Resonance peak in neutron scattering experiments on the cuprates revisited: The case of exciton versus π-resonance and magnetic plasmon

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We reanalyze the issue whether the resonance peak observed in neutron scattering experiments on the cuprates is an exciton, a π-resonance, or a magnetic plasmon. We consider a toy model on-site Hubbard U and nearest-neighbor interaction in both charge and spin channels. We find that the mixing between π and spin channels is not negligible, but the resonance remains predominantly an exciton even if the magnetic interaction is absent and the d-wave pairing originates from attractive density-density interaction. Our results indicate that it may be difficult to distinguish between spin- and charge-mediated pairing interactions by just looking at the resonance peak in the spin susceptibility.

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I. INTRODUCTION

The origin of the (π,π) spin resonance in the cuprates continue to attract interest of the high-T_c community. The resonance has been observed in four different classes of high-T_c compounds, YBCO, Bi2212, Tl2201, and Hg1201,[1] and the doping variation in its energy follows closely the doping dependence of T_c. Magnetic resonances have been also recently observed in heavy-fermion materials[2] and in Fe pnictides.[3]

It is widely accepted that the resonance at $\mathbf{Q}=(\pi,\pi)$ is a feedback from the opening of a d-wave pairing gap in the fermionic spectrum. There is no consensus, however, about the driving force. The simplest and most transparent idea put forward by various groups[4] is that the neutron resonance is a spin exciton, that is, a resonance mode in the spin response function, which emerges due to an attractive residual spin interaction between quasiparticles in a d-wave superconductor. To obtain this mode, one can either compute the susceptibility within the low-energy model with spin interaction only (no charge component),[5] or calculate the spin susceptibility within a conventional random-phase approximation (RPA) for the underlying Hubbard model[6]—either way one obtains a δ-functional excitonic peak at a finite frequency below 2Δ, where Δ is the amplitude of gap at "hot spots"—k_F points separated by $\mathbf{Q}$.

This simple approach, however, is incomplete as it neglects the fact that in a d-wave superconductor the staggered particle hole, charge zero-spin variable $\mathbf{S}^a_Q=(1/2\sqrt{N})\Sigma_k c^\dagger_{k,\alpha}\sigma^a_{\alpha\beta}c_{k+Q,\beta}$ is mixed with the staggered d-wave particle-particle charge ± 2 variables π^a_Q and $(\pi^a_Q)^*$, where $\pi^a_Q=(1/\sqrt{N})\Sigma_k d_k c^\dagger_{k,\alpha}(\sigma^a\sigma^y)_{\alpha\beta}c_{k+Q,\beta}$, and $d_k=\cos k_x-\cos k_y$ (Refs. 7–9). Diagrammatically, the mixed $\langle S\pi\rangle$ response function is given by $d_k G_k F_{k+Q}$ bubbles made out of normal (G) and anomalous (F) Green's functions.[8] Such terms are finite in a d-wave superconductor at $\Omega\neq 0$.

Because spin and π responses are coupled, the full spin response function is obtained by solving the full 3×3 set of coupled generalized RPA equations for $\langle SS\rangle$, $\langle \pi,\pi\rangle$, and $\langle S\pi\rangle$ correlators (Ref. 10). As a consequence, the resonance mode emerges simultaneously in spin and π channels and its location $\Omega=\Omega_{res}$ is in general the solution of

$$\chi_s^{-1}(\Omega)\chi_\pi^{-1}(\Omega)-\Omega^2C_\Omega^2=0, \tag{1}$$

where $\chi_s^{-1}\propto(\Omega-\Omega_s)$ and $\chi_\pi^{-1}\propto(\Omega-\Omega_\pi)$ are inverse RPA susceptibilities in s and π channels, each resonating at its own frequency, and ΩC_Ω is the mixing GF term. If $C_\Omega=0$, s and π channels are decoupled, and the spin and π resonances occur at Ω_s and Ω_π, respectively, and are not affected by each other. In general, however, the resonance frequency Ω_{res} is the solution of Eq. (1) and the full spin and π susceptibilities near the resonance are given by $\chi_s=Z_s/(\Omega-\Omega_{res}),\chi_\pi=Z_\pi/(\Omega-\Omega_{res})$ [we normalize Z such that for $C_\Omega=0$, $Z_s=1,Z_\pi=0$ at $\omega=\Omega_s$ and $Z_\pi=1,Z_s=0$ at $\Omega=\Omega_\pi$].

Equation (1) shows that, in general, there are three possibilities for the neutron resonance. It can be an exciton, which is the case when $\Omega_{res}\approx\Omega_s$ and $Z_s\gg Z_\pi$ (Refs. 4–6). It can also be π resonance,[7] which holds when $\Omega_{res}\approx\Omega_\pi$ and $Z_\pi\gg Z_s$, and finally, it can be a magnetic plasmon,[9] which is the case when $\chi_s(\Omega)$ and $\chi_\pi(\Omega)$ weakly depend on frequency, and the resonance emerges due to the mixing between the two channels. In this last case, $\Omega_{res}\approx[\chi_s^{-1}(0)\chi_\pi^{-1}(0)/C_0^2]^{1/2}$ and is generally different from both Ω_s and Ω_π.

The interplay between an exciton, a π mode, and a plasmon has been considered in earlier works but the results remain controversial. The idea that the resonance may be a π mode was put forward by Demler *et al.*[7] Tchernyshov *et al.*[8] considered a model with nearest-neighbor spin- and charge-repulsive interactions and argued that the resonance keeps predominantly excitonic character. This is somewhat expected as for repulsive interactions a π mode is antiresonance (it appears above two-particle continuum). Lee *et al.*[9] addressed this issue recently and argued that the resonance is predominantly a plasmon, particularly when the pairing comes from nearest-neighbor density-density attraction. The attractive density-density interaction was not considered in Ref. 8.

In this paper, we reanalyze this issue and compare the two cases—when the d-wave pairing comes from spin-spin interaction[5] and when it comes from density-density interaction.[11] We follow earlier works, use BCS approximation, and model the attractive spin-dependent interaction by nearest-neighbor Heisenberg exchange term $J>0$, (Ref. 8) and a d-wave interaction in the charge channel by nearest-neighbor density-density interaction V (Ref. 9). Using BCS theory with a frequency-independent gap is indeed an approximation as the effective spin and charge interactions are frequency dependent, and to obtain T_c and the resonance frequency one has to solve a set of coupled integral equations in ω and k spaces for bosonic and fermionic self-energies and the pairing vertex, which all depend on frequency and on the momentum component along the Fermi surface.[5] However, the spin resonance is a generic property of a d-wave superconductor, and it exists even if one models the interactions by frequency-independent constants and solve for the pairing and the spin response in the superconducting state within the BCS approximation using a cutoff imposed by the lattice dispersion instead of a frequency cutoff imposed by the interaction. As our goal is to distinguish between different scenarios for the resonance, we will restrict with the BCS approximation.

For a repulsive charge interaction ($V>0$), there is no π resonance (i.e., no pole in χ_π below 2Δ),[8] hence the neutron resonance can be either an exciton or a plasmon. For negative V, both χ_s and χ_π have poles below 2Δ, and the resonance can be an exciton, a π-resonance, or a plasmon. To distinguish between them, we solved the full 3×3 matrix equation for χ, compare the residues in spin and π channels (this determines whether the resonance is an exciton or a π resonance), and also compare the location of the pole with Ω_s, (this determines whether or not the resonance is a plasmon). We follow earlier work[9] and require that the value of a d-wave gap should agree with ARPES experiments.[12]

Our results show that, to a surprisingly good accuracy, the resonance remains an exciton no matter whether the pairing is in the spin or in the charge channel. For both cases, we found that neither π-resonance nor the mixture between s and π channels affect the location and the residue of the resonance residue in any substantial way, although the corrections due to mixture are larger for the case $|V|\gg J$. Furthermore, we find that Z_s can be large enough and the resonance frequency can be the experimental 40 meV without placing the system too close to an antiferromagnetic instability.

Our results disagree with the idea about the dominance of the π-resonance,[7] and also disagree to a certain extent with the idea[9] that the resonance is a plasmon rather than an exciton. Still, we find, in agreement with Ref. 9, that the mixing between spin and π channels is not negligible and has to be taken into account in quantitative studies of the cuprates.

We caution that for the charge-mediated pairing, the results strongly depend on the magnitude of nearest-neighbor attraction V. We have chosen $|V|$ which yields a BCS gap of 35 meV. This $|V|$ turns out to be too small to give rise to π-resonance. For larger $|V|$, the structure of $\chi_s(\Omega)$ will differ more from an exciton.

A related issue which we also consider is a potential relation between the spin resonance and the "glue" for a d-wave superconductivity, at least at and above optimal doping, where the system falls into moderate coupling regime.[13] Lee *et al.*[9] argued that the study of the resonance can distinguish between spin and charge mechanisms in favor of the former. We found that the resonance is only weakly sensitive to the form of the pairing glue, and it may be difficult to distinguish from the measurements of the resonance alone between spin-mediated and charge-mediated pairings.

The structure of the paper is the following. In Sec. II we introduce the model. In Sec. III we introduce generalized RPA susceptibilities and discuss the coupling between particle-hole and particle-particle channels. In Sec. IV we present the results of our calculations for the location of the resonance and the residues of various contributions to the resonance. In Sec. V we present our conclusions.

II. MODEL

We consider the same model as in previous works (Ref. 9), with on-site Hubbard repulsion and nearest-neighbor density-density and spin-spin interactions,

$$H=\sum_{\mathbf{k},\sigma}(\epsilon_{\mathbf{k}}-\mu)a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}+\sum_i Un_{i\uparrow}n_{i\downarrow}+\sum_{\langle ij\rangle}(Vn_in_j+J\mathbf{S}_i\cdot\mathbf{S}_j), \tag{2}$$

where $\epsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y$, $n_{i\sigma}=c^\dagger_{i\sigma}c_{i\sigma}$, and $\mathbf{S}_i=(1/2)c^\dagger_{i\sigma}\sigma_i c_{i\sigma}$ are the particle and spin operators on site i (each interaction is counted once). A similar model but without U term has been earlier considered by Tchernyshov *et al.*[8]

The soft modes of the system are singlet pairs on nearest-neighbor bonds, $\psi_{ij}=a_{i\alpha}\sigma^y_{\alpha\beta}a_{j\beta}$, spin fluctuations $\vec{S}_{ij}=(1/2)a^\dagger_{i\alpha}\vec{\sigma}_{\alpha\beta}a_{j\beta}$, and triplet pairs $\vec{\pi}_{ij}=a_{i\alpha}(\vec{\sigma}\sigma^y)_{\alpha\beta}a_{j\beta}$. The gap $\Delta_{\mathbf{k}}=\Delta g_{\mathbf{k}}$ with $g_{\mathbf{k}}=(\cos k_x-\cos k_y)/2$ is determined from the standard equation

$$-\frac{V_\psi}{2}\int\frac{d^2k}{(2\pi)^2}\frac{g^2_{\mathbf{k}}}{\sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+\Delta^2 g^2_{\mathbf{k}}}}=1, \tag{3}$$

where $V_\psi=V-3J/4$. Choosing $x=0.12$ ($\mu=-0.94t$), $t'/t=-0.3$, and $t=0.433$ eV to match the observed shape of the Fermi surface, the nodal Fermi velocity,[14] and setting the maximum gap to be $\Delta=35$ meV, we find $V_\psi=V-3J/4=-0.60t$, in agreement with Ref. 9.

III. GENERALIZED RPA SUSCEPTIBILITIES

We use V_ψ and Δ as inputs and compute dynamic susceptibilities within a generalized RPA scheme which, we remind, takes into account the fact that a particle-hole and a particle-particle channels are mixed in the presence of a charged condensate of Cooper pairs. The derivation of the generalized RPA equations is rather straightforward and has been described before.[7–9] Because of SU(2) spin symmetry, it is sufficient to probe only one spin component, e.g., restrict in momentum space with $A_0(q)=S^+(q)$, $A_1(q)=[\pi^y(q)+i\pi^x(q)]/2$, and $A_2(q)=A^*_1(q)$. These three operators create bosonic excitations with the same momentum and spin $S_z=1$ but with different charges, 0 and ± 2, respectively. For

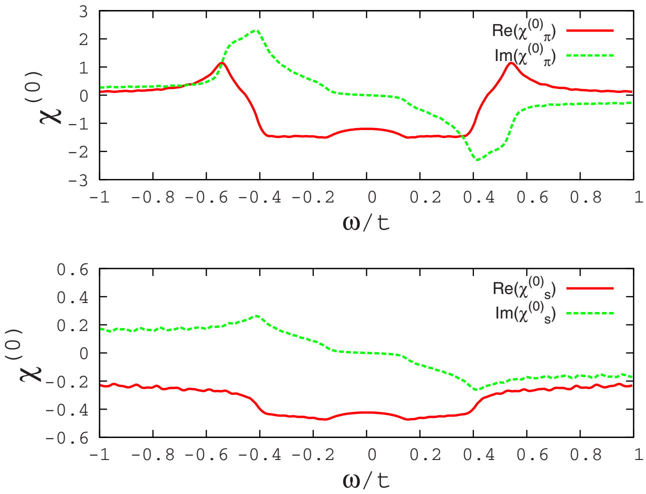

FIG. 1. (Color online) The bare susceptibilities in the spin and π channels, $\chi_s^0(\Omega)$ and $\chi_\pi^0(\Omega)$, respectively (in units of $1/t$). The features at $\pm 0.16t$ are 2Δ effects, features at higher Ω are Van Hove singularities. Note that χ_s^0 has more variation than χ_π^0 Note also the difference in vertical scales, χ_π^0 is larger than χ_s^0.

definiteness, we restrict with antiferromagnetic $q=Q=(\pi,\pi)$.

Generalized RPA equations relate bare and full susceptibilities,

$$\chi_{a,b}(\Omega) = \chi_{a,b}^0(\Omega) + \chi_{a,c}^0(\Omega)\Gamma_{c,d}\chi_{d,b}(\Omega), \qquad (4)$$

where $a,b=0,1,2$, and $\chi_{a,b}^0(\Omega)$ are linear-response functions for the noninteracting system—the Fourier transforms of $-i\theta(t)\langle[A_\alpha(t),A_\beta^\dagger(0)]\rangle$, where the averaging is over free fermion ground state. Diagrammatically, $\chi_{aa}^0(\Omega)$ are the convolutions of *GG* and *FF* terms, while nondiagonal $\chi_{a,b}^0(\Omega)$ are *GF* terms. All nine elements of $\chi_{a,b}^0(\Omega)$ are nonzero but nondiagonal terms vanish at zero frequency. It is convenient to rotate the basis in π,π^* plane and introduce, instead of $A_{1,2}$, $\bar{A}_{1,2}=(A_1 \mp A_2)/\sqrt{2}$ [same notations have been used in earlier works (Refs. 8 and 9)]. In this basis, the interaction matrix $\Gamma_{a,b}$ is diagonal due to charge conservation, and its diagonal elements are $V_0=-U-2J$ and $V_{1,2}=(V+J/4)/2$, i.e., without mixing $\chi_s=\chi_s^0/(1-V_0\chi_s^0)$ and $\chi_\pi=\chi_\pi^0/(1-V_{1,2}\chi_\pi^0)$.

In Fig. 1 we show real and imaginary parts of the bare $\chi_s^0(\Omega)$ and $\chi_\pi^0(\Omega)$. Note that, in our notations, static $\chi_{s,\pi}^0$ are negative. Sharp features at $\pm 0.16t$ (± 70 meV) are 2Δ effects, the features at higher energies are Van Hove singularities.

IV. RESULTS

We present the results for the two extreme cases, $V=0$ and $J=0$. In the first case, *d*-wave superconductivity is magnetically mediated and $V_\psi=-3J/4$. In the second it emerges due to an attraction in the charge channel and $V_\psi=V$. For both cases, we used on-site Hubbard U as an extra parameter that drives the system toward an antiferromagnetic instability and brings the resonance frequency down.

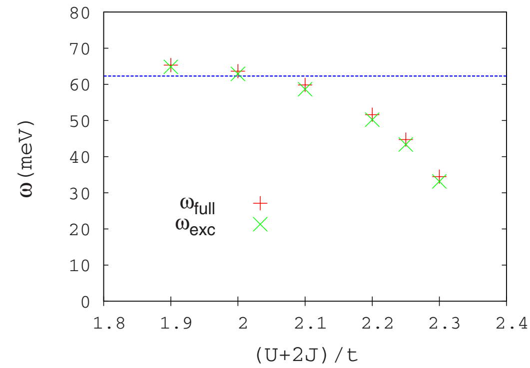

FIG. 2. (Color online) The resonance positions for $V=0$ and $J=0.8t$ for different U. $\omega_{\rm full}$ is the solution of the full 3×3 set, $\omega_{\rm exc}$ is the energy of a spin exciton. The blue dashed line is the edge of two-particle continuum. Antiferromagnetism emerges at $|V_0|=2.38t$.

A. $V=0$, $J\neq 0$

In this case $V_0=-(U+1.6t)$, $V_{1,2}=0.1t>0$, and π susceptibility taken alone only develops an antiresonance above the upper edge of two-hole continuum.[8] The issue for this case is whether the resonance is an exciton or a plasmon. In Fig. 2 we present the results of our calculations of the resonance frequency using the full 3×3 set and compare them with the RPA result for spin-only channel. We see that the energies match nearly perfectly, which we believe is a strong indication that the resonance is indeed an exciton. Observe that $\omega_{\rm full}\geq\omega_{\rm exc}$, although the two are rather close. We verified the sign of $\omega_{\rm full}-\omega_{\rm exc}$ analytically and found that it is determined by the sign of $V_{12}=(V+J/2)/4$, and that $\omega_{\rm full}$ is larger than $\omega_{\rm exc}$ when $V_{12}>0$. This is indeed the case when $V=0$ and $V_{12}=J/8>0$.

In Fig. 3 we plot the residues of the resonance in spin and π channels, Z_s and Z_π, respectively, together with the residue of a pure exciton, $Z_{\rm exc}$, which we obtained by eliminating the mixing between spin and π channels. We used a finite broadening $\gamma=0.002$ which explains why $Z<1$ even for the case of a pure exciton. We see that for all U, the residue of the resonance is much larger in the spin channel than in the π channel. If the resonance was a plasmon, the residue in the spin and π channels would be comparable. As an indepen-

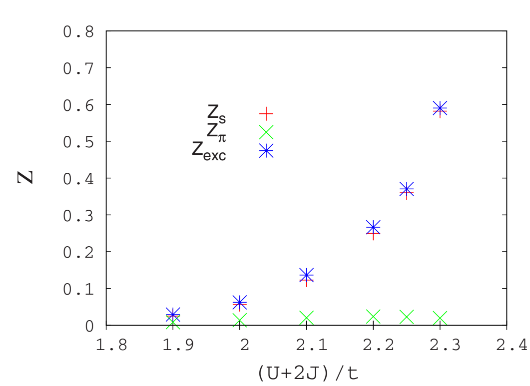

FIG. 3. (Color online) The residues Z_s and Z_π from the full 3×3 set, and the residue of an exciton $Z_{\rm exc}$ for different U.

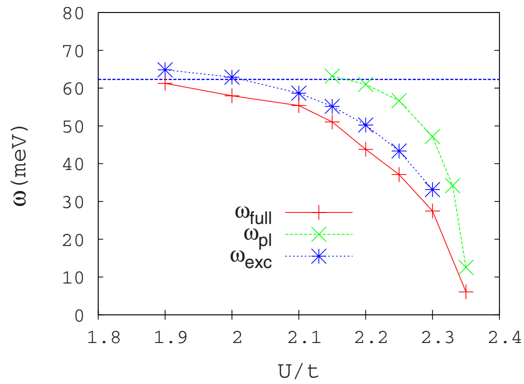

FIG. 4. (Color online) The energy of the resonance from the solution of the full 3×3 set (ω_{full}), and the energies of an exciton and a lasmon (ω_{exc} and ω_{pl}) for the case of nearest-neighbor charge interaction $J=0$ and $V=-0.6t$ as functions of U (see text). The blue dashed line is the edge of the two-particle continuum.

dent check, we solved a 3×3 set with diagonal $\chi^0_{aa}(\Omega)$ replaced by their static values. The solution in this case would be a plasmon [see Eq. (1)] but we didn't find a resonance.

On a more careful look, we found that the dominant mixing term is χ_{01} and that the correction due to mixing is only 3%. This not due to smallness of $\chi_{10}=C\omega$ per se (we found $C\sim1.3t$) but rather due to the fact that a frequency of 50 meV is only 0.12 in units of t, which, we remind, was chosen to reproduce the Fermi velocity measured by ARPES. Lee *et al.*[9] used a much smaller t, in which case the mixing term is indeed larger.

Figure 2 also shows that the resonance shifts down from 2Δ (and becomes strong) when $|V_0|$ exceeds roughly 80% of the critical $|V_0|=2.38t$. beyond which antiferromagnetic order emerges. Using $\xi\propto(\xi/a)^2$, where ξ is the correlation length and a is interatomic spacing, we find that this corresponds to $\xi\sim2.5a$. A correlation length of about $3.7a$ is necessary for the resonance frequency Ω_{res} to be 40 meV.

B. $J=0$, $V\neq0$

In this case $V=-0.6t$, i.e., $V_0=-U$ and $V_{1,2}=-0.3t$. The results of the calculations are presented in Figs. 4 and 5. Now π channel becomes attractive, and exciton, plasmon, and π-resonance are all competing for the dominant contribution to the resonance in the full spin susceptibility. The three sets of points in Fig. 4 are the solution of the full 3×3 set and two approximate sets in which we (i) considered the spin channel only (the resonance is an exciton) and (ii) approximated diagonal $\chi^0_{aa}(\omega)$ by their static values (the resonance is a plasmon). We see that the position of the actual resonance (the full solution) is rather close to the position of the spin exciton and the two follow the same trend with U, although there is a clearly visible difference of about 5 %–10 %. The plasmon has different dependence on U and is located below 2Δ only in a narrow range of U. It approaches the exciton near the critical $U/t=2.38$ at which the system orders antiferromagnetically, but this is merely the consequence of the fact that at this U, the energies of an exciton and a plasmon vanish. Note that $\omega_{\text{full}}<\omega_{\text{exc}},\omega_{pl}$, as it indeed should be [see Eq. (1)]. Observe that $\omega_{\text{full}}<\omega_{\text{exc}}$ is consistent with the fact that for $J=0$ and $V<0$, V_{12}, which determines the sign of $\omega_{\text{full}}-\omega_{\text{exc}}$ is negative.

In Fig. 5 we show the residues of the spin and π components of the full susceptibilities near Ω_{res} and compare them with the residue of a pure spin exciton [the case (i) above]. We see that, when the resonance shifts below 2Δ and becomes measurable, its residue in the spin channel is larger than in the π channel and practically coincides with the residue of an exciton. Note that the same $\xi/a\sim3.7$ as in the first case is required for the resonance to be at 40 meV.

These results imply that even if the pairing is due to an attractive nearest-neighbor density-density interaction, the resonance in the spin susceptibility still has predominantly excitonic character. We caution, however, the absence of a substantial π component of the neutron resonance is a numerical rather than a fundamental effect. Namely, for $V=-0.6$ eV extracted from the gap equation, π-resonance in the absence of broadening is close to 2Δ, and a small broadening washes it out. We also note that a plasmon does exist in this case, in agreement with Ref. 9 but in a narrow range of U near an antiferromagnetic instability.

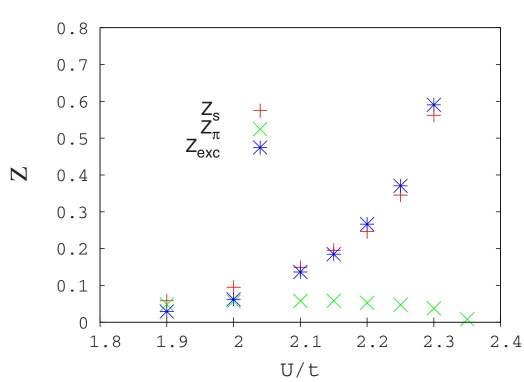

FIG. 5. (Color online) The residues Z_s, Z_π, and Z_{exc} for the case $J=0, V=-0.6t$ for different U.

C. $J\neq0$, $V\neq0$

We also performed calculations for several J and V in between the two limits, still keeping $V_\psi=V-3J/4=-0.6t$ to match the gap value. For all cases we found that the resonance is predominantly an exciton. The situation changes if we abandon BCS gap equation and take larger $|V|$. The larger $|V|$ is, the stronger the resonance differs the exciton. We also found empirically that the plasmon solution (like the one in Fig. 4) only exists when $V_{1,2}<0$. This agrees with the result of Ref. 8.

V. CONCLUSIONS

To conclude, in this paper we reanalyzed whether the resonance peak observed in neutron scattering experiments on the cuprates is an exciton, a π-resonance, or a magnetic plasmon. We considered a model with on-site Hubbard U and nearest-neighbor interaction in both charge and spin channels and found that the resonance is predominantly an exciton, even if d-wave pairing originates from attractive density-density interaction rather than spin-spin interaction. Our results indicate that one cannot distinguish between spin-mediated and charge-mediated pairing by just looking at the resonance peak in the spin susceptibility. Other probes like, e.g., dispersion anomalies[15] or Raman scattering[16] are more useful in this regard

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