Search for the π Resonance in Two-Particle Tunneling Experiments of YBCO Superconductors

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A recent theory of the resonant neutron scattering peaks in YBCO superconductors predicts the existence of a sharp spin-triplet two-particle collective mode (the "π resonance") in the normal state. In this paper, we propose an experiment in which the π resonance could be probed directly in a two-particle tunneling measurement. [S0031-9007(97)03952-5]

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Recent spin polarized inelastic neutron scattering experiments [1–3] of the YBCO superconductor revealed the existence of a sharp collective mode. This collective mode has spin one, carries momentum (π, π), and has well-defined energies of 41, 33, and 25 meV, respectively, for materials with $T_c = 92$, 67, and 52 K [1]. Most strikingly, this feature is only observed in the neutron scattering experiment below the superconducting transition temperature.

A number of theoretical explanations has been offered for this unique feature [4,5]. In particular, two of us [4] proposed that there exists a sharp spin-triplet particle-particle collective mode in a wide class of strongly correlated models, including the Hubbard and the t-J model. This collective mode, called the triplet π mode or simply the π resonance [6], is created by a two-particle operator

$$\pi^\dagger = \sum_k (\cos k_x - \cos k_y)\, c^\dagger_{k+Q,\uparrow} c^\dagger_{-k,\uparrow}, \qquad Q = (\pi, \pi) \,. \tag{1}$$

It carries spin one, momentum (π, π), and its energy scale is determined by J, the spin exchange energy. This collective mode exists both in the normal and the superconducting states. In the normal state, it does not couple to the neutron scattering probe because of its particle-particle nature. However, below the superconducting transition temperature T_c, this particle-particle collective mode can mix into the particle hole channel and couple to the neutron scattering amplitude. Since the mixing amplitude is proportional to the superconducting order parameter, this theory offers a unique explanation why the resonant neutron scattering peak disappears above the superconducting transition temperature. There is a fundamental difference between this theory and the possible alternative explanations based on the excitonic bound states inside the superconducting gap. In the former case, the existence of the collective mode is not dependent on the superconducting order, only the coupling to neutron is, while in the later case, the collective mode will disappear entirely from the physical spectrum when the superconducting gap disappears.

More recently, a unified theory of antiferromagnetism (AF) and d-wave superconductivity (SC) in the high T_c superconductors has been proposed [6]. This theory is based on a SO(5) symmetry generated by the total spin, total charge, and the π operators which rotate AF order parameters into the SC order parameters and vice versa. Within this theory, the resonant neutron scattering peak is interpreted as the pseudo-Goldstone boson associated with the spontaneous breaking of the SO(5) symmetry, reflecting the tendency of a SC state to fluctuate into the AF direction. The SO(5) symmetry is based on the assumption that the π operator is an approximate eigenoperator of the microscopic Hamiltonian. Although there are both analytical [4] and numerical [7] calculations in support of this assumption, it is certainly desirable to test it in direct experiments.

Therefore, in order to distinguish among the various theoretical explanations of the resonant neutron peak, and to test the SO(5) theory of high T_c superconductivity, it is crucial to search for the signature of the π resonance in the normal state of the YBCO superconductor. In the classic theoretical work of Scalapino [8] and the subsequent experimental confirmation by Goldman and coworkers [9], a superconductor with a higher T_c was used to probe the pairing fluctuation of a lower T_c material in the normal state. Inspired by their ideas, we propose a similar tunneling experiment to probe the π resonance in both the superconducting and the normal states. The proposed experimental geometry is depicted in Fig. 1. The proposed sample consists of a Josephson junction made out of a lower T_c superconductor (layer C), a thin (less than the coherence length) layer of a antiferromagnetic insulator (layer B), and a bulk higher T_c material (A), on the other side of the junction. The lower T_c and higher T_c pairs of superconductors can consist of a pair of

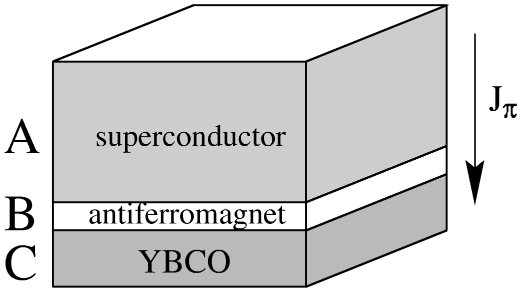

FIG. 1. Setting of the suggested experiment.

underdoped and optimally doped YBCO superconductors or a pair of optimally doped YBCO and Ta or Bi doped BCO superconductors. The antiferromagnetic insulator can be realized by the parent YBCO insulator or the Pr doped BCO insulator. All layers have their *ab* plane perpendicular to the tunneling direction. A voltage V is applied in the tunneling direction.

The basic idea is that when the temperature is in between the two superconducting transition temperatures, the BCS pairing condensate of the bulk superconductor A acts as a classical external field coupling to the two-particle quantum operators in the normal state of layer C. The antiferromagnetic layer is needed to transfer a center of mass momentum of (π, π) to the Cooper pair and flip its spin at the same time, so that it has exactly the same quantum number as the π resonance on the other side of the junction.

To start with, let us consider the effective tunneling matrix element between A and C, mediated through the antiferromagnetic insulator. We can model the antiferromagnetic insulating layer B by a positive U Hubbard model at half-filling, with a one-particle Green's function given by [10]

$$G_{\mathrm{AF}}(k, p; \alpha, \beta; \omega) = \frac{(\omega + \epsilon_k)\delta_{\alpha\beta}\delta_{kp} + \Delta_{\mathrm{SDW}}\delta_{\alpha,-\beta}\delta_{k,p+Q}}{\omega^2 - \Delta_{\mathrm{SDW}}^2 - \epsilon_k^2}, \quad (2)$$

where Δ_{SDW} is the spin-density-wave gap. We assume that the chemical potentials of both A and C layers are within Δ_{SDW}; the tunneling process is therefore nonresonant. From (2) we see explicitly that electrons can tunnel either via a direct channel preserving its spin and transverse momentum or via a spin flip channel changing its transverse momentum by Q. Consequently, we can model the tunneling from A to C by the following effective Hamiltonian:

$$H_T = \sum_{pk\sigma} T_{pk}^{d} a_{p\sigma}^{\dagger} c_{k\sigma} e^{iVt} + T_{pk}^{f} a_{p+Q\sigma}^{\dagger} c_{k-\sigma} e^{iVt} + \mathrm{H.c.}, \quad (3)$$

where V is the applied voltage, and the $a_{p\alpha}$ and $c_{k\alpha}$ operators refer to the electronic operators in A and C with momenta p and k. The ratio of the spin flip matrix element T_{pk}^{f} to the direct matrix element T_{pk}^{d} is on the order of Δ_{SDW}/U. In the summation above p is the usual three dimensional momentum of electrons in bulk superconductor A. We model layer C as a two dimensional film with a 2D momentum vector k.

We consider a particular case of a perfectly specular scattering which conserves the momentum parallel to the interface

$$T_{kp}^{d,f} = T^{d,f}\delta_{k,p_{\parallel}}. \quad (4)$$

The δ symbol above is a Kroneker delta of the discrete momenta, and $T^{d,f}$ are assumed to be constant. In what follows we use common approximations in the theory of specular tunneling [11]

$$\sum_{k} \to \mathcal{A} N_C(0) \int d\epsilon_k, \quad (5)$$

$$\sum_{p\perp} \to \rho_A(0) d_A \int d\epsilon_p, \quad (6)$$

where $\mathcal{A}$ is the area of the junction, d_A is a width of layer A, $N_C(0)$ is a two dimensional density of states in layer C, and $\rho_A(0)$ is a one dimensional density of electrons in layer A. Equations (3)–(6) serve as the starting point for our discussion of the tunneling measurement of the π resonance.

Being a collective mode, the π resonance is represented by a pole in the four-leg vertex. Its first contribution comes in the third order of perturbation theory (from now on we will use a finite-temperature Matsubara technique),

$$J^{(3)}(\tau_0) = -\frac{1}{6}\int_0^{1/T} d\tau_1\, d\tau_2\, d\tau_3 \times \langle T_\tau\{H_T(\tau_1)H_T(\tau_2)H_T(\tau_3)J(\tau_0)\}\rangle, \quad (7)$$

with

$$J(\tau) = -e\sum_{kp,\alpha\beta}[T_{kp}^{\alpha\beta} a_{k\alpha}^{\dagger}(\tau) c_{p\beta}(\tau) e^{i\Omega\tau} - T_{pk}^{\beta\alpha *} c_{p\beta}^{\dagger}(\tau) a_{k\alpha}(\tau) e^{-i\Omega\tau}]_{i\Omega\to eV}. \quad (8)$$

Expression (7) has many terms, each containing four a and four c operators. The resonant contribution describes the coupling of the BCS condensate in A to the π resonance in C, and is given by the terms which have anomalous two-particle Green's function K_L on the superconducting side, and the two-particle Green's function K_R on the normal-metal side that takes into account the multiple scattering of the particles of each other. The anomalous K_L has total momentum zero and total spin zero and the singular part of K_R, as shown in [4], corresponds to the two particles having the center of mass momentum Q and spin one. This mismatch is compensated by the matrix elements T^f which flip the spin and add momentum Q to the pair. Disposing all momentum, spin, and energy conservation properties of the bulk Green's function we come to the π resonance contribution to the tunneling current,

$$J_\pi = -\frac{4e}{N}\,\mathrm{Im}\Bigg[\Bigg(\sum_{kpk''p''} T_{kp}^{d} T_{k''p''}^{d*} T_{-p-k}^{f} T_{-p''-k''}^{f*} \Gamma_{\uparrow}(k, k''; 2i\Omega, Q) T \sum_{\omega_1} F_p(i\omega_1) G_k(-i\omega_1 - i\Omega) G_{Q-k}(i\omega_1 - i\Omega) T \times \sum_{\omega_2} F_{p''}(i\omega_2) G_{k''}(-i\omega_2 - \Omega) G_{Q-k''}(i\omega_2 - \Omega)\Bigg)_{i\Omega\to eV}\Bigg], \quad (9)$$

where $\Gamma_{\uparrow}(k, k', E, Q)$ is the vertex for all spins up with total energy E and momentum Q. $N = \mathcal{A}/a^2$ with a being a unit cell size of YBCO. A similar expression has been studied in [11] in connection with the problem of the fluctuational contribution to the tunneling currents in conventional superconductors. Diagrammatically expression (9) is shown on Fig. 2.

We assume that the normal metal is described by the t-J Hamiltonian and the triplet vertex $\Gamma_{\uparrow}$ may be found from the Dyson's equation

$$\Gamma_{\uparrow}(k; k''; 2i\Omega, Q) = J \sum_{\alpha} g_{\alpha}(k) g_{\alpha}(k'') - JT \sum_{k'\nu\alpha} g_{\alpha}(k) g_{\alpha}(k') G_{k'}(i\nu) G_{Q-k'}(2i\Omega - i\nu) \Gamma_{\uparrow}(k', k''; 2i\Omega, Q), \qquad (10)$$

where α is an index that may be $+$ or $-$ and $g_{\pm}(k) = \cos k_x \pm \cos k_y$.

The t-J Hamiltonian possesses two remarkable properties. Namely, the two-particle continuum collapses to a point when their center of mass momentum is Q, and second there is repulsive interaction between the two particles in a triplet state sitting on the neighboring sites. This leads to the existence of an antibonding state of two electrons with center of mass momentum Q and energy $\omega_0 = J(1 - n)/2 - 2\mu$—the π resonance [4]. Identifying this energy with the observed resonant neutron scattering peaks give $\omega_0 = 41$ or 33 meV depending on the T_c of layer C. This antibonding state appears up as a sharp pole in $\Gamma_{\uparrow}(k, k', 2i\Omega, Q)$ when $2i\Omega = \omega_0$. So, we can write a solution to (10) as

$$\Gamma_{\uparrow}(k; k''; 2i\Omega, Q) = J g_{-}(k) g_{-}(k'') \frac{2i\Omega + 2\mu}{2i\Omega - \omega_0} + \Gamma_{\uparrow}^{reg}. \qquad (11)$$

Putting together Eqs. (9) and (10) and noticing that the anisotropic gap of the superconductor may be written as $\Delta_p = \Delta g_{-}(p_{||})$ we get

$$J_{\pi}(V) = 2eJ\Delta^2 \,\mathrm{Im}\left[\left(\frac{2i\Omega + 2\mu}{2i\Omega - \omega_0} \frac{1}{N} \sum_{kpk''p''} T^{d}_{kp} T^{d*}_{k''p''} T^{f}_{-p-k} T^{f*}_{-p''-k''} g_{-}(k'') g_{-}(p''_{||}) g_{-}(k) g_{-}(p_{||}) R(i\Omega, E_p, \epsilon_k) \right.\right.$$
$$\left.\left. \times R(i\Omega, E_{p''}, \epsilon_{k''}) \right)_{i\Omega \to eV} \right], \qquad (12)$$

where

$$R(i\Omega, E_p, \epsilon_k) = \frac{\tanh(E_p/T)}{E_p(E_p - \epsilon_k - i\Omega)(E_p - 2\mu - \epsilon_k + i\Omega)} + \frac{\tanh(\epsilon_k/T)}{(E_p - \epsilon_k - i\Omega)(E_p - 2\mu - \epsilon_k + i\Omega)(2\mu - 2i\Omega)},$$
$$E_p = \sqrt{\epsilon_p^2 + \Delta_p^2}. \qquad (13)$$

In the expression above the angular dependence comes from g_{-} functions as well as from the anisotropy of Δ_p in the expressions for E_p. It is easy to convince oneself that the later does not have any significant effect on the result. So, we can neglect the anisotropy of Δ_p^2 and replace it by the average value Δ^2. Then integrating over directions of k and k'' may be done explicitly giving the average values of $\langle g_{-}^2(k) \rangle \approx 1$. Finally we arrive at the following expression for J_{π}

$$J_{\pi} = \frac{2eJ\Delta^2}{N} [T^d T^f A d_A \rho_A(0) N_C(0)]^2 \,\mathrm{Im}\left[\frac{2eV + 2\mu}{2eV - \omega_0 + i0} \left(\int d\epsilon_p \, d\epsilon_k \, R(eV + i0, E_p, \epsilon_k) \right)^2 \right]. \qquad (14)$$

In Fig. 3 we present the characteristic V dependence of j_{π}. One can see that it does have a resonant feature when $eV_0 = \omega_0/2$ which, if found, will be a clear indication of the existence of the π excitation in YBCO materials.

We can do a simple estimate of the integrated spectral weight of the π resonance. The usual expression for the normal-to-normal tunneling current is given by

$$J_N = e \sum_{pk} |T^{d}_{pk}|^2 \delta(eV + \epsilon_k - \epsilon_p) [n_F(\epsilon_k) - n_F(\epsilon_p)]$$
$$= d_A \mathcal{A} |T^d|^2 \rho_C(0) N_A(0) e^2 V. \qquad (15)$$

Then, assuming that the characteristic scale of ϵ_p's and ϵ_k's in Eq. (14) is set by J we can obtain after a few straightforward manipulations

$$\int J_{\pi} \, dV \cong \left| \frac{T^f}{T^d} \right|^2 \frac{\hbar a^2 \mathcal{A} \Delta^2}{e^4} \left(\frac{1}{R_N \mathcal{A}} \right)^2. \qquad (16)$$

To get an idea of the magnitude of this effect we take the numbers characteristic to the experiments of Goldman *et al.* on the fluctuational contribution to the S-N current in low temperature superconductors [9]. $\mathcal{A} \approx 10^{-4}$ cm^2, $R_N \approx 10^{-1}$ Ω, and characteristic to YBCO gap $\Delta = 20$ meV and $a = 4.8 \times 10^{-8}$ cm. For $T^f/T^d \approx 1$ this gives us

$$\int J_{\pi} \, dV \approx 10 \ \mu\mathrm{A} \, \mu\mathrm{V},$$

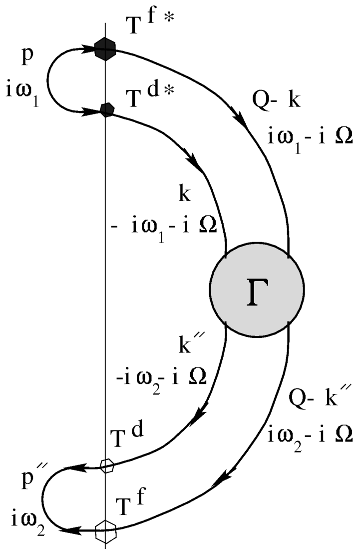

FIG. 2. Second order tunneling diagram.

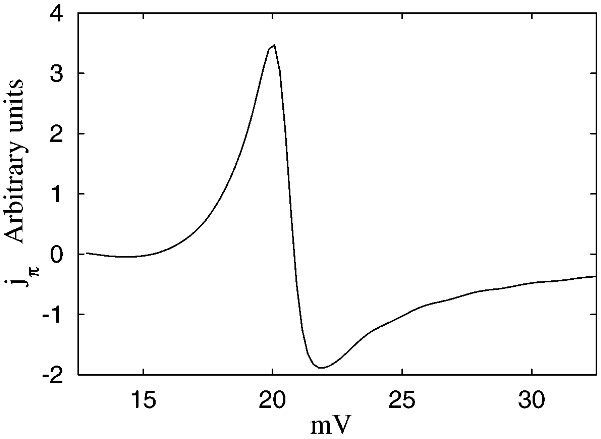

FIG. 3. j_π as a function of V for $\omega_0 = 41$ meV.

which is the effect of the same order of magnitude as measured by Goldman and co-workers [9].

It was noted to us by B. Janko that the use of a tunneling Hamiltonian for the two-particle tunneling is not completely justified. This difficulty does not alter the physical picture of the tunneling into the π-mode manifesting itself as a sharp peak at $V = \hbar\Omega_0/2e$, but may change the magnitude of the peak in question. We rely on the observation of the two-particle contribution in the experiments reported in [9] to suggest that in the present case observation of the peak can also be within the possibilities of an experiment.

In conclusion, we have proposed a concrete two-particle tunneling experiment to probe the π resonance of the high T_c superconductors. Identification of this mode could uniquely distinguish among the various theoretical explanations of the resonant neutron scattering peaks, lend direct experimental support of the SO(5) theory, and deepen our understanding of the symmetry relationship between antiferromagnetic and superconducting phases in the high T_c superconductors.

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