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Finite-temperature conductivity in the t–J model with spin frustration

Zhan-Hai Dong[1,2,3] **and Shi-Wei Gu**[2]

[1] Institute of Condensed Matter Physics, Department of Applied Physics, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China
[2] Department of Physics, Yanbei Normal College, Datong 037000, People's Republic of China

E-mail: zhdong803@mail1.sjtu.edu.cn

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Abstract

We use an alternative operator transform to study hole motion against a frustrated antiferromagnet background described by the t–J model with next-nearest-neighbour exchange energy. Using the self-consistent Born approximation, the optical conductivity and direct-current resistivity are evaluated, and their dependences on the next-nearest-neighbour exchange energy are discussed.

1. Introduction

It is believed that undoped copper oxide materials are antiferromagnetic Mott insulators, and most of the normal-state electronic properties are closely related to the strong antiferromagnetic correlations in their CuO_2 planes which are common to all high-T_c materials. Moreover, one of the most striking characteristics of these antiferromagnets is the spin frustration that arises from the special geometry of the lattice, for example on the triangular lattice [1, 2], or from the competition between the nearest-neighbour and next-nearest-neighbour interactions. In the early days of the studies of hole motion in an antiferromagnet, it was suggested that the effect of doping could be described by introducing second- and sometimes third-nearest-neighbour couplings in the undoped Hamiltonian [3, 4]. However, by studying the t–J model and the frustrated Heisenberg J–J' model, Nori *et al* have found that doped systems cannot be accurately modelled by a pure frustrated spin model [5, 6], i.e., the effect of doping could not be mimicked by the frustration. Nonetheless, this does not mean that the frustration makes no contribution to the carrier motion. A hole moving against an antiferromagnetically correlated background is heavily normalized due to the existence of spin fluctuation which is closely related to the nearest-neighbour and the long-range spin couplings. Thus, the next-nearest-neighbour interaction, termed J', should have a relationship with the charge dynamics which is manifested by the optical conductivity $\sigma(\omega)$ and by the dc resistivity ρ. Now extensive studies, both experimental and theoretical, have revealed that the optical conductivity in the

[3] Author to whom any correspondence should be addressed.

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low-energy region is not of the usual Drude type, but seems to be composed of at least two components, a Drude-like narrow band centred at $\omega = 0$ and a broad band centred in the mid-infrared region [7]. It is the purpose of this paper to study how the frustration affects these optical conductivity features.

In the following we consider the t–J model with next-nearest-neighbour spin exchange energy, i.e., the spin frustration is considered. The Hamiltonian, termed the t–J–J' model, reads as follows:

$$H = -t \sum_{\langle ij\rangle_1\sigma} C^\dagger_{i\sigma} C_{j\sigma} + J \sum_{\langle ij\rangle_1} P_i \boldsymbol{s}_i \cdot \boldsymbol{s}_j P_j + J' \sum_{\langle ij\rangle_2} P_i \boldsymbol{s}_i \cdot \boldsymbol{s}_j P_j \tag{1.1}$$

where the $P_i = 1 - h^\dagger_i h_i$ are projection operators, and the summations over $\langle i, j\rangle_1$ and $\langle i, j\rangle_2$ run over the first- and second-neighbour pairs, respectively. $C_{i\sigma}$ is the constrained annihilation operator for an electron with spin σ on the lattice site i. The single-occupancy constraint $\sum_\sigma C^\dagger_{i\sigma} C_{i\sigma} \leqslant 1$ is imposed at each site.

In order to implement the single-occupancy constraint, various representations of slave-particle techniques have been developed [8–10]. Schmitt-Rink *et al* have proposed a spin-polaron picture to describe the hole dynamics in the t–J model [11], and obtained good results. In the present paper, an alternative electron operator transform, which can be reduced to that of the spin-polaron picture in the linear spin-wave approximation, is used to evaluate the optical conductivity of an electron moving against a frustrated antiferromagnet background.

2. The effective Hamiltonian

We introduce hole operators h_i and two-component vectors $\boldsymbol{\beta}_i$ which are defined in terms of a bosonic operator a_i:

$$\boldsymbol{\beta}_i = \begin{cases} \dfrac{1}{\sqrt{2S}} \begin{pmatrix} \sqrt{2S - a^\dagger_i a_i} \\ a_i \end{pmatrix} & i \in \text{spin-up sublattice} \\ \dfrac{1}{\sqrt{2S}} \begin{pmatrix} a_i \\ \sqrt{2S - a^\dagger_i a_i} \end{pmatrix} & i \in \text{spin-down sublattice} \end{cases} \tag{2.1}$$

their conjugate vectors being [12]

$$\frac{1}{\sqrt{2S}}(\sqrt{2S - a^\dagger_i a_i}, a^\dagger_i) \qquad \text{and} \qquad \frac{1}{\sqrt{2S}}(a^\dagger_i, \sqrt{2S - a^\dagger_i a_i}).$$

The vectors $\boldsymbol{\beta}_i$ obey the normalization condition

$$\boldsymbol{\beta}^\dagger_i \boldsymbol{\beta}_i = 1 \qquad (\text{on any site } i). \tag{2.2}$$

In terms of $\boldsymbol{\beta}_i$, the spin operators $\boldsymbol{s}_i$ can be expressed as $\boldsymbol{s}_i = S\boldsymbol{\beta}^\dagger_i \boldsymbol{\sigma} \boldsymbol{\beta}_i$ ($\boldsymbol{\sigma}$ is a Pauli matrix), which is just the Holstein–Primakoff transform. The suggested form of the electron operator transform is

$$\sum_\sigma C^\dagger_{i\sigma} C_{j\sigma} = h_i \boldsymbol{\beta}^\dagger_i h^\dagger_j \boldsymbol{\beta}_j. \tag{2.3}$$

With this electronic operator transform,

(1) the no-double-occupancy constraint, $\sum_\sigma C^\dagger_{i\sigma} C_{i\sigma} = h_i \boldsymbol{\beta}^\dagger_i h^\dagger_i \boldsymbol{\beta}_i = h_i h^\dagger_i = 1 - h^\dagger_i h_i \leqslant 1$, is satisfied automatically; this differs from the case for the slave-particle representation where an additional condition is added to the Hamiltonian to implement the no-double-occupancy constraint, and

(2) the t–J model with any spin can be treated, which differs from the case for the Fermi-spin theory which works only for the spin-half system [10].

Moreover, within linear spin-wave theory the present transform can be deduced from the transform given by Gerardo Martinez and Peter Horsch [13], i.e., the present transform reduces to theirs for low-energy excitation.

In the following discussion the projection operator P_i is ignored since the consideration of this operator leads only to the effective exchange parameter J or J' changing into $J_{eff} = J(1-\delta)^2$ or $J'_{eff} = J'(1-\delta)^2$ (δ is the hole density). Also the spin-wave excitation is treated as an ideal boson gas. Using the Holstein–Primakoff transform, the Heisenberg exchange Hamiltonian $H_{JJ'}$ can be expressed in terms of the boson operator a_i. After space Fourier transformation, we arrive at

$$H_{JJ'} = \frac{1}{2} JSz \sum_k \left[2(1-\rho_k) a_k^\dagger a_k + \gamma_k (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger) \right] \tag{2.4}$$

where a_k is the Fourier transform of the operator a_i and

$$\rho_k = \frac{J'}{J}(1-\gamma_k^{(2)})$$

Also, $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$ and $\gamma_k^{(2)} = \cos k_x \cos k_y$, and z is the coordination number of the lattice. After carrying out the Bogoliubov transformation, $a_k = u_k \alpha_k + v_k \alpha_{-k}^\dagger$, the Hamiltonian $H_{JJ'}$ can be diagonalized:

$$H_{JJ'} = \sum_k \omega_k \alpha_k^\dagger \alpha_k + E_{J0} \tag{2.5}$$

where

$$\omega_k = JSz\sqrt{(1-\rho_k)^2 - \gamma_k^2}$$

is the spin-wave dispersion and E_{J0} is a constant. The parameters u_k and v_k satisfy

$$u_k = \left[\frac{1}{2} \left(1 + \frac{1-\rho_k}{\sqrt{(1-\rho_k)^2 - \gamma_k^2}} \right) \right]^{1/2} \tag{2.6}$$

$$v_k = -\mathrm{sgn}(\gamma_k) \left[\frac{1}{2} \left(\frac{1-\rho_k}{\sqrt{(1-\rho_k)^2 - \gamma_k^2}} - 1 \right) \right]^{1/2}. \tag{2.7}$$

Using the electron operator transform (2.3) and retaining only the terms linear in a_i, we can express the hopping Hamiltonian H_t as

$$H_t = -\frac{t}{\sqrt{2S}} \sum_{\langle ij \rangle_1} h_i h_j^\dagger (a_i^\dagger + a_j). \tag{2.8}$$

After performing the Bogoliubov transformation, this hopping Hamiltonian H_t can be expressed in momentum space as

$$H_t = \frac{tz}{\sqrt{2SN}} \sum_{kq} h_{k-q}^\dagger h_k (\gamma_{k-q} u_q + \gamma_k v_q) \alpha_q^\dagger + \mathrm{H.c.} \tag{2.9}$$

Equations (2.5) and (2.9) constitute the effective Hamiltonian.

3. Optical conductivity and dc resistivity

The single-hole Green's function is defined as

$$G(k,t) = -\mathrm{i}\langle 0|Th_k(t)h_k^{\dagger}(0)|0\rangle \tag{3.1}$$

where $|0\rangle$ is the ground state of the AF Heisenberg part of the Hamiltonian and T is a time-ordering operator. The Dyson's equation for the hole propagator $G(k,\omega)$ is

$$G(k,\omega) = \frac{1}{\omega - \Sigma(k,\omega)} \tag{3.2}$$

where $\Sigma(k,\omega)$ is the self-energy resulting from the incoherent hole motion. In the limit $J \ll t$, the vertex correction can be neglected [14, 15]. Then, using the self-consistent Born approximation (SCBA), one finds for the self-energy

$$\Sigma(k,\omega) = \frac{z^2t^2}{2SN}\sum_q M^2(k,q)G(k-q,\omega-\omega_q) \tag{3.3}$$

where $M^2(k,q) = (u_q\gamma_{k-q} + v_q\gamma_k)^2$. The spectral function is

$$A(k,\omega) = -2\,\mathrm{Im}\,G(k,\omega). \tag{3.4}$$

Using the linear response theory and in terms of the spectral function $A(\boldsymbol{k},\omega)$, the optical conductivity can be expressed as [16]

$$\begin{aligned}\sigma(\omega) &= -\frac{\mathrm{Im}[\pi(\omega)]}{\omega} \\ &= \frac{\sigma_0}{\omega}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}\,[n_F(\omega') - n_F(\omega'+\omega)]\frac{1}{N}\sum_k(\sin k_x)^2A(\boldsymbol{k},\omega')A(\boldsymbol{k},\omega'+\omega)\end{aligned} \tag{3.5}$$

where $\pi(\omega)$ is the Fourier transform of the current–current correlation function

$$\pi(\tau) = -\frac{1}{N}\langle T_\tau j^{\dagger}(\tau)j\rangle. \tag{3.6}$$

Here, j is the current operator

$$j = \mathrm{i}e_0ta_0\sum_{ij}(h_i^{\dagger}h_j - h_j^{\dagger}h_i). \tag{3.7}$$

Also, $n_F(\omega) = [1+\exp(\omega/k_BT)]^{-1}$ is the Fermi distribution function and $\sigma_0 = (2e_0ta_0)^2$ is a constant.

The dc resistivity $\rho(T)$ is given by the following limit for $\omega \to 0$:

$$\rho(T) = -\lim_{\omega\to 0}\frac{\omega}{\mathrm{Im}[\pi(\omega)]}. \tag{3.8}$$

Equations (3.2) and (3.3) constitute a self-consistent equation set for determining the spectral function $A(\boldsymbol{k},\omega)$, and are solved by means of an iterative method. We start from an arbitrary initial function $G(k,\omega)$ for all wave vectors $\boldsymbol{k}$, belonging to the first Brillouin zone of a 16×16 cluster, and 1000 points of frequency ω, and use this equation set to iterate until convergence is achieved. In order to clarify the contribution of the frustration, the nearest-neighbour exchange parameter is fixed at $J/t = 0.4$ in the calculation. In addition, it should be stressed that the present operator transform cannot give significantly better results than the existing ones due to already using the linear approximation.

4. Results and discussion

Let us first show the dependence of the optical conductivity on the spin frustration manifested by the next-nearest-neighbour exchange parameter J'. In figure 1 we present the spectra $\sigma(\omega)$ against ω/t with the parameters given in the caption. In the absence of frustration ($J' = 0$), the spectrum exhibits a rapid rise at low frequencies that can be attributed to the appearance of a Drude-like band centred at $\omega = 0$, and a mid-infrared (MIR) band centred at $\omega \approx t$ that may be attributed to the spin excitation surrounding the hole carriers. When $\omega > 5t$, the spectral weight is nearly unchanged. Using the Lanczos method, Dagotto evaluated the optical conductivity of the one-band Hubbard model at $U/t = 10$ on a 4×4 cluster; the finding was that the MIR band is located near $\omega \approx 2t$ for doping $x = 0.125$ [4]. Also Stephan and Horsch [17] obtained a MIR band centred at $\omega \approx 1.5t$ using the t–J model on a 4×4 cluster. Therefore, the present result is in qualitative agreement with those obtained by these groups.

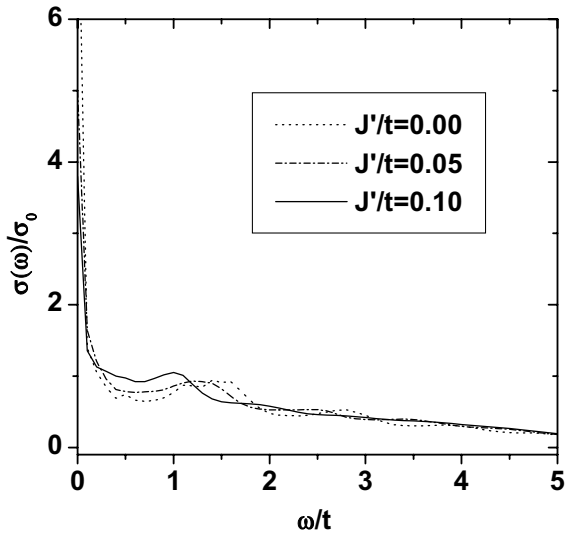

Figure 1. Optical conductivity $\sigma(\omega)/\sigma_0$ against ω/t at temperature $T = t$ for different values of J': $J' = 0.00$ (dotted line), 0.05 (dash–dotted line), and 0.10 (solid line).

When the frustration is taken into account, the optical conductivity continues to consist of a Drude-like band and a MIR band. However, with increasing J' the spectral weight decreases below $\omega = 0.1t$. The lost weight is transferred to higher energy. This indicates that the consideration of the frustration leads to further deviation of the optical conductivity from the ω^{-2}-behaviour in the far-infrared region. Cooper *et al* and Uchida *et al* have studied the doping dependence of the optical conductivity, and revealed that, with increasing doping x, spectral weight grows in the far-infrared Drude-like band peaked at $\omega = 0$, while it decreases in the region above the charge-transfer absorption band [7,18] (above the CT gap). Comparing with their results, it can be concluded that the decreasing spin frustration is equivalent to the increasing doping. Here we only compare the contributions of the frustration and the doping to the conductivity, and by no means support the claim that the doping can be completely mimicked by the frustration. When $\omega > 5t$ the spectra for different frustrations overlap, which may correspond to the so-called 'isosbestic' point [4].

Now we evaluate the order of magnitude of the resistivity ρ. In the numerical calculation we have used units with $e_0 = \hbar = k_B = a_0 = 1$ as well as the next-nearest-neighbour hopping

energy $t = 1$. In these units, σ_0 and $\rho_0 = 1/\sigma_0$ are of order 1. Then, in international units, the order of ρ_0 should be $\hbar a_0/e_0^2 \sim 10^{-5}$ Ω m which is of the same order as the experimental magnitude of the ab-plane resistivity in single-crystal $La_{2-x}Sr_xCuO_4$ [7]. If t takes the value 0.4 eV suggested in some calculations [4], then the MIR band is located at $\hbar\omega \sim 0.4$ eV, similar to that observed experimentally by Uchida *et al* [7].

In figure 2 we display the temperature dependence of the dc resistivity $\rho(T)$ for $J' = 0.00$ (solid line), 0.05 (dotted line), 0.10 (dash–dotted line). The resistivity exhibits a sharp drop as temperature $T \to 0$. Throughout the temperature range the resistivity increases with the rise of the next-nearest-neighbour exchange energy J'. Its line shape is very similar to that measured by Uchida *et al* [7] who have experimentally investigated the doping dependence of the dc resistivity, and found that the ab-plane resistivity reduces with increasing doping. Jaklič and Prelovšek have studied the dependence on J (the nearest-neighbour exchange energy) of the dc resistivity (figure 12 in reference [19]), and revealed that the larger the nearest-neighbour exchange energy, the larger the dc resistivity, although $\rho(T)$ is weakly influenced by J. Therefore, the contributions of the nearest- and next-nearest-neighbour exchanges to the dc resistivity are the same. However, this is not true when $\omega \neq 0$.

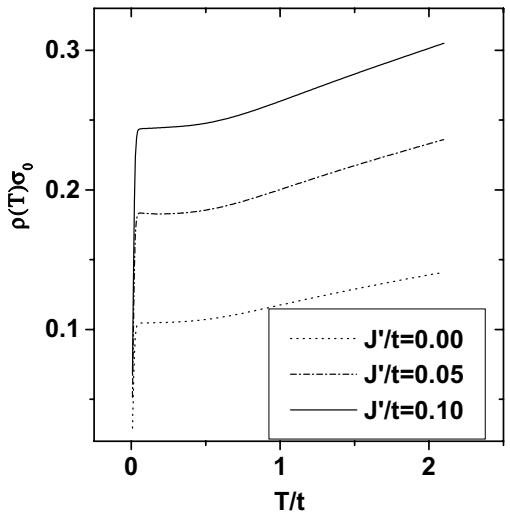

Figure 2. The temperature dependence of the dc resistivity $\rho(T)$ for $J' = 0.00$ (dotted line), 0.05 (dash–dotted line), 0.10 (solid line).

5. Conclusions

We use an alternative operator transform, for which the no-double-occupancy constraint is satisfied automatically and with which hole motion against an AF background with any spin can be treated, to treat a t–J model with next-nearest-neighbour exchange J'. Using the self-consistent Born approximation, the optical conductivity and dc resistivity are evaluated, and their dependences on J' are discussed. We find that the main features of the optical conductivity are not qualitatively changed by the consideration of the spin frustration. The optical conductivity continues to consist of two components: a Drude-like band and an infrared band. The consideration of spin frustration is equivalent to minimizing doping. Spin frustration raises the dc resistivity throughout the temperature range.

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