Journal of Magnetism and Magnetic Materials 468 (2018) 269–272

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Research articles

Transition to disordered phase and spin dynamics in the two-dimensional ferrimagnetic model

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A B S T R A C T

The effect of transition to disordered phase on AC conductivity in the two-dimensional frustrated ferrimagnetic model in the square lattice at $T = 0$ is investigated. The spin conductivity, $\sigma^{reg}(\omega)$ is determined for different values of frustration parameters J_{2S} and J_{2s} that separates the different phases such as the ferrimagnetic phase and the collinear phase. We obtain a small influence of this phase transition on spin conductivity. Furthermore, we present the behavior of the half-width of $S(\vec{q}, \omega)$ that gives the information about the scattering of magnons at long wavelength range.

1. Introduction

Frustration in quantum spin systems plays an important role in the understanding of physical properties of novel magnetic materials [1]. It can arise either due to the geometry of the lattice, as in the triangular and hexagonal lattices [2–8], or due to competing interactions, such as in the antiferromagnetic model in the square lattice with interactions on diagonal [9–11]. The main effects of frustrating interactions in the neighborhood of a Néel state are the increase of the coupling and the decreasing of the spin-wave velocity [12]. Another type of frustrated spin system is the spin chain mixed with different values of spins [13]. Brehemer et al. [14] has showed that the absolute ground state of this model has a ferrimagnetic long-range order. Moreover, he has obtained the low-lying excitations by using the spin wave theory (SWT) and quantum Monte Carlo method (QMC), where his results have been confirmed by Kolezhuk et al. [15] by using the matrix product approach. Besides, Yamamoto et al. [16] has used the modified spin wave theory (MSWT), the density matrix renormalization group method DMRG and quantum Monte Carlo method QMC to calculate the thermodynamic quantities. From an experimental point of view, results for magnetic and transport properties of Ni_xGe, that presents ferrimagnetic correlations, have been obtained in [17–30].

Although much has been learned about the properties independent on time of frustrated magnetic systems using both analytic and numerical tools, the dynamical properties of this model have not been well understood yet. The dynamic experiments such as inelastic neutron scattering NMR are the basic tools to determine the detailed nature of the interactions in these spin systems [31]. Being in an insulating magnet, the magnetization may be transported by excitations such as magnons without the transport of electric charge.

The spin transport has been studied since much time ago and it is well known that the spin conductivity is very sensitive to phase transitions [32]. An important question that must be answered in studies of spin transport is whether the spin transport in the system is ballistic or diffusive. The aim here is to verify the effect of the quantum phase transition from disordered phase to ferrimagnetic phase on spin transport in the ferrimagnetic model in the square lattice. The work is divided in the following way. In Section 2, we discuss about the model. In Section 3, we present the results using the linear spin wave approach. In the last section, Section 4, we present our conclusions and final remarks.

2. The model

The model in the ferrimagnetic phase is defined by the Hamiltonian [12]

$$\mathscr{H} = \sum_{i,j} J_{ij}\sigma_i \cdot \mathbf{s}_j. \tag{1}$$

$J_{ij} = J_1$ means the exchange interaction for the nearest neighbor in the x and y directions on the lattice. $J_{ij} = J_{2S}$ and $J_{ij} = J_{2s}$ are the two possibilities of frustrating coupling on diagonal. σ_i are the spins operators in the sublattice A that assume value $S = 1$ and s_i are the spins operators in the sublattice B that assume the value $s = 1/2$. The Holstein-Primakoff representation of spin operators expanded in first order in $1/S$ powers for the model is given as [33]

$$\begin{aligned} &\sigma_i^{+(A)} \simeq \sqrt{2S}\,a_i, \quad \sigma_i^{-(A)} \simeq \sqrt{2S}\,a_i^{\dagger},\\ &s_i^{+(B)} \simeq \sqrt{2s}\,b_i^{\dagger}, \quad s_i^{-(B)} \simeq \sqrt{2s}\,b_i,\\ &\sigma_i^{z(A)} = S - a_i^{\dagger}a_i, \quad s_i^{z(B)} = -s + b_i^{\dagger}b_i. \end{aligned} \tag{2}$$

a_i and b_i are boson operators for the sublattices A (up) and B (down)

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https://doi.org/10.1016/j.jmmm.2018.08.020
Received 3 January 2018; Received in revised form 8 June 2018; Accepted 9 August 2018
Available online 10 August 2018

respectively. We consider $J_1 > 0$ as the (nn) exchange interaction in the x and y directions, while $J_{2S} > 0$, $J_{2s} > 0$ the (nnn) exchange interactions along the diagonal directions. The Hamiltonian (1) can be written as [12]

$$\mathscr{H} = \mathscr{H}^0 + \mathscr{H}^1 \tag{3}$$

The classical ground state energy $\mathscr{H}^0$ and the contribution of the quadratic terms $\mathscr{H}^1$ are given as

$$\mathscr{H}^0 = -NJ_1 Ss\left[2-\alpha_1\left(\frac{S^2+s^2}{Ss}-\Delta\frac{S}{s}\right)\right], \tag{4}$$

$$\mathscr{H}^1 = J_1\sum_k \mathscr{A}_k a_k^\dagger a_k + \mathscr{B}_k b_k^\dagger b_k + \mathscr{C}_k(a_k b_k + a_k^\dagger b_k^\dagger), \tag{5}$$

where N is the number of sites of the lattice, being the approach used accurate in the limit of large N.

$$\mathscr{A}_k = 4S + 4(1-\Delta)\alpha_1 s[\cos k_x \cos k_y - 1], \tag{6}$$

$$\mathscr{B}_k = 4s + 4\alpha_1 S[\cos k_x \cos k_y - 1], \tag{7}$$

$$\mathscr{C}_k = 2\sqrt{Ss}[\cos k_x + \cos k_y]. \tag{8}$$

To simplify the equations, we define the parameters: $\alpha_1 = J_{2S}/J_1$ and $\alpha_2 = J_{2s}/J_1$. We consider two cases where the exchange interactions are $J_{2s} = (1-\Delta)J_{2S}$ and $J_{2S} = (1-\Delta)J_{2s}$. In the first case, Δ reinforces the frustration α_1 of the spins σ_i, while in the second case, Δ reinforces the frustration α_2 of the spins s_i.

The Hamiltonian in the diagonal form is given by

$$\mathscr{H} = J_1\sum_k [(\varepsilon_k^{(\alpha)}\alpha_k^\dagger\alpha_k + \varepsilon_k^{(\beta)}\beta_k^\dagger\beta_k) + \Lambda_k], \tag{9}$$

where α_k and β_k are the boson operators in the sublattices A and B respectively. We consider $\varepsilon_k^{(\alpha)} = \varepsilon_k^{(\beta)} = \varepsilon_k$ and

$$\Lambda_k = \left[\frac{\Delta_k}{2}(\Gamma_k - 1) + \frac{2C_k^2}{\varepsilon_k}\right], \tag{10}$$

$$\Delta_k = \mathscr{A}_k + \mathscr{B}_k \tag{11}$$

$$\Gamma_k = \frac{\Delta_k}{\varepsilon_k}. \tag{12}$$

The dispersion relation is given by

$$\varepsilon_k = \sqrt{\Delta_k^2 - 4\mathscr{C}_k^2}. \tag{13}$$

ε_k is monotonic into the first Brillouin zone $-\pi \leqslant k \leqslant \pi$. At zero temperature the system will be in a ground state; at higher temperatures one has a superposition of excited states. Moreover, the system considered here is infinite which is described most in the language of C*-algebras [34]. This is true for the Heisenberg model at nonzero temperature; but because we can explicitly describe the ground state of the Heisenberg model, we can avoid C*-allebgraic in this case. Even here, there are other ideas that are physically interesting such as the phenomenon of spontaneously broken symmetry, which require C*-algebras.

For the model for finitely many spins. Let Λ be a finite subset of $\mathbb{Z}^3$. For each $\alpha \in \Lambda$ we associate a copy of $\mathbb{C}^2$, calling it $\mathbb{C}^2_\alpha$. The Hilbert space for finitely many spins $\mathfrak{H}_A$, one at each point of Λ, is $\mathfrak{H}_A = \otimes_{\alpha\in A}\mathbb{C}^2_\alpha$. The set of vectors $\otimes_{\alpha\in\Lambda}e^{(\alpha)}$ is a basis for $\mathfrak{H}_A$.

3. Spin dynamics

The dynamical structure factor $S(\vec{q},\omega)$ or spectral function is defined as the Fourier transform of the time depend correlation function:

$$S(\vec{q},\omega) = \int_{-\infty}^{\infty} e^{-i\omega t}\langle\sigma_q(t)\cdot s_{-q}(0)\rangle dt. \tag{14}$$

It relates with the inelastic neutrons scattering experiments in the magnetic sample through the differential cross section of scattering.

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\vec{q},\omega), \tag{15}$$

where $\vec{q}$ and ω are the wavevectors of momentum and the energy of the spin excitations. For a particular wave-vector $\vec{q}$, the peak of the correlation function $S(\vec{q},\omega)$ occurring for a value of ω leads to energy of the magnetic excitation. Moreover, $S(\vec{q},\omega)$ is the probability that a magnon has momentum q and energy ω. For a free or noninteracting particle we have that $S(\vec{q},\omega)$ is just a delta function. When we compute $S(\vec{q},\omega)$ for interacting systems, we typically find the broad distribution. In this case, there is a band of ω values for each $\vec{q}$, because when the electron scatters, it has a finite mean free path and there is some uncertainty in its momentum or both. Thus, we must treat $\vec{q}$ and ω as separate variables and sum over them both when evaluating physical quantities.

Using the linear spin wave approximation, LSWT, we obtain the expression for $S(\vec{q},\omega)$ as

$$S(\vec{q},\omega) = \frac{\sqrt{Ss}}{4}u_q v_q[\delta(\omega-\varepsilon_q) + \delta(\omega+\varepsilon_q)] + \sum_k u_{k-q}^2 v_{k-q}^2\delta(\omega - 2\varepsilon_{k-q}), \tag{16}$$

where

$$u_k = \sqrt{\frac{\Delta_k+\varepsilon_k}{2\varepsilon_k}},\quad v_k = -\mathrm{sgn}(\varepsilon_k)\sqrt{\frac{\Delta_k-\varepsilon_k}{2\varepsilon_k}}. \tag{17}$$

The behavior of the half-width of the spectral function $S(\vec{q},\omega)$ is showed in Fig. 1. The first term in the Eq. (16) generates a contribution due to one magnon processes and the second term the contribution due to two magnon processes. Hence, the main contribution is due to the second term in the Eq. (16) (two magnon processes) since the first term generates only a thin line in the spectral function $S(\vec{q},\omega)$ and the half-width is zero in this case. We obtain an larger damping in the range of low $q = \|\vec{q}\|$ and therefore, a larger scattering of magnons in this range of long wavelength.

Another kind of spin dynamics in a magnetic system is the spin transport. The spin current responses to an external magnetic field h^z, where $h^z = g\mu_B B$ is $\langle\mathscr{J}\rangle = \sigma\nabla h^z$. Where we suppose the spin diffusion obeying the Fick's Law. In this case, the flow of spin current will go in the same direction of the gradient of external magnetic field, and if it is weak, it may be approached by the first term of the Taylor series. In the limit $\vec{q} \to 0$ we have that [35–39]

$$\langle\mathscr{J}(\vec{q},\omega)\rangle = -\frac{\langle\mathscr{K}\rangle - \mathscr{G}(\vec{q},\omega)}{i(\omega+i0^+)}iq_x h^z(\vec{q},\omega), \tag{18}$$

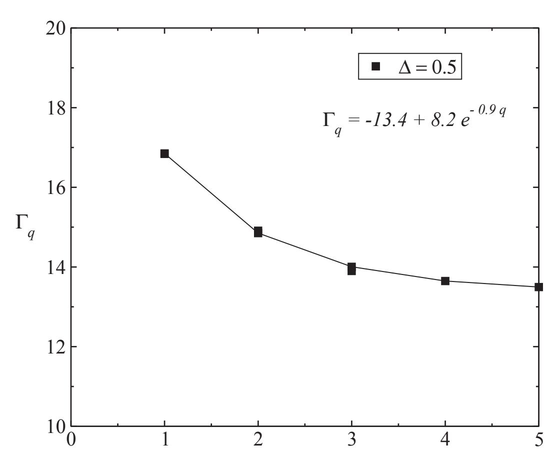

Fig. 1. Behavior of the half-width of magnons Γ_q, at $T = 0$, for values $\Delta = 0.5$ and $\alpha_{2c} = \alpha_c = 0.77$. We obtain a exponential decreasing in the damping of magnons with $q = \|\vec{q}\|$. We obtain an exponential fit to the data as indicated in the figure.