of Arovas and Auerbach [3], was formulated by Takahashi [4] 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. Results obtained using the MSW formalism agree with those obtained with the NLSM. The dynamics of the 1DAF with spin $S = 1$ was studied by Pires and Gouvea using the MSW technique [5].

Although the thermodynamics of the 1DAF model is now well understood, there are still open questions regarding spin transport. Sachdev and Damle [6] showed that a semiclassical analysis of the 1D NLSM gives a diffusive behavior. However, Fujimoto and Kawakami [7] studying the same model, using the Bethe ansatz method, found that the spin transport at finite temperatures is ballistic and therefore there is no spin diffusion in this system. Buragohain and Sachdev [8] criticized the approach used by Fujimoto and Kawakami, claiming that the calculation of the Drude weight from the finite size spectrum might not give the correct thermodynamic limit at finite temperatures. Fujimoto, in a subsequent paper [9], studied the spin–spin correlation function using the $1/N$ expansion method for the NLSM. He found that a cancelation of the self-energy corrections with vertex corrections of the Green function leads to a ballistic behavior of the spin–spin correlation function. He concluded that the quasiparticle damping did not give rise to a diffusive behavior, if one takes into account the vertex corrections which preserve the current conservation law. He attributed the spin diffusion observed experimentally [10] in the $S = 1$ 1DAF $AgVP_2S_6$ to spin–phonon interactions. The result of Fujimoto was confirmed by Konik [11], who also found a ballistic behavior for the 1D NLSM using a truncated ‘form factor’ expansion. Konik found as well no additional regular contribution to the spin conductivity near $\omega = 0$—only the Drude term was present. He obtained, however, a regular contribution for $\omega > 2m$, even in the zero-temperature limit. He pointed out that it was the integrability of the NLSM and the existence of an infinite number of conserved quantities that leads to a finite Drude weight. But the subject is still controversial. Karadamoglou and Zotos [12] using the exact diagonalization and microcanonical Lanczos method obtained a diffusive, rather than ballistic behavior, in the high-temperature limit of the $S = 1$ 1DAF.

The study of spin transport is also important for understanding the relaxation and non-equilibrium phenomena in strongly correlated electron systems [13]. Practical applications in spintronics have also been proposed [14]. In the present paper we extend early results [15] and consider the effect of magnon–magnon interactions. We calculate the spin conductivity for the 1DAF using the MSW approach and the Kubo formula for transport.

2. Spin conductivity

Spin currents flow in response to a magnetic field gradient. Therefore, we will add to the Hamiltonian

$$H = J\sum_n \vec{S}_n \cdot \vec{S}_{n+1}, \tag{1}$$

an external space and time dependent magnetic field $B(x,t)$ applied along the z-direction. We assume a magnetic field gradient along the x direction.

From the continuity equation

$$j_{n+1} - j_n = -\frac{\partial S_n^z}{\partial t}, \tag{2}$$

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

$$j_x(l) = \frac{\mathrm{i}J}{2}(S_l^+ S_{l+1}^- - S_l^- S_{l+1}^+), \tag{3}$$

where $l+1$ is the nearest-neighbor site of site l in the positive x direction. The spin current response to an external magnetic field gradient is given by [16]

$$\langle j(q,\omega)\rangle = \chi_{jS}(q,\omega)h(q,\omega), \tag{4}$$

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

$$\chi_{jS}(q,\omega) = \frac{\mathrm{i}}{N}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle[j(q,t), S^z(-q,0)]\rangle. \tag{5}$$

From equations (2)–(4) we obtain

$$\langle j(\vec{q},\omega)\rangle = \frac{K(q,\omega)}{\omega} q_x h(\vec{q},\omega), \tag{6}$$

where the current response function is defined by

$$K(q,\omega) = \langle K\rangle + \Lambda(q,\omega), \tag{7}$$

with

$$\langle K\rangle = \frac{J}{\hbar N}\sum_n \langle S_n^+ S_{n+a}^- + S_n^- S_{n+a}^+\rangle, \tag{8}$$

and

$$\Lambda(q,\omega) = \frac{\mathrm{i}}{N}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle[j(q,t), j(-q,0)]\rangle. \tag{9}$$

The current–current correlation function $\Lambda(q,\omega+\mathrm{i}0^+)$ is analytic in the upper half of the complex ω-plane and the extrapolation along the imaginary axis can be reliably done.

In the Kubo formalism [17], the frequency dependent spin conductivity $\sigma(\omega)$ is given by

$$\sigma(\omega) = (g\mu_B)^2 \lim_{q\to 0}\frac{K(q,\omega)}{\mathrm{i}(\omega + \mathrm{i}0^+)}. \tag{10}$$

The real part of the conductivity can be written as

$$\sigma'(\omega) = \sigma_0(\omega) + \sigma^{\mathrm{reg}}(\omega), \tag{11}$$

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

$$D = -\pi \lim_{\omega\to 0, q\to 0} K'(q,\omega). \tag{12}$$

The regular part is given by

$$\sigma^{\mathrm{reg}}(\omega) = \frac{1}{\omega}P(\omega), \tag{13}$$

where

$$P(\omega) = \lim_{q\to 0}\Lambda''(q,\omega). \tag{14}$$

The regular part, $\sigma^{\mathrm{reg}}(\omega)$, 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, i.e. the system is a perfect conductor with an infinite static conductivity. The Drude weight is a probe for transport properties; it measures the ability of the system to sustain a current without dissipation.

We can also define a spin stiffness by [18]

$$\rho = \lim_{q\to 0, \omega\to 0} K(q,\omega). \tag{15}$$

The spin stiffness corresponds to a time independent spiral twist of the spins in the limit that the wavelength of the spiral becomes infinitely large. If the system has long-range spin correlations, ρ is finite; otherwise it is zero [18].

Using the continuity equation we find [19, 20]

$$P(\omega) = \lim_{q\to 0}\frac{\omega}{2}(1 - \mathrm{e}^{-\beta\omega})\frac{S(q,\omega)}{q^2}, \tag{16}$$

where $S(q,\omega)$ is the dynamic structure factor for the spin–spin correlation function. Let us suppose that we have diffusion. In this case we can write [19]

$$S(q,\omega) = \frac{2\chi\omega}{1 - \mathrm{e}^{-\beta\omega}}\frac{\mathsf{D}q^2}{(\mathsf{D}q^2)^2 + \omega^2}, \tag{17}$$

where D is the spin diffusion coefficient and χ is the uniform susceptibility. From equations (12), (16) and (17) and using the fact that ρ is zero for the 1DAF, we can show that spin diffusion implies the vanishing of the Drude weight [19].

3. Modified spin wave theory

In the MSW formalism the constraint of zero sublattice magnetization is introduced in the Hamiltonian through a Lagrangian multiplier. The diagonalization of the quadratic part leads to a spin wave energy that has a gap, in agreement with the Haldane conjecture. The results of the MSW and Schwinger boson methods are qualitatively similar and the choice of one method over the other is largely a question of taste [21]. Following [4], we define boson operators in each sublattice according to

$$S_n^+ = \sqrt{2S}a_n, \qquad S_n^- = \sqrt{2S}a_n^+, \tag{18}$$

for the spin up sublattice, and by

$$S_m^+ = \sqrt{2S}b_m^+, \qquad S_m^- = \sqrt{2S}b_m, \tag{19}$$

for the spin down sublattice. Taking the Fourier transform and following [4], we introduce the following Bogoliubov transformation:

$$a_k = u_k\alpha_k + v_k\beta_k^+, \qquad b_k = u_k\beta_k + v_k\alpha_k^+, \tag{20}$$

where the coefficients u_k and v_k are given by

$$u_k = \sqrt{\frac{\lambda+\omega_k}{2\omega_k}}, \qquad v_k = \sqrt{\frac{\lambda-\omega_k}{2\omega_k}}, \tag{21}$$

with

$$\omega_k = \lambda\sqrt{1-\eta^2\cos^2 k}. \tag{22}$$

The temperature dependent parameters λ and η are obtained by solving simultaneously the self-consistent equations

$$S+\frac{1}{2} = \frac{1}{N}\sum_k \frac{1}{2(1-\eta^2\cos^2 k)^{1/2}} \times \coth\left[\frac{\lambda}{2T}(1-\eta^2\cos^2 k)^{1/2}\right], \tag{23}$$

$$\frac{\eta^2\lambda}{2J} = \frac{1}{N}\sum_k \frac{\eta^2\gamma_k^2}{2(1-\eta^2\cos^2 k)^{1/2}} \times \coth\left[\frac{\lambda}{2T}(1-\eta^2\cos^2 k)^{1/2}\right]. \tag{24}$$

The temperature dependence of λ and η is discussed in [4].

4. Green function formalism

4.1. Basic theory

From equations (3), (19) and (20) the spin current $j_0 = \sum_l j_x(l)$ can be written as

$$j_0 = \frac{\lambda^2}{2}\sum_k \frac{\sin k}{\omega_k}[\eta\cos k(\alpha_k^+\alpha_k + \beta_k^+\beta_k) - (\alpha_k^+\beta_k^+ + \alpha_k\beta_k)]. \tag{25}$$

We have to add to j_0 a term coming from the four-magnon term in the Hamiltonian. All the details of the calculations are presented in [16, 22–24]. In those references the calculations were performed in 3D and 2D using the standard spin wave procedure, but the details are the same as for the one used for the MSW. We refer the reader to those references and present here only the final result. We remark that only multimagnon excitations with vanishing total momentum contribute to the spin conductivity.

Following the cited references, we start with the spin current Green function defined by

$$G_j(t) \equiv -\frac{\mathrm{i}}{\hbar N}\langle 0|Tj(t)j(0)|0\rangle, \tag{26}$$

where T is the time ordering operator and $|0\rangle$ is the ground state. The magnon propagators are

$$\begin{aligned} G_{\alpha\alpha}(k,t) &= -\mathrm{i}\langle 0|T\alpha_k(t)\alpha_k^+(0)|0\rangle, \\ G_{\beta\beta}(k,t) &= -\mathrm{i}\langle 0|T\beta_k^+(t)\beta_k(0)|0\rangle, \end{aligned} \tag{27}$$

while the Fourier-transformed propagators for the free magnons have the formula

$$G^0_{\alpha\alpha}(k,\omega) = \frac{1}{\omega-\omega_k+\mathrm{i}\delta}, \qquad G^0_{\beta\beta}(k,\omega) = \frac{-1}{\omega+\omega_k-\mathrm{i}\delta}. \tag{28}$$

After a straightforward calculation we obtain

$$G_j(\omega) = \frac{\lambda^4}{4}\sum_{k,k'}\frac{\sin k\sin k'}{\omega_k\omega_{k'}}\Pi_{kk'}(\omega), \tag{29}$$

where

$$\Pi_{kk'}(t) = -\mathrm{i}\langle 0|T\alpha_k(t)\beta_k(t)\alpha_{k'}^+(0)\beta_{k'}^+(0)|0\rangle, \tag{30}$$

is the two-magnon Green function. From now on the calculation is very long, but all the steps can be found in [16, 22]. The final result is

$$\Pi_{kk'}(\omega) = \mathrm{i}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{2\pi}G_{\alpha\alpha}(k,\omega+\omega')G_{\beta\beta}(k,\omega')\Gamma_{kk'}(\omega,\omega'), \tag{31}$$

where $\Gamma_{kk'}(\omega,\omega')$ is the vertex function.

4.2. Noninteracting magnons

In a first step we neglect magnon–magnon interaction. In this case the calculations can be performed easily. This amounts to the replacement of the one-particle Green function, $G\to G^0$, and we obtain

$$G_j(\omega) = \frac{\lambda^4}{4}\sum_k\frac{\sin^2 k}{\omega_k^2}\Pi_{kk}(\omega), \tag{32}$$

where

$$\Pi_{kk}(\omega) = \mathrm{i}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{2\pi}G^0_{\alpha\alpha}(k,\omega+\omega')G^0_{\beta\beta}(k,\omega'). \tag{33}$$

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

$$\frac{1}{2\pi}\int \to \mathrm{i}T\sum_n.$$

After performing the sum using $\sum_n(\mathrm{i}\omega_n - x)^{-1} = (\mathrm{e}^{x/T}-1)^{-1}/T$, a simple analytical continuation yields the frequency and temperature dependent Green function [17]. The final result is

$$\Lambda(q=0,\omega) = G_j(\omega) = \frac{\lambda^4}{8}\int\frac{\mathrm{d}k}{2\pi}\frac{\sin^2 k[1+2n(k)]}{\omega_k^2} \times \frac{1}{\omega-2\omega_k}, \tag{34}$$

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

$$\sigma^{\mathrm{reg}}(\omega) = (g\mu_{\mathrm{B}})^2\frac{\Lambda''(q=0,\omega)}{\omega} = (g\mu_{\mathrm{B}})^2\frac{\pi\lambda^4}{16} \times \int\frac{\mathrm{d}k}{2\pi}\frac{[1+2n(k)]\sin^2 k}{\omega_k^3}\delta(\omega-2\omega_k). \tag{35}$$

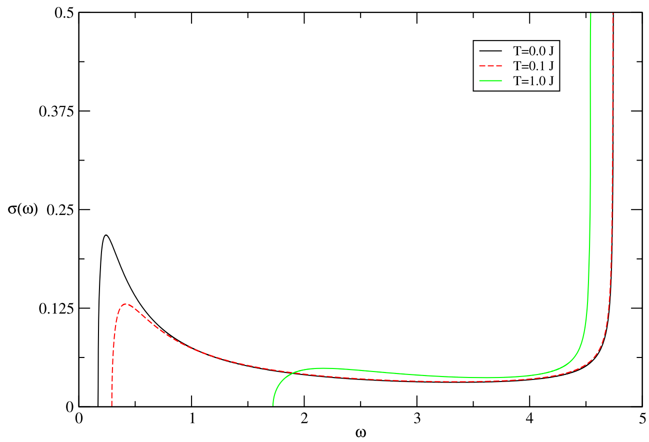

Figure 1. Regular part of the spin conductivity, for the noninteracting magnons, for three values of temperatures. (This figure is in colour only in the electronic version)

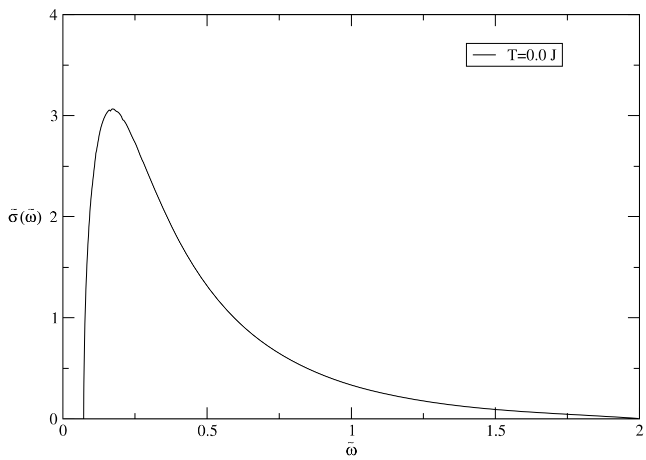

Figure 2. Regular part of the spin conductivity, at $T = 0$, within the ladder approximation.

The delta function $\delta(\omega - 2\omega_k)$ accounts for two-magnon excitations at energy ω_k. We can solve the integral (35) exactly and obtain

$$\sigma^{\mathrm{reg}}(\omega) = \frac{(g\mu_{\mathrm{B}})^2\lambda^2}{16\eta^2}[1 + 2n(\omega/2)]\theta(|\omega| - 2m)$$
$$\times \frac{1}{\omega^2}\sqrt{\frac{\omega^2 - 4m^2}{4\lambda^2 - \omega^2}}, \tag{36}$$

where $m = \lambda\sqrt{1 - \eta^2}$ is the gap. The regular part of the conductivity vanishes below a threshold frequency for $\omega < \omega_c$, where $\omega_c = 2m$ is the sum of the excitation gaps for an α magnon and a β magnon excitation. Above the threshold frequency α–β magnons can be created, and $\sigma^{\mathrm{reg}}(\omega)$ is finite. This means that propagating modes can be excited. $\sigma^{\mathrm{reg}}(\omega)$ diverges at the maximum two-magnon energy ($\omega = 2\lambda$). This singularity will be rounded out when higher-order corrections are included.

For $T \gg \omega$ we find

$$\sigma^{\mathrm{reg}}(\omega) = \frac{(g\mu_{\mathrm{B}})^2\lambda^2}{4\eta^2}\frac{T}{\omega^3}\sqrt{\frac{\omega^2 - 4m^2}{4\lambda^2 - \omega^2}}. \tag{37}$$

In figure 1 we show $\sigma^{\mathrm{reg}}(\omega)$ for the noninteracting model for three values of temperatures.

4.3. Drude weight

The Drude weight can be calculated using equation (12). We find

$$D = \frac{\eta^2\pi}{8T}\int\frac{\mathrm{d}k}{2\pi}\frac{\gamma_k^2\sin^2 k_x}{\omega_k^2\sinh^2(\omega_k/2T)}. \tag{38}$$

For small values of the temperature we obtain

$$D \propto \sqrt{T}\mathrm{e}^{-m/T}. \tag{39}$$

For $T \gg \omega_k$ we find $D \propto T$. It may appear peculiar that the 1DAF which is insulating at $T = 0$ turns into a perfect spin conductor at finite temperature. There are hidden conservation laws that make it impossible to relax the current to zero and thus the conductivity is infinite [25].

4.4. Ladder approximation

Treating the interactions within a ladder approximation for $T = 0$ [16] we find

$$\sigma^{\mathrm{reg}}(\omega) = -\frac{(g\mu_{\mathrm{B}})^2\lambda^2}{16\eta^2\tilde{\omega}}$$
$$\times \operatorname{Im}\frac{r^{(2)} - \lambda^{-1}(r^{(1)}r^{(1)} - r^{(0)}r^{(2)})}{1 + \lambda^{-1}(r^{(0)} + r^{(2)}) - \lambda^{-2}(r^{(1)}r^{(1)} - r^{(0)}r^{(2)})}, \tag{40}$$

where

$$r^{(m)} = \frac{2}{\pi}\int_0^{\pi}\mathrm{d}k\frac{\sin^2 k}{\varepsilon_k^m}\frac{1}{\tilde{\omega} - 2\varepsilon_k}, \tag{41}$$

and $\varepsilon_k = \sqrt{1 - \eta^2\cos^2 q}$, $\tilde{\omega} = \omega/\lambda$. The imaginary part of $r^{(m)}$ can be calculated analytically. We find

$$\operatorname{Im} r^{(m)}(\tilde{\omega}) = \frac{1}{\eta^2}\left(\frac{\tilde{\omega}}{2}\right)^{1-m}\sqrt{\frac{4(\eta^2 - 1) + \tilde{\omega}^2}{4 - \tilde{\omega}^2}}. \tag{42}$$

In figure 2 we show $\tilde{\sigma}^{\mathrm{reg}}(\tilde{\omega})$ as a function of $\tilde{\omega}$ within the ladder approximation. The magnon–magnon interaction removes the divergence of the noninteracting theory at $\omega = 2\lambda$. The behavior of $\tilde{\sigma}^{\mathrm{reg}}(\tilde{\omega})$ shown in figure 2 agrees qualitatively with the behavior of the conductivity of interacting fermions in a one-dimensional lattice as discussed by Giamarchi [25].

5. Conclusions

We have studied spin transport in the quantum one-dimensional antiferromagnet with $S = 1$. The spin conductivity was calculated, at zero temperature, using a modified spin wave theory and the Kubo formalism, within the ladder approximation. We have found a nonzero Drude weight at finite temperatures, indicating ballistic transport, in agreement with Fujimoto [9] and Konik [11]. As pointed out by Sentef [16], the spin conductivity can be determined experimentally by means of measurements of magnetization currents and appears experimentally feasible.

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