TRIPLET HOLE PROPAGATION AND HIGH- T_c SUPERCONDUCTIVITY

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We investigate the dynamics of a triplet hole in the d^9 background by using Born approximation. It is found that the coherent propagation by the hopping t is renormalized by the coupling between the hole and spin waves and that the Fermi liquid picture is lost. Arguments are given that triplet holes might give rise to superconductivity with a high value of T_c .

The main difficulty in the theoretical description of the high T_c superconductivity lies in the proximity of these systems to the metal-insulator transition. It is commonly accepted that the undoped materials are Mott-Hubbard (M-H) insulators and are well described by the isotropic spin- $\frac{1}{2}$ Heisenberg model. The main effort is therefore concentrated on the understanding of the dynamics of holes added by doping to the antiferromagnetic (AF) background stabilized in CuO_2 planes by strong correlations on Cu -sites. Up to now it has been assumed that the added hole forms locally a singlet of Zhang-Rice type,¹ with the dynamics described in terms of the $t-J$ model.²

The recent spectral weight transfer experiments³ gave support to the notion that the $t-J$ model suffices for the description of the low energy physics. However, the results of the photoemission experiments by Bianconi *et al.*⁴ indicate that a significant fraction of the holes have $3d_{3z^2-r^2}$ (d_{z^2}) character and may form a *local triplet*. Motivated by this, we analyze the dynamics of a triplet hole in an AF d^9 background of Cu spins, starting from the effective Hamiltonian derived in the strong correlation limit,⁵

$$H = t_z \sum_{\langle ij \rangle, \sigma} d_{i\sigma}^+ f_{j,\alpha(\sigma)}^+ f_{i,\alpha(\sigma)} d_{j\sigma} + \frac{t_z}{\sqrt{2}} \sum_{\langle ij \rangle, \sigma} (d_{i\sigma}^+ f_{j,0}^+ f_{i,\alpha(\sigma)} d_{j\sigma, -\sigma} + h.c.) + \frac{t_z}{2} \sum_{\langle ij \rangle, \sigma} d_{i\sigma}^+ f_{j,0}^+ f_{i,0} d_{j\sigma, \sigma} + J \sum_{\langle ij \rangle} \tilde{S}_i \tilde{S}_j. \quad (1)$$

Here t_z stands for the hopping of the added hole of d_{z^2} symmetry and is smaller by a factor ~ 3 than the usually considered hopping of $3d_{x^2-y^2}$ (d_{x^2}) holes. J is the AF exchange interaction between Cu spins. The operators $f_{i,m}^+$ and $d_{i\sigma}^+$ create a component $m = 1, 0, -1$ of the triplet ($\alpha(\sigma) = 1, -1$ for $\sigma = \uparrow, \downarrow$),

and a hole of spin σ in d_{x^2} orbital at site i , respectively. There are three elementary hopping processes for a triplet hole: $(1_i, \uparrow_j \rightarrow \uparrow_i, 1_j)$, $(1_i, \downarrow_j \rightarrow \uparrow_i, 0_j)$, $(0_i, \uparrow_j \rightarrow \uparrow_i, 0_j)$, with hopping amplitudes $t, t/\sqrt{2}$ and $t/2$, respectively (i and j denote nn lattice sites; the other 5 hops can be obtained by time- and/or spin reversal). In the singlet $t-J$ model, only the third type of hopping exists; the other two are a consequence of the internal degree of freedom of the triplet hole.

We study the dynamics of the triplet hole by using the linear spin wave (LSW) approach of Schmitt-Rink *et al.*,⁶ which proved to be very successful in the case of the singlet $t-J$ model with a single hole.⁷ After rewriting the Hamiltonian (1) in terms of Schwinger bosons and making the standard mean-field approximation for a two-sublattice AF system,⁸ one finds

$$H^{LSW} = \sum_{\vec{k}, \sigma = \pm 1/2} \varepsilon_{\vec{k}} \xi_{\vec{k}\sigma}^\dagger \xi_{\vec{k}\sigma} + \sum_{\vec{q}} \omega_{\vec{q}} \beta_{\vec{q}}^\dagger \beta_{\vec{q}} - \frac{zt_z}{4\sqrt{N}} \sum_{\vec{k}, \vec{q}} \{ \xi_{\frac{1}{2}, \vec{k}} \xi_{-\frac{1}{2}, \vec{k}-\vec{q}}^\dagger [(\gamma_{\vec{k}-\vec{q}} u_{\vec{q}} + \gamma_{\vec{k}} v_{\vec{q}}) \beta_{\vec{q}}^\dagger + (\gamma_{\vec{k}-\vec{q}} v_{\vec{q}} + \gamma_{\vec{k}} u_{\vec{q}}) \beta_{-\vec{q}}] + 2 \sum_{\pm} \xi_{\pm \frac{1}{2}, \vec{k}} \xi_{\pm \frac{1}{2}, \vec{k}-\vec{q}}^\dagger \gamma_{\vec{k}} (v_{\vec{q}} \beta_{\vec{q}}^\dagger + u_{\vec{q}} \beta_{-\vec{q}}) + h.c. \}. \quad (2)$$

Here, $\varepsilon_{\vec{k}} = -zt_z \gamma_{\vec{k}} / \sqrt{2}$, $\omega_{\vec{q}}$ and $\beta_{\vec{q}}^\dagger$ are the magnon dispersion and creation operator, respectively, and $u_{\vec{k}}, v_{\vec{k}}$ are the LSW coherence factors.⁶ This equation is considerably more complicated than the equivalent expression for the singlet model. First, we note that the number of hole degrees of freedom is doubled. Calling the up (down) spin sublattice A (B), and adding a hole of spin $1/2$ ($-1/2$) creates the triplet states of $M_s = 1$ on A and of $M_s = 0$ on B (or 0 on A and -1 on B), respectively. This corresponds to a physical hole added to the Néel state and is labelled with $\xi_{\pm \frac{1}{2}, \vec{k}}$, respectively. In addition, a $M_s = 1$ state can be created on sublattice

tice B (or -1 on A), corresponding to a total z th spin component $3/2$ ($-3/2$) and labelled by $\xi_{\pm\frac{3}{2},\vec{k}}$. Second difference between the present problem and the singlet hole is the presence of a free propagation term $\sim \varepsilon_{\vec{k}}$. It reflects the possibility of the triplet hole propagation without disturbing the underlying spin background, as, for example, by $1_A \rightarrow 0_B \rightarrow 1_A \rightarrow \dots$ processes. But like in the singlet $t-J$ model, the coupling to magnons is present in the processes $0_A \rightarrow 0_B \rightarrow \dots$

Using the self-consistent Born approximation,^{6,8} we find the $1/2$ and $3/2$ hole Greens functions of the form $G_{1/2}(\vec{k}, \omega) = [z - \varepsilon_{\vec{k}} - \Sigma(\vec{k}, \omega) - \Pi(\vec{k}, \omega)]^{-1}$, and $G_{3/2}(\vec{k}, \omega) = [z - R(\vec{k}, \omega)]^{-1}$, with the selfenergies,

$$\Sigma(\vec{k}, \omega) = \left(\frac{zt_z}{4}\right)^2 \frac{1}{N} \sum_{\vec{q}} f(\vec{k}, \vec{q}) G_{1/2}(\vec{k} - \vec{q}, \omega - \omega_{\vec{q}}),$$

$$\Pi(\vec{k}, \omega) = \left(\frac{zt_z}{2}\right)^2 \frac{1}{N} \sum_{\vec{q}} \gamma_{\vec{k}}^2 \gamma_{\vec{q}}^2 G_{3/2}(\vec{k} - \vec{q}, \omega - \omega_{\vec{q}}),$$

$$R(\vec{k}, \omega) = \left(\frac{zt_z}{2}\right)^2 \frac{1}{N} \sum_{\vec{q}} \gamma_{\vec{k}-\vec{q}}^2 u_{\vec{q}}^2 G_{1/2}(\vec{k} - \vec{q}, \omega - \omega_{\vec{q}}),$$

where $f(\vec{k}, \vec{q}) = (\gamma_{\vec{k}-\vec{q}} u_{\vec{q}} + \gamma_{\vec{k}} v_{\vec{q}})^2$. We have solved this system of integral equations numerically in 2D on a 16×16 lattice. In the Ising limit there is no coupling of the $1/2$ hole to the $3/2$ defects. It suffices therefore to iterate the selfenergy $\Sigma(\vec{k}, \omega)$ alone, and the problem resembles the singlet $t-J$ model,⁷ but the free propagation $\varepsilon_{\vec{k}}$ is added. It determines the main features of the spectral function $A(\vec{k}, \omega) = \frac{1}{\pi} \text{Im} G_{1/2}(\vec{k}, \omega)$, with the sharp quasiparticle (QP) surviving at finite J only at the bottom of the band, while in the rest of the Brillouin zone, the QPs are strongly damped. If we turn on the coupling between the $1/2$ and $3/2$ holes, the above picture is altered in a subtle, but important way. First, one finds that the $3/2$ spectral function, $B(\vec{k}, \omega) = \frac{1}{\pi} \text{Im} G_{3/2}(\vec{k}, \omega)$, is completely incoherent

and no bound state develops. This can be understood qualitatively by considering again the Ising limit, where the $3/2$ hole splits into a delocalized $1/2$ hole, and a localized spin-flip, i.e. it appears as composite particle. As a consequence of the incoherency of the $3/2$ hole, the QP character of the physical $1/2$ hole is destroyed even at low energy and wavelength due to the coupling to the zero-energy magnons with $\vec{q} = (\pi, \pi)$. In Fig. 1 we show a typical result for the physical hole spectral function $A(\vec{k}, \omega)$. Thus, in contrary to the singlet $t-J$ model, QP behaviour is weakened by the spin background and is reminiscent of the divergence discussed in the spin-fermion model.⁹

It may be shown that the delocalization of triplet holes leads at finite hole concentration to a strong interaction with crystal field excitations which, in turn, is responsible for a qualitatively new pairing mechanism, with the attractive interaction being here of purely kinetic origin. The hopping of triplet holes becomes easier when some of the d_{x^2} holes are excited and the d_{x^2} holes may hop. Therefore, one expects that the moving triplet hole is dressed by the $d_{x^2} \rightarrow d_{z^2}$ orbital excitations. Higher values of T_c are obtained for increasing energy of the charge transfer excitation, E_z , as suggested by the experimental data.^{4,10}

Summarizing, we have shown that the triplet holes exhibit qualitatively different behaviour from the singlet ones. We believe that the experimental evidence that triplet holes are present in high- T_c superconductors may be of crucial importance for the theoretical understanding of the origin of superconductivity.

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FIGURE 1

Spectral function $A(\vec{k}, \omega)$, as obtained for $J = t_z = 1$ for five values of $\vec{k} = n(\frac{\pi}{4}, \frac{\pi}{4})$, with $n = 0, 1, 2, 3, 4$.

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