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Effect of quantum phase transition on spin transport in the spatially frustrated Heisenberg model

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ABSTRACT

We have used the Schwinger's boson theory to study the spin transport in the anisotropic two-dimensional spatially frustrated Heisenberg antiferromagnetic model in the square lattice. Our results show a sudden change in the *AC* spin conductivity $\sigma^{reg}(\omega)$ in the quantum phase transition point, where we have the gap of the system going to zero at critical point D_c=0. We have found a sudden change for a superconductor state in the *DC* limit $\omega \to 0$ independent of the value of the Drude's weight found in the quantum phase transition point. Away from it, we have obtained that the behavior of the spin conductivity changes for single peak at $\omega = \omega_p$ and in this case, $\sigma^{reg}(\omega)$ goes to zero in small ω and large ω limits.

1. Introduction

Quantum frustrated magnets have been an important subject in condensed matter physics. These have been studied using several techniques such as quantum Monte Carlo (QMC), Renormalization Group Density Matrix (DMRG) and so on [1]. One model that presents a particular interest is the two-dimensional Heisenberg model with antiferromagnetic exchange coupling J_1 and J_2. This model has been less studied for S=1 despite the potential relevance for the iron-pnictides [2,3]. For S=1, the Berry phases act in favor of the formation of spin chains singlets that can stack either along the x or y directions on the square lattice, yielding a twofold degenerate ground state [2].

Recently, a large experimental effort has been made in the tentative to measure the spin current with the aim to use the spin degree of freedom to improve electronic devices. Magnonic devices based not on the flow of electrical charges but on the flow of quantized excitations of the spin system, such as magnons and excitons, were proposed for the transmission and processing of information. Hence, the structures studied such as frustrated quantum spin systems promise to have various applications in spintronics [4–8]. Moreover, the spin superfluid transport is a phenomena well known since 30 year ago when it was discovered in ^{3}He superfluid [9,12,10,11,13]. The ^{3}He superfluid is an antiferromagnet where all magnetic properties including magnon Bose-Einstein condensation (BEC) and spin superfluidity are indeed the properties of a magnetically ordered system. Since ^{3}He has a small relaxation rate, this simplified the discovery of BEC and the spin supercurrent. Later, these phenomenas were also found in many other systems, like in antiferromagnets with the Suhl-Nakamura interaction [14] and YIG films [15], being the spin superfluidity in these systems generated by the gradients of the wave function of excited magnons. This is the quantum transport of magnetization by magnons.

Recently, the spin transport in the two-dimensional Heisenberg model has been studied theoretically, as for instance, in the Refs. [16-26]. Experimentally, there has been a growing interest in phenomena based on pure spin currents, which allow to move from charge to spin based logic gates [6], in addition to research of the quantum Hall effect for spins [4–8].

The model that we are interested is represented in the Fig. 1 and is defined by the Hamiltonian

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

where $J_{ij} = J_x$ for all horizontal bonds, $J_{ij} = J_y$ for the vertical bonds and $J_{ij} = J_2$ for the next-nearest neighbors in the diagonal. We consider the value of spin S=1 where the local spin order parameter $\langle \vec{S} \rangle$ has a quadrupole spin nematic order parameter [3]. The frustration here is due to a J different in the x and y directions in the square lattice. The isotropic model with D=0 has an ordered ground state. In the limit of large D, the model will be in a disordered ground state with total magnetization null separated by a gap from the first excited states, where there is a critical value D_c denoting a quantum phase transition describing the condensation of magnons, from the large D phase to an ordered phase. The quadupole phase presents no magnetic order, but has a nonzero quadrupole order parameter $Q = \langle S_z^2 - 2/3 \rangle$, where this order is different from the conventional paramagnetic state. For $D < D_c$ and positive, the system is in a gapless ordered Néel phase at T=0. Consequently, a quantum phase transition (QPT) takes place at $D = D_c$ [3].

The aim of this paper is to verify the influence of the quantum phase transition on the spin transport in the two-dimensional spatially frustrated Heisenberg model in the square lattice using the SU(3) Schwinger's boson approximation. Recently, we have obtained an

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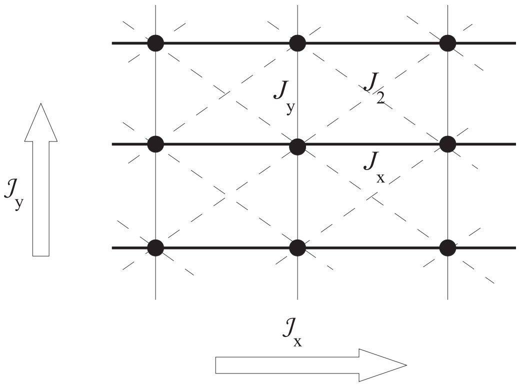

Fig. 1. Representation of a square lattice spatially anisotropic with J_x and J_y interactions. A flow of a spin current is depicted in the x and y directions in the square lattice.

influence of the QPT on the spin conductivity in other quantum frustrated spin systems [27–30]. The critical properties of this model were studied using this method in [3]. This work is divided in the following way. In Section 2 we discuss about the method employed, in Section 3, we develop the Kubo formalism of the linear response theory to calculate the spin conductivity for this model and in the last section, Section 4 is dedicated to our conclusions and final remarks.

2. SU(3) Schwinger boson approximation

The SU(3) Schwinger boson formalism is a generalization of the SU(2) formalism and has been derived to treat systems with single ion anisotropy by Papanicolau [31–33]. In this formalism is chosen the following basis for the eigenstates $|n\rangle$ of S^z

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

The spin operators are written via a set of three boson operators t_α ($\alpha = x, y, z$) defined by [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 vacuum state. We also impose the constraint condition $t_x^\dagger t_x + t_y^\dagger t_y + t_z^\dagger t_z = 1$.

In terms of the t operators, we can write the x, y and z components of the spin operators as

$$S^x = -i(t_y^\dagger t_z - t_z^\dagger t_y), \quad S^y = -i(t_z^\dagger t_x - t_x^\dagger t_z), \quad S^z = -i(t_x^\dagger t_y - t_y^\dagger t_x) \tag{3}$$

where $t_x^\dagger|v\rangle$ and $t_y^\dagger|v\rangle$ consist of eigenstates of $S^z = \pm 1$ and we have the mean value $\langle S^z\rangle = 0$. This property will preserve the disorder of the ground state. Is also convenient to introduce other two bosonic operators $u^\dagger$ and $d^\dagger$ [31] to study the disordered phases as

$$u^\dagger = -\frac{1}{\sqrt{2}}(t_x^\dagger + it_y^\dagger), \quad d^\dagger = \frac{1}{\sqrt{2}}(t_x^\dagger - it_y^\dagger), \tag{4}$$

thus

$$|1\rangle = u^\dagger|v\rangle, \quad |0\rangle = t_z^\dagger|v\rangle, \quad |-1\rangle = d^\dagger|v\rangle, \tag{5}$$

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

$$S^+ = \sqrt{2}(t_z^\dagger d + u^\dagger t_z), \quad S^- = \sqrt{2}(d^\dagger t_z + t_z^\dagger u), \quad S^z = u^\dagger u + d^\dagger d. \tag{6}$$

Substituting (6) into the Eq. (1) we obtain

$$\begin{aligned}\mathcal{H} = {}& \frac{J_{1x}}{2}\sum_{i,\delta_x} t^2[(d_i^\dagger d_{i+\delta_x} + u_{i+\delta_x}^\dagger u_i + u_i^\dagger d_{i+\delta_x} + d_i^\dagger u_{i+\delta_x}^\dagger + H.\,c.) \\ & + (u_i^\dagger u_i - d_i^\dagger d_i)(u_{i+\delta_x}^\dagger u_{i+\delta_x} - d_{i+\delta_x}^\dagger d_{i+\delta_x})] \\ & + \frac{J_{1y}}{2}\sum_{i,\delta_y} t^2\left[\left(d_i^\dagger d_{i+\delta_y} + u_{i+\delta_y}^\dagger u_i + u_i^\dagger d_{i+\delta_y} + d_i^\dagger u_{i+\delta_y}^\dagger + H.\,c.\right)\right. \\ & \left. + (u_i^\dagger u_r - d_i^\dagger d_i)\left(u_{i+\delta_y}^\dagger u_{i+\delta_y} - d_{i+\delta_y}^\dagger d_{i+\delta_y}\right)\right] \\ & + \frac{J_2}{2}\sum_{i,d} t^2[(d_i^\dagger d_{i+d} + u_{i+d}^\dagger u_i + u_i^\dagger d_{i+d} + d_i^\dagger u_{i+d}^\dagger + H.\,c.) \\ & + (u_i^\dagger u_i - d_i^\dagger d_i)(u_{i+d}^\dagger u_{i+d} - d_{i+d}^\dagger d_{i+d})] + D\sum_i (u_i^\dagger u_i - d_i^\dagger d_i) \\ & - \sum_i (u_i^\dagger u_i - d_i^\dagger d_i + t^2 - 1),\end{aligned} \tag{7}$$

where δ_x, δ_y and d, not showed in the Fig. 1, connect each site with the first neighbors on the x, y and diagonal directions respectively. Using the mean field theory, we can assume the chemical potential $\mu_i = \mu$ and the remaining terms, we make the mean field decoupling $\langle d_i^\dagger u_{i+\delta_x}^\dagger\rangle = \langle d_i u_{i+\delta_x}\rangle = p_x$, $\langle d_i^\dagger u_{i+\delta_y}^\dagger\rangle = \langle d_i u_{i+\delta_y}\rangle = p_y$, $\langle d_i^\dagger u_{i+d}^\dagger\rangle = \langle d_i u_{i+d}\rangle = \tilde{p}$. In following we make the Fourier transformation followed by the Bogoliubov transformation

$$u_k = \chi_k\alpha_k - \rho_k\beta_k^\dagger, \quad d_k = \chi_k\beta_{-k} - \rho_k\alpha_{-k}^\dagger \tag{8}$$

with

$$\chi_k = \sqrt{\frac{\Lambda_k + \omega_k}{2\omega_k}}, \quad \rho_k = \sqrt{\frac{\Lambda_k - \omega_k}{2\omega_k}}. \tag{9}$$

Moreover, we make the supposition that the t_z bosons are condensed, i.e. $\langle t_z\rangle = \langle t_z^\dagger\rangle = t$. After the steps above, we obtain the Hamiltonian in the diagonal form as [32]

$$\mathcal{H} = \sum_k \omega_k(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k) + \sum_k(\omega_k - \Lambda_k) + C. \tag{10}$$

The temperature dependent chemical potential μ_i is introduced together with the local constraint $S_i^2 = S(S+1) = 2$. The α and η parameters are defined as $\alpha = J_x/J_y$, $\eta = J_2/J_x$ and the dispersion relation of the excitons is given as

$$\omega_k = \sqrt{\Lambda_k^2 - \Delta_k^2}, \tag{11}$$

$$\Lambda_k = -\mu + D + (1 - t^2)(1 + \alpha + 2\eta) + 4t^2 g(k_x, k_y), \tag{12}$$

$$\Delta_k = 4t^2 g(k_x, k_y) - 2(\alpha p_x\cos k_x + p_y\cos k_y) - 4\eta\tilde{p}\tilde{\gamma}_k, \tag{13}$$

where z is the coordinator number and

$$\gamma_k = \frac{1}{2}(\alpha\cos k_x + \cos k_y), \tag{14}$$

$$\tilde{\gamma}_k = \cos k_x\cos k_y, \tag{15}$$

$$g(k_x, k_y) = \gamma_k + \eta\tilde{\gamma}_k, \tag{16}$$

$$C = \mu N(1 - t^2) - \frac{N(1 + \alpha)(1 - t^2)^2}{2 + \eta} + 2N(\alpha p_x^2 + p_y^2 + \tilde{p}^2). \tag{17}$$

N is the number of sites of the lattice. The t^2, μ, p_x, p_y and $\tilde{p}$ parameters are given by the self-consistent equations Ref. [3]

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

$$\mu = \frac{4}{N}\sum_k \frac{\Lambda_k - \Delta_k}{\omega_k} g(k_1, k_2)\coth\left(\frac{\beta\omega_k}{2}\right), \tag{19}$$

$$p_x = -\frac{1}{2N}\sum_k \frac{\Delta_k\cos k_x}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{20}$$

$$p_y = -\frac{1}{2N}\sum_k \frac{\Delta_k \cos k_y}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{21}$$

$$\tilde{p} = -\frac{1}{2N}\sum_k \frac{\Delta_k \tilde{\gamma}_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right). \tag{22}$$

The above equations are solved numerically [32]. The critical parameter D_c is the value of D where the excitation gap goes to zero signaling the QPT.

3. Quantum phase transition and Spin Transport

We use the SU(3) Schwinger's boson approach with objective to determine the regular part of the spin conductivity (*AC* conductivity) or continuum conductivity at T=0. A flow of spin current appears if there is a difference $\Delta\vec{B}$ between two magnetic fields at the two ends of the sample [5,4].

In the Kubo formalism [34,35,17,19] of spin transport, the components of the spin conductivity tensor are given by

$$\sigma_{\alpha\alpha}(\omega) = \lim_{\vec{q}\to 0}\frac{\langle\mathcal{K}\rangle + \Lambda_{\alpha\alpha}(\vec{q},\omega)}{i(\omega + i0^+)}, \tag{23}$$

where $\alpha = x, y$. $\langle\mathcal{K}\rangle$ is the kinetic energy and $\Lambda_{\alpha\alpha}(\vec{q},\omega)$ is the current-current correlation function defined as

$$\Lambda_{xx}(\vec{q},\omega) = \frac{i}{\hbar N}\int_0^\infty dte^{i\omega t}\langle[\mathcal{J}_x(\vec{q},t), \mathcal{J}_x(-\vec{q},0)]\rangle, \Lambda_{yy}(\vec{q},\omega) = \frac{i}{\hbar N}\int_0^\infty dte^{i\omega t}\langle[\mathcal{J}_y(\vec{q},t), \mathcal{J}_y(-\vec{q},0)]\rangle. \tag{24}$$

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

From the Heisenberg equation of motion $\dot{S}_n^z = i[\mathcal{H}, S_n^z]$ and from the horizontal and vertical differences of the spin current, as the divergence operator in the continuum version, we obtain the spin current operators for the x and y directions as

$$\mathcal{J}_x(\vec{q}) = -J_x\frac{t^2}{2}\sum_k \frac{[(1+\alpha)\sin k_x + \eta\sin\sqrt{2}k_x]}{\omega_k}(\alpha_k + \beta_k)(\alpha_k^\dagger + \beta_k^\dagger), \tag{25}$$

$$\mathcal{J}_y(\vec{q}) = -J_y\frac{t^2}{2}\sum_k \frac{[(1+\frac{1}{\alpha})\sin k_y + \zeta\sin\sqrt{2}k_y]}{\omega_k}(\alpha_k + \beta_k)(\alpha_k^\dagger + \beta_k^\dagger), \tag{26}$$

where we have defined the ζ parameter as $\zeta = J_2/J_y$.

The Green's function for the non-interacting excitons is given by

$$G(k, i\omega_n) = \frac{1}{i\omega_n - \omega}, \tag{27}$$

where ω_n is the Matsubara frequency. We obtain the temperature dependent Green's function that is obtained from the zero-temperature Green's function by replacing ω by $i\omega_n$, with $\omega_n = 2\pi nT$, $\beta = 1/T$. The analytical continuation yields the frequency and temperature dependent Green's function making $z = i\omega$.

The real part of $\sigma(\omega)$, $\sigma'(\omega)$ can be written in a standard form as [35]

$$\sigma'(\omega) = \sigma_0(\omega) + \sigma^{reg}(\omega), \tag{28}$$

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

$$D_S = \pi[\langle\mathcal{K}\rangle + \Lambda'(\vec{q} = 0, \omega \to \vec{0})]. \tag{29}$$

and $\sigma^{reg}(\omega)$, the regular part of $\sigma'(\omega)$, is given by [35]

$$\sigma^{reg}(\omega) = \frac{\Lambda''(\vec{q} = 0, \omega)}{\omega}. \tag{30}$$

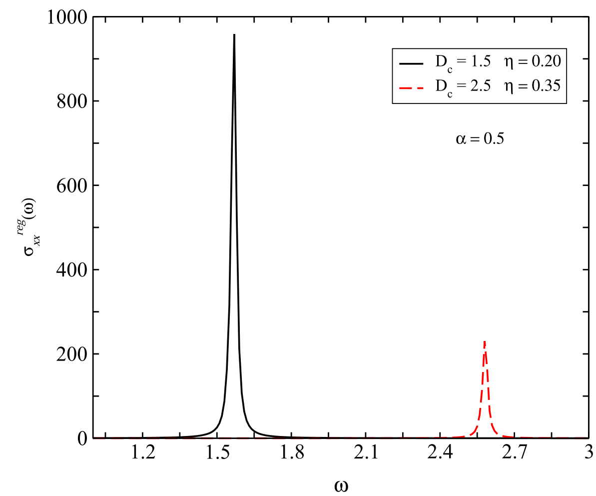

Fig. 2. Behavior of $\sigma_{xx}^{reg}(\omega)$ for $\alpha = 0.5$ and for the values D_c=1.5, $\eta = 0.20$ and D_c=2.5, $\eta = 0.35$. We have gotten a single peak for the *AC* spin conductivity at $\omega = \omega_p$ in consequence of the gap of the system.

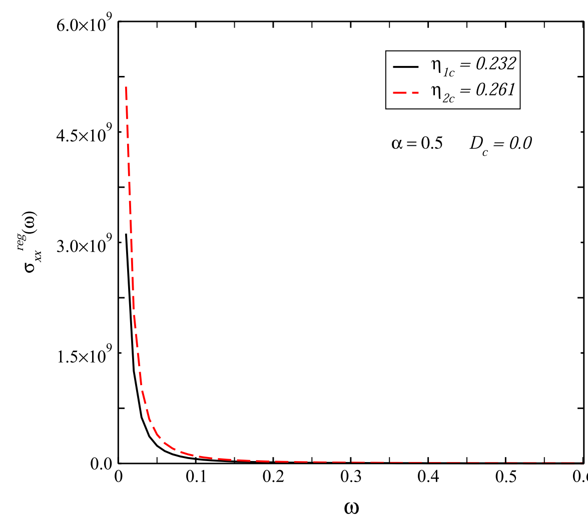

Fig. 3. Behavior of σ_{xx}^{reg} in the neighborhood of the quantum phase transition $\eta_{1c} = 0.232$ and $\eta_{2c} = 0.261$. In these points, the gap of the system goes to zero and D_c=0 and hence, we have gotten the spin conductivity tending to infinity in the limit $\omega \to 0$. Therefore we have, in this case, an ideal spin conductor in the neighborhood of the QTP in the limit $\omega \to 0$. We have found the behavior of the conductivity changes suddenly near of the QTP. We have made the calculations for a value of α such as $\alpha = 0.5$.

It represents the continuum contribution for the conductivity. In the Eqs. (29) and (30), Λ' and Λ'' stand for the real and imaginary part of Λ.

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

$$\sigma_{xx}^{reg}(\omega) = \frac{\Lambda_{xx}(k=0,\omega)}{\omega} = (g\mu_B)^2\frac{\pi J_x^2}{\hbar} \times \int_0^\pi\int_0^\pi \frac{d^2k}{(2\pi)^2}\frac{[(1+\alpha)\sin k_x + \eta\sin\sqrt{2}k_x]^2}{\omega_k^3}\delta(\omega - \omega_k), \tag{31}$$

$$\sigma_{yy}^{reg}(\omega) = \frac{\Lambda_{yy}(k=0,\omega)}{\omega} = (g\mu_B)^2\frac{\pi J_y^2}{\hbar} \times \int_0^\pi\int_0^\pi \frac{d^2k}{(2\pi)^2}\frac{[(1+\frac{1}{\alpha})\sin k_y + \zeta\sin\sqrt{2}k_y]^2}{\omega_k^3}\delta(\omega - \omega_k). \tag{32}$$

In the Fig. 2, we present the behavior of $\sigma_{xx}^{reg}(\omega)$ for $\alpha = 0.5$ and for

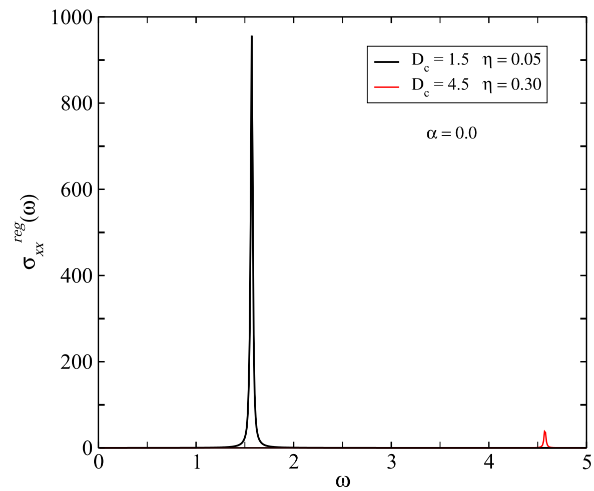

Fig. 4. Behavior of $\sigma_{xx}^{reg}(\omega)$ for $\alpha = 0.0$, for a small value of D_c such as D_c=1.5 and for a large value of D_c, such as D_c=4.5. The η value employed is $\eta = 0.30$. We have gotten in this case the behavior the height of the peak decreases with D_c and η. Due the system present a gap in this range of D_c (large D_c), we have gotten a peak for the *AC* conductivity at $\omega = \omega_p$, and hence the *AC* conductivity going to zero in the limits $\omega \to 0$ and $\omega \to \infty$.

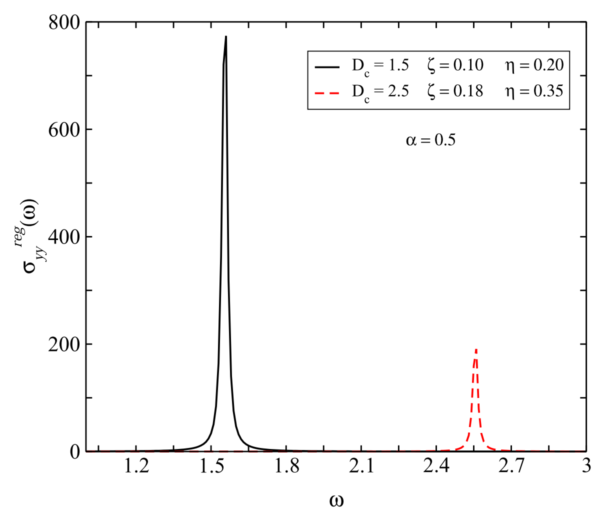

Fig. 5. Behavior of $\sigma_{yy}^{reg}(\omega)$ for $\alpha = 0.5$ and for the values D_c=1.5, $\zeta = 0.10$, $\eta = 0.20$ and D_c=2.5, $\eta = 0.18$, $\eta = 0.35$. In consequence of the gap, in this case, the behavior of the *AC* spin conductivity presents a peak at $\omega = \omega_p$ tending to zero in the limits $\omega \to 0$ and $\omega \to \infty$.

different values of D_c: D_c=1.5, $\eta = 0.20$ and D_c=2.5, $\eta = 0.35$. As we can see, the behavior of the *AC* spin conductivity presents a peak at $\omega = \omega_p$, tending to zero in the limits $\omega \to 0$ and $\omega \to \infty$ that is a consequence of the gap of the system in this range of D_c. In Figs. 3–7, we present the behavior of $\sigma_{xx}^{reg}(\omega)$ and $\sigma_{yy}^{reg}(\omega)$ in the neighborhood of the QPT points: $\eta_{1c} = 0.232$ and $\eta_{2c} = 0.261$. In these points, the gap of the system goes to zero and D_c=0 hence, in this case, the spin conductivity tends to infinity in the *DC* limit. The value of α employed in the our calculations is $\alpha = 0.5$. We have gotten so a sudden change in the behavior of the *AC* conductivity in the neighborhood of the QPT as obtained for other frustrated quantum spin systems [27–30], where the curve of the conductivity $\sigma^{reg}(\omega)$ suffers a change in the neighborhood of the QPT.

In Fig. 4 we present the behavior of $\sigma_{xx}^{reg}(\omega)$ for $\alpha = 0.0$ and for a small value of D_c as D_c=1.5, and in following, for a large value of D_c as D_c=4.5. The η value employed is $\eta = 0.30$. We also have getting peaks for the conductivity in these points as in the Fig. 1 since we are away from the QPT points and in this range the system presents gap. We have found the behavior of the spin conductivity varies with D_c, where

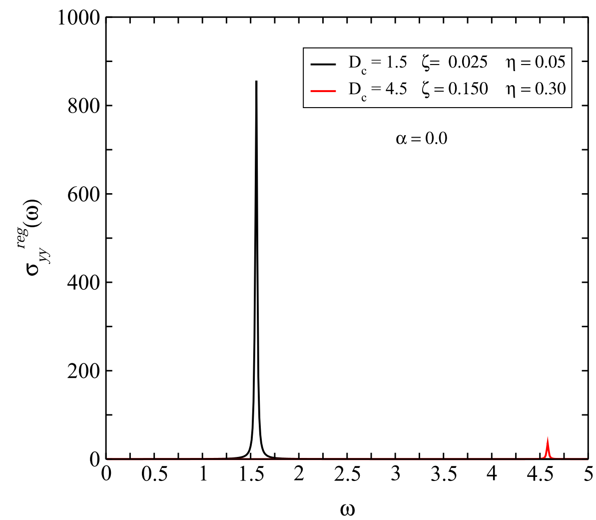

Fig. 6. Behavior of $\sigma_{yy}^{reg}(\omega)$ for $\alpha = 0.0$, for a small value of D_c as D_c=1.5 and $\eta = 0.050$, $\zeta = 0.025$, and for large value of D_c as D_c=4.5 for $\eta = 0.30$, $\zeta = 0.15$. We have gotten the height of the peak decreases with D_c and η. Due to the gap in this range, we have obtained a peak for the *AC* conductivity at $\omega = \omega_p$ and hence the *AC* conductivity going to zero in the limits $\omega \to 0$ and $\omega \to \infty$.

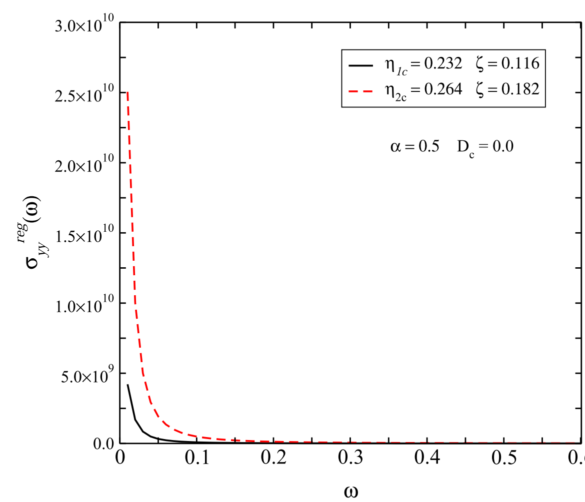

Fig. 7. Behavior of $\sigma_{yy}^{reg}(\omega)$ near of the QTP point $\eta_{1c} = 0.232$ and $\eta_{2c} = 0.261$. In these points, the gap of the system goes to zero and D_c=0. Therefore, the behavior of the *AC* conductivity tends to infinity when $\omega \to 0$ and we have an ideal spin conductor in this limit. The value of α employed is $\alpha = 0.5$. The values of ζ constant that correspondents to each η points are $\zeta_{1c} = 0.116$ and $\zeta_{2c} = 0.132$.

the height of the peak decreases with D_c and η. Hence, we have gotten a single peak for the *AC* conductivity at $\omega = \omega_p$ and the *AC* conductivity going to zero in the limits $\omega \to 0$ and $\omega \to \infty$ so as in the other cases analysed.

4. Conclusions and final remarks

We have studied the influence of the quantum phase transition on the spin transport in the two-dimensional spatially frustrated Heisenberg model in the square lattice using the SU(3) Schwinger's boson theory. How has been obtained for other frustrated spin systems [27–30], we have obtained an influence of the quantum phase transition on the behavior of the spin conductivity. We have gotten the *AC* conductivity changing suddenly to zero in the limit $\omega \to 0$, in the points far from the QPT point. In the neighborhood of the QPT, we have the spin conductivity tending to infinity in the limit $\omega \to 0$.

From a general way, one of the most important problems in condensed matter physics in the actuality is the understand of the relation between antiferromagnetism and superconductivity, where the two-dimensional Heisenberg model has a important role. For it is well known that superconductors materials such as La_2CO_4 in the insulating phase Mott are two-dimensional antiferromagnets [36,37].

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