Bethe-Salpeter equations for the collective modes of the *t-U-V-J* model with *d*-wave pairing: Analysis of the photoemission resonance of $Bi_2Sr_2CaCu_2O_8$

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(Received 30 June 2010; published 21 July 2010)

The Bethe-Salpeter equations for the collective modes of a *t-U-V-J* model are used to analyze the resonance peak observed at $\mathbf{Q}=(\pi,\pi)$ 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 angle-resolved photoemission spectroscopy data and reproduces the resonance peak at 40 meV in Bi2212 compound. We find that the resonance is predominantly a spin exciton.

DOI: 10.1103/PhysRevB.82.014528 PACS number(s): 71.10.Ca, 74.20.Fg, 74.25.Ha

I. 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 $\Delta_{\mathbf{k}}=\Delta(\cos k_x-\cos k_y)]/2$, where Δ is the maximum value of the energy gap (lattice constant $a=1$). The corresponding BCS gap equation is

$$1=\frac{V_\psi}{2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{d\mathbf{k}}{(2\pi)^2}\frac{d_{\mathbf{k}}^2}{\sqrt{\bar{\varepsilon}_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}}, \tag{1}$$

where $V_\psi=2V+3J/2$ and $E(\mathbf{k})=\sqrt{\bar{\varepsilon}_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$. The mean-field electron energy $\bar{\varepsilon}_{\mathbf{k}}$ has a tight-binding form

$$\begin{aligned}\bar{\varepsilon}_{\mathbf{k}}=&t_1(\cos k_x+\cos k_y)/2+t_2\cos k_x\cos k_y+t_3(\cos 2k_x\\&+\cos 2k_y)/2+t_4(\cos 2k_x\cos k_y+\cos 2k_y\cos k_x)/2\\&+t_5\cos 2k_x\cos 2k_y-\mu\end{aligned} \tag{2}$$

obtained by fitting the ARPES data with a chemical potential μ and hopping amplitudes t_i for first to fifth nearest neighbors on a square lattice. Δ, $t_1,\ldots,t_5$ and μ should all be thought of as an effective set of parameters, while V_ψ has to be determined by the gap equation. For Bi2212 compound, there are two possible sets of parameters with all tight-binding basis functions involved (see Table I in Ref. 1). Assuming $\Delta=35$ meV, we obtain $V_\psi^{(1)}=115.2$ meV with set 1, and $V_\psi^{(2)}=87.9$ meV with set 2. Hao and Chubukov[2] have used another set of parameters (we shall call it H&C) for Bi2212 compound with a doping concentration $x=0.12$: $t_1=-4t$, $t_2=1.2t$, $t=0.433$ eV, $\mu=-0.94t$, $\Delta=35$ meV, and $V_\psi=0.6t$. The parameters U, V, and J should be adjusted in such a way that the sharp collective mode which appears at wave vector $\mathbf{Q}_0=(\pi,\pi)$ in inelastic neutron-scattering resonance (INSR) studies[3–10] occurs at energy which corresponds to the lowest collective mode of the corresponding Hamiltonian. In the random phase approximation (RPA) the resonance is determined by the pole of the spin correlation function, which in the case of $J=0$ (the phase diagram at half filling shows an "island" in U-V space where *d*-wave pairing exists[11]) is

$$\chi_s(\omega)=\chi_{00}^0(\mathbf{Q}_0,\omega)/[1+U\chi_{00}^0(\mathbf{Q}_0,\omega)],$$

where $\chi_{00}^0=I_{\tilde{\gamma}\tilde{\gamma}}$ is the bare spin correlation function[1,12] ($I_{\tilde{\gamma}\tilde{\gamma}}$ is defined later in the text). Using the H&C set of parameters[2] and a resonance energy of 40 meV, we calculate the RPA value of U of about 1.16 eV. Sets 1 and 2 provide $U^{(1)}=0.533$ eV and $U^{(2)}=0.418$ eV, respectively.

The coupling of the spin channel with other channels should change the RPA results for U. For example, we can take into consideration two π channels[13–15] with bare π susceptibilities $\chi_{11}^0=I_{ll}^{22}$ and $\chi_{22}^0=I_{\gamma\gamma}^{22}$, respectively. The susceptibilities $I_{\gamma\tilde{\gamma}}^2, J_{l\tilde{\gamma}}^2, J_{l\gamma}^{22}$ represent the mixing of the spin and two π channels. Thus, the coupling of the spin and two π channels (a three-channel response-function theory) leads in the generalized random phase approximation (GRPA) to a set of three coupled equations,[2] and the value of U is reduced from 1.16 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. 16 $U\approx 300$ meV is required in the case when $V_\psi=0.260$ 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 $\det|\hat{\chi}^{-1}-\hat{V}|=0$, where the mean-field response function $\hat{\chi}$ and the interaction $\hat{V}$ are 20×20 matrices. The secular determinant can be rewritten as

$$\det|\hat{\chi}^{-1}-\hat{V}|=\det\begin{vmatrix}A & B\\ B^T & C\end{vmatrix}=\det|C|\det|A-BC^{-1}B^T|.$$

In the case of the four-channel response-function theory,[16,17] A is a 4×4 matrix while the mixing with the other 16 chan-

nels is represented by a 4×4 matrix $BC^{-1}B^T$. We emphasize that none of the previous theoretical interpretations of the INSR feature at $\mathbf{Q}_0$ have accounted properly for the mixing term $BC^{-1}B^T$.

II. COLLECTIVE EXCITATIONS OF THE *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 antiferromagnetic interaction J,

$$H = -\sum_{i,j,\sigma} t_{ij}\psi^{\dagger}_{i,\sigma}\psi_{j,\sigma} - \mu\sum_{i,\sigma}\hat{n}_{i,\sigma} + U\sum_{i}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} - V\sum_{\langle i,j\rangle\sigma\sigma'}\hat{n}_{i,\sigma}\hat{n}_{j,\sigma'} + J\sum_{\langle i,j\rangle}\vec{\mathbf{S}}_i.\vec{\mathbf{S}}_j. \quad (3)$$

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

$$J_1 = \frac{J}{4}\sum_{\langle i,j\rangle}[\hat{n}_{i,\uparrow}\hat{n}_{j,\uparrow} + \hat{n}_{i,\downarrow}\hat{n}_{j,\downarrow} - \hat{n}_{i,\uparrow}\hat{n}_{j,\downarrow} - \hat{n}_{i,\downarrow}\hat{n}_{j,\uparrow}]$$

and

$$J_2 = \frac{J}{2}\sum_{\langle i,j\rangle}[\psi^{\dagger}_{i,\uparrow}\psi_{i,\downarrow}\psi^{\dagger}_{j,\downarrow}\psi_{j,\uparrow} + \psi^{\dagger}_{i,\downarrow}\psi_{i,\uparrow}\psi^{\dagger}_{j,\uparrow}\psi_{j,\downarrow}].$$

It is useful to introduce four-component Nambu fermion fields $\hat{\bar{\psi}}(y)=[\psi^{\dagger}_{\uparrow}(y)\psi^{\dagger}_{\downarrow}(y)\psi_{\uparrow}(y)\psi_{\downarrow}(y)]$ and $\hat{\psi}(x)=[\psi^{\dagger}_{\uparrow}(x)\psi^{\dagger}_{\downarrow}(x)\psi_{\uparrow}(x)\psi_{\downarrow}(x)]^T$, 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,[18,19]

$$\int DA e^{[(1/2)A_\alpha(z)D^{(0)-1}_{\alpha\beta}(z,z')A_\beta(z)+\hat{\bar{\psi}}(y)\hat{\Gamma}^{(0)}_{\alpha}(y;x|z)\hat{\psi}(x)A_\alpha(z)]} = e^{-(1/2)\hat{\bar{\psi}}(y)\hat{\Gamma}^{(0)}_{\alpha}(y;x|z)\hat{\psi}(x)D^{(0)}_{\alpha\beta}(z,z')\hat{\bar{\psi}}(y')\hat{\Gamma}^{(0)}_{\beta}(y';x'|z')\hat{\psi}(x')}. \quad (4)$$

The last equation is used to define the 4×4 matrices $\hat{D}^{(0)}_{\alpha\beta}$ and $\hat{\Gamma}^{(0)}_{\alpha}$ ($\alpha,\beta=1,2,3,4$). Their Fourier transforms, written in terms of the Pauli σ_i, Dirac γ^0 and alpha[20,21] matrices, are as follows:

$$\hat{D}^{(0)} = \begin{pmatrix} \hat{D}_1 & 0 \\ 0 & \hat{D}_2 \end{pmatrix}, \quad \alpha_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_y\sigma_i\sigma_y \end{pmatrix},$$

$$\hat{\Gamma}^{(0)}_{1,2} = (\gamma^0 \pm \alpha_z)/2, \quad \hat{\Gamma}^{(0)}_{3,4} = (\alpha_x \pm \imath\alpha_y)/2,$$

where

$$\hat{D}_1 = [J(\mathbf{k}) - V(\mathbf{k})]\sigma_0 + [U - J(\mathbf{k}) - V(\mathbf{k})]\sigma_x,$$

$$\hat{D}_2 = 2J(\mathbf{k})\sigma_x.$$

The nearest-neighbor interactions for the case of a square lattice are

$$V(\mathbf{k}) = 4V[\cos(k_x) + \cos(k_y)],$$

$$J(\mathbf{k}) = J[\cos(k_x) + \cos(k_y)].$$

Now, we can establish a one-to-one correspondence between the system under consideration and a system which consists of a four-component boson field $A_\alpha(z)$ interacting with fermion fields $\hat{\bar{\psi}}(y)$ and $\hat{\psi}(x)$. The action of the model system is $S=S^{(e)}_0+S^{(A)}_0+S^{(e-A)}$ where

$$S^{(e)}_0 = \hat{\bar{\psi}}(y)\hat{G}^{(0)-1}(y;x)\hat{\psi}(x),$$

$$S^{(A)}_0 = \frac{1}{2}A_\alpha(z)D^{(0)-1}_{\alpha\beta}(z,z')A_\beta(z'),$$

$$S^{(e-A)} = \hat{\bar{\psi}}(y)\hat{\Gamma}^{(0)}_{\alpha}(y,x|z)\hat{\psi}(x)A_\alpha(z).$$

Here, we have used composite variables $x,y,z=\{\mathbf{r}_i,u\}$, where $\mathbf{r}_i$ is a lattice site vector, and variable u range from 0 to $\beta=1/k_BT$ (T and k_B are the temperature and the Boltzmann constant). We set $\hbar=1$ and we use the summation-integration convention: that repeated variables are summed up or integrated over.

Let us first briefly discuss the existing methods for calculating the excitation spectra of collective modes in the case when $V=J=0$ (the Hubbard model). Belkhir and Randeria[22] obtained the collective modes by linearizing the Anderson-Rickayzen (AR) equations.[23,24] This method leads to a set of three homogeneous equations and the collective spectrum can be obtained by setting the corresponding 3×3 secular determinant equal to zero. Côté and Griffin[25] obtained the collective excitations of the Hubbard model from the poles of the density and spin response functions in the GRPA. Density (spin) response describes how the total density (spin) of the system changes as a result of a sharp change in the external field assuming that it is coupled with density (spin). The corresponding secular determinant is a 4×4 determinant with six independent elements. In the third approach, referred to as BS formalism, the collective excitations are obtained by solving the BS equations for the poles of the two-particle Green's in the GRPA. The corresponding secular determinant is a 4×4 determinant, but with nine independent elements.[18] The Belkhir and Randeria secular determinant appears as a cofactor of the $I_{\tilde{\gamma}\tilde{\gamma}}$ element. The advantage of the BS formalism over the response-function approach lies not only in the ability to obtain the poles of density and spin response functions in a uniform manner, but it can be generalized to the case of extended Hubbard model ($V\neq0$, $J=0$) as well.[18]

In this paper we extend the BS formalism to the *t-U-V-J* model. Following the same steps as in Refs. 18, 19, 25, and 26, we can derive a set of 16 BS equations for the collective mode $\omega(\mathbf{Q})$ and BS amplitudes $\Psi^{\mathbf{Q}}_{n_1 n_2}(\mathbf{k})$ $(n_1, n_2 = 1,2,3,4)$. Their matrix representation at zero temperature is

$$\hat{\Psi}^{\mathbf{Q}}(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}} \int \frac{d\Omega}{2\pi}\{-\hat{D}^{(0)}_{\alpha\beta}(\mathbf{k}-\mathbf{q})\hat{G}(\mathbf{k}+\mathbf{Q};\Omega+\omega) \times \hat{\Gamma}^{(0)}_{\alpha}\hat{\Psi}^{\mathbf{Q}}(\mathbf{q})\hat{\Gamma}^{(0)}_{\beta}\hat{G}(\mathbf{k};\Omega) + \hat{D}^{(0)}_{\alpha\beta}(\mathbf{Q})\hat{G}(\mathbf{k}+\mathbf{Q};\Omega+\omega) \times \hat{\Gamma}^{(0)}_{\alpha}\hat{G}(\mathbf{k};\Omega)\mathrm{Tr}[\hat{\Gamma}^{(0)}_{\beta}\hat{\Psi}^{\mathbf{Q}}(\mathbf{q})]\}, \tag{5}$$

where $\hat{G}(\mathbf{k};\omega)$ is the BCS Green's function.[20,21] The direct $\hat{D}^{(0)}_{\alpha\beta}(\mathbf{k}-\mathbf{q})\hat{\Gamma}^{(0)}_{\alpha}\hat{\Gamma}^{(0)}_{\beta}$ and exchange $\hat{D}^{(0)}_{\alpha\beta}(\mathbf{Q})\hat{\Gamma}^{(0)}_{\alpha}\hat{\Gamma}^{(0)}_{\beta}$ interactions mix all 16 BS amplitudes. The BS equations in the presence of a spin-dependent antiferromagnetic interaction are more complicated than the BS equations in the case of an extended Hubbard model.[19] We may greatly simplify BS Eqs. (5) using the fact that in the RPA the susceptibilities at $\mathbf{Q}_0$ are convolutions of two single-particle Green's functions $\hat{G}$, and the equation for the collective mode in the RPA is

$$\chi_1^{(0)-1}(\omega)\chi_2^{(0)-1}(\omega) - C_{12}(\omega) = 0,$$

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 appear in the case of spin triplet pairing states where the order parameter $\Delta_{\alpha\beta}(\mathbf{k})$ is a 2×2 matrix. For a singlet superconductivity and *d*-wave pairing $\Delta_{\alpha\beta}(\mathbf{k}) = i(\sigma_y)_{\alpha\beta}\Delta(\mathbf{k})$, $C_{12}(\omega) = 0$, and the equation for collective modes becomes

$$[1 + (U + 4J)I_{\tilde{\gamma}\tilde{\gamma}}][1 + 4JI_{\tilde{\gamma}\tilde{\gamma}}] = 0.$$

Since in RPA the J_1 and J_2 terms contribute separately to the collective modes, we shall neglect all contributions due to the J_2 term in Eqs. (5). 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. 25 and 26,

$$\begin{aligned}[\omega(\mathbf{Q}) - \varepsilon(\mathbf{k},\mathbf{Q})]G^{+}(\mathbf{k},\mathbf{Q}) &= \frac{U}{2N}\sum_{\mathbf{q}}[(\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} + l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q}) - (\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} - l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q})] \\ &- \frac{1}{2N}\sum_{\mathbf{q}}[V(\mathbf{k}-\mathbf{q}) + J(\mathbf{k}-\mathbf{q})][(\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} + l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q}) - (\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} - l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q})] \\ &- \frac{1}{2N}\sum_{\mathbf{q}}[V(\mathbf{k}-\mathbf{q}) - J(\mathbf{k}-\mathbf{q})][(\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}} + m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q}) - (\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}} - m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q})] \\ &- \frac{U - 2J(\mathbf{Q})}{2N}\sum_{\mathbf{q}}\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}}(G^{+}(\mathbf{q},\mathbf{Q}) - G^{-}(\mathbf{q},\mathbf{Q})) + \frac{U - 2V(\mathbf{Q})}{2N}\sum_{\mathbf{q}} m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}}[G^{+}(\mathbf{q},\mathbf{Q}) + G^{-}(\mathbf{q},\mathbf{Q})],\end{aligned} \tag{6}$$

$$\begin{aligned}[\omega(\mathbf{Q}) + \varepsilon(\mathbf{k},\mathbf{Q})]G^{+}(\mathbf{k},\mathbf{Q}) &= -\frac{U}{2N}\sum_{\mathbf{q}}[(\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} + l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q}) - (\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} - l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q})] \\ &+ \frac{1}{2N}\sum_{\mathbf{q}}[V(\mathbf{k}-\mathbf{q}) + J(\mathbf{k}-\mathbf{q})][(\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} + l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q}) - (\gamma_{\mathbf{k},\mathbf{Q}}\gamma_{\mathbf{q},\mathbf{Q}} - l_{\mathbf{k},\mathbf{Q}}l_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q})] \\ &+ \frac{1}{2N}\sum_{\mathbf{q}}[V(\mathbf{k}-\mathbf{q}) - J(\mathbf{k}-\mathbf{q})][(\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}} + m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}})G^{-}(\mathbf{q},\mathbf{Q}) - (\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}} - m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}})G^{+}(\mathbf{q},\mathbf{Q})] \\ &- \frac{U - 2J(\mathbf{Q})}{2N}\sum_{\mathbf{q}}\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}\tilde{\gamma}_{\mathbf{q},\mathbf{Q}}(G^{+}(\mathbf{q},\mathbf{Q}) - G^{-}(\mathbf{q},\mathbf{Q})) - \frac{U - 2V(\mathbf{Q})}{2N}\sum_{\mathbf{q}} m_{\mathbf{k},\mathbf{Q}}m_{\mathbf{q},\mathbf{Q}}[G^{+}(\mathbf{q},\mathbf{Q}) + G^{-}(\mathbf{q},\mathbf{Q})].\end{aligned} \tag{7}$$

Here $\varepsilon(\mathbf{k},\mathbf{Q}) = E(\mathbf{k}+\mathbf{Q}) + E(\mathbf{k})$, and we use the same form factors as in Ref. 25, $\gamma_{\mathbf{k},\mathbf{Q}} = u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{Q}} + v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{Q}}$, $l_{\mathbf{k},\mathbf{Q}} = u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{Q}} - v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{Q}}$, $\tilde{\gamma}_{\mathbf{k},\mathbf{Q}} = u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{Q}} - u_{\mathbf{k}+\mathbf{Q}}v_{\mathbf{k}}$, and $m_{\mathbf{k},\mathbf{Q}} = u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{Q}} + u_{\mathbf{k}+\mathbf{Q}}v_{\mathbf{k}}$ where $u_{\mathbf{k}}^2 = 1 - v_{\mathbf{k}}^2 = [1 + \bar{\varepsilon}(\mathbf{k})/E(\mathbf{k})]/2$.

It is worth mentioning that in the case of an extended Hubbard model $(J=0)$, Eqs. (6) and (7) 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 $\mathbf{Q}=0$. The last statement corresponds to the so-called trivial solution of the BS equations: $G^+(\mathbf{k},\mathbf{Q}=0)=-G^-(\mathbf{k},\mathbf{Q}=0)=\Delta_\mathbf{k}/2E(\mathbf{k})$, and the gap equation[27]

$$\Delta_\mathbf{k}=\frac{1}{N}\sum_\mathbf{q}[-U+V(\mathbf{k}-\mathbf{q})]\frac{\Delta_\mathbf{q}}{2E(\mathbf{q})}$$

is recovered from our BS equations.

The Fourier transforms of V and J interactions are separable, i.e., $V(\mathbf{k}-\mathbf{q})=2V\hat{\lambda}_\mathbf{k}\hat{\lambda}_\mathbf{q}^T$ and $J(\mathbf{k}-\mathbf{q})=J\hat{\lambda}_\mathbf{k}\hat{\lambda}_\mathbf{q}^T/2$, and therefore, Eqs. (6) and (7) can be solved analytically. Here $\hat{\lambda}_\mathbf{k}=(s_\mathbf{k},d_\mathbf{k},ss_\mathbf{k},sd_\mathbf{k})$ is an 1×4 matrix, and we have used the following notations: $s_\mathbf{k}=\cos(k_x)+\cos(k_y)$, $d_\mathbf{k}=\cos(k_x)-\cos(k_y)$, $ss_\mathbf{k}=\sin(k_x)+\sin(k_y)$ and $cd_\mathbf{k}=\sin(k_x)-\sin(k_y)$. Thus, we obtain a set of 20 coupled linear homogeneous equations for the dispersion of the collective excitations. The existence of a nontrivial solution requires that the secular determinant $\det\|\hat{\chi}^{-1}-\hat{V}\|$ is equal to zero, where the bare mean-field-quasiparticle response function $\hat{\chi}=\left(\begin{smallmatrix}P & Q\\ Q^T & R\end{smallmatrix}\right)$ and the interaction $\hat{V}=\mathrm{diag}(U,U,-(U+4J),U+16V,-(2V+J/2),\ldots,-(2V+J/2),-(2V-J/2),\ldots,-(2V-J/2))$ are 20×20 matrices. P and Q are 4×4 and 4×16 blocks, respectively, while R is 16×16 block (in what follows $i,j=1,2,3,4$),

$$P=\begin{vmatrix} I_{\gamma,\gamma} & J_{\gamma,l} & I_{\gamma,\tilde{\gamma}} & J_{\gamma,m}\\ J_{\gamma,l} & I_{l,l} & J_{l,\tilde{\gamma}} & I_{l,m}\\ I_{\gamma,\tilde{\gamma}} & J_{l,\tilde{\gamma}} & I_{\tilde{\gamma},\tilde{\gamma}} & J_{\tilde{\gamma},m}\\ J_{\gamma,m} & I_{l,m} & J_{\tilde{\gamma},m} & I_{m,m}\end{vmatrix},$$

$$Q=\begin{vmatrix} I^i_{\gamma,\gamma} & J^i_{\gamma,l} & I^i_{\gamma,\tilde{\gamma}} & J^i_{\gamma,m}\\ J^i_{\gamma,l} & I^i_{l,l} & J^i_{l,\tilde{\gamma}} & I^i_{l,m}\\ I^i_{\gamma,\tilde{\gamma}} & J^i_{l,\tilde{\gamma}} & I^i_{\tilde{\gamma},\tilde{\gamma}} & J^i_{\tilde{\gamma},m}\\ J^i_{\gamma,m} & I^i_{l,m} & J^i_{\tilde{\gamma},m} & I^i_{m,m}\end{vmatrix},$$

$$R=\begin{vmatrix} I^{ij}_{\gamma,\gamma} & J^{ij}_{\gamma,l} & I^{ij}_{\gamma,\tilde{\gamma}} & J^{ij}_{\gamma,m}\\ J^{ij}_{\gamma,l} & I^{ij}_{l,l} & J^{ij}_{l,\tilde{\gamma}} & I^{ij}_{l,m}\\ I^{ij}_{\gamma\tilde{\gamma}} & J^{ij}_{l,\tilde{\gamma}} & I^{ij}_{\tilde{\gamma},\tilde{\gamma}} & J^{ij}_{\tilde{\gamma},m}\\ J^{ij}_{\gamma,m} & I^{ij}_{l,m} & J^{ij}_{\tilde{\gamma},m} & I^{ij}_{m,m}\end{vmatrix}.$$

The quantities $I_{a,b}=F_{a,b}(\varepsilon(\mathbf{k},\mathbf{Q}))$ and $J_{a,b}=F_{a,b}(\omega)$, the 1×4 matrices $I^i_{a,b}=F^i_{a,b}(\varepsilon(\mathbf{k},\mathbf{Q}))$ and $J^i_{a,b}=F^i_{a,b}(\omega)$, and the 4×4 matrices $I^{ij}_{a,b}=F^{ij}_{a,b}(\varepsilon(\mathbf{k},\mathbf{Q}))$ and $J^{ij}_{a,b}=F^{ij}_{a,b}(\omega)$ are defined as follows [the quantities $a(\mathbf{k},\mathbf{Q})$ and $b(\mathbf{k},\mathbf{Q})=l_{\mathbf{k},\mathbf{Q}},m_{\mathbf{k},\mathbf{Q}},\gamma_{\mathbf{k},\mathbf{Q}}$ or $\tilde{\gamma}_{\mathbf{k},\mathbf{Q}}$],

$$F_{a,b}(x)\equiv\frac{1}{N}\sum_\mathbf{k}\frac{xa(\mathbf{k},\mathbf{Q})b(\mathbf{k},\mathbf{Q})}{\omega^2-\varepsilon^2(\mathbf{k},\mathbf{Q})},$$

$$F^i_{a,b}(x)\equiv\frac{1}{N}\sum_\mathbf{k}\frac{xa(\mathbf{k},\mathbf{Q})b(\mathbf{k},\mathbf{Q})\hat{\lambda}^i_\mathbf{k}}{\omega^2-\varepsilon^2(\mathbf{k},\mathbf{Q})},$$

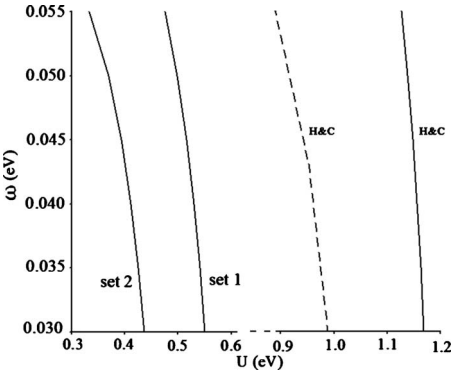

FIG. 1. The energy of the resonance obtained from the BS equations when $J=0$. The curves are plotted using parameters given in Table I in Ref. 1 (set 1 and set 2), and the Hao and Chubukov parameters (curves H&C). The dashed curve represents the three-channel energy (Fig. 4 in Ref. 2).

$$F^{ij}_{a,b}(x)\equiv\frac{1}{N}\sum_\mathbf{k}\frac{xa(\mathbf{k},\mathbf{Q})b(\mathbf{k},\mathbf{Q})}{\omega^2-\varepsilon^2(\mathbf{k},\mathbf{Q})}(\hat{\lambda}^T_\mathbf{k}\hat{\lambda}_\mathbf{k})_{ij}.$$

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 $\mathbf{Q}_0$, $I^i_{a,b}$ and $J^i_{a,b}$ with $i=3,4$ involve sine functions, and therefore, all vanish. $I^2_{a,b}$ and $J^2_{a,b}$ also vanish because $\varepsilon(\mathbf{k},\mathbf{Q}_0)$ is symmetric with respect to exchange $k_x\leftrightarrow k_y$. Similarly, the nondiagonal elements of $I^{ij}_{a,b}$ and $J^{ij}_{a,b}$ with $i\neq j$ all vanish. Thus, blocks P and Q, each has ten different nonzero elements, while R has 40 nonzero elements. In other words, the ω dependence of $\hat{\chi}$ (or $\hat{\chi}^{-1}$) comes from these 60 nonzero elements. It is worth mentioning that within the four-channel theory[16] the collective mode energy has been calculated by using a 4×4 symmetric matrix $\hat{\chi}$ which has only six nonzero elements at $\mathbf{Q}_0$: $\hat{\chi}_{11}=I_{\tilde{\gamma}\tilde{\gamma}}$, $\hat{\chi}_{22}=I^{11}_{mm}$, $\hat{\chi}_{33}=I^{22}_{\gamma\gamma}$, $\hat{\chi}_{44}=I^{22}_{ll}$, $\hat{\chi}_{12}=J^1_{m\tilde{\gamma}}$ and $\hat{\chi}_{34}=J^{22}_{l\gamma}$ (the other 4 elements $\hat{\chi}_{13}=I^2_{\gamma\tilde{\gamma}}$, $\hat{\chi}_{14}=J^2_{l\tilde{\gamma}}$, $\hat{\chi}_{23}=J^{12}_{m\gamma}$ and $\hat{\chi}_{24}=I^{12}_{ml}$ vanish).

In Fig. 1 we present the results of our calculations of the lowest collective mode of the extended Hubbard model ($J=0$) using 49×49 $\mathbf{k}$ points in the Brillouin zone and three possible sets of parameters: sets 1 and 2 include all tight-binding basis functions (see Table I in Ref. 1), while the third set (H&C) is used by Hao and Chubukov.[2] 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 Figs. 2 and 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 exciton.

III. SUMMARY

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.

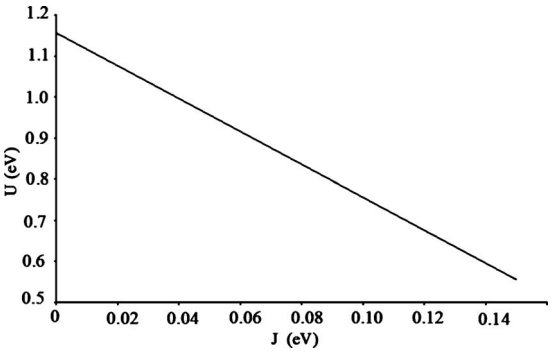

FIG. 2. Line in U,J parameter space which reproduce the INSR energy of 0.04 eV. Note that $V=V_\psi/2-3J/4$ where $V_\psi=0.6t=259.8$ meV is calculated from the gap equation by using the set of parameters given in Ref. 2.

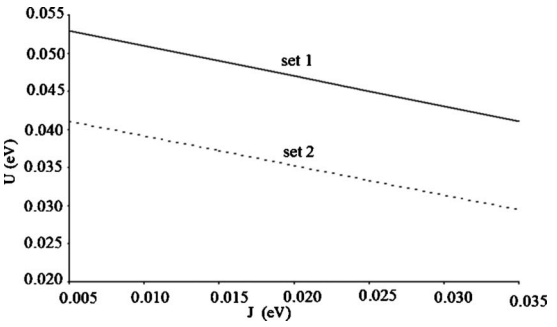

FIG. 3. Line in U,J parameter space which reproduce the INSR energy of 0.04 eV. The V value is $V=V_\psi/2-3J/4$ where $V_\psi^{(1)}=115.2$ meV and $V_\psi^{(2)}=87.9$ meV are calculated by using two sets of parameters given in Ref. 1.

These equations have been used to analyze the resonance (commensurate) peak in Bi2212. The BS equations describe also the dispersion of the collective modes at incommensurate wave vectors from the Brillouin zone. Perhaps due to the limited size of single crystals currently available, no incommensurate peaks in Bi2212 samples have been reported so far. It is possible to obtain the exact strengths of the interactions in Bi2212 by using the energy and the position of one incommensurate peak.

It is interesting to note that the trivial solution of the BS Eqs. (6) and (7) leads to an equation similar to the gap equation but with $V_\psi=2V+J/2$ instead of $V_\psi=2V+3J/2$. 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 16 BS equations.

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[1] M. R. Norman, Phys. Rev. B **61**, 14751 (2000).
[2] Z. Hao and A. V. Chubukov, Phys. Rev. B **79**, 224513 (2009).
[3] J. Rossat-Mignond, L. P. Regnault, C. Vettier, P. Bourges, P. Burlet, J. Bossy, J. Y. Henry, and G. Lapertot, Physica C **185-189**, 86 (1991).
[4] H. A. Mook, M. Yethiraj, G. Aeppli, T. E. Mason, and T. Armstrong, Phys. Rev. Lett. **70**, 3490 (1993).
[5] P. Dai, H. A. Mook, R. D. Hunt, and F. Dogan, Phys. Rev. B **63**, 054525 (2001).
[6] H. F. Fong, B. Keimer, D. Reznik, D. L. Milius, and I. A. Aksay, Phys. Rev. B **54**, 6708 (1996).
[7] H. F. Fong, P. Bourges, Y. Sidis, L. P. Regnault, A. Ivanov, G. D. Gu, N. Koshizuka, and B. Keimer, Nature (London) **398**, 588 (1999).
[8] H. F. Fong, P. Bourges, Y. Sidis, L. P. Regnault, J. Bossy, A. Ivanov, D. L. Milius, I. A. Aksay, and B. Keimer, Phys. Rev. B **61**, 14773 (2000).
[9] P. Bourges, Y. Sidis, H. F. Fong, L. P. Regnault, J. Bossy, A. Ivanov, and B. Keimer, Science **288**, 1234 (2000).
[10] H. He, P. Bourges, Y. Sidis, C. Ulrich, L. P. Regnault, S. Pailhes, N. S. Berzigiarova, N. N. Kolesnikov, and B. Keimer, Science **295**, 1045 (2002).
[11] E. Dagotto, J. Riera, Y. C. Chen, A. Moreo, A. Nazarenko, F. Alcaraz, and F. Ortolani, Phys. Rev. B **49**, 3548 (1994).
[12] N. Bulut and D. J. Scalapino, Phys. Rev. B **53**, 5149 (1996).
[13] E. Demler and S. C. Zhang, Phys. Rev. Lett. **75**, 4126 (1995).
[14] E. Demler, H. Kohno, and S. C. Zhang, Phys. Rev. B **58**, 5719 (1998).
[15] O. Tchernyshyov, M. R. Norman, and A. V. Chubukov, Phys. Rev. B **63**, 144507 (2001).
[16] W. C. Lee and A. H. MacDonald, Phys. Rev. B **78**, 174506 (2008).
[17] W. C. Lee, J. Sinova, A. A. Burkov, Y. Joglekar, and A. H. MacDonald, Phys. Rev. B **77**, 214518 (2008).
[18] Z. Koinov, Phys. Status Solidi B **247**, 140 (2010).
[19] Z. Koinov, Physica C **470**, 144 (2010).
[20] M. Yakiyama and Y. Hasegawa, Phys. Rev. B **67**, 014512 (2003).
[21] W. F. Brinkman, J. W. Serene, and P. W. Anderson, Phys. Rev. A **10**, 2386 (1974).
[22] L. Belkhir and M. Randeria, Phys. Rev. B **49**, 6829 (1994).
[23] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).
[24] G. Rickayzen, Phys. Rev. **115**, 795 (1959).
[25] R. Côté and A. Griffin, Phys. Rev. B **48**, 10404 (1993).
[26] Z. Koinov, Phys. Rev. B **72**, 085203 (2005).
[27] R. Micnas, J. Ranninger, S. Robaszkiewicz, and S. Tabor, Phys. Rev. B **37**, 9410 (1988).