Resonant neutron peak and the symmetry of the superconducting order parameter in $YBa_2Cu_3O_7$

Tao Li and Zi-Zhao Gan
Department of Physics, Peking University, Beijing 100871, People's Republic of China
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It is shown that the $s^{\pm}$-wave pairing state proposed to interpret the resonant neutron peak observed in $YBa_2Cu_3O_7$ corresponds to an interlayer pairing state and it has a drastically different magnetic behavior (in the odd channel) in the long wavelength limit as compared to the $d_{x^2-y^2}$-wave state. It is found that the $d_{x^2-y^2}$-wave state provides a more natural interpretation for the resonant peak, especially its sharpness in the momentum space which is a direct consequence of the d-wave symmetry of the order parameter. An experiment is proposed to decide which kind of pairing state is actually realized in $YBa_2Cu_3O_7$.
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It is widely believed that the essential physics of high-temperature superconductors is contained in the single CuO_2 planes and the strong two-dimensional antiferromagnetic spin fluctuation in it plays a crucial role in both the anomalous normal state behavior and the occurrence of high T_c. In recent years, various kinds of experiments indicate that high-T_c superconductors may have a $d_{x^2-y^2}$-wave symmetry order parameter. This result is fully consistent with the picture based on the antiferromagnon exchange, although it may still be too early to conclude that this is really the correct origin of high T_c.

Neutron scattering is a very powerful tool in the study of high-T_c superconductors. It can provide the most detailed information on the magnetic response of the system through the measurement of the full momentum and frequency dependence of the dynamic spin susceptibility and thus contains important information on both the normal state spin fluctuation (which might be the origin of superconducting pairing) and the symmetry of the order parameter in the superconducting state. In recent neutron scattering experiments on superconducting $YBa_2Cu_3O_7$, a sharp feature located at 41 meV and centered at $Q=(\pi,\pi)$ in momentum space is observed.[1–4] The peak is peculiar in that it appears only in the superconducting state and is sharply peaked in both the momentum and the energy space (hence it is sometimes called a resonant neutron peak). Furthermore, it displays sinusoidal modulation along the c axis with a period of π/c (c is the interlayer spacing in the Cu_2O_4 bilayer).

Much theoretical effort has been devoted to the interpretation of this remarkable observation. Most of these theories assume the peak occurs due to spin-flip electron excitations across the superconducting gap,[5–13] although an interpretation based on a collective mode in the particle-particle channel[14] (rather than the particle-hole channel mentioned above) is also possible. Since magnetic scattering is odd with respect to time reversal, the BCS coherence factor in the magnetic response function vanishes on the Fermi surface unless the order parameter has opposite sign for momentum $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ ($\mathbf{q}$ is the momentum transfer of the scattered neutron), i.e.,

$$\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}}<0. \tag{1}$$

Obviously, this requirement is satisfied in the $d_{x^2-y^2}$-wave state for $\mathbf{q}=\mathbf{Q}$, while in a s-wave state it can never be satisfied. It is thus suggested that the resonant neutron peak at $\mathbf{Q}=(\pi,\pi)$ is a manifestation of $d_{x^2-y^2}$-wave pairing in $YBa_2Cu_3O_7$.

However, what really exists in $YBa_2Cu_3O_7$ is a Cu_2O_4 bilayer rather than a single CuO_2 plane. Due to the interlayer coupling in the bilayer, the electronic band will split into the bonding and antibonding bands. As will be shown below, the magnetic response observed in neutron experiments is mainly due to the interband transitions. Hence it is important to know the relative sign of the superconducting order parameter in these two bands. In the theories based on $d_{x^2-y^2}$ pairing within single CuO_2 planes, it is implicitly assumed that the order parameter in these two bands have the same sign. However, these single plane based theories have difficulties in explaining the c-axis modulation observed in experiments. In view of this, Mazin and Yakovenko proposed an alternative pairing symmetry. They argued that the superconducting order parameter in $YBa_2Cu_3O_7$ should have s-wave symmetry and an opposite sign in the bonding and antibonding bands and called it an $s^{\pm}$ state.[5,13,15–17]

Here we show that the $s^{\pm}$ state they proposed actually corresponds to a interlayer pairing state and its magnetic response in the long wavelength limit is drastically different from that of the $d_{x^2-y^2}$ state. We find it is more natural to interpret the resonant neutron peak within the $d_{x^2-y^2}$-wave picture and the sharpness of the resonant neutron peak in momentum space is a direct consequence of the $d_{x^2-y^2}$-wave symmetry of the order parameter. We find the c-axis modulation is consistent with the $d_{x^2-y^2}$-wave picture, although a quantitative comparison with experiment may be difficult. Finally, we propose a simple experiment to decide which kind of pairing state is realized in $YBa_2Cu_3O_7$.

The neutron scattering cross section is proportional to the imaginary part of the spin susceptibility $\chi(\mathbf{q},q_z,\omega)$. For the bilayer case, the total magnetic response is given by

$$\chi(\mathbf{q},q_z,\omega)=\sum_{m,n}\exp[iq_z(z_m-z_n)]\chi^{(m,n)}(\mathbf{q},\omega), \tag{2}$$

where m and n are layer indexes and

$$\chi^{(m,n)}(\mathbf{q},\tau)=\langle T_\tau M_m^z(\mathbf{q},\tau)M_n^z(-\mathbf{q},0)\rangle.$$

$M_m^z(\mathbf{q},\tau)$ is the magnetization in the z direction in the mth layer. If we introduce the in-phase and the out of phase magnetization

$$M_+^z(\mathbf{q},\tau)=M_m^z(\mathbf{q},\tau)+M_n^z(\mathbf{q},\tau),$$

$$M_-^z(\mathbf{q},\tau)=M_m^z(\mathbf{q},\tau)-M_n^z(\mathbf{q},\tau),$$

then $\chi(\mathbf{q},q_z,\omega)$ simplifies to[17]

$$\chi(\mathbf{q},q_z,\omega)=\chi^+(\mathbf{q},\omega)\cos^2(q_zc/2)+\chi^-(\mathbf{q},\omega)\sin^2(q_zc/2). \tag{3}$$

Here χ^+ and χ^- are the susceptibility in the even and the odd channel,

$$\chi^+(\mathbf{q},\tau)=\langle T_\tau M_+^z(\mathbf{q},\tau)M_+^z(-\mathbf{q},0)\rangle,$$

$$\chi^-(\mathbf{q},\tau)=\langle T_\tau M_-^z(\mathbf{q},\tau)M_-^z(-\mathbf{q},0)\rangle. \tag{4}$$

When expressed in the bonding and the antibonding band representations, χ^+ and χ^- reads

$$\chi^+(\mathbf{q},\omega)=\chi^{(bb)}(\mathbf{q},\omega)+\chi^{(aa)}(\mathbf{q},\omega),$$

$$\chi^-(\mathbf{q},\omega)=\chi^{(ba)}(\mathbf{q},\omega)+\chi^{(ab)}(\mathbf{q},\omega). \tag{5}$$

Here b and a refer to the bonding and the antibonding band. We see χ^+ and χ^- correspond to intraband and interband transitions, respectively.

In BCS theory, the susceptibility is (for simplicity, we only consider the zero temperature case)[18]

$$\chi_0^{(ij)}(\mathbf{q},\omega)=\frac{1}{2}\sum_{\mathbf{k}}\left(1-\frac{\xi_{\mathbf{k+q}}\xi_{\mathbf{k}}+\Delta_{\mathbf{k+q}}^{(i)}\Delta_{\mathbf{k}}^{(j)}}{E_{\mathbf{k+q}}E_{\mathbf{k}}}\right)\times\left(\frac{1}{\omega+E_{\mathbf{k+q}}+E_{\mathbf{k}}+i\delta}-\frac{1}{\omega-E_{\mathbf{k+q}}-E_{\mathbf{k}}+i\delta}\right), \tag{6}$$

where $E_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$, i and j are the band index. From this expression we see the coherence factor vanishes for $\xi\ll\Delta$ unless $\Delta_{\mathbf{k}}^i$ and $\Delta_{\mathbf{k+q}}^j$ has opposite sign. This is a direct consequence of superconducting pairing and the singlet nature of the BCS ground state. For a conventional s-wave superconductor, when the wavelength of the external field is much longer than the coherence length of the superconducting pairs, the magnetic response of the system will be greatly suppressed by the coherence factor. However, here we have two almost degenerate bands and the situation is more subtle.

Since only the second term in Eq. (3) is observed experimentally, it is argued in Ref. 13 that χ^+, the susceptibility in the even channel which involves only the intraband transition, should be suppressed upon entering the superconducting state, while the odd channel susceptibility, which involve interband transition χ^- should not be affected. Following the coherence factor argument, they conclude that the order parameter in the bonding and the antibonding band $\Delta^{(b)}$ and $\Delta^{(a)}$ have s-wave symmetry but opposite sign. Thus the system has a $s^{\pm}$-wave order parameter.

To make the physical picture more clear, let us re-express the bonding and the anti-bonding band operator $c_{\mathbf{k}}^b$ and $c_{\mathbf{k}}^a$ in the layer representation, i.e.,

$$c_{\mathbf{k}}^b=\frac{1}{\sqrt{2}}(c_{\mathbf{k}}^{(1)}+c_{\mathbf{k}}^{(2)}),$$

$$c_{\mathbf{k}}^a=\frac{1}{\sqrt{2}}(c_{\mathbf{k}}^{(1)}-c_{\mathbf{k}}^{(2)}). \tag{7}$$

Here $c_{\mathbf{k}}^{(1)}$ and $c_{\mathbf{k}}^{(2)}$ represent the annihilation operator in the upper and lower layer in the Cu_2O_4 bilayer. With the help of Eq. (7), we can express the pairing amplitude of the bonding and the antibonding band in terms of the intralayer and interlayer pairing amplitude

$$\langle c_{\mathbf{k}}^b c_{-\mathbf{k}}^b\rangle=\frac{1}{2}(\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(1)}\rangle+\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(2)}\rangle+\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(2)}\rangle+\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(1)}\rangle),$$

$$\langle c_{\mathbf{k}}^a c_{-\mathbf{k}}^a\rangle=\frac{1}{2}(\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(1)}\rangle+\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(2)}\rangle-\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(2)}\rangle-\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(1)}\rangle). \tag{8}$$

Making use of the fact that $\langle c_{\mathbf{k}}^a c_{-\mathbf{k}}^b\rangle=\langle c_{\mathbf{k}}^b c_{-\mathbf{k}}^a\rangle=0$, we have

$$\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(1)}\rangle=\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(2)}\rangle. \tag{9}$$

Hence, if $\Delta_{\mathbf{k}}^a=-\Delta_{\mathbf{k}}^b$ (as assumed in Ref. 13), then we get

$$\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(1)}\rangle=\langle c_{\mathbf{k}}^{(2)}c_{-\mathbf{k}}^{(2)}\rangle=0 \tag{10}$$

and

$$\Delta_{\mathbf{k}}^{(i,j)}\propto\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(2)}\rangle,$$

that is, the system is dominated by interlayer pairing and there is no pairing amplitude within the layers. Thus the pairing force must come from interlayer process and has no relation with the antiferromagnetic spin fluctuation within each CuO_2 planes. On the other hand, if we assume $\Delta_{\mathbf{k}}^a=\Delta_{\mathbf{k}}^b$ (as implicitly assumed in the $d_{x^2-y^2}$-wave picture), then

$$\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(2)}\rangle=0 \tag{11}$$

and

$$\Delta_{\mathbf{k}}^{(i,j)}\propto\langle c_{\mathbf{k}}^{(1)}c_{-\mathbf{k}}^{(1)}\rangle,$$

thus the system is dominated by intralayer pairing and there is no pairing amplitude between the layers. Thus we must conclude that the pairing force comes from an intralayer process. The most possible source of this force is the exchange of antiferromagnetic spin fluctuation. If this is the case, then it is natural to understand why $d_{x^2-y^2}$-wave pairing dominates. From this discussion, we see the physical picture for $d_{x^2-y^2}$-wave and $s^{\pm}$-wave pairing states is quite different.

A direct consequence of this difference is the drastically different magnetic response of the system (in the odd channel) in the long wavelength limit. For a conventional *s*-wave superconductor, when the wavelength of the external field is much larger than the coherence length of the superconducting pairs, the magnetic response of the system will be greatly suppressed as compared to the normal state due to the singlet nature of the superconducting pairs [more directly, due to the coherence factor in Eq. (6)]. For the $d_{x^2-y^2}$-wave state discussed above, the pairing occurs totally within each planes. Hence when the in-plane wavelength of the external field approaches infinity, their magnetic response will be suppressed correspondingly, no matter how small the out of plane wavelength is. While in the $s^{\pm}$-wave state proposed in Ref. 13, the pairing occurs predominately between the two layers of the Cu_2O_4 bilayer. The intralayer pairing amplitude is rather small, thus the magnetic response will not be suppressed when the in-plane wavelength approaches infinity, as long as the out of plane wavelength remains finite. This is indeed the case. As shown in Ref. 13, when $\mathbf{q}\rightarrow 0$, $\chi_0''(\mathbf{q},\omega)$ increase to a much higher value than that at $\mathbf{q}=\mathbf{Q}$ in the $s^{\pm}$-wave state and there is only a rather weak peak around $\mathbf{q}=\mathbf{Q}$. In fact, to account for the sharpness of the resonance peak in the momentum space, these authors have introduced a strongly momentum dependent antiferromagnetic interaction $J(\mathbf{q})=J(\cos q_x+\cos q_y)$ which peaks at $\mathbf{q}=\mathbf{Q}$ and conclude that the position of the neutron peak in $\mathbf{q}$ space is set by $J(\mathbf{q})$ and has no relation with the symmetry of the order parameter. We note that even with such a momentum dependent $J(\mathbf{q})$, the peak around $\mathbf{q}=\mathbf{Q}$ is still rather broad. More importantly, the long wavelength magnetic response in the odd channel is still quite large. On the other hand, in the $d_{x^2-y^2}$-wave state which has dominate pairing within each individual CuO_2 planes, the long wavelength response is prohibited in both the even and the odd channel, hence the peak at $\mathbf{q}=\mathbf{Q}$ is intrinsically more sharp than that in the $s^{\pm}$-wave state. We think the sharpness of the neutron peak in momentum space comes mainly from the symmetry of the order parameter, rather than the antiferromagnetic coupling.

We now turn to the *c*-axis modulation. From Eq. (3), we see the sinusoidal modulation will persist (but with a reduced amplitude $\chi^- - \chi^+$) as long as $\chi^- > \chi^+$. The nonzero response in the even channel only produce a constant background. As is clear from Eq. (4), if there exists antiferromagnetic interlayer coupling, the magnetic response in the odd channel will be larger than that in the even channel below some characteristic energy. Obviously, this characteristic energy should be of the same order as the energy of the optical spin wave. Hence we conclude that the frequency of optical spin wave must be larger than the energy of the resonant neutron peak. Indeed, experiments have failed to observe the optical spin wave below 60 meV, although its absence may have a more profound origin.

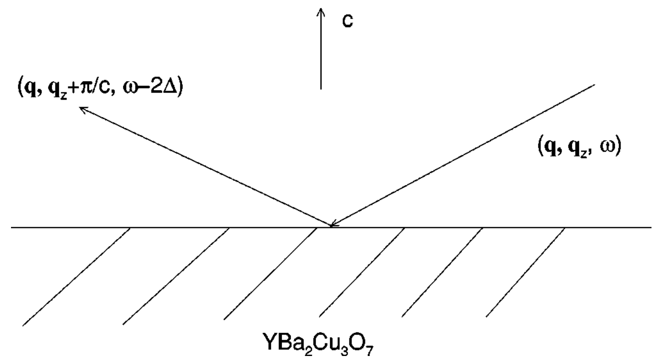

FIG. 1. Schematic drawing of the experimental setting.

Since the $d_{x^2-y^2}$-wave and $s^{\pm}$-wave states have drastically different magnetic responses in the long wavelength limit, we can devise a simple experiment to decide which one is actually realized in $YBa_2Cu_3O_7$ by detecting the scattered neutron with a momentum transfer $\mathbf{q}=(0,0,\pi)$ and energy transfer $\omega=2\Delta_{\max}$. The experimental setting is shown in Fig. 1. Making use of the energy and the momentum conservation, we see at once the *z* component of the incident momentum of the scattered neutron should be kept at

$$q_z=\frac{1}{2}\frac{\pi}{c}+\frac{2m}{\hbar^2}\frac{\Delta_{\max}}{\pi/c}, \tag{12}$$

where *m* is the neutron mass.

In conclusion, we show the $s^{\pm}$-wave state proposed to interpret the resonant neutron peak corresponds to an interlayer pairing state and it has drastically different magnetic response in the long wavelength limit as compared to the $d_{x^2-y^2}$-wave state which has dominate pairing within each individual CuO_2 planes. We find it is more natural to interpret the neutron peak within the $d_{x^2-y^2}$-wave picture, especially its sharpness in the momentum space which we think is a direct consequence of the $d_{x^2-y^2}$-wave symmetry of the order parameter. We also proposed an experiment to decide which kind of pairing is actually realized in $YBa_2Cu_3O_7$.

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