Magnetic resonance in the cuprates – exciton, plasmon, or $\pi$–mode

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We re-analyzed the issue whether the resonance peak observed in neutron scattering experiments on the cuprates is an exciton, a $\pi$–resonance, or a magnetic plasmon. We considered a toy model with on-site Hubbard $U$ and nearest-neighbor interactions in both charge and spin channels. We found that the resonance is predominantly an exciton, even if magnetic interaction is absent and $d$–wave pairing originates from attractive density-density interaction. Our results indicate that one cannot distinguish between spin and charge-mediated pairing interactions by just looking at the resonance peak in the dynamic spin susceptibility.

Introduction. The origin of the $(\pi, \pi)$ 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, and the doping variation of its energy follows closely the doping dependence. Magnetic resonances have been also recently observed in heavy-fermion materials and in Fe-pnictides.

It is widely accepted that the resonance at $Q = (\pi, \pi)$ is a feedback from the opening of a $d$–wave pairing gap in the fermionic system. There is no consensus, however, about the driving force. The simplest and most transparent idea put forward by various groups 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), or just calculate the spin susceptibility within a conventional RPA for the underlying Hubbard model – either way one obtains a $\delta$–functional excitonic peak at a finite frequency below $2\Delta$, where $\Delta$ is the amplitude of gap at “hot spots” – $k_F$ points separated by $Q$.

This simple approach, however, is incomplete as it neglects the fact that in a $d$–wave superconductor the staggered particle-hole, charge 0 spin variable $S_Q^\alpha = (1/2\sqrt{N}) \sum_k c_{k,\alpha}^\dagger c_{k+Q,\beta}^\dagger$ is mixed with the staggered $d$–wave particle–particle charge $\pm 2$ variables $\pi_Q^\alpha$ and $(\pi_Q^\alpha)^*$, where $\pi_Q^\alpha = (1/\sqrt{N}) \sum_k d_{k,\alpha} c_{k,\sigma^y,\alpha} c_{k+Q,\beta}$, and $d_k = \cos k_x - \cos k_y$ (Refs. 7 and 8). Diagrammatically, mixed $< S\pi >$ response function is given by $d_k G_k F_{k+Q}$ bubbles made out of normal $(G)$ and anomalous $(F)$ Green’s functions. Such terms are finite in a $d$–wave superconductor at $\omega \neq 0$.

Because spin and $\pi$ responses are coupled, the full spin response function is obtained by solving the full $3 \times 3$ set of coupled generalized RPA equations for $< SS >$, $< \pi, \pi >$ and $< S\pi >$ correlators (Ref. 9). As a consequence, the resonance mode emerges simultaneously in spin and $\pi$ channels, and for the case when both $s$ and $\pi$ resonances are present, its location $\omega = \omega_{res}$ is in general the solution of

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

where $\chi_s^{-1}(\omega - \omega_{exc})$ and $\chi_{\pi}^{-1}(\omega - \omega_{\pi})$ are inverse RPA susceptibilities in $s$ and $\pi$ channels, each resonating at its own frequency, and $\omega_{exc}$ is the mixing $GF$ terms. If $\omega_{exc} = 0$, $s$ and $\pi$ channels are decoupled, and the spin and $\pi$ resonances occur at $\omega_{exc}$ and $\omega_\pi$, respectively, and are not affected by each other. In general, however, the resonance frequency $\omega_{res}$ is the solution of Eq. 1, and the full spin and $\pi$ 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 $C_\omega = Z_s = 1, Z_\pi = 0$ at $\omega = \omega_{exc}$, and $Z_s = 1, Z_\pi = 0$ at $\omega = \omega_{\pi}$].

Eq. 1 shows that, in general, there are three possibilities for the neutron resonance. It can be an exciton, which is the case when $\omega_{res} \approx \omega_{exc}$ and $Z_s \gg Z_\pi$ (Refs. 10 and 11). It can also be a $\pi$ resonance, which holds when $\omega_{res} \approx \omega_{\pi}$, and $Z_\pi \gg Z_s$. And, finally, it can be a magnetic plasmon, 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, $\omega_{res} \approx \chi_s^{-1}(0)\chi_{\pi}^{-1}(0)C_\omega^2/2$ and is generally different from both $\omega_{exc}$ and $\omega_\pi$.

Another issue which we consider is the 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. The pairing can be magnetically-mediated, or it can be mediated by a $d$–wave attraction in the charge channel. We will analyze whether the location and the residue of the resonance can distinguish between the two cases.

We follow earlier works, use BCS approximation, and model the attractive spin-dependent interaction by nearest-neighbor Heisenberg exchange term $J > 0$, (Ref. 12), and a $d$–wave interaction in the charge channel by nearest-neighbor density-density interaction $V$ (Ref. 13). For a repulsive charge interaction ($V > 0$),
there is no \( \pi \) resonance (i.e., no pole in \( \chi_\pi \) below \( 2\Delta \)), hence the neutron resonance can be either an exciton or a plasmon. For negative \( V \), both \( \chi_s \) and \( \chi_\pi \) have poles below \( 2\Delta \), and the resonance can be an exciton, a \( \pi \)-resonance, or a plasmon. To distinguish between them, we will solve the full \( 3 \times 3 \) matrix equation for \( \chi \), compare the residues in spin and \( \pi \) channels, (this should show whether the resonance is an exciton or a \( \pi \) resonance), and also compare the location of the pole with \( \omega_{\text{exc}} \) (this should show whether or not the resonance is a plasmon). We follow earlier work and require that the value of a \( d \)-wave gap should agree with ARPES experiments.

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 \( \pi \)-resonance nor the mixture between \( s \) and \( \pi \) 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 \( 40\,\text{meV} \) without placing the system too close to an antiferromagnetic instability.

Our results disagree with the idea about the dominance of the \( \pi \) resonance\(^{10}\), and also somewhat disagree with the recent study\(^{11}\) which associated the resonance with a plasmon rather than an exciton. That work also found that the study of the resonance can distinguish between spin and charge mechanisms in favor of the former. We, on the contrary, found that the resonance is only weakly sensitive to the form of the pairing glue. Still, we find, in agreement with Ref. \(^{10}\), that the mixing between spin and \( \pi \) channels is not completely negligible and has to be taking 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 \( 35\,\text{meV} \). This \( |V| \) turns out to be too small to give rise to \( \pi \) resonance. For larger \( |V| \), the structure of \( \chi_s(\omega) \) will differ more from an exciton.

\textbf{The model.} We consider the same model as Lee et al\.(Ref. \(^{10}\)), with on-site Hubbard repulsion and nearest-neighbor density-density and spin-spin interactions,

\[
H = \sum_{\mathbf{k},\sigma} (\epsilon_k - \mu) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{\langle ij \rangle} (V n_{i\uparrow} n_{j\downarrow} + J S_i \cdot S_j),
\]

where \( \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \), \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), and \( S_i = (1/2) c_{i\uparrow}^\dagger \sigma_{\alpha\beta} c_{i\beta} \) 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 Norman and one of us\(^{25}\).

The soft modes of the system are singlet pairs on nearest-neighbor bonds, \( \psi_{ij} = a_{i\sigma}^\dagger \sigma_{\alpha\beta} a_{j\beta} \), spin fluctuations \( S_{ij} = (1/2) a_{i\sigma}^\dagger \sigma_{\alpha\beta} a_{j\beta} \), and triplet pairs \( \pi_{ij} = a_{i\sigma} (\bar{\sigma} \sigma_{\alpha}^\dagger a_{j\beta} \). The gap \( \Delta_k = \Delta g_k \) with \( g_k = (\cos k_x - \cos k_y)/2 \) is determined from the standard equation

\[
-\frac{V_\psi}{2} \int \frac{d^2k}{(2\pi)^2} \frac{g_k^2}{\sqrt{\epsilon_k - \mu)^2 + \Delta^2 g_k^2}} = 1.
\]

where \( V_\psi = V - 3J/4 \). Choosing \( x = 0.12 \) \((\mu = -0.94t)\), \( t'/t = -0.3 \) and \( t = 0.433 \,\text{eV} \) to match the observed shape of the Fermi surface and the nodal Fermi velocity\(^{15}\), and setting the maximum gap to be \( \Delta = 35\,\text{meV} \), we find \( V_\psi = V - 3J/4 = -0.60t \), in agreement with\(^{10}\).

\textbf{Generalized RPA susceptibilities} We use \( V_\psi \) and \( \Delta \) 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\(^{7,8,10}\). 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 \( \pm 2 \), respectively. For definiteness, we restrict with antiferromagnetic \( q = (\pi, \pi) \).

Generalized RPA equations relate bare and full susceptibilities:

\[
\chi_{a,b}(q) = \chi_{a,b}^0(q) + \chi_{a,c}^0(q) \Gamma_{c,d} \chi_{d,b}(q),
\]

where \( a,b = 0, 1, 2 \), and \( \chi_{a,c}^0(q) \) are linear response functions for the noninteracting system – the Fourier transforms of \(-i\theta(t)[A_a(t), A_b^\dagger(0)]\) where the averaging is over free fermion ground state. Diagrammatically, \( \chi_{a,c}^0(q) \) are the convolutions of \( GG \) and \( FF \) terms,
while non-diagonal \( \chi^{0}_{a,b}(\omega) \) are GF terms. All 9 elements of \( \chi^{0}_{a,b}(\omega) \) are nonzero, but non-diagonal terms \( \chi^{0}_{01} \) and \( \chi^{0}_{12} \) vanish at zero frequency, and \( \chi^{0}_{00} \) is nonzero only because of the curvature of the fermionic dispersion near \( k_F \). It is convenient to rotate the basis in \( \pi, \pi^* \) plane and introduce, instead of \( A_{1,2}, A_{1,2}(A_{1} \mp A_{2})/\sqrt{2} \) (same notations have been used in earlier works \(^{8,10}\)). In this basis, the interaction matrix \( \Gamma_{a,b} \) is diagonal due to charge conservation, and its diagonal elements are \( V_0 = -U - 2J, V_{1,2} = (V + J)/2 \), i.e., without mixing \( \chi_\alpha = \chi^{0}_\alpha/(1 - V_0 \chi^{0}_\alpha), \chi_\pi = \chi^{0}_\pi/(1 - V_{1,2} \chi^{0}_\pi) \).

In Fig. 1 we show real and imaginary parts of the bare \( \chi^{0}_0(\omega) \) and \( \chi^{0}_1(\omega) \) (a phase mode of the \( \pi \) field). The bare \( \chi^{0}_2 \) is smaller than \( \chi^{0}_1 \). Note that in our notations, static \( \chi^{0}_\alpha \) are negative. Sharp features at \( \pm 0.16 \) ( \( \pm 700 \) meV) are 2\( \Delta \) effects, the features at higher energies are Van Hove singularities.

The 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 towards an antiferromagnetic instability and brings the resonance frequency down.

For the first case, \( V_0 = -(U + 1.6)t, V_{1,2} = 0.1t > 0 \), and \( \pi - \pi \)-susceptibility taken alone only develops an antiresonance above the upper edge of two-hole continuum \(^2\). 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 \( 3 \times 3 \) 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 the exciton. On a more careful look, we found that a near-perfect match is not the consequence of the small mixing amplitude \( C_\omega \) in \(^1\) is roughly \( 1.3t \) but rather the consequence of the fact that \( \omega = 50 \) meV is only \( 0.12t \). In Fig. 3 we plot the residues of the resonance in spin and \( \pi \) channels, \( Z_s \) and \( Z_\pi \), respectively, together with the residue of a pure exciton, \( Z_{exc} \), which we obtained by eliminating the mixing between spin and \( \pi \) 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 \( \pi \) channel. If the resonance was a plasmon, the residue in the spin and \( \pi \) channels would be comparable. As an independent check, we solved a \( 3 \times 3 \) set with diagonal \( \chi^{0}_{a,a}(\omega) \) replaced by their static values. The solution in this case would be a plasmon (see Eq. \(^1\)), but we didn’t find a resonance.

Fig. 2 also shows that the resonance shifts down from \( 2\Delta \) (and becomes strong) when \( |V_0| \) exceeds roughly 80% of the critical \( |V_0| = 2.8t \), beyond which antiferromagnetic order emerges. Using \( \xi \propto (\xi/a)^2 \), where \( \xi \) is the correlation length and \( a \) is interatomic spacing, we find that this corresponds to \( \xi \propto 2.5a \), while \( \xi \propto 3.7a \) is necessary for the resonance frequency \( \omega_{exc} \) to be \( 40 \) meV.

The results for the second case, \( J = 0, V = -0.6t \), i.e., \( V_0 = -U, V_{1,2} = -0.3t \), are presented in Figs. 4 and 5. Now \( \pi \)-channel becomes are attractive, and exciton, plasmon, and \( \pi \) 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 \( 3 \times 3 \) set and two approximate sets in which we (i) considered the spin channel only (the resonance is an exciton) and (ii) approximated diagonal \( \chi^{0}_{a,a}(\omega) \) 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 \( 2\Delta \) only in a narrow range of \( U \). Note that \( \omega_{full} < \omega_{exc}, \omega_{pl} \), as it indeed should be (see Eq. \(^1\)). In Fig. 6 we show the residues of the spin and \( \pi \) components of the full sus-
when the resonance shifts below \(2\Delta\) and becomes measurable, its residue in the spin channel is larger than in the \(\pi\) channel and practically coincides with the residue of an exciton. Note that the same \(\xi/a\sim 3.7\) as in the first case is required for the resonance to be at \(40\text{meV}\).

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 \(\pi\) component of the neutron resonance is as a numerical rather than a fundamental effect. Namely, for \(V = -0.6eV\) extracted from the gap equation, \(\pi\)-resonance in the absence of broadening is close to \(2\Delta\), and a small broadening washes it out. We also note that a plasmon does exist in this case, in agreement with Ref. 10, but in a narrow range of \(U\) near an antiferromagnetic instability.

We also performed calculations for several \(J\) and \(V\) in between the two limits, still keeping \(V_{\phi} = V - 3J/4 = -0.6t\) 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.

To conclude, in this paper we re-analyzed whether the resonance peak observed in neutron scattering experiments on the cuprates is an exciton, a \(\pi\)-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 and charge-mediated pairings by looking at the resonance peak in the spin susceptibility. Other probes like e.g., dispersion anomalies, or Raman scattering are more useful in this regard.

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