Neutron resonance in high-$T_c$ superconductors is not the $\pi$ particle

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We discuss the interplay of particle-particle and particle-hole spin-triplet channels in high-$T_c$ superconductors using a quasiparticle dispersion motivated by angle-resolved photoemission. Within a generalized random-phase approximation, we find a well-defined antibound state of two holes, the $\pi$ resonance of Demler and Zhang, as well as a bound state of a particle and a hole, the spin exciton. We show that the energy of the $\pi$ resonance always exceeds $2\Delta$, twice the maximum $d$-wave gap, therefore the neutron resonance observed in the cuprates around energy $\Delta$ is most likely a spin exciton. At the same time, we speculate that the $\pi$ particle can exist at higher energies and might be observed in neutron scattering around 100 meV.

Reflecting our poor understanding of high-$T_c$ superconductivity in general, theoretical debates continue on virtually every aspect of it. A good example is the resonance observed in inelastic neutron scattering at energies 25–43 meV in $\text{YBa}_2\text{Cu}_3\text{O}_7$, and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. Measurements using polarized neutrons indicate that the observed excitation is magnetic in nature. Theoretical proposals include a van Hove singularity in the Stoner continuum, a bound state (spin exciton) in the particle-hole channel, and an antibound state in the particle-particle channel ($\pi$ resonance). Deciding between these approaches is somewhat difficult since in all theories the resonance mode is an excited pair of quasiparticles with total lattice momentum $Q = (\pi/a, \pi/a)$ and spin $S = 1$.

In this paper, we use available experimental data and a simple kinematic argument to demonstrate that a particle-hole bound state is the most likely explanation for the resonance. In a nutshell, our reasoning goes as follows. Angle-resolved photoemission spectroscopy (ARPES) directly measures the dispersion of fermonic quasiparticles $E_k$ in the superconducting state. From this, one can deduce information about the continuum of states of two quasiparticles with total momentum $Q$ and, in particular, determine its energy bounds. An analysis of ARPES data in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ shows that the two-quasiparticle continuum starts at $E_{\text{min}} = 2\Delta$, where $\Delta$ is the maximum value of the superconducting gap at the Fermi surface. The commensurate neutron resonance in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ resides at $E_{\text{res}} \approx \Delta$, definitely below the lower edge of the continuum. The resonance then can only be a bound state of two quasiparticles, not an antibound state.

This argument—that the lower edge of the two-particle continuum is determined by $\Delta$ and not by the chemical potential $\mu$ as in Ref. 13—is based on the analysis of the Fermi surface inferred from ARPES data (Fig. 1). We have verified that for this Fermi surface, $E_{\text{min}}$ is determined not by electrons along zone diagonals $k_p = k_\parallel$, but rather by electrons near the hot spots (points at $\mathbf{k} = k_F$ separated by $Q$). The latter are located close to $(0, \pi)$ and symmetry related points, and in the superconducting state have a gap $\Delta(k_{\text{ps}}) \approx \Delta$. This yields a threshold at $E_{\text{min}} = 2\Delta$ for the total momentum of two particles $(\pi, \pi)$. Note that this argument also invalidates the interpretation of the resonance as a van Hove singularity in the two-quasiparticle continuum.

Does it mean that the $\pi$ resonance does not exist? Not necessarily. In our model calculations, the spin exciton and the $\pi$ resonance are found to coexist at intermediate coupling strengths, similar to earlier findings. Furthermore, in a situation where the continuum of states with two holes is narrow and has a sharp upper edge, we find that the $\pi$ resonance is rather sharp. To what extent these conditions are satisfied in the cuprates is not clear because self-energy effects could wash out the upper edge of the continuum. We therefore can only speculate that the $\pi$ resonance might be discovered in neutron scattering at energies above $E_{\text{min}}$ (60 meV in optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$), more likely around 100 meV.

To proceed, we need a model treating all spin-triplet excitations (with charges 0 and $\pm 2$) on an equal footing. The simplest approach is an adaptation of Anderson’s treatment of phase fluctuations and plasmons in a superconductor to

FIG. 1. “Hot spots” are points $k_{\text{ps}}$ on the Fermi surface connected by the wave vector $Q = (\pi/a, \pi/a)$ or those equivalent to it. Equivalently, they are given by intersections of the Fermi surface with the magnetic zone boundary (dashed lines).
the spin-triplet channel. Precisely this method, known as generalized random-phase approximation (RPA),\textsuperscript{18,19} was used by Demler \textit{et al.}\textsuperscript{14} To make the approach self-consistent, we make a quasiparticle approximation with a dispersion\textsuperscript{20} fitted to peak positions in the ARPES data in the superconducting state of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. As the measured dispersion is flat near $(0,\pi)$, our calculation yields a strikingly narrow two-hole continuum with a width of about 10 meV. This narrowness is caused by the proximity of the hot spots to the van Hove points at $(\pi,0)$.

This quasiparticle model is a “best case” scenario for the antibound state. This model assumes that one has a superfluid Fermi liquid, which appears to be consistent with transport and ARPES data, at least at low temperatures. Within this approximation, the upper edge of the two-hole continuum is sharp, which is favorable for the formation of the $\pi$ resonance. By making such an approximation, we essentially neglect the large incoherent part of the electron spectral function known to exist from photoemission. On the other hand, this incoherent part is absent below the energy scale $\Delta + E_{\text{cns}}$ set by the spin resonance.\textsuperscript{11,21} so the fermionic incoherence affects the two-particle propagators only at energies above $2\Delta + E_{\text{cns}}$. Thus the $\pi$ resonance can, in principle, live below this threshold. We make no attempt to explain why the quasiparticle dispersion is so remarkably flat near $(\pi,0)$. A number of authors\textsuperscript{21–23} have pointed out that this flatness most likely results from a strongly $\omega$-dependent self-energy that renormalizes the bare dispersion. Also note that the extreme narrowness of the two-particle continuum is not a crucial part of our argument: we have observed similar behavior with a much wider (70-meV) two-particle continuum based on normal-state dispersions.

We now proceed with the calculations. Consider a system of fermions described by a Hamiltonian that consists of kinetic energy and nearest-neighbor interactions involving both spin and charge:

$$H = \sum_{k,\sigma} \epsilon_k \hat{a}^\dagger_{k\sigma} \hat{a}_{k\sigma} + \sum_{\langle ij \rangle} \left[J \left(S_i \cdot S_j - \frac{n_{i\uparrow} n_{j\uparrow}}{4}\right) + V n_i n_j \right].$$

(1)

The one-particle energy $\epsilon_k$ has a tight-binding form obtained by fitting ARPES data (see Ref. 20 for details) with the following chemical potential and hopping amplitudes for first through fifth nearest neighbors on a square lattice (the units are meV): $\mu = -87.9$, $t_{10} = -138.7$, $t_{11} = 33.2$, $t_{20} = 3.3$, $t_{21} = -46.2$, and $t_{22} = 6.6$. The $J$ term in Eq. (1) gives rise to an attraction in the particle-particle $d$-wave singlet channel and in the particle-hole triplet channel, where it can induce a spin exciton. The $V$ term accounts for repulsion in the triplet-pairing channel and gives rise to the $\pi$ resonance. In the conventional $t$-$J$ model, $V = 0$. Following Refs. 13 and 24, we consider a more general interaction and treat $V$ and $J$ as independent parameters.

Although we are interested in spin susceptibility, in a superconducting ground state an operator of spin has the same quantum numbers as an operator creating a spin-triplet pair. We therefore analyze the linear response for the set of three operators\textsuperscript{14}

$$S_\pi = N^{-1/2} \sum_k a^\dagger_{k\uparrow} a_{k+Q\downarrow},$$

$$\pi = N^{-1/2} \sum_k g_k \hat{a}_{Q-k\downarrow} a_{k\uparrow},$$

$$\bar{\pi} = N^{-1/2} \sum_k g_k \hat{a}_{Q-k\downarrow} a^\dagger_{k\uparrow}.$$  

(2)

(3)

(4)

Here $a_{k,\sigma}$ is an electron annihilation operator and $g_k = \cos(k_y a) - \cos(k_x a)$. Operators $S_\pi$, $\pi$ and $\bar{\pi}$ destroy a bosonic excitation with the same momentum $Q = (\pi/a, \pi/a)$ and spin $S_z = -1$, but with different charges $0$ and $\pm 2$, respectively.

As a warmup exercise, consider first a hypothetical (Fermi liquid) nonsuperconducting ground state. The triplet channels $(2–4)$ are decoupled by virtue of a charge $U(1)$ symmetry. The Fourier transform of the bare pair susceptibility

$$\chi^0_\pi(t) = -i \theta(t) \langle[\pi(t), \pi^\dagger(0)]\rangle_{V=J=0}$$

(5)

is shown in Fig. 2(a). As anticipated, the two-hole continuum ($\omega < 0$) is strikingly narrow: its upper edge is at $|E_{\text{max}}| \approx 10$ meV. The $\omega^{-1/2}$ divergence near $E_{\text{max}}$ is a van Hove-type singularity associated with the $(\pi,0)$ points. Observe that, at $|\omega| > |E_{\text{max}}|$, $\chi^0_\pi(\omega)$ is purely real. On the other hand, the bare spin susceptibility $\chi^0_S(\omega)$ [shown in the inset of Fig. 2(a)] is complex for all frequencies.

Within the generalized RPA approximation, the full susceptibilities are given by

$$\chi_\pi(\omega) = \chi^0_\pi(\omega) \frac{1}{1 - V \chi^0_\pi(\omega)}, \quad \chi_S(\omega) = \frac{\chi^0_S(\omega)}{1 + 2J \chi^0_\pi(\omega)}.$$  

(6)

Note the opposite signs of the interaction terms: attractive in the particle-hole channel, repulsive in the particle-particle channels. Because $\chi^0_\pi(\omega) = 1/V$ has a solution for any $V > 0$ [Fig. 2(a)], the full $\pi$ susceptibility $\chi_\pi(\omega)$ acquires a pole above the upper edge of the continuum. This pole is the $\pi$ resonance. In contrast, no pole occurs in the RPA response for $S_\pi$. This is a consequence of the fact that the particle-hole continuum [and, hence, $\text{Im} \chi_S(\omega)$] extends to the lowest energies.

We now turn to the superconducting state. To facilitate the RPA treatment, we assume that the superconducting state is of the BCS type with a $d$-wave gap $\Delta(k) = \Delta \cos(k_x a) - \cos(k_y a)/2$. We treat $\Delta$ as another input parameter in the problem. In principle, the gap has to be computed self-consistently, but for our purposes this is not necessary as we are not concerned with response functions in the singlet channel at small momenta.

Since in a superconductor, charge is defined modulo 2, all three operators $(2–4)$ now carry identical quantum numbers and one can use any superposition of these. It is customary to choose

$$\chi^0_S(\omega) = \frac{1}{1 + 2J \chi^0_\pi(\omega)}.$$
FIG. 2. The bare response function \( \pi \) in a hypothetical Fermi liquid (a) and a \( d \)-wave superconductor with \( \Delta_{\text{max}} = 35 \text{ meV} \) (b) at \( Q \). Solid line: real part, dashed line: imaginary part. Inset: spin susceptibility in the normal state (note the difference in vertical scales). A broadening of \( \Gamma = 0.5 \text{ meV} \) was employed. Solution of the equation \( \chi_{s}^{0}(\omega) = 1/\nu \) gives the RPA energy of the \( \pi \) resonance \( \omega = -E_{s} \). The notations “2 electrons” and “2 holes” refer to continua of d-particle states with both particles, respectively, inside and outside the closed hole Fermi surface centered at \( (\pi, \pi) \) (see Fig. 1).

\[
A_{0} = S_{+}, \quad A_{1} = \frac{\pi - \bar{\pi}}{\sqrt{2}}, \quad A_{2} = \frac{\pi + \bar{\pi}}{\sqrt{2}}.
\]

(7)

The operators \( A_{1} \) and \( A_{2} \) describe fluctuations of the phase and the amplitude of the \( \pi \) mode, respectively. The bare susceptibilities \( \chi_{qq'}^{0}(\omega) \) are defined, similarly to Eq. (5), as the Fourier transforms of

\[
\chi_{qq'}^{0}(t) = -i \theta(t) \langle [A_{q'}(t), A_{q}(0)] \rangle |_{\nu = J = 0}.
\]

(8)

They can be written as components of a \( 3 \times 3 \) matrix \( \chi^{0} \). At \( T = 0 \), we have

\[
\chi_{qq'}^{0}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \left( \frac{\phi_{q} \phi_{q'}}{\omega - E_{\mathbf{k}} - E_{\mathbf{k'}}} - \frac{(1)^{q+q'} \phi_{q} \phi_{q'}}{\omega + E_{\mathbf{k}} + E_{\mathbf{k'}}} \right),
\]

(9)

where \( E_{\mathbf{k}}^{2} = \epsilon_{\mathbf{k}}^{2} + \Delta_{\mathbf{k}}^{2} \), \( \mathbf{k}' = \mathbf{Q} - \mathbf{k} \), and \( \phi_{q} \) are components of the vector.
gap opens up. We stress once again that the lower boundary of the two-hole continuum \(E_{\text{min}}\) is produced by fermions with momenta near hot spots, hence \(E_{\text{min}} \approx 2\Delta\). Certainly, an antibound state in the particle-particle triplet channel is located above \(2\Delta\). How much above \(2\Delta\) depends on the width of the two-electron continuum and the coupling strength.

The bare \(\pi-\pi\) response function in a superconducting state is presented in Fig. 2(b). It has two step-like discontinuities at \(E_{\text{min}}\) and \(E_{\text{max}}\) that are seen in both hole-hole (\(\omega < 0\)) and particle-particle (\(\omega > 0\)) spectra. The location of the \(\pi\) resonance in a superconductor is, however, not simply given by Eq. (6), but is a solution of the secular equation

\[
\det \begin{pmatrix}
X_{11}(\omega) & X_{12}(\omega) \\
X_{21}(\omega) & X_{22}(\omega)
\end{pmatrix} - \frac{1}{V} = 0.
\]

All four matrix elements \(X_{qq'}^{0}\) for \(q=1,2\) have the same thresholds as \(X_{\pi-\pi}^{0}\) in Fig 2(b). We solved this equation numerically and found that the \(\pi\) resonance indeed moves to an energy higher than \(2\Delta\). For \(V = 40\) meV, the resonance moves from 22 meV in the normal state [Fig. 2(a)] to 82 meV in the superconducting state with \(2\Delta = 70\) meV [Fig. 2(b)]. Reasoning similar to that above implies that the \(\pi\) resonance shows up in the spin channel.

\(J \neq 0, V \neq 0\)

The general case interpolates between the two limits. Fig. 3 presents our results for the spin susceptibility at various ratios of the coupling strengths \(V/J\). Interestingly enough, for comparable couplings, we found that the response functions contain two peaks at different energies. One, above \(E_{\text{max}}\), is the \(\pi\) resonance, the other, below \(E_{\text{min}}\), is the bound state in the particle-hole channel (Fig. 4 shows a particularly striking example). As \(V\) is increased, the high-energy resonance pulls away from the upper edge of the two-hole continuum and strengthens. At the same time, the low-energy resonance approaches the lower edge and enters into the two-electron continuum, where it broadens and finally becomes invisible. In the opposite limit, as \(V\) gets progressively smaller, the \(\pi\) resonance weakens, merges with the outer edge of the continuum, and disappears.

**DISCUSSION**

Direct comparison of neutron and ARPES data for \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8\) shows that the neutron resonance is located well below \(2\Delta\). We believe that the same holds true for \(\text{YBa}_2\text{Cu}_3\text{O}_7\). Because the lower continuum edge \(E_{\text{min}}\) is just below \(2\Delta\), the resonance almost certainly occurs below this edge. This point can be verified by analyzing ARPES data at the hot spots. In a slightly overdoped \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8\) sample with \(T_c = 87\) K, the gap value at the hot spots is \(32 \pm 3\) meV,\(^{27}\) and \(E_{\text{min}} \approx 58\) meV. The neutron resonance at \(Q = (\pi/\alpha, \pi/\alpha)\) in the overdoped \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8\) with similar \(T_c = 83\) K is observed at \(E = 38\) meV,\(^{28}\) i.e., well below \(E_{\text{min}}\). We thus conclude that the neutron resonance is an exciton-like bound state in the particle-hole channel, not an antibound state, such as the \(\pi\) resonance.

It has been previously remarked that particle-hole mixing may mask the origin of the neutron resonance,\(^{10,14,15}\) a spin resonance mixes into triplet-pair channels and vice versa. We rely on a continuity argument to make the unambiguous identification of the experimental neutron peak that is observed below the continuum edge \(E_{\text{min}} \approx 2\Delta\), as expected for \(V < J\). As the pair-triplet coupling \(V\) is turned off, the low-energy peak stays below the edge and continuously evolves into the usual RPA spin resonance at \(V = 0\). On the other hand, there is no collective mode below \(E_{\text{min}}\) in the limit \(V \gg J\), in which the \(\pi\) resonance can be defined unambiguously. Moving the high-energy \(\pi\) resonance across the continuum involves a discontinuous change. For this reason, the neutron resonance should not be associated with the \(\pi\) resonance.
We feel that a more realistic analysis will not change this general conclusion because our argument does not rely on detailed dynamics of the resonances, but is based on measured kinematics of low-energy fermion excitations and on general properties of bound states. If one wishes to find the \( \pi \) resonance in neutron scattering, the search should be confined to energies above the two-hole continuum. As its true upper edge is not known experimentally, we can only suggest that this energy exceeds \( 2\Delta \). On the other hand, because of the large incoherent parts of the spectral function observed in ARPES data for energies beyond \( \Delta \), there may be no true upper edge to the continuum,24 and it is quite possible that the \( \pi \) resonance will be strongly damped, or perhaps even absent, in neutron data.

To keep our discussion focused, we have left out some interesting avenues that deserve further exploration, notably the interplane coupling in bilayer materials. It is known that the neutron resonance is observed in the odd channel, at lattice momentum \((\pi, \pi, \pi)\), but not in the even one \((\pi, \pi, 0)\). Noting in passing that the resonance in the even channel may simply be closer to the continuum boundary and therefore have a much smaller amplitude, we refer the interested reader to the available literature on the subject.20,29

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16 The behavior of the threshold at other total momenta is discussed in M. R. Norman, cond-mat/0010298 (unpublished); A. V. Chubukov, B. Jankó, and O. Tchernyshyov, cond-mat/0012065 (unpublished).
20 M. R. Norman, Phys. Rev. B 61, 14751 (2000). Note dispersion ''two'' of Table I of that paper is used here, with the exception of Fig. 4, where we used dispersion ''one.''