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HOLE QUASIPARTICLE DYNAMICS IN THE DOPED 2D QUANTUM ANTIFERROMAGNET

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The spectrum of hole quasiparticles and the role of magnetic correlations are investigated in the self-consistent Irreducible Green Functions formalism motivated from Strongly Correlated Electron systems in the framework of spin-fermion model. It was clearly pointed out on the self-energy level, beyond Hartree–Fock approximation, how the one- and two-magnon processes define the true nature of carriers in HTSC.

A vast amount of theoretical searches for the relevant mechanism of high temperature superconductivity (HTSC) deals with the strongly correlated electron models.[1–5] The understanding of the true nature of the electronic states in HTSC are one of the central topics of the current experimental and theoretical efforts in the field. The plenty of experimental and theoretical results shows that the charge and spin fluctuations induced in the carrier hopping lead to the drastic renormalization of the single-particle electronic states due to the strong correlation. It makes the problem of constructing of the correct ground state wave functions and description the real many-body dynamics of the relevant correlated models of HTSC quite difficult.[1–12] The right picture of dynamical properties is very important because of the most important experimental data of HTSC have a dynamical nature, i.e. depends on frequency.[1] The dramatic change of the electronic structure caused by the carrier doping is found in the one-particle spectral density.[13]

As far as the CuO_2-planes in the HTSC compounds are concerned, it was argued[14–17] that a suitable workable model with which one can start to discuss the dynamical properties of copper oxides is the spin-fermion (or Kondo–Heisenberg model).[17–23] This model allows for motion of doped holes and results from d-p model

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Hamiltonian with using of the strong coupling unitary transformation.[3,4,15] A number of perturbation approaches have been used[17–27] to describe the spin and carrier dynamics of HTSC. In the present paper we use novel nonperturbative method to attack the same problem. This method of Irreducible Green Functions (IGF)[28,29] rely on a unified self-consistent calculation of one-particle fermion and spin Green Functions (GF) including damping effects and finite lifetimes and gives the correct results both for the weak and strong coupling. The approach we suggest is founded on the number of studies and has proved to be valuable for the s-f model,[30,31] Heisenberg antiferromagnet,[32] Anderson model,[33,34] and Hubbard model.[35,36]

We consider the interacting hole-spin model for a copper-oxide planar system described by the Hamiltonian

$$H = H_t + H_{\mathrm{K}} + H_J\,, \tag{1}$$

where H_t is the doped hole Hamiltonian

$$H_t = -\sum_{\langle ij\rangle\sigma}(ta^+_{i\sigma}a_{j\sigma} + \mathrm{h.c.}) = \sum_{k\sigma}\epsilon(k)a^+_{k\sigma}a_{k\sigma}\,, \tag{2}$$

where $a^+_{i\sigma}$ and $a_{i\sigma}$ are the creation and annihilation second quantized fermion operators, respectively for itinerant carriers with energy spectrum

$$\epsilon(q) = -4t\cos(1/2q_x)\cos(1/2q_y) = t\gamma_1(q). \tag{3}$$

The term H_J in (1) denotes Heisenberg superexchange Hamiltonian

$$H_J = \sum_{\langle mn\rangle} J\mathbf{S}_m\mathbf{S}_n = \frac{1}{2N}\sum_q J(q)\mathbf{S}_q\mathbf{S}_{-q}\,. \tag{4}$$

Here $\mathbf{S}_n$ is the operator for a spin at copper site $\mathbf{r}_n$ and J is the nearest neighbor (n.n.) superexchange interaction

$$J(q) = 2J[\cos(q_x) + \cos(q_y)] = J\gamma_2(q)\,. \tag{5}$$

Finally, the hole-spin (Kondo type) interaction H_{K} may be written as (for one-doped hole)

$$H_{\mathrm{K}} = \sum_i K\sigma_i\mathbf{S}_i = N^{-1/2}\sum_{kq}\sum_{\sigma}K(q)[S^{-\sigma}_{-q}a^+_{k\sigma}a_{k+q-\sigma} + z_\sigma S^z_{-q}a^+_{k\sigma}a_{k+q\sigma}]\,. \tag{6}$$

This part of the Hamiltonian was written as the sum of a dynamic (or spin-flip) part and a static one. Here $K(q)$ is hole-spin interaction energy

$$K(q) = K[\cos(1/2q_x) + \cos(1/2q_y)] = K\gamma_3(q) \tag{7}$$

and sign factor z_σ is given by

$$z_\sigma = (+\ \text{or}\ -) \quad \text{for} \quad \sigma = (\uparrow\ \text{or}\ \downarrow)\,.$$

We start in this paper with the one-doped hole model (1), which is considered to have captured the essential physics of the multi-band strongly correlated Hubbard model in the most interesting parameters regime $t > J, |K|$. We apply the IGF method to spin-fermion model (1). We are able to give a much more detailed and self-consistent description of the fermion and spin excitation spectra than in papers,[17-23] including the damping effects and finite lifetimes.

The two-time thermodynamic Green Functions to be studied here are given by

$$G(k\sigma, t-t') = \langle\langle a_{k\sigma}(t), a^{+}_{k\sigma}(t')\rangle\rangle = -i\theta(t-t')\langle[a_{k\sigma}(t), a^{+}_{k\sigma}(t')]_{+}\rangle\,, \qquad (8)$$

$$\chi^{+-}(mn, t-t') = \langle\langle S^{+}_{m}(t), S^{-}_{n}(t')\rangle\rangle = -i\theta(t-t')\langle[S^{+}_{m}(t), S^{-}_{n}(t')]_{-}\rangle\,. \qquad (9)$$

In order to evaluate the GFs (8) and (9) we need use the suitable information about a ground state of the system. For the 2D spin 1/2 quantum antiferromagnet in a square lattice the calculation of the exact ground state is a very difficult problem.[1,12] In this paper we assume the two-sublattice Neel ground state. According to Neel model, the spin Hamiltonian (4) may be expressed as[32]

$$H_J = \sum_{(mn)}\sum_{\alpha,\beta} J^{\alpha\beta}\mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\,. \qquad (10)$$

Here $(\alpha, \beta) = (a, b)$ are the sublattice indices.

To calculate the electronic states induced by hole-doping in the spin-fermion model approach we need to calculate the energies of a hole introduced in the Neel antiferromagnet. To be consistent with (10) we define the single-particle fermion GF as

$$G(k\sigma, \omega) = \begin{pmatrix} \langle\langle a_a(k\sigma)|a^{+}_{a}(k\sigma)\rangle\rangle & \langle\langle a_a(k\sigma)|a^{+}_{b}(k\sigma)\rangle\rangle \\ \langle\langle a_b(k\sigma)|a^{+}_{a}(k\sigma)\rangle\rangle & \langle\langle a_b(k\sigma)|a^{+}_{b}(k\sigma)\rangle\rangle \end{pmatrix}. \qquad (11)$$

Note, that the same fermion operators $a_\alpha(i\sigma)$, annihilates a fermion with spin σ on the (α)-sublattice in the ith unit cell has been used in Ref. 18. The equation of motion for the Fourier transform of the elements of GF (11) are written as

$$\sum_{\gamma}(\omega\delta_{\alpha\gamma} - \epsilon^{\alpha\beta}(k))\langle\langle a_\gamma(k\sigma)|a^{+}_{\beta}(k\sigma)\rangle\rangle = \delta_{\alpha\beta} - \langle\langle A(k\sigma, \alpha)|a^{+}_{\beta}\rangle\rangle\,, \qquad (12)$$

where

$$A(k\sigma, \alpha) = N^{-1/2}\sum_{p} K(p)(S^{-\sigma}_{-p\alpha}a_\alpha(k+p-\sigma) + z_\sigma S^{z}_{-p\alpha}a_\alpha(k+p\sigma))\,. \qquad (13)$$

We make use of the general Irreducible Green Function(IGF) approach[28,29] to threat the the equation of motion (12). It may be shown after much straightforward(c.f. Refs. 30 and 31) but tedious manipulation that the equation (13) can be rewritten as the Dyson equation for two-time thermodynamic retarded GF

$$G(k\sigma, \omega) = G_0(k\sigma, \omega) + G_0(k\sigma, \omega)M(k\sigma, \omega)G(k\sigma, \omega)\,. \qquad (14)$$

Here $G_0(k\sigma,\omega) = \Omega^{-1}$ describes the behavior of the electronic subsystem in the Generalized Mean-Field(GMF) approximation (for the detailed discussion of the GMF concept, see Refs. 29 and 36). The Ω matrix have the form

$$\Omega(k\sigma,\omega) = \begin{pmatrix} (\omega - \epsilon_a(k\sigma)) & -\epsilon^{ab}(k) \\ -\epsilon^{ba}(k) & (\omega - \epsilon_b(k\sigma)) \end{pmatrix}, \tag{15}$$

where

$$\epsilon_\alpha(k\sigma) = \epsilon^{\alpha\alpha}(k) - z_\sigma N^{-1/2}\sum_p K(p)\langle S^z_{p\alpha}\rangle\delta_{p,0} = \epsilon^{\alpha\alpha}(k) - z_\sigma K S_z\,, \tag{16}$$

$$S_z = N^{-1/2}\langle S^z_{0\alpha}\rangle\,,$$

is the renormalized band energy of the holes.

The elements of the matrix GF $G_0(k\sigma,\omega)$ are found to be

$$G_0^{aa}(k\sigma,\omega) = \frac{u^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{v^2(k\sigma)}{\omega - \epsilon_-(k\sigma)}\,, \tag{17}$$

$$G_0^{ab}(k\sigma,\omega) = \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_+(k\sigma)} - \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_-(k\sigma)} = G_0^{ba}(k\sigma,\omega)\,, \tag{18}$$

$$G_0^{bb}(k\sigma,\omega) = \frac{v^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{u^2(k\sigma)}{\omega - \epsilon_-(k\sigma)}\,, \tag{19}$$

where

$$u^2(k\sigma) = 1/2\left(1 - z_\sigma\frac{KS_z}{R(k)}\right); v^2(k\sigma) = 1/2\left(1 + z_\sigma\frac{KS_z}{R(k)}\right), \tag{20}$$

$$\epsilon_\pm(k\sigma) = \pm R(k) = ((\epsilon^{ab}(k)^2 + K^2S_z^2)^{1/2}\,, \tag{21}$$

the simplest assumption is that each sublattice is s.c. and $\epsilon^{\alpha\alpha}(k) = 0(\alpha = a, b)$. Although we have worked in the GFs formalism, our expressions (17)–(21) are in accordance with the results of the Bogolubov (u,v)-transformation for fermions, but, of course, the present derivation is more general.

The mass operator M in Dyson equation (14), which describes hole–magnon scattering processes, is given by as a "proper" part[28] of the irreducible matrix GF of higher order

$$M(k\sigma,\omega) = \begin{pmatrix} {}^{(\mathrm{ir})}\langle\langle A(k\sigma,a)|A^+(k\sigma,a)\rangle\rangle^{(\mathrm{ir})} & {}^{(\mathrm{ir})}\langle\langle A(k\sigma,a)|A^+(k\sigma,b)\rangle\rangle^{(\mathrm{ir})} \\ {}^{(\mathrm{ir})}\langle\langle A(k\sigma,b)|A^+(k\sigma,a)\rangle\rangle^{(\mathrm{ir})} & {}^{(\mathrm{ir})}\langle\langle A(k\sigma,b)|A^+(k\sigma,b)\rangle\rangle^{(\mathrm{ir})} \end{pmatrix}. \tag{22}$$

To find the renormalization of the spectra $\epsilon_\pm(k\sigma)$ and the damping of the quasiparticles it is necessary to determine the self-energy for each type of excitations. The formal solution of the Dyson equation (14) can be written as

$$G = ((G_0)^{-1} - M)^{-1}\,. \tag{23}$$

From (23) one immediately obtain

$$G_{\pm}(k\sigma) = (\omega - \epsilon_{\pm}(k\sigma) - \Sigma^{\pm}(k\sigma,\omega))^{-1}. \tag{24}$$

Here the self-energy operator is given by

$$\Sigma^{\pm}(k\sigma,\omega) = A^{\pm}M^{aa} \pm B(M^{ab} + M^{ba}) + A^{\mp}M^{bb}, \tag{25}$$

where

$$A^{\pm} = \begin{pmatrix} u^2(k\sigma) \\ v^2(k\sigma) \end{pmatrix},$$
$$B = u(k\sigma)v(k\sigma).$$

Equations (24) determines the quasiparticle spectrum with damping ($\omega = E - i\Gamma$) for the hole in the AFM background. Contrary to the simplified calculations of the hole GF for doped HTSC, the self-energy (25) is proportional K^2 but not t^2

$$M^{\alpha\beta}(k\sigma,\omega) = N^{-1}K^2 \sum_q \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \times \left[F^{\sigma,-\sigma}_{\alpha\beta}(q,\omega_1) g_{\alpha\beta}(k+q-\sigma,\omega_2) + F^{zz}_{\alpha\beta}(q,\omega_1) g_{\alpha\beta}(k+q,\omega_2)\right]. \tag{26}$$

Here functions $N(\omega)$ and $n(\omega)$ are Bose and Fermi distributions, respectively, and the following notations have been used for spectral intensities

$$F^{ij}_{\alpha\beta}(q,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\langle\langle S^i_{q\alpha} | S^j_{-q\beta}\rangle\rangle_\omega, \quad g_{\alpha\beta}(k\sigma,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\langle\langle a_\alpha(k\sigma) | a^+_\beta(k\sigma)\rangle\rangle_\omega, \quad i,j = (+,-,z). \tag{27}$$

The equations (27) and (24) forms the self-consistent set of equations for the determining of the GF (22). It need hardly be remarked that the advantages of the present formulation permits:

(i) to make much more exact statements about interacting hole-spin system;
(ii) to calculate in controlled manner beyond the Hartree–Fock approximation;
(iii) with IGF method we can make a one-to-one correspondence between each complete set of contractions arising in each term of diagrammatic expansion(c.f. Refs. 18 and 19).

The Coupled equations (24) can be solved analytically by suitable iteration procedure. In principle, we can use, in the right-hand side of (26) any workable first iteration step for of the relevant GFs and find a solution by repeated iteration. It is most convenient to choose as the first iteration step the simplest two-pole expressions, corresponding to the GF structure for a mean field, in the following form

$$g_{\alpha\beta}(k\sigma,\omega) = R_+\delta(\omega - E_+(k\sigma)) + R_-\delta(\omega - E_-(k\sigma)), \tag{28}$$

where $R_\pm$ are the certain coefficients depending on $u(k\sigma)$ and $v(k\sigma)$. The magnetic excitation spectrum corresponds to the frequency poles of the GFs in (27). In view of the discussion elsewhere of the spin dynamics of the present model, we shall content ourselves with the simplest initial approximation for the spin GF occurring in (26) (c.f. Ref. 32)

$$\frac{1}{2z_\sigma S_z} F^{\sigma-\sigma}_{\alpha\beta}(q,\omega) = L_+ \delta(\omega - z_\sigma \omega_q) - L_- \delta(\omega + z_\sigma \omega_q)\,. \tag{29}$$

Here ω_q is the energy of the antiferromagnetic magnons and $L_\pm$ are the certain coefficients.[32] We are now in a position to find an explicit solution of coupled equations obtained so far. This is achieved by using (28) and (29) in the right-handside of (26). Then the hole self-energy in 2D quantum antiferromagnet for the low-energy quasiparticle band $E_-(k\sigma)$ is

$$\begin{aligned}
&\Sigma^-(k\sigma,\omega) \\
&= \frac{K^2 S_z}{2N} \sum_q C_-^2 \left[\frac{1 + N(\omega_q) - n(E_-(k-q))}{\omega - \omega_q - E_-(k-q)} + \frac{N(\omega) + n(E_-(k+q))}{\omega + \omega_q - E_-(k+q)} \right] \\
&\quad + \frac{2K^2 S_z^2}{N} \sum_{qp} D_-^2 \frac{N(\omega_{q+p})(1 + N(\omega_q)) + n(E_-(k+p))(N(\omega_q) - N(\omega_{q+p}))}{\omega + \omega_{q+p} - \omega_q - E_-(k+p)}\,.
\end{aligned} \tag{30}$$

Here we have used the notations

$$C_-^2 = (U_q + V_q)^2\,, \quad D_-^2 = (U_q U_{q+p} - V_q V_{q+p})^2\,,$$

where the coefficients U_q and V_q appears as a results of explicit calculation of the mean-field magnon GF (9).[32]

A very remarkable feature of this result is that our expression (30) accounts for the hole-magnon inelastic scattering processes with the participation of one or two magnons. It will be important for the consideration of Cooper pairing processes as we will show elsewhere.

The self-energy representation in a self-consistent form (26) provide a possibility to model the relevant spin dynamics by selecting spin-diagonal or spin-off-diagonal coupling as a dominating or having different characteristic frequency scales. As a workable pattern, we consider now the static trial approximation for the correlation functions of the magnon subsystem[32] in the expression (26). Then the following expression is readily obtained

$$\begin{aligned}
M^{\alpha\beta}(k\sigma,\omega) = \frac{K^2}{N} \sum_q \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} \Big[&\langle S^{-\sigma}_{-q\beta} S^{\sigma}_{q\alpha} \rangle g_{\alpha\beta}(k+q-\sigma,\omega') \\
&+ \langle (S^z_{-q\beta})^{\mathrm{ir}} (S^z_{q\alpha})^{\mathrm{ir}} \rangle g_{\alpha\beta}(k+q\sigma,\omega') \Big]\,.
\end{aligned} \tag{31}$$

Taking into account (25) we find the following approximative form

$$\Sigma^{-}(k\sigma,\omega) \approx \frac{K^2}{2N}\sum_q \frac{\chi^{-+}(q)+\chi^{z,z}(q)}{\omega - E_{-}(k+q)}(1-\gamma_1(q))\,. \qquad (32)$$

The dynamics of spin-1/2 Heisenberg antiferromagnet with nearest-neighbor exchange constant J, on a two-dimensional square lattice deserves a more detailed discussion. This will be done in the near future.

It should be noted, however, that in order to make this kind of study valuable as one of the directions to studying the mechanism of HTSC the binding of quasiparticles must be taking into account. This very important problem[15,18,23] deserves the separate consideration. In spite of formal analogy of the our model (1) with that of a Kondo lattice, the physics are different. There is a dense system of spins interacting with a smaller concentration of holes. As many authors have mentioned, for the obtaining the magnon exchange mediated superconductivity (of the non-s-wave character most probably) the suitable effective interactions between two fermions, which is relevant for the case, is two-magnon exchange-type of interaction. Whese the fermion-magnon bound state formation has to be suppressed or not for promotion of the appearance of the superconductivity is not quite clear problem. This question is in close relation with the right definition of the magnon vacuum for the case when $K \neq 0$.

In summary, in this paper we have presented calculations for normal phase of HTSC, which are describable in terms of the spin-fermion model. We have characterized the true quasiparticle nature of the carriers and the role of magnetic correlations. It was shown that the physics of spin-fermion model can be understood in terms of competition between antiferromagnetic order on the CuO_2-plane preferred by superexchange J and the itinerant motion of carriers. In the present paper we do not presented all the details as regards for different possibilities of the definition of the relevant generalized mean fields in this formalism. Carrying this procedure to other possibilities leads to a much more rich set of solutions for the spin-fermion model. In the light of this situation it is clearly of interest to explore in details whether the hole motion is expressed as that of the Zhang–Rice singlet in the framework of the present formalism. Considering that the carrier-doping results in the HTSC for the realistic parameters range $t \gg J, K$, corresponding the situation in oxide superconductors, the careful examination of the collective behavior of the carriers for a moderately doped system must be performed. It seems that this behavior can be very different from that of single hole case. The problem of the coexistence of the suitable Fermi-surface of mobile fermions and the antiferromagnetic long range or short range order(c.f. Refs. 6, 18, and 19) has to be clarified. Finally, in the present paper we have considered the simplified spin-fermion model (1), taking into account a Kondo-like spin coupling K (6) between the oxygen hole and two nearest copper spins, arising from the strong *d–p* hybridization of the three-band extended Hubbard model.[1–4] However hybridization induces effective spin-preserving hopping and spin-exchanging hopping terms also,[1–4,37] implicitly taking into account the charge-transfer processes. Work is in progress to refine the present approach for calculating of two-hole dynamics and the binding of quasiparticles for more general models.

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