Solid State Communications 250 (2017) 49–52

Contents lists available at ScienceDirect

Solid State Communications

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

Communication

Influence of quantum phase transition on spin conductivity in the anisotropic three-dimensional ferromagnetic model

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A B S T R A C T

We use the SU(3) Schwinger boson formalism to study the spin transport in the three-dimensional S=1 Heisenberg ferromagnet in the cubic lattice with an easy plane crystal field, considering first-, second- and third-neighbor interactions. We have got one single peak for the spin conductivity for this system at $\omega = \omega_k$ and a variation of the height of the peak with the parameters D_c and η, and hence an influence of the quantum phase transition, between the disordered paramagnetic phase and the ordered ones, on the spin conductivity of this system. We have considered the exchange interaction J_1 as ferromagnetic and the interactions J_2 and J_3 as antiferromagnetic.

1. Introduction

The frustrated Heisenberg model is an important model in the actuality [1], where the study of the quantum phase transition (QPT) in quantum ferromagnets and antiferromagnets is an important subject in condensed matter physics. It is well known that the long range order of the spin system can be destroyed by frustration caused, for example, by second neighbor interactions and by geometry of the lattice [2–10].

On the other hand, the spin superfluidity is a phenomenon arising due to spontaneous breaking of the $U(1)$ symmetry in a spin system that is represented by the symmetry group $SU(2)$ of spin rotations about direction of the magnetic field. The Bose–Einstein condensation (BEC) of quasiparticles such as magnons and excitons whose number is not conserved is presently one of the most debated phenomena in condensed matter physics [11]. In atomic BEC and helium superfluid the symmetry breaking leads to a non-zero value of the superfluid rigidity or the superfluid density ρ_S, which enters into the non-dissipative supercurrent of quasi-particles and thus in the magnon supercurrent. The prototypical superfluid, liquid ^{4}He, is also a Bose–Einstein condensate. Although the two concepts, superfluidity and BEC, are not equivalent, nor is one necessarily a consequence of the other, they are intimately related. In the spintronics, the spin-superfluidity refers to the capacity for spin currents to be carried without dissipation by a metastable configuration of a magnetic condensate, rather than by an electron or magnon quasi-particle current.

Recently, the advances in the studies of pure spin currents which is a flow of spin angular momentum not accompanied by the electric current have opened new horizons for the emerging of new technologies based on the electron spin degree of freedom, such as spintronics and magnonics. The main advantage of pure spin current, as compared to the spin-polarized electric current, is the possibility to exert spin transfer torque on the magnetization in thin magnetic films without electrical current flowing through the material. In addition to minimizing Joule heating and electromigration effects, this characteristic enables the implementation of spin torque devices based on the low-loss insulating magnetic materials, and offers an unprecedented geometric flexibility [12].

The spin superfluidity and spin transport has also been studied a lot theoretically in the last years [11,13–21]. In the three-dimensional Heisenberg model we have that Sentef et al. [22] have studied the spin transport in this model using the standard spin wave theory and more recently the quantum frustrated three-dimensional XY model has been analyzed using the Schwinger boson approximation and diagrammatic expansion for Green's function [23].

Moreover, the gradients of the excited magnons wave function lead to spin superfluidity, that is the quantum transport of magnetization by magnons. From a general way, the spin transport properties of materials are the corner stones for many applications. Once having these properties been determined, it is possible to calculate the parameters for many devices which can operate on the basis of these structures. Recently, the transport phenomenon by magnetic excitations such as magnons, excitons and so on has been much studied due to its connection with spintronics [12,24–27]. The injection of a spin current into a magnetic film can generate a spin-transfer torque that acts on the magnetization collinearly to the damping torque [25].

From an experimental point of view, recently, there has been also

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http://dx.doi.org/10.1016/j.ssc.2016.11.014
Received 20 October 2016; Accepted 13 November 2016
Available online 16 November 2016

an intense research about the quantum spin Hall effect [24–27]. In these studies, often only sign differences between related quantities like magnetic fields and generated spin and charge currents can be determined. There has been also a large experimental effort in the generation and detection of spin (polarized) currents in the tentative to measure the spin current [24–28] with the aim to use the spin degree of freedom to improve electronic devices. In particular magnonic devices based not on the flow of electrical charges but on the flow of quantized excitations of the spin system (magnons and excitons) have been considered for the transmission and processing of information [28].

The aim of this paper is to study the spin transport in the three-dimensional frustrated ferromagnetic Heisenberg model on the cubic lattice with easy-plane anisotropy using the mean field Schwinger boson approach. This formalism has been shown to be very well successful, describing the magnetism in various quantum systems. Results qualitatively correct are mostly obtained even in the mean-field approximation. As pointed out by Timm and Jensen [29] there are basically two reasons why the Schwinger boson mean-field theory (SBMFT) works well even in low dimensions: first, since the bosonic spin degrees of freedom are integrated over a functional integral, the spin fluctuations are taken into account and second, this approach does not constitute an expansion around an ordered state, and thus works well for both ordered and disordered ground states.

This work is divided into the following way. In Section 2, we discuss about the method employed, in Section 3, we present the analytical results and in Section 4, is dedicated to our conclusions and final remarks.

The model that we are interested is defined by the following Hamiltonian:

$$\mathcal{H} = \sum_{\langle i,j\rangle} J_{ij}\vec{S}_i\cdot\vec{S}_j + D\sum_i (S_i^z)^2. \tag{1}$$

J_{ij} is the exchange constant, where $J_{ij} = J_1$ for the nearest-neighbor interaction, $J_{ij} = J_2$ for the second neighbor interactions on diagonal in plane and $J_{ij} = J_3$ for the inter-plane coupling on diagonal of the cubic lattice. We consider the value of spin S=1. The model is depicted in Fig. 1.

2. Schwinger boson approach

The SU(3) Schwinger boson formalism has been derived to treat systems with single ion anisotropy D by Papanicolau [30,31], being a generalization of the SU(2) formalism. In this formalism we choose the following basis:

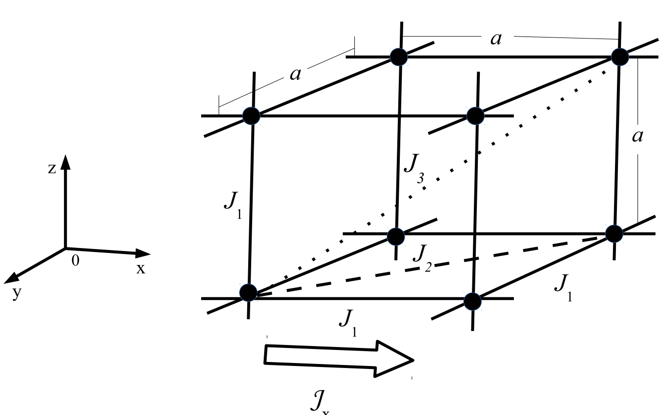

Fig. 1. Representation of the model with the direction of the flow of the spin current depicted, which flows in the x direction through a three-dimensional cubic lattice with diagonal inter-plane coupling J_3. We consider the lattice spacing a as a=1.

$$|1\rangle = \frac{1}{\sqrt{2}}(|y\rangle - i|x\rangle),\quad |-1\rangle = \frac{1}{\sqrt{2}}(|y\rangle + i|x\rangle),\quad |0\rangle = i|z\rangle,$$

where $|n\rangle$ are eigenstates of S^z. The spin operators are written via a set of three boson operators t_α ($\alpha = x, y, z$) defined as [32]

$$|x\rangle = t_x^\dagger|v\rangle,\quad |y\rangle = t_y^\dagger|v\rangle,\quad |z\rangle = t_z^\dagger|v\rangle, \tag{2}$$

where $|v\rangle$ is the vacuo state. We also impose the constraint condition $t_x^\dagger t_x + t_y^\dagger t_y + t_z^\dagger t_z = 1$.

The states $t_x^\dagger|v\rangle$ and $t_y^\dagger|v\rangle$ both consist of eigenstates $S^z = \pm 1$ and have the mean value $\langle S^z\rangle = 0$. This property will preserve the disorder of the ground state. To study disordered phases, it is convenient to introduce the other two bosonic operators $u^\dagger$ and $d^\dagger$ [32]:

$$u^\dagger = -\frac{1}{\sqrt{2}}(t_x^\dagger + it_y^\dagger),\quad d^\dagger = \frac{1}{\sqrt{2}}(t_x^\dagger - it_y^\dagger), \tag{3}$$

and so

$$|1\rangle = u^\dagger|v\rangle,\quad |0\rangle = t_z^\dagger|v\rangle,\quad |-1\rangle = d^\dagger|v\rangle, \tag{4}$$

with the constraint $u^\dagger u + d^\dagger d + t_z^\dagger t_z = 1$. The spin operators can be written in terms of the u and d operators as [32]

$$S^x = \frac{1}{\sqrt{2}}[(u^\dagger + d^\dagger)t_z + t_z^\dagger(u + d)],$$
$$S^y = \frac{1}{\sqrt{2}}[(u^\dagger - d^\dagger)t_z - t_z^\dagger(u - d)],\quad S^z = u^\dagger u - d^\dagger d. \tag{5}$$

We can write the Hamiltonian in the momentum space, in the diagonal form as [32]

$$\mathcal{H} = \sum_{\vec{k}}\omega_k(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k) + \sum_k(\omega_k - \Lambda_k) + C, \tag{6}$$

where

$$C = \frac{N(1-t^2)}{4}(z_1 - \eta z_2 - \alpha z_3) + N\mu(1-t^2) + N(-z_1p_1^2 - \eta z_2p_2^2 + \alpha z_3p_3^2). \tag{7}$$

The η and α parameters are defined as $\eta = J_2/J_1$ and $\alpha = J_3/J_1$, where $J_1 = 1$. The dispersion relation is given as

$$\omega_k = \sqrt{\Lambda_k^2 - \Delta_k^2} \tag{8}$$

where

$$\Lambda_k = -\tfrac{1}{2}(1-t^2)(-z_1 + \eta z_2 + \alpha z_3) + g_kt^2 + D - \mu, \tag{9}$$

$$\Delta_k = t^2g_k - f_k, \tag{10}$$

and

$$f_k = -z_1\gamma_{k_1}p_1 + \eta z_2\gamma_{k_2}p_2 + \alpha z_3\gamma_{k_3}p_3, \tag{11}$$

$$g_k = -z_1\gamma_{k_1} + \eta z_2\gamma_{k_2} + \alpha z_3\gamma_{k_3}. \tag{12}$$

where

$$\gamma_{k_1} = \tfrac{1}{3}[\cos(k_x) + \cos(k_y) + \cos(k_z)], \tag{13}$$

$$\gamma_{k_2} = \tfrac{1}{3}[\cos(k_x)\cos(k_y) + \cos(k_x)\cos(k_z) + \cos(k_y)\cos(k_z)], \tag{14}$$

$$\gamma_{k_3} = \cos(k_x)\cos(k_y)\cos(k_z). \tag{15}$$

The ground state energy per site is given by

$$e_0 = (1/N)\sum_k[\omega_k - \Lambda_k] + (1/N)C, \tag{16}$$

where the energy gaps occur at $\vec{k_0} = (\pi, \pi, \pi)$ or $\vec{k_0} = (0, \pi, \pi)$, $\Delta_{k_0} = \omega(\vec{k_0})$. A quantum phase transition between the large D phase ($D > D_c$) and the ordered phase occurs when the gap ω_{k_0} goes to zero at a specified wave-vector k_0. Replacing the sum by the integrals on the first Brillouin zone, the self-consistent equations can be written as [32]

$$\mu = \frac{1}{N}\sum_{\vec{k}}\frac{\Lambda_k - \Delta_k}{\omega_k} g(\vec{k})\coth\left(\frac{\beta\omega_k}{2}\right), \tag{17}$$

$$2 - t^2 = \frac{1}{N}\sum_{\vec{k}}\frac{\Lambda_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{18}$$

$$p_i = -\frac{1}{2N}\sum_{\vec{k}}\frac{\Lambda_k}{\omega_k}\gamma_{k_i}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{19}$$

with $i = 1, 2, 3$. The integration region is $[-\pi, \pi]$. At k_0, where the gap energy goes to zero, which indicates a phase transition from a large D phase to an ordered phase. When $D < D_c$ the system enters into the ordered state. We assume that the excitations are condensed at k_0. Keeping $\omega_0 = 0$, we solve the self-consistent equations in a Bose–Einstein condensation (BEC) that amounts to n_0 to be extracted. When D=0 the model presents two ordered phases at zero temperature: a ferromagnetic phase, characterized by $\vec{k}_F = (0, 0, 0)$; a collinear anti-ferromagnetic phase, characterized by $\vec{k}_{AF} = (0, 0, \pi)$ or $\vec{k}_{AF} = (0, \pi, 0)$ or $\vec{k}_{AF} = (\pi, 0, 0)$. Being in contrast to the classical J_1–J_2–J_3 antiferromagnetic Heisenberg model, the collinear antiferromagnetic phase is never stable in its ferromagnetic counterpart [32].

3. Quantum phase transition and transport properties

A gradient of magnetic field $\nabla\vec{B}$, through the system induces a spin current in the system. If we connect a low dimensional magnet with two bulk ferromagnets, they will act as reservoirs of spins [26,27]. One flow of a spin current appears, if there is a difference, $\nabla\vec{B}$, between the magnetic fields between the two ends of the sample. As we are interested in the calculus of the longitudinal spin conductivity, we will add an external magnetic field depending on space and time, $\vec{B}(x, t)$, applied along the axis $\hat{z}$, direction of the Hamiltonian equation (1).

In the Kubo formalism [22,33–35] the spin conductivity is given by the following formula:

$$\sigma(\omega) = \lim_{\vec{q}\to 0}\frac{\langle\mathcal{K}\rangle + \Lambda(\vec{q}, \omega)}{i(\omega + i0^+)}, \tag{20}$$

where $\langle\mathcal{K}\rangle$ is the kinetic energy and $\Lambda(\vec{q}, \omega)$ is the current–current correlation function, defined by

$$\Lambda(\vec{q}, \omega) = \frac{i}{\hbar N}\int_0^\infty dt e^{i\omega t}\langle[\mathcal{J}(\vec{q}, t), \mathcal{J}(-\vec{q}, 0)]\rangle. \tag{21}$$

$\Lambda(\vec{q}, \omega + i0^+)$ is analytic in the upper half of the complex plane and the extrapolation along the imaginary axis can be reliably done.

The continuity equation for the lattice allows us to write the discrete version of the spin current as

$$\mathcal{J}_{n+x} - \mathcal{J}_n = -\frac{\partial S_n^z}{\partial t}, \tag{22}$$

where $n + x$ is the nearest neighbor site of the site n in the positive x direction. The Heisenberg equation of motion, $\dot{S}_n^z = i[\mathcal{H}, S_n^z]$, can be used together with Eq. (22) to obtain the spin current operator as

$$\mathcal{J} = -\frac{J_1 t^2}{2}\sum_k\left[\frac{\sin k_x + \eta\sin(\sqrt{2}k_x) + \alpha\sin(\sqrt{3}k_x)}{\omega_k}\right](\alpha_k + \beta_k)(\alpha_k^\dagger + \beta_k^\dagger). \tag{23}$$

The real part of $\sigma(\omega)$, $\sigma'(\omega)$ can be written in the standard form as [34]

$$\sigma'(\omega) = \sigma_0(\omega) + \sigma^{reg}(\omega), \tag{24}$$

where $\sigma_0(\omega)$ gives a measure of the ballistic transport being given by $\sigma_0(\omega) = D_S\delta(\omega)$, where D_S is Drude's weight

$$D_S = \pi[\langle\mathcal{K}\rangle + \Lambda'(\vec{q} = 0, \omega \to \vec{0})]. \tag{25}$$

and $\sigma^{reg}(\omega)$, the regular part of $\sigma'(\omega)$, is given by [34]

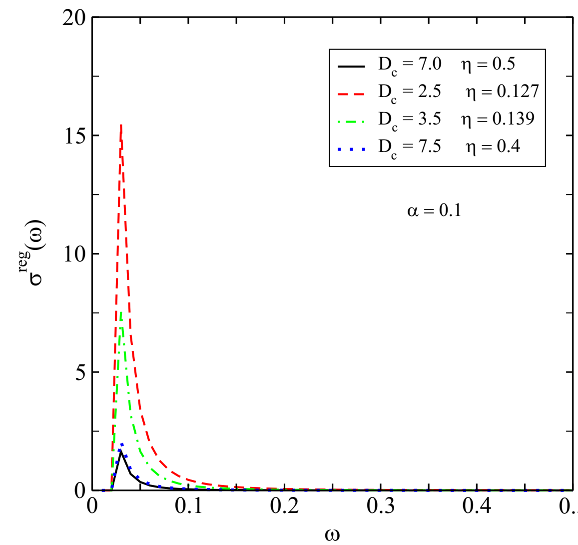

Fig. 2. Behavior of $\sigma^{reg}(\omega)$ for $\alpha = 0.1$ and different values of η and D_c. We have got a sudden change in the behavior of the spin conductivity in the neighbor of the quantum phase transition, or in the range where D_c tends to zero abruptly. We have obtained that the height of the peak changes abruptly at this range.

$$\sigma^{reg}(\omega) = \frac{\Lambda''(\vec{q} = 0, \omega)}{\omega}, \tag{26}$$

that represents the continuum contribution to the conductivity. In Eqs. (25) and (26), Λ' and Λ'' stand for the real and imaginary parts of Λ respectively.

Using Matsubara's Green's function, we obtain $\sigma^{reg}(\omega)$ as

$$\sigma^{reg}(\omega) = \frac{\Lambda(k = 0, \omega)}{\omega} = \frac{(g\mu_B)^2}{8\pi^2 w^3}\int_0^\pi\int_0^\pi\int_0^\pi d^3k[\sin k_x + \eta\sin(\sqrt{2}k_x) + \alpha\sin(\sqrt{3}k_x)]^2\delta(\omega - \omega_k). \tag{27}$$

In Figs. 2 and 3, we present the behavior of $\sigma^{reg}(\omega)$ with ω. As we can see, the behavior of the AC conductivity presents a single peak at $\omega = \omega_0$. The height of the peak varies with η and D_c parameters, where in the neighbor of the region where D_c falls to zero suddenly, the height

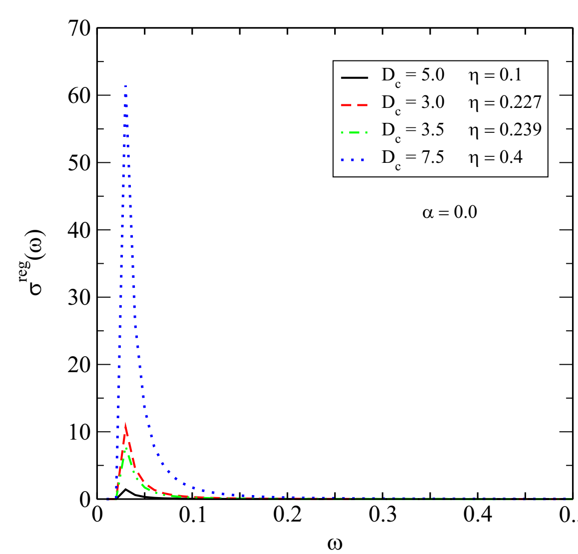

Fig. 3. Behavior of $\sigma^{reg}(\omega)$ for $\alpha = 0.0$ and different values of η and D_c. We have got a sudden change in the behavior of the spin conductivity in the neighbor of the range where D_c tends to zero abruptly and the system presents a quantum phase transition. We have found that the height of peak changes abruptly at this range indicating an influence of the QTP on spin conductivity.

of the peak suffers an abrupt change, indicating so an influence of the quantum phase transition induced by the frustration on the spin conductivity. We have also got the *AC* conductivity tending to zero in the *DC* limit ($\omega \to 0$) and for large values ω.

4. Conclusions and final remarks

In summary, we have studied the spin transport in the frustrated three-dimensional ferromagnetic Heisenberg model on the cubic lattice with an easy-plane crystalline field using the Schwinger boson approach. Our calculations show a small influence of the frustration parameters on the spin transport, and hence an influence of the phase transition on it. We have gotten a sudden variation of the height of the peak of the spin conductivity in the neighbor of the region where the D_c parameter falls suddenly to zero in the graphic D_c vs. η. The behavior of the *AC* spin conductivity is sensible so to behavior of D_c as a function of η (graphic of Ref. [32]), and hence we have found an influence of the QTP on the spin conductivity in this system. Experimental results for the spin transport can be compared with our theoretical results when available for the studied model.

Finally, we have that, recently, there has been a large experimental effort in the tentative to measure the spin current [24–28] with the aim to use the spin degree of freedom to improve electronic devices. In particular magnonic devices based not on the flow of electrical charges but on the flow of quantized excitations of the spin system (magnons and excitons) have been considered for the transmission and processing of information [28].

Acknowledgment

I am grateful to Brazilian agencies FAPEMIG, CEFET-MG and CNPq.

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