ISSN 1063-7834, Physics of the Solid State, 2011, Vol. 53, No. 10, pp. 1997–2000. © Pleiades Publishing, Ltd., 2011.
Original Russian Text © V.V. Val'kov, A.A. Shklyaev, M.M. Korovushkin, A.F. Barabanov, 2011, published in Fizika Tverdogo Tela, 2011, Vol. 53, No. 10, pp. 1895–1898.

SUPERCONDUCTIVITY

Influence of Triplet States on the Spectrum of Collective Spin-Polaron Excitations in a 2D Kondo Lattice

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Received April 5, 2011

Abstract—The normal and superconducting phases of the ensemble of spin polarons in a two-dimensional Kondo lattice have been considered under the conditions when the hopping integral is comparable to the *s–d* exchange interaction energy. The polaron excitation spectrum and the superconducting transition temperature have been found taking into account upper triplet states. The change in the concentration dependence of the critical temperature of the transition to the superconducting phase with the relation between the hopping integral and the integral of the *s–d* exchange coupling has been analyzed.

DOI: 10.1134/S1063783411100337

The electronic structure of the CuO_2 plane of high-T_c superconductors is quite well reproduced by the Emery model [1]. In the weakly doped region, it proves possible to switch to the effective Hamiltonian, for which the states of copper ions are homopolar, characterized by spin $S = 1/2$, and coupled to each other by indirect exchange interaction. The hole charge carriers of the oxygen subsystem interact with localized spin moments of the copper ions via the *s–d* exchange coupling. As a result, the energy spectrum of Fermi excitations is described by the two-dimensional Kondo lattice. If the *s–d* exchange coupling constant is comparable to or greater than the hopping integral, fining the spectrum of the Kondo lattice is based on the concept of a spin polaron [2, 3], according to which the elementary excitation in a 2D antiferromagnet is regarded as a hole- or electron-type charge carriers surrounded by a cloud of spin fluctuations. This approach reproduces the pseudogap behavior of high-T_c superconductors [4] and allows one to find the region of existence of the superconducting phase [5–7].

The Hamiltonian of the Kondo lattice includes the on-site *s–d* exchange interaction $J > 0$ between the spins $\mathbf{s}_f$ ($s_f^+ = c_{f\uparrow}^+ c_{f\downarrow}$, $s_f^z = (\hat{n}_{f\uparrow} - \hat{n}_{f\downarrow})/2$) and $\mathbf{S}_f$ of the hole and the localized ion, the Hubbard on-site repulsion of two holes with the energy U, as well as the motion of holes with the hopping energy t_{fg} and the Heisenberg term with the antiferromagnetic interaction integral of the localized ions

$$\begin{aligned}\hat{H} &= J\sum_f \mathbf{S}_f\mathbf{s}_f + U\sum_f \hat{n}_{f\uparrow}\hat{n}_{f\downarrow} + H_{\text{int}},\\ \hat{H}_{\text{int}} &= \sum_{fg,\alpha} t_{fg}c_{f\alpha}^+ c_{g\alpha} + \frac{1}{2}\sum_{fg} I_{fg}\mathbf{S}_f\mathbf{S}_g,\end{aligned} \quad (1)$$

where $\hat{n}_{f\alpha} = c_{f\alpha}^+ c_{f\alpha}$ are expressed in term of the Fermi creation and annihilation operators $c_{f\alpha}^+$ and $c_{f\alpha}$ of a hole with the spin α on the site f.

The eigenstates of the single-site Hamiltonian with the neglect of hopping and exchange interactions between the localized spins form an eight-dimensional space. In the absence of a hole, an ion can have two, spin-up $|\uparrow\rangle$ and spin-down $|\downarrow\rangle$, states. In the presence of a hole on the site, the magnetic interaction results in the formation of the singlet $|S\rangle = \frac{1}{\sqrt{2}}(c_\downarrow^+|\uparrow\rangle - c_\uparrow^+|\downarrow\rangle)$ with zero projection of the total spin or one of the triplet states $|-1\rangle = c_\downarrow^+|\downarrow\rangle$, $|0\rangle = \frac{1}{\sqrt{2}}(c_\downarrow^+|\uparrow\rangle + c_\uparrow^+|\downarrow\rangle)$, $|1\rangle = c_\uparrow^+|\uparrow\rangle$.

The energy of the triplet single-site states lies above the singlet by the *s–d* exchange interaction energy J. In the case of two holes on the site, the system appears in the state $|+\rangle = c_\uparrow^+ c_\downarrow^+|\uparrow\rangle$ or $|-\rangle = c_\uparrow^+ c_\downarrow^+|\downarrow\rangle$ with the positive or negative projection of the total spin, respec-

tively, depending on the orientation of the magnetic moment of the ion. In terms of the Hubbard operators for the above basis, the Fermi creation and annihilation operators of a hole take the form

$$c_{f\uparrow}^{+} = X_f^{1\uparrow} + \frac{1}{\sqrt{2}}(X_f^{0\downarrow} - X_f^{S\downarrow} + X_f^{+S} + X_f^{+0}) + X_f^{--1},$$
$$c_{f\downarrow}^{+} = X_f^{-1\downarrow} + \frac{1}{\sqrt{2}}(X_f^{0\uparrow} + X_f^{S\uparrow} + X_f^{-S} - X_f^{-0}) + X_f^{+1}. \quad (2)$$

Similarly, for the spin operators, we have

$$S_f^{+} = X_f^{\uparrow\downarrow} + \frac{1}{\sqrt{2}}(X_f^{S-1} + S_f^{0-1} + X_f^{10} - X_f^{1S}) + X_f^{+-},$$
$$S_f^{z} = \frac{1}{2}(X_f^{\uparrow\uparrow} - X_f^{\downarrow\downarrow} + X_f^{0S} + X_f^{S0} + X_f^{11} - X_f^{-1-1} \quad (3)$$
$$- X_f^{++} - X_f^{--}).$$

Hereinafter, we consider the system with weak doping in the $U=\infty$ limit and, therefore, neglect the two-hole states $|+\rangle$ and $|-\rangle$.

In the previous works [2–4, 6, 7], the normal and superconducting phases of the spin polaron on the Kondo lattice were studied under the assumption that the magnitude of the s–d exchange interaction is much greater than the hopping integral. Thus, the triplet state could be neglected or they were taken into account with the use of the perturbation operators. However, consideration of the contributions of upper energy levels expressed in terms of the additional two- and three-site components of the effective Hamiltonian indicate that the said contributions significantly affect the phase diagram of the transition of spin polarons to the superconducting state. This effect increases with a decrease in the ratio of the integral of the s–d exchange interaction to the hopping integral. It becomes clear that the perturbation theory can be insufficient to describe the ensemble of spin polarons at J close to t. The exact inclusion of the triplet states changes the structure of polaron because the multilevel system opens additional opportunities for the formation of Cooper pairs.

In the case of the s–d exchange interaction energy J comparable with the hopping integral t, the description of the system should equally take into account the transitions to the triplet states and to the singlet level. We disregard the two-hole states assuming that the Hubbard repulsion parameter is much greater than other energy parameters of the system. In terms of the Hubbard operators, Hamiltonian (1) involving the triplet states takes the form

$$H = -\frac{3}{4}J\sum_f X_f^{SS} + \frac{1}{4}J\sum_f (X_f^{00} + X_f^{11} + X_f^{-1-1}) + \hat{T} + \hat{I}, \quad (4)$$
$$\hat{T} = \sum_{fg} t_{fg}(c_{f\uparrow}^{+}c_{g\uparrow} + c_{f\downarrow}^{+}c_{g\downarrow}), \quad \hat{I} = \frac{1}{2}\sum_{fg} I_{fg}(\mathbf{S}_f\mathbf{S}_g),$$

where $\hat{T}$ corresponds to the kinetic part of the intersite interaction Hamiltonian and $\hat{I}$ describes the magnetic subsystem of the localized ions.

To study the normal and superconducting phases of the ensemble of spin polarons we choose the following basic Fermi annihilation operators: $a_{f\uparrow} = X_f^{\downarrow S}$, $b_{f\uparrow} = X_f^{\downarrow 0} + \sqrt{2}X_f^{\uparrow 1}$ for spin-up and $a_{f\downarrow} = X_f^{\uparrow S}$, $b_{f\downarrow} = X_f^{\uparrow 0} + \sqrt{2}X_f^{\downarrow -1}$ for spin-down quasiparticles. The hole annihilation operators are expressed in terms of the new operators in the following manner: $c_{f\uparrow} = \frac{1}{\sqrt{2}}(b_{f\uparrow} - a_{f\uparrow})$, $c_{f\downarrow} = \frac{1}{\sqrt{2}}(b_{f\downarrow} + a_{f\uparrow})$. The operators $a_{f\uparrow}$ and $a_{f\downarrow}$ correspond to the annihilation of a hole in the singlet state, whereas the operators $b_{f\uparrow}$ and $b_{f\downarrow}$ describe the transitions from the triplet states.

The equations of motion for the Green's functions constructed from the basic operators were separated with the use of the Zwanzig–Mori projection-operator technique [8–10]. This yields the set of equations for the normal $G_1(k) = \langle\langle a_{k\uparrow}|a_{k\uparrow}^{+}\rangle\rangle$, $G_2(k) = \langle\langle b_{k\uparrow}|b_{k\uparrow}^{+}\rangle\rangle$ and anomalous $F_1(k) = \langle\langle a_{-k\downarrow}^{+}|a_{k\uparrow}^{+}\rangle\rangle$, $F_2(k) = \langle\langle b_{-k\downarrow}^{+}|b_{k\uparrow}^{+}\rangle\rangle$ Green's functions in the Hartree–Fock approximation

$$(\omega - \varepsilon_{1k})G_1(k) + \frac{1}{4}t_kG_2(k) + \Delta_kF_1(k) - \frac{1}{3}\Delta_kF_2(k) = \frac{1}{2},$$
$$\frac{3}{4}t_kG_1(k) + (\omega - \varepsilon_{2k})G_2(k) + \Delta_kF_1(k) - \frac{1}{3}\Delta_kF_2(k) = 0,$$
$$\Delta_kG_1(k) + \frac{1}{3}\Delta_kG_2(k) + (\omega + \varepsilon_{1k})F_1(k) - \frac{1}{4}t_kF_2(k) = 0, \quad (5)$$
$$-\Delta_kG_1(k) - \frac{1}{3}\Delta_kG_2(k) - \frac{3}{4}t_kF_1(k)$$
$$+ (\omega + \varepsilon_{2k})F_2(k) = 0.$$

The bare spectra of the triplet and singlet levels have the respective form

$$\varepsilon_{1k} = -\frac{3}{4}J + \frac{1}{4}t_k, \quad \varepsilon_{2k} = \frac{1}{4}J + \frac{3}{4}t_k, \quad (6)$$

and the superconducting order parameter Δ_k is defined in terms of the anomalous averages

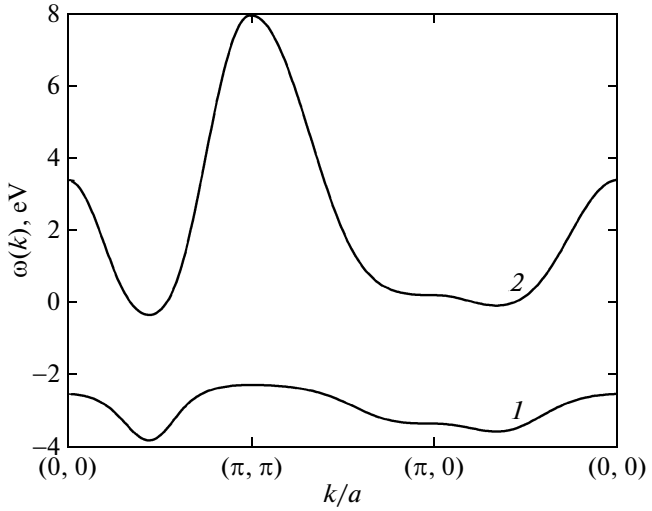

Fig. 1. Dispersion curves of (*1*) spin-singlet and (*2*) spin-triplet polarons for the parameters $J = 4$ eV, $t_1 = -0.6$ eV, $t_2 = 0.8$ eV, and $t_3 = 0.5$ eV.

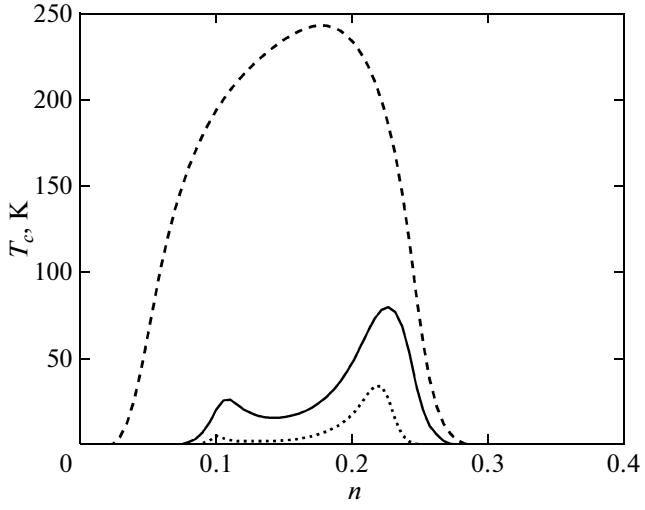

Fig. 2. Concentration dependences of the critical temperature calculated taking into account (dashed line) only singlet polarons (the $J = \infty$ limit), (solid line) singlet and triplet polarons, and (dotted line) contribution of triplet polarons found perturbatively.

$$\Delta_k = \frac{1}{N}\sum_q I_{k-q}\left(-\frac{3}{2}\langle a_{-q\downarrow}a_{q\uparrow}\rangle - \langle a_{-q\downarrow}b_{q\uparrow}\rangle\right) \qquad (7)$$

When writing the anomalous averages that appear in the Mori projecting procedure we took into account the averages corresponding to singlet–singlet and singlet–triplet pairing. The triplet–triplet averages were disregarded in the superconducting order parameter because the statistical weight of such pairings at thermodynamic equilibrium is quadratic in the concentration of triplet polarons. Thus, under usual conditions, such a quadratic contribution can be neglected as compared to the linear one.

Solving the dispersion relation for system (5) in the normal phase ($\Delta_k = 0$), we find two branches of the spectrum, which correspond to the (ω_{1k}) singlet and (ω_{2k}) triplet levels.

$$\begin{aligned}\omega_{1k} &= -\frac{1}{4}J + \frac{1}{2}t_k - \frac{1}{2}\sqrt{J^2 + Jt_k + t_k^2},\\ \omega_{2k} &= -\frac{1}{4}J + \frac{1}{2}t_k + \frac{1}{2}\sqrt{J^2 + Jt_k + t_k^2}.\end{aligned} \qquad (8)$$

The spin-polaron spectrum involving hopping up to the third coordination sphere is shown in Fig. 1.As is seen, the distance between the bands is comparable with the width of the lower band, whereas the value of the *s*–*d* exchange integral is relatively high, as compared to the hopping parameters.

Note, that when taking into account the triplet states, we could choose the basis built on the Hubbard operators $X_f^{\downarrow S}$, $X_f^{\downarrow 0}$, and $X_f^{\uparrow 1}$. In this case, finding the spin-polaron spectrum requires solving a cubic equation and two branches of the spectrum coincide with those given above, whereas the third one is dispersionless and corresponds to the triplet level $J/4$.

For the *d*-type symmetry of the order parameter, the equation for the critical temperature of the superconducting transition reads as

$$1 = \frac{1}{N}\sum_q I(\cos q_x - \cos q_y)^2 A(q, T_c), \qquad (9)$$

where

$$\begin{aligned}A(q, T) = &\left[\frac{3}{4}\left((\varepsilon_{2q}-\mu)^2 - (\omega_{1q}-\mu)^2 - \frac{1}{16}t_q^2\right)\right.\\ &\left.+\frac{1}{2}\left((\omega_{1q}-\mu)^2 - \left(\varepsilon_{1q}-\mu-\frac{3}{4}t_q\right)\left(\varepsilon_{2q}-\mu+\frac{1}{4}t_q\right)\right)\right]\\ &\times\left[2(\omega_{1q}-\mu)((\omega_{2q}-\mu)^2 - (\omega_{1q}-\mu)^2)\right]^{-1}\tanh\frac{\omega_{1q}-\mu}{2T}\\ &-\left[\frac{3}{4}\left((\varepsilon_{2q}-\mu)^2 - (\omega_{2q}-\mu)^2 + \frac{1}{16}t_q^2\right)\right.\\ &\left.+\frac{1}{2}\left((\omega_{2q}-\mu)^2 - \left(\varepsilon_{1q}-\mu-\frac{3}{4}t_q\right)\left(\varepsilon_{2q}-\mu+\frac{1}{4}t_q\right)\right)\right]\\ &\times\left[2(\omega_{2q}-\mu)((\omega_{2q}-\mu)^2 - (\omega_{1q}-\mu)^2)\right]^{-1}\tanh\frac{\omega_{2q}-\mu}{2T}.\end{aligned} \qquad (10)$$

Figure 2 presents the phase diagrams built with the use of different approaches to take into account the single-site states for the following parameters: $J = 4$ eV, $t_1 = -0.6$ eV, $t_2 = 0.8$ eV, $t_3 = 0.5$ eV, $I = 0.2$ eV.

Thus, the equations for the Green's functions of the normal and superconducting phases of the ensem-

ble of spin polarons taking into account both singlet and triplet single-hole states have been derived with the use of the Mori projection-operator technique. The spectrum of spin polarons in the normal phase (Fig. 1) has been found analytically. Clearly, at comparable values of the s–d exchange integral and the hopping parameters, the singlet branch of the polaronic excitations lies in the same energy interval as the one corresponding to the triplet states.

According to the analysis of the effect of the triplet states, the role of these states substantially increases with the relative contribution of the hopping integral. At the same time, the contribution of singlet–triplet paring to the concentration dependence of the superconducting transition temperature becomes important and leads to a difference with the results obtained perturbatively. It should be emphasized that, in this approach, the numerical results show an increase in the critical temperature.

ACKNOWLEDGMENTS

This study was supported by the Presidium of the Russian Academy of Sciences (Program "Quantum Physics of Condensed Matter"), the Siberian Branch of the Russian Academy of Sciences (Interdisciplinary Integration project no. 53), the Ministry of Education and Science of the Russian Federation (Russian Federal Targeted Program "Scientific and Scientific–Pedagogical Personnel of the Innovative Russia" in 2009–2013), and the Russian Foundation for Basic Research (projects nos. 09-02-00127, 10-02-00614).

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Translated by A. Safonov