Bethe-Salpeter equations for the collective modes of the $t-U-V-J$ model with d-wave pairing

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The Bethe-Salpeter equations for the collective modes of a $t-U-V-J$ model are used to analyze the resonance peak observed at $Q = (\pi, \pi)$ in neutron scattering experiments on the cuprates. We assume that the resonance emerges due to the mixing between the spin channel and 19 other channels. We have calculated the energy of the lowest mode of the extended Hubbard model ($J = 0$) vs the on-site repulsive interaction $U$, as well as the $UJ$ lines in the interaction parameter space which are consistent with the ARPES data and reproduces the resonance peak at 40 meV in Bi2212 compound. We find that the resonance is predominantly a spin exciton.

PACS numbers: 71.10.Ca, 74.20.Fg, 74.25.Ha

Introduction. It is widely accepted that: (i) the angle-resolved photoemission spectroscopy (ARPES) data produce evidences for the opening of a d-wave pairing gap in cuprates compounds described at low energies and temperatures by a BCS theory, and (ii) the basic pairing mechanism arises from the antiferromagnetic exchange correlations, but the charge fluctuations associated with double occupancy of a site also play an essential role in doped systems. The simplest model that is consistent with the last statements is the $t-U-V-J$ model. In the case of d-pairing the gap function is $\Delta_k = \Delta d_k/2$, where $\Delta$ is the maximum value of the energy gap and $d_k = (\cos k_x - \cos k_y)$ (lattice constant $= 1$). The BCS gap equation is $1 = \frac{V^2}{2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d^2 \mathbf{k}}{(2\pi)^2} \sqrt{\Delta^2 + \Delta_k^2}$, where $V_\phi = 2V + 3J/2$, $E(k) = \sqrt{\Delta^2 + \Delta_k^2}$. The mean-field electron energy $E_k$ has a tight-binding form $E_k = t_1 (\cos k_x + \cos k_y)/2 + t_2 (\cos 2k_x \cos k_y + \cos 2k_y) + t_3 (\cos 2k_x + \cos 2k_y)/2 + t_4 (\cos 2k_x \cos k_y + \cos 2k_y)/2 + t_5 \cos 2k_x \cos 2k_y - \mu$. The coupling of the spin channel with other channels should change the RPA results for $U$. For example, we have two $\pi$ channels with bare $\pi$ susceptibilities $\chi^{(2)}_{\pi} = \frac{2}{\pi} I_{\gamma\gamma}^{2} J_{\gamma\gamma}^{2}$, respectively. The susceptibilities $I_{\gamma\gamma}^{2}$, $J_{\gamma\gamma}^{2}$, $J_{\gamma\gamma}^{2}$ represent the mixing of the spin and two $\pi$ channels. Thus, the coupling of the spin and two $\pi$ channels (a three-channel response-function theory) leads in the generalized random phase approximation (GRPA) to a set of three coupled equations and the value of $U$ is reduced from 1.16 eV to 0.974 eV. When the extended spin channel is added to the previous three channels, we have a set of four coupled equations (a four-channel theory), and according to Ref. $U \approx 300$ meV is required in the case when $V_\phi = 0.260 eV$ and $J = 0$.

In what follows, the energy of the resonance is obtained from the solution of 20 coupled Bethe-Salpeter (BS) equations for the collective modes in GRPA, i.e. the resonance emerges due to the mixing between the spin channel and other 19 channels. In our approach the INSR energy solves $det[\chi^{-1} - \hat{V}] = 0$, where the mean-field response function $\chi$ and the interaction $\hat{V}$ are $20 \times 20$ matrices. The secular determinant can be rewritten as $det[\chi^{-1} - \hat{V}] = det [\hat{A} \hat{B}]$, where $A = det[C|det|A - BC^{-1}B^T|]$. In the case of the four-channel response-function theory $A$ is a $4 \times 4$ matrix while the mixing with the other 16 channels is represented by a $4 \times 4$ matrix $BC^{-1}B^T$. We emphasize that none of the previous theoretical interpretations of the INSR feature at $Q_0$ have accounted properly for the mixing term $BC^{-1}B^T$.

$t-U-V-J$ model. The Hamiltonian of the $t-U-V-J$ model consists of $t$ and $U$ terms representing the hopping of electrons between sites of the lattice and their on-site repulsive interaction, as well as the spin-independent attractive interaction $V$ and the spin-dependent antiferro-
magnetic interaction $J$:  

$$H = -\sum_{i,j,\sigma} t_{ij} \hat{\psi}_{i,\sigma}^\dagger \hat{\psi}_{j,\sigma} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - V \sum_{<i,j>\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'} + J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j. \tag{1}$$

Here, the Fermi operator $\hat{\psi}_{i,\sigma}^\dagger$ ($\hat{\psi}_{i,\sigma}$) creates (destroys) a fermion on the lattice site $i$ with spin projection $\sigma = \uparrow, \downarrow$ along a specified direction and $\hat{n}_{i,\sigma} = \hat{\psi}_{i,\sigma}^\dagger \hat{\psi}_{i,\sigma}$ is the density operator on site $i$ with a position vector $r_i$. The symbol $\sum_{<i,j>}$ means sum over nearest-neighbor sites. $t_{ij}$ is the single electron hopping integral. The antiferromagnetic spin-dependent interaction $J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j = J_1 + J_2$ consists of two terms:  

$$J_1 = \sum_{<i,j>\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,,\sigma'} - \hat{n}_{i,\uparrow} \hat{n}_{j,\downarrow} - \hat{n}_{i,\downarrow} \hat{n}_{j,\uparrow}, \quad \text{and} \quad J_2 = \sum_{<i,j>} \left[ \hat{n}_{i,\uparrow} \hat{n}_{j,\downarrow} \hat{\psi}_{i,\downarrow} \hat{\psi}_{j,\uparrow} + \hat{n}_{i,\downarrow} \hat{n}_{j,\uparrow} \hat{\psi}_{i,\uparrow} \hat{\psi}_{j,\downarrow} \right].$$

It is useful to introduce four-component Nambu fermion fields $\vec{\psi}(y)$ and $\hat{\psi}(x)$ as $\left(\psi_i^\dagger(y) \psi_i(x) \psi_i(y) \psi_i^\dagger(x)\right)^T$, where $x$ and $y$ are composite variables and the field operators obey anticommutation relations. The "hat" symbol over any quantity $\hat{O}$ means that this quantity is a matrix.

The interaction part of the extended Hubbard Hamiltonian is quartic in the Grassmann fermion fields so the functional integrals cannot be evaluated exactly. However, we can transform the quartic terms to a quadratic form by applying the Hubbard-Stratonovich transformation for the electron operators $\hat{A}_{\alpha}(z)$:

$$\int D\hat{A}_\alpha(z) D\hat{A}_\beta(z') \gamma_{\alpha\beta}(z,z') \psi(z) \psi(z') = e^{-\frac{1}{2} \langle \hat{\psi}(y) \hat{\psi}(x) \rangle D_{\alpha\beta}^{(0)}(y,x)} D_{\alpha\beta}^{(0)}(z,z') \langle \hat{\psi}(y) \hat{\psi}(x) \rangle \delta(z-z').$$

The last equation is used to define the $4 \times 4$ matrices $\hat{D}_\alpha^{(0)}$ and $\hat{\Gamma}_\alpha^{(0)}(\alpha, \beta = 1, 2, 3, 4)$. Their Fourier transforms, written in terms of the Pauli matrices $\sigma_i$, Dirac $\gamma^0$ and alpha matrices, are as follows: $\hat{\Gamma}_\alpha^{(0)} = \left( \begin{array}{cc} \hat{D}_{1} & 0 \\ 0 & \hat{D}_{2} \end{array} \right)$, $\hat{\Gamma}_\alpha^{(0)} = (\gamma^0 \pm \alpha_i)/2$ and $\hat{\Gamma}_3^{(0)} = (\alpha_x \pm i\alpha_y)/2$, where $\alpha_i = \left( \begin{array}{cc} \sigma_i & 0 \\ 0 & -\sigma_i \end{array} \right)$. Following the same steps as in Refs. [12,13], we can derive a set of sixteen BS equations for the collective modes $\omega(Q)$ and BS amplitudes $\Psi_{n_1 n_2}(k)$ ($n_1, n_2 = 1, 2, 3, 4$). Their matrix representation at zero temperature is:

$$\hat{\Psi}(Q) = \frac{1}{N} \sum_q \int \frac{d\Omega}{2\pi} \langle -\hat{\Gamma}_\alpha^{(0)}(q-k) \hat{G}(k+Q; \Omega + \omega) \rangle \hat{\Psi}(Q) \hat{G}(k; \Omega) Tr[\hat{\Gamma}_\beta^{(0)} \hat{\Psi}(Q)]$$

where $\hat{G}(k; \Omega)$ is the BCS Green’s function. The di-
rect \( \tilde{\Gamma}^{(0)}_{\alpha\beta} (k-q) \tilde{\Gamma}^{(0)}_{\alpha\beta} \) and exchange \( \tilde{\Gamma}^{(0)}_{\alpha\beta} (Q) \tilde{\Gamma}^{(0)}_{\alpha\beta} \) interactions mix all sixteen BS amplitudes. We can greatly simplify Eqs. [2] using the fact that in the RPA the susceptibilities at \( Q_0 \) are convolutions of two single-particle Green's functions \( \tilde{G} \), and the equation for the collective mode in the RPA is: \( \chi_1^{(0)\dagger}(\omega) \chi_2^{(0)}(\omega) - C_{12}(\omega) = 0 \), where the susceptibilities \( \chi_1^{(0)} \) and \( \chi_2^{(0)} \) originate from \( (U, J_1) \) and \( J_2 \) interactions, respectively. The term \( C_{12} \) mixes the \( J_1 \) and \( J_2 \) interactions, but it is proportional to convolutions which involve the anomalous Green's functions \( G_{13} \) and \( G_{24} \). The two Green's functions appears in the case of spin triplet pairing states where the order parameter \( \Delta_{\alpha\beta}(k) \) is a \( 2 \times 2 \) matrix. For a singlet superconductivity and d-wave pairing \( \Delta_{\alpha\beta}(k) = i(\sigma_y)_{\alpha\beta} \Delta(k) \), \( C_{12}(\omega) = 0 \), and the equation for collective modes becomes \( [1 + (U + 4J)I_{\tilde{\chi}_1}] [1 + 4JI\tilde{\chi}_1] = 0 \), i.e. \( J_1 \) and \( J_2 \) terms contribute separately to the collective modes. Thus, we shall neglect all contributions due to the \( J_2 \) term in Eqs. [2]. In this approximation we have a set of four equations, which can be further simplified to a set of two equations in the same manner as in Refs. [12][13]:

\[
[\omega(Q) - \varepsilon(k, Q)] G_+^{\dagger}(k, Q) = \frac{U}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + l_{k,Q} l_{k,Q} \right] G_+^{\dagger}(q, Q) - \frac{U}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - l_{k,Q} l_{k,Q} \right] G_-^{\dagger}(q, Q)
- \frac{1}{2N} \sum_q \left[ V(k - q) + J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + l_{k,Q} l_{k,Q} \right] G_+^{\dagger}(q, Q)
- \frac{1}{2N} \sum_q \left[ V(k - q) - J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + m_{k,Q} m_{k,Q} \right] G_+^{\dagger}(q, Q)
+ \frac{1}{2N} \sum_q \left[ V(k - q) + J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - l_{k,Q} l_{k,Q} \right] G_-^{\dagger}(q, Q)
+ \frac{1}{2N} \sum_q \left[ V(k - q) - J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - m_{k,Q} m_{k,Q} \right] G_-^{\dagger}(q, Q)
- \frac{U - 2J(Q)}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} \left( G_+^{\dagger}(q, Q) - G_-^{\dagger}(q, Q) \right) \right] + \frac{U - 2V(Q)}{2N} \sum_q \left[ m_{k,Q} m_{k,Q} \left[ G_+^{\dagger}(q, Q) + G_-^{\dagger}(q, Q) \right] \right],
\]

\[
[\omega(Q) + \varepsilon(k, Q)] G_-^{\dagger}(k, Q) = -\frac{U}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + l_{k,Q} l_{k,Q} \right] G_-^{\dagger}(q, Q) + \frac{U}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - l_{k,Q} l_{k,Q} \right] G_+^{\dagger}(q, Q)
+ \frac{1}{2N} \sum_q \left[ V(k - q) + J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + l_{k,Q} l_{k,Q} \right] G_-^{\dagger}(q, Q)
+ \frac{1}{2N} \sum_q \left[ V(k - q) - J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} + m_{k,Q} m_{k,Q} \right] G_-^{\dagger}(q, Q)
- \frac{1}{2N} \sum_q \left[ V(k - q) + J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - l_{k,Q} l_{k,Q} \right] G_+^{\dagger}(q, Q)
- \frac{1}{2N} \sum_q \left[ V(k - q) - J(k - q) \right] \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} - m_{k,Q} m_{k,Q} \right] G_+^{\dagger}(q, Q)
- \frac{U - 2J(Q)}{2N} \sum_q \left[ \tilde{\gamma}_{k,Q} \tilde{\gamma}_{k,Q} \left( G_+^{\dagger}(q, Q) - G_-^{\dagger}(q, Q) \right) \right] - \frac{U - 2V(Q)}{2N} \sum_q \left[ m_{k,Q} m_{k,Q} \left[ G_+^{\dagger}(q, Q) + G_-^{\dagger}(q, Q) \right] \right].
\]
Here $\varepsilon(k, Q) = E(k + Q) + E(k)$, and we use the same form factors as in Ref.\[12\]: $\gamma_{k, Q} = u_k u_{k+Q} + v_k v_{k+Q}$, $b_{k, Q} = u_k u_{k+Q} - v_k v_{k+Q}$, $\gamma_{k, Q} = u_k v_{k+Q} - u_{k+Q} v_k$, and $m_{k, Q} = u_k v_{k+Q} + u_{k+Q} v_k$ where $u_k^* = 1 - v_k^* = [1 + \varepsilon(k)/E(k)]/2$.

It is worth mentioning that in the case of an extended Hubbard model ($J = 0$), Eqs. (8) and (9) are the exact BS equations in the GRPA. They are in accordance with the Goldstone theorem which says that the gauge invariance is restored by the existence of the Goldstone mode whose energy approaches zero at $Q = 0$. The last statement corresponds to the so-called trivial solution of the BS equations: $G^+(k, Q = 0) = G^-(k, Q = 0) = \Delta_k/2E(k)$, and the gap equation $\Delta_k = \frac{1}{N} \sum_q [-U + V(k - q)] \Delta_q / 2E(q)$ is recovered from our BS equations.

The Fourier transforms of $V$ and $J$ interactions are separable, i.e., $V(k - q) = 2V(\hat{\lambda}_k \hat{\gamma}_q)$ and $J(k - q) = J(\hat{\lambda}_k \hat{\gamma}_q)^2/2$, and therefore, Eqs. (8) and (9) can be solved analytically. Here $\hat{\lambda}_k = (s_k d_k, s_k s_k, s_k d_k)$ is an $1 \times 4$ matrix, and we have used the following notations: $s_k = \cos(k_x) + \cos(k_y)$, $d_k = \cos(k_x) - \cos(k_y)$, $s_k = \sin(k_x) + \sin(k_y)$, and $c_d = \sin(k_x) - \sin(k_y)$.

Thus, we obtain a set of 20 coupled linear equations for the dispersion of the collective excitations. The existence of a non-trivial solution requires that the secular determinant $\det(\hat{\chi}^{-1} - \hat{V})$ is equal to zero, where the bare mean-field-quasiparticle response function $\hat{\chi} = \left( \begin{array}{cc} P & Q \\ Q^T & R \end{array} \right)$ and the interaction $\hat{V} = \text{diag}(U, U, -(U + 4J), U + 16V, -(2V + J/2), ..., -(2V + J/2), -(2V - J/2), ..., -(2V - J/2))$ are 20 by 20 matrices.

The quantities $I_{a,b} = F_{a,b}(\varepsilon(k, Q))$ and $J_{a,b} = F_{a,b}(\omega)$, the $1 \times 4$ matrices $I_{a,b}^i = F_{a,b}(\varepsilon(k, Q))$ and $J_{a,b}^i = F_{a,b}(\omega)$ are defined as follows (the quantities $a(k, Q)$ and $b(k, Q) = l_{a,k}, m_{a,k}, \gamma_k, \chi_k$ or $\tilde{\chi}_k$):

$$F_{a,b}(x) = \frac{1}{N} \sum_k \frac{xa(k, Q)b(k, Q)}{\omega^2 - \varepsilon^2(k, Q)}, F_{a,b}^i(x) = \frac{1}{N} \sum_k \frac{xa(k, Q)b(k, Q)\tilde{\chi}_k}{\omega^2 - \varepsilon^2(k, Q)} (\tilde{\lambda}_k \tilde{\lambda}_k)^{ij}.$$

The elements of $P, Q$ and $R$ blocks are convolutions of conventional two normal $GG$, two anomalous $FF$ Green’s functions or $FG$ terms. At the high-symmetry wave vector $Q_0$, $V_{a,b}$ and $J_{a,b}$ with $i = 3, 4$ involve sine functions, and therefore, all vanish. $I_{a,b}^2$ and $J_{a,b}^2$ also vanish because $\varepsilon(k, Q_0)$ is symmetric with respect to exchange $k_x \leftrightarrow k_y$.

Similarly, the non-diagonal elements of $I_{a,b}^i$ and $J_{a,b}^i$ with $i \neq j$ vanish. Thus, blocks $P$ and $Q$ each contain 10 different non-zero elements, while $R$ has 40 non-zero elements. In other words, the $\omega$ dependence of $\hat{\chi}$ (or $\tilde{\chi}^{-1}$) comes from these 60 non-zero elements. It is worth mentioning that within the four-channel theory the collective mode energy has been calculated by using a $4 \times 4$ symmetric matrix $\tilde{\chi}$ which has only 6 non-zero elements at $Q_0$: $\tilde{\chi}_{11} = I_{33} \tilde{\gamma}_3 \tilde{\gamma}_3 = I_{33}, \tilde{\chi}_{33} = I_{22} \tilde{\gamma}_2 \tilde{\gamma}_2 = I_{22}, \tilde{\chi}_{14} = I_{14} \tilde{\gamma}_1 \tilde{\gamma}_4 = I_{14}$ and $\tilde{\chi}_{13} = I_{13} \tilde{\gamma}_1 \tilde{\gamma}_3 = I_{13}$ (the other 4 elements $\tilde{\chi}_{13} = I_{13} \tilde{\gamma}_1 \tilde{\gamma}_3 = I_{13}, \tilde{\chi}_{12} = I_{12} \tilde{\gamma}_1 \tilde{\gamma}_2 = I_{12}$).

In Ref. [1], while the third set (H&C) is used by Hao and Chubukov. As can be seen in Fig. 1, BS equations provide energies which are significantly different from those obtained according to the three-channel theory (see Fig. 4 in Ref. [2]). In Fig. 2 and Fig. 3 we present the results of our calculations of the lines in $U, J$ parameter space which reproduce the INSr energy of 40 meV using all twenty channels. We see that the RPA spin correlation function and the BS equations in GRPA, both provide very similar results for $U$ at point $J = 0$. This indicates that the resonance remains predominantly a spin excitation.

In summary, we have derived a set of four coupled BS equations for the collective modes of the $t - U - V - J$ model including the $J_1$ part of the antiferromagnetic interaction. These equations have been used to analyze the resonance peak in Bi2212. It is interesting to note that the trivial solution of the BS equations (8) and (9) leads to an equation similar to the gap equation but with $V_0 = 2V + J/2$ instead of $V_0 = 2V + 3J/2$. The Goldstone mode, which is expected on physical grounds as the symmetry is spontaneously broken by the condensate, does exist as a trivial solution of the sixteen BS equations.
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