One Spin-Polaron Problem in the Two-Dimensional Kondo-Lattice

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Within the frameworks of spin-polaron concept and the spherically symmetric state for the antiferromagnetic spin background, the one-particle motion is studied for two-dimensional Kondo-lattice. The elementary excitations are represented as a Bloch superposition of four one-site electron states: two local states - a bare electron state and a local spin-polaron of small radius, and two states of delocalized polarons which correspond to the coupling of local states to the antiferromagnetic spin wave with momentum $Q = (\pi, \pi)$, so called Q-polarons. As a remarkable result we show that the lowest band of elementary excitations is essentially determined by Q-polaron states in strongly coupled regime. The account of Q-polarons shifts the band bottom from $(\pi, \pi)$ to $(0, 0)$. The spectral weight of a bare particle in the lowest band states can greatly differ from 1. This may lead to a large Fermi surface for relatively small particle concentration.

71.27.+a,71.10.Fd,75.30.Mb

In order to understand the nature of high temperature superconductors it is important to describe properly the motion of a hole in the $CuO_2$ plane. This motion takes place on the antiferromagnetic spin background of copper spins and it must be treated as a correlated motion of a hole coupled to spin excitations (a spin polaron). Usually the spin polaron is studied within the frameworks of the t-J model and the three-band Hubbard model. These models seem to be rather complex because the effective spin-fermion coupling appears there only through the fermion hopping. Moreover, in the case of t-J model it is difficult to take into account the local constraint which represents the strong on-site fermion repulsion. We shall study the formation of the spin polaron within the frameworks of the more simple Kondo-lattice model. Note, that a generalized variant of the model leads to description of low-lying states in the three-band Hubbard model.

Treating this model Schrieffer replaced the spin subsystem by a classic field with a doubled lattice period and described the elementary excitations as the superposition of electronic states with the momenta $p$ and $p + Q$, where $Q = (\pi, \pi)$ is the antiferromagnetic vector. Such a description is deficient for the two-dimensional $S = \frac{1}{2}$ antiferromagnet because of strong spin fluctuations. Moreover, it becomes impossible if the spin subsystem is found in the homogeneous spherically symmetric state with long range order but with zero value of the average site spin $< S^\alpha > = 0$ (the homogeneous Neel state). The homogeneous Neel state seems more adequate, then the usual two-sublattice Neel state, for treating the ground state of the doped $CuO_2$ plane.

The distinctive feature of the present investigation consists in considering of the one-electron motion on the background of the homogeneous Neel state of the Kondo lattice. This motion is described by a spin polaron with the spectrum periodicity relative to the full Brillouin zone. Note that the conventional two-sublattice spin approach leads to periodicity relative to the magnetic Brillouin zone.

Another distinctive feature of our investigation consists in treating the spin-polaron as a complex quasiparticle accounted for a coherent superposition of a bare electron, of a local polaron and of two types of antiferromagnetic delocalized polarons. A local polaron can be attributed to the local singlet (an analogous of Zang-Rice polaron in the three-band Hubbard model) and such a polaron represents the lowest band in the limit of the strong Kondo interaction $J$. As to the antiferromagnetic delocalized polaron it is a bound state of an electron (or of a local polaron) with a spin wave with the momentum $Q$. As we know such bound states were not investigated previously. If the spin subsystem is found in the state with the antiferromagnetic long range order then the amplitude $S_Q$ of the spin wave with $q = Q$ (the Q-wave) has the macroscopic large value and has the properties analogous to the amplitude of a Bose particle with the zero momentum in the superfluid Bose-gas. As a result for many problems this amplitude can be treated as a $c-$number. Then the coupling of the $Q$-wave to local electron states does
not represent new states but leads, as mentioned above, to mixing of the states with the momenta \( p \) and \( p + Q \). But this treatment fails in the case of the homogeneous Neel state. In this background the average value \( < S_Q > = 0 \) and only \( < S_Q S_Q > \) can be treated as a macroscopic value. Then the coupling of a particle local state to \( S_Q \) corresponds to a new delocalized state. It will be shown that it is important to take into account such a quantum nature of the spin \( Q \)-wave because the transitions between the local polaron states and the delocalized polaron states essentially determine the spin polaron bands.

The Kondo-lattice Hamiltonian has the form

\[
H^{tot} = H_0 + H_1 + H_2,
\]

\[
H_0 = \sum_{rg} t_g a_{r+g}^\dagger a_r = \sum_p \epsilon_p a^\dagger_p a_p,
\]

\[
H_1 = J \sum_r a_r^\dagger \tilde{S}_r a_r,
\]

\[
H_2 = \frac{1}{2} I \sum_{rg} S^\dagger_{r+g} S^\alpha_r. \tag{4}
\]

Here the sums run over the sites \( r \) of a square lattice and over the nearest neighbors with the lattice spacing \( |g| = 1 \). For short we miss the spin index for creation \( a^\dagger_r \) and annihilation \( a_r \) operators of the Fermi particles (we shall name them as electrons) and in the Hamiltonian of Kondo-interaction \( H_1 \) we take the notation \( \tilde{S}_r = S^\dagger_r \sigma^\alpha \).

Let us represent the first two equations of the infinite chain of equations for the retarded Green’s functions, which describe the motion of one particle in the antiferromagnetic spin background. In the present paper we restrict ourself mainly to the analysis of the spectrum of the quasiparticles. That is why for simplicity of notations we shall simply write operators \( a \) instead of the Green’s functions \( \langle \langle a \mid b^\dagger \rangle \rangle \) and shall miss the nonhomogeneous terms \( < a, b^\dagger > \). The equations have the form

\[
(\omega - \epsilon_p) a_p = J b_p, \quad b_p = N^{-\frac{1}{2}} \sum_r b_r e^{-ipr}, \quad b_r = \tilde{S}_r a_r, \tag{5}
\]

\[
\omega \tilde{S}_{r+R} a_r = [\tilde{S}_{r+R} a_r, H_0 + H_1 + H_2] = \sum_g t_g \tilde{S}_{r+R} a_{r+g} + J \tilde{S}_{r+R} \tilde{S}_r a_r + i \epsilon \sigma_{\alpha} \sum_g \sigma_{\alpha} S^{\beta}_{r+R} a_{r+R} + \tilde{S}_r a_r. \tag{6}
\]

In Ref. [8] the mean-field approach was taken for the Neel lattice and the spins were treated as the classical vectors:

\[
S^\alpha_r = \delta_{az} S_0 e^{iQr}, \quad S_0 = const, \quad Q = (\pm \pi, \pm \pi). \tag{7}
\]

In this approximation the Kondo-interaction Hamiltonian \( H_1 \) takes the form of the potential energy with the doublet period and the equation \( \Box \) has a closed form:

\[
(\omega - \epsilon_p) a_p = \sigma J S_0 a_{p-Q}. \tag{8}
\]

Here \( p \) is in the Brillouin zone with the periods \( (2\pi, 0), (0, 2\pi) \), but the spectrum has the periodicity of the magnetic Brillouin zone:

\[
E_{ap} = \pm \sqrt{\epsilon_p^2 + \Delta^2}, \quad \Delta = S_0 J. \tag{9}
\]

In \( \Box \) and below we suppose the spectrum model with the ”nesting”:

\[
\epsilon_p = -\epsilon_{p+Q} = -2t(cosp_x + cosp_y) \tag{10}
\]

In the case of the \( S = \frac{1}{2} \) spin system the quantum fluctuations are important and the equation \( \Box \) must be used in order to find the last term in Eq. \( \Box \). In one’s turn the equation \( \Box \) hasn’t a closed form. In order to close the chain of equations we use the standard Mori-Zwanzig projection technique \( \Box \). In our case this means that we must approximate the last two terms in the right-hand side of \( \Box \) by their
projections on the restricted space of bases operators. The choice of the restricted set of basis operators
must be dictated by the physics of the problem under discussion.

For a paramagnetic spin subsystem state the simplest set of basis operators may be taken as two
operators that appear in the first equation (5), that are the operator of a "bare" electron \( a_r \) and the
annihilation operator of an one-site spin polaron \( b_r \). The local polaron excitations in the Kondo lattice
were previously discussed in Ref. \[7\].

Now let the spin subsystem to be found in the homogeneous Neel state with the tensor parameter of
the long range order:

\[
< S^\alpha_r > = 0, 
\tag{11}
\]

\[
C^{\alpha\beta}_{R} = < S^\alpha_r S^{\beta}_{r+R} > = M^{\alpha\beta} e^{iQR}, \quad |R| >> 1. 
\tag{12}
\]

Then it will be consecutively to introduce the operators which take into account the correlation of the
electron and the local polaron with the antiferromagnetic \( Q \)-wave

\[
c_r = \tilde{Q} r a_r, \quad c_p = \tilde{Q} a_{p+Q}, 
\tag{13}
\]

\[
\tilde{Q} r = N^{-1} \sum_R e^{iQR} \tilde{S} r+R = e^{iQR} \tilde{Q} \text{.} 
\tag{14}
\]

\[
d_r = \tilde{Q} r \tilde{S} r a_r, \quad d_p = \tilde{Q} a_{p+Q}. 
\tag{15}
\]

Note, that the operators \( c_r \) and \( d_r \) allow for distant correlations between the spin and the electron
(| \( R \) | >> 1). So, in a sense our approach is alternative to the widely used \( t-J \) model investigations based
on the decoupling of an on-site Fermi operator into a spinless fermion and an antiferromagnetic magnon
operator \[13–16\].

It is substantial that the adopted set of the basis operators is closed relative to the Kondo-interaction
Hamiltonian:

\[
[a_r, H_1] = J b_r , \\
[b_r, H_1] = J (\frac{3}{4} a_r - b_r) , \\
c_r, H_1 = J d_r , \\
[d_r, H_1] = J (\frac{3}{4} c_r - d_r). 
\tag{16}
\]

Taking into account Eq.(6) this gives,in particular,

\[
(\omega - \epsilon_{p+Q}) c_p = J d_p . 
\tag{17}
\]

In order to get a closed form for the Green’s functions equations we shall project the corresponding
commutators on the following orthonormal set of basis operators:

\[
B_1 r = a_r , \\
B_2 r = \frac{1}{\sqrt{f_2}} b' r , \quad b_r = b_r - c_r , \\
f_2 = < [b'_r, b'_r]^+ > = \frac{3}{4} - M, \quad M = M^{\alpha\alpha} , \\
B_3 r = \frac{1}{\sqrt{f_3}} c_r , \\
f_3 = < [c_r, c_r]^+ > = M , \\
B_4 r = \frac{1}{\sqrt{f_4}} d'_r , \quad d'_r = d_r - M a_r + \frac{M}{f_2} (b_r - c_r) , \\
f_4 = < [d'_r, d'_r]^+ > = M (f_2 - \frac{M}{f_2}) . 
\tag{18}
\]
The coefficients of the projection relations
\[ [B_i, H] = \sum_j a_{ij} B_j \]  
are determined as
\[ a_{ij} = \langle [B_i, H], B_j^+ \rangle _+ . \]  

Taking into account the equations (17), (18) and (20), we obtain in momentum representation a simple system of four equations
\[ \omega B_{i,p} = \sum_j a_{ij} B_{j,p} \]  
The matrix elements of the spectral matrix \( a_{ij} \) are equal
\[ a(1, 1) = \epsilon_p, \quad a(1, 2) = J\sqrt{f_2}, \quad a(1, 3) = J\sqrt{M}, \quad a(1, 4) = 0, \]
\[ a(2, 2) = \frac{1}{f_2} [(C + M)\epsilon_p - J(f_2 - M) - 4IC], \]
\[ a(2, 3) = -J\sqrt{\frac{M}{f_2}}, \]
\[ a(2, 4) = \frac{M}{f_2} (C + M)\epsilon_p - Jf_4 - 2IM(1 + \frac{2C}{f_2}) \frac{1}{\sqrt{f_2f_4}}; \]
\[ a(3, 3) = -\epsilon_p, \quad a(3, 4) = J\sqrt{\frac{4}{M}}; \]
\[ a(4, 4) = \frac{M}{f_4} [(C + M)\frac{M}{f_2} - (C + \frac{M}{3})\epsilon_p - \frac{3J}{4f_2} + \frac{IM}{f_4}\frac{8M}{3} - 4C(1 + \frac{M}{f_2}) - \frac{4M}{f_2}]. \]

Here \( C = C^\alpha_{R=1} < 0 \). To obtain these expressions we used the following approximation of Takahashi [17] for four different-site spin correlation functions
\[ < S^i_{r_1} S^j_{r_2} S^k_{r_3} S^l_{r_4} >= C^{ij}_{r_1-r_2} C^{kl}_{r_3-r_4} + C^{ik}_{r_1-r_3} C^{jl}_{r_2-r_4} + C^{il}_{r_1-r_4} C^{jk}_{r_2-r_3}, r_1 \neq r_2 \neq r_3 \neq r_4. \]  

Hence, in the adopted approximation the electron motion in the antiferromagnetic background is described by the quasiparticle that is a coherent superposition of four Fermi fields - the field of the bare electron \( a_p \), the field of the delocalized polaron \( \epsilon_p \) and two fields of the localized polaron \( b_p \) and \( d_p \), which are hybridized mainly due to the Kondo-interaction. The system of equations (21) can be treated as the system of the Schrodinger equations where the matrix elements \( a_{ij} \) reproduce the amplitude of the transitions from the state \( j \) to the state \( i \). The presence of the nondiagonal matrix elements underlines the quantum nature of the spin \( S \) and the \( Q \)-waves. The eigenfunctions and the eigenvalues of Eqs. (21) describe the elementary excitations which generate four bands. The form of the bands depends on the state of the magnetic subsystem (the quantities \( M \) and \( C \)) and the relations between the energetic parameters \( t, J, I \). Below we take the following typical values for the quantities \( M \) and \( C \): \( M = 0.1 \) and \( C = -0.335 \) [18][19][20][21].

In the adopted model all the spectra depend on momentum only through \( \epsilon_p \). Let us mention that calculating the matrix elements (24) we took the approximation of low density of Fermi particles, i.e., \( < a_p^\dagger a_p > \rightarrow 0 \).

It is essential that the resulting four bands are only approximately symmetric relative to the magnetic Brillouin zone boundary. In the momentum space the distance between two quasiparticle states with the equal energy can differ from the antiferromagnetic vector \( Q \). This means that dictated by these bands the "shadow band" effect can be other than the usual one displaced by \( Q \) vector in the two-sublattice Neel antiferromagnet [19].

Four waves of the quasiparticle spectrum \( E^{(i)}(p), i = 1 - 4 \), given by the eigenvalues of the system of equations (21), have a clear physical meaning in the cases when one of energetic parameters \( t, J, I \) is much greater than the others. The bands for these cases are represented in Figs. 1-3(a). In Figs. 1-3(b) we also represent the values of the electron Green’s function residues \( Z^{(i)}_p \), which correspond to the poles E^{(i)}(p).
In the low density limit the residues $Z_p^{(i)}$ are determined by the solution of the equations of motion for Green's functions $<< B_{1,p} | B_{1,p}^+ >>$ when the nonhomogeneous terms are equal to $W_{1,1} = << B_{1,p} | B_{1,p}^+ >>$. The $Z_p^{(i)}$ values represent one-particle spectral function $A(p, \omega) = \sum_i Z_p^{(i)} \delta(\omega - E^{(i)}(p))$. Each of these values $Z_p^{(i)}$ characterizes the contribution (weight) of a bare particle state $a_p$ to the quasiparticle state with the energy $E^{(i)}(p)$. For this reason $\sum_i Z_p^{(i)} = 1$.

First, if the energy of the antiferromagnetic exchange is the largest energetic parameter ($I >> J, t$) then the formation of the local polaron $b_p$ is energetically disadvantageous because this formation leads to the disintegrating of antiferromagnetic correlations between spins $S_r$ and $S_{r+q}$. In Fig. 3 the quasiparticle spectra $E^{(i)}(p)$ are given along the symmetry line $p = (p_x, p_y)$ for $I = 5, J = t = 1$. The local polaron bands (they represent the motions of $b_p$ and $d_r$) lie essentially higher by energy then two other bands which correspond to the hybridized spectra (11) with the gap $\Delta = J\sqrt{M}$. Two higher bands are characterized by a small weight of spectral function $A(p, \omega)$ (see Fig. 3(b)). As to two lowest bands, the spectral function weight is close to 1 when the band represents mainly the motion of a bare particle and is close to zero for the Q-polaron band. In the region of strong hybridization, $p$ close to $\pi/2$, the spectral weight is of the same order for both bands. It may be seen, that these two lowest bands have the symmetry close to the symmetry given by the magnetic Brillouin zone, but the corresponding quasiparticles have the full Brillouin zone symmetry.

Now let us discuss the second case, represented in Fig. 3 by the spectrum for $J = I = 0.1t$, when the spin interactions are small relative to the kinetic energy of the electron, $t >> J, I$. In this case all quasiparticles are approximately independent: the free motion of the bare electron $B_{1,p} = a_p$ is described by the band $E_1 \equiv \epsilon_p$ and the antiferromagnetic polaron $B_{3p}$ moves in the band $E_3 \equiv \epsilon_{p+r} = -\epsilon_p$. As to the local polaron $B_{2p}$ it has it’s own dispersion $E_2 \equiv a(2,2)$, (22). The absolute value of the multiplier $(- | C_1 | + M)/f_2$ of the term with $\epsilon_p$ in the expression for $a(2,2)$ characterizes the essential band narrowing, i.e. the increase of the local polaron mass relative to the mass of the bare electron. Finally, the $B_{4p}$ polaron band $E_4 \equiv a(4,4)$ also demonstrates a strong, but different renormalization of the mass. The difference in the renormalization is one of the reasons why the resulting hybridized spectra are asymmetrical relative to the magnetic Brillouin zone boundary. The crossing of the nonhybridized spectra takes place close to this boundary where $\epsilon_p = 0$. Out of this region one of the bands explicitly represents the motion of the bare particle and has the spectral weight $Z_p$ close to 1.

Fig.3 describes the case $J >> t, I$. The lowest bands (with the center at $E^{(s)} \cong -\frac{3}{2}J$) correspond to the motion of the local polaron in a singlet state $b^{(s)} = b - \frac{1}{2}a$ and to the motion of such a polaron coupled to the Q-wave. The upper bands (centered at $E^{(t)} \cong \frac{3}{2}J$) describe the motion of the local polaron in a triplet state $b^{(t)} = b + \frac{1}{2}a$ and also its coupling to the Q-wave. The "singlet" and "triplet" terminology suppose, that acting on the spin subsystem state, the operators $b^{(s)}_r$, $b^{(t)}_r$ create accordingly a singlet or triplet spin-electron pair in the site $r$.

The qualitative and important difference of this case from the previous ones is the following. For two first cases the bottom of the lowest band is determined mainly either by the motion of the bare particle or by the motion of Q-polaron $c_p$, the residues being close to 1 and zero correspondingly. In the present case the bottom of the spectrum of the elementary excitations turns out to be substantially determined by the $b_p$ and $d_p$-states. At the same time, as it may be seen from Fig.3 (b) (the solid line), the possible filling of each $p$ state by a particle with a fixed spin is not too small for the lowest band and is close to 0.1. Let us mind that such a strong deviation of filling from 1 must lead to relatively great Fermi surface even at small filling.

The present case demonstrates the importance of taking into account the Q-polaron $d_p$. In order to illustrate this circumstance, in Fig. 4 we show the spectrum of the elementary excitations calculated for the same values of energetic parameters as in Fig.3, but using the basis of the first three operators $a_p, b_p, c_p$. As it may be seen by comparison of Figs.3 and 4, this leads to the shift of the lowest band from the point $p = (0, 0)$ to the point $p = (\pi, \pi)$. At the same time the value of the residue $Z_p$ for the band bottom is close to 0.1 as in Fig.3.

Finally, if three energetic parameters are of the same order of magnitude then the elementary excitation in any of four bands is a coherent superposition of the states $a, b, c, d$ and these states have relatively the same weight. It is notable that the presence of the long range order doesn’t lead to the periodicity of the spectrum relative to the magnetic Brillouin zone.
Let us mind that the described above properties of the spin polaron are mainly preserved if we suppose that the spin subsystem has no long range order but the spin correlation length is large. This must lead to the replacement of (12) with the following relation which is true for 2D antiferromagnet at $T \neq 0$:

$$C_{\alpha \beta}^{\gamma \delta} = \langle S_{\alpha}^{\gamma} S_{\beta}^{\delta} \rangle = M_{\alpha \beta}^{\gamma \delta} e^{iQR} e^{-\frac{R}{L}}, \quad L > > 1.$$  

In this case the delocalized polaron is described by the relation

$$c_r = L^{-3} \sum_R e^{iQR} e^{-\frac{R}{L}} S_{r+R} a_r.$$  

In conclusion we want to make several notes. First, above we investigated the elementary excitations of the system - one electron plus the AFM spin subsystem. It may be seen that all the results for the system with one hole may be obtained from the discussed above case by substituting $(-t_g)$ instead of $t_g$ in the kinetic Hamiltonian.

Secondly, the ignoring of the Q-polarons, i.e., the states $c$ and $d$, leads to the disappearance of bands, and can change essentially the remaining bands. We think that it is important to take into account Q-polarons in such models as $t-J$ and three-band Hubbard model, where the particle motion is strongly coupled to the spin subsystem.

Finally, let us mention once more that our calculations are performed in the limit of low filling. Nevertheless the calculated upper bands have physical meaning if we shall study the electron transitions. In general case it may be seen that the one-particle spectral density strongly depends on filling.

ACKNOWLEDGMENTS

We are grateful to L.B.Litinski for valuable discussions and comments. This work was supported, in part, by the INTAS-PFBR (project No. 95-0591), by RSFR (Grant No. 95-02-04239-a), by Russian National program on Superconductivity (Grant No. 93080), ISI Foundation and EU NTAS Network 1010-CT930055.

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FIG. 1. (a) The quasiparticle spectra $E_i(p)$ for $I = 5 \gg J = t = 1$ along the symmetry line $p = p_x = p_y$; (b) the values of the electron Green’s function $\langle \langle a_{\rho\sigma} | a_{\rho\sigma}^+ \rangle \rangle$ residues $Z_p^{(i)}$ which correspond to the poles $E_i(p)$. Different line types represent four bands and corresponding residues.

FIG. 2. (a) The quasiparticle spectra $E_i(p)$ for $t = 1 \gg I = J = 0.1$ along the symmetry line $p = p_x = p_y$; (b) the values of the electron Green’s function $\langle \langle a_{\rho\sigma} | a_{\rho\sigma}^+ \rangle \rangle$ residues $Z_p^{(i)}$ which correspond to the poles $E_i(p)$, $Z_p^{(i)}$ are shown for the interval close to $p = \pi/2$. Different line types represent four bands and corresponding residues.

FIG. 3. (a) The quasiparticle spectra $E_i(p)$ for $J = 5 \gg t, I, t = 1, I = 0.1$ along the symmetry line $p = p_x = p_y$; (b) the values of the electron Green’s function $\langle \langle a_{\rho\sigma} | a_{\rho\sigma}^+ \rangle \rangle$ residues $Z_p^{(i)}$ which correspond to the poles $E_i(p)$. Different line types represent four bands and corresponding residues.

FIG. 4. The same as in Fig. 3, but for truncated basis of three operators $a_p, b_p, c_p$. 
