Theory of sinusoidal modulation of the resonant neutron scattering in high-temperature superconductors

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A model with interlayer pairing is proposed to explain the sinusoidal modulation of the resonant neutron scattering in high-temperature superconductors. It is found that the interlayer pairing has *s*-wave symmetry in the CuO_2 plane and has comparable magnitude with the *d*-wave intralayer pairing. It is also found that the interlayer pairing mainly affects momentum close to the hot spots on the Fermi surface while its effect on the gap nodes is negligible. It is pointed out that these characteristics of the interlayer pairing can be understood in a model in which the superconducting pairing originates from the exchange of the antiferromagnetic spin fluctuation.

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The discovery of the resonant neutron scattering is one of the most important in the high-T_c field in recent years.[1–5] This resonance, also called (π,π) resonance, has many interesting characteristics and has attracted much theoretical attention.[6–18] The *c*-axis modulation is an interesting and intriguing problem that occurs when explaining the (π,π) resonance. In experiments, only the odd-channel magnetic response $(q_c=\pi)$ has been observed in the CuO_2 bilayer systems (the sinusoidal modulation), while in most single CuO_2 plane-based random-phase-approximation (RPA) theories, the interlayer exchange is far too small to distinguish the even from the odd channel.[11–13,16,18]

Physically, the momentum dependence of the magnetic response is closely related to the internal structure of the superconducting Cooper pair. For pointlike *s*-wave pairing, the magnetic response is generally momentum independent and is suppressed due to the singlet nature of the pair. While for *d*-wave pairing that takes place between nearest-neighbor sites on a plane, the magnetic response is strongly momentum dependent. In fact, here we can take the Cooper pair roughly as the coherent superposition of two antiferromagnetic spin configurations. Thus, if we look at the pair with a momentum transfer of the order (π,π), we will find an enhanced magnetic response. Similarly, if there exists interlayer pairing between the two CuO_2 planes in the CuO_2 bilayer, the odd-channel magnetic response $(q_c=\pi)$ will be enhanced while the even-channel response $(q_c=0)$ will be suppressed. Although such pairing is obviously favored by the interlayer exchange coupling, it is totally neglected in the single CuO_2 plane-based theories.

In this paper, we find that the sinusoidal modulation of the (π,π) resonance can be naturally explained with the inclusion of the interlayer pairing. We find that the interlayer pairing has *s*-wave symmetry in the CuO_2 plane and has comparable magnitude with the intralayer *d*-wave pairing. We find that the interlayer pairing mainly affects momentum close to the hot spots on the Fermi surface and has a negligible effect on the gap nodes.

To model the CuO_2 bilayer with interlayer pairing, we take the following mean-field Hamiltonian:[19]

$$H_{MF}=\sum_{k,n,\sigma}\xi_k c_{k\sigma}^{(n)\dagger}c_{k\sigma}^{(n)}+\sum_{k,n}\left(\Delta_k c_{k\uparrow}^{(n)\dagger}c_{-k\downarrow}^{(n)\dagger}+\text{H.c.}\right)+\sum_k\left[\Delta_k'\left(c_{k\uparrow}^{(1)\dagger}c_{-k\downarrow}^{(2)\dagger}+c_{k\uparrow}^{(2)\dagger}c_{-k\downarrow}^{(1)\dagger}\right)+\text{H.c.}\right], \tag{1}$$

in which $n=1,2$ is the layer index and ξ_k is the dispersion in the CuO_2 plane. Here we use the dispersion derived from fitting the angle-resolved photoemission spectroscopy result in $Bi_2Sr_2CaCu_2O_8$,[18,20,21] $\xi_k=-t(\cos k_x+\cos k_y)-t'\cos k_x\cos k_y-t''(\cos 2k_x+\cos 2k_y)-t'''(\cos 2k_x\cos k_y+\cos k_x\cos 2k_y)-t''''\cos 2k_x\cos 2k_y-\mu$, $t=0.2975$ eV, $t'=-0.1636$ eV, $t''=0.02595$ eV, $t'''=0.05585$ eV, $t''''=-0.0510$ eV, and μ is the chemical potential. Note that we have neglected the interlayer hopping term in the dispersion since no band splitting is observed in experiment. $\Delta_k=\Delta_0/2(\cos k_x-\cos k_y)$ is the intralayer *d*-wave pairing function and Δ_k' is the interlayer pairing function. As will be shown later, Δ_k' has strong momentum dependence in the CuO_2 plane. However, such momentum dependence is not essential for the discussion of the (π,π) resonance since the low-energy magnetic response at $q=(\pi,\pi)$ is determined mainly by the electronic transition between the hot spots on the Fermi surface (see Fig. 1). For the sake of simplicity, we will take Δ_k' as being momentum independent for the moment. The relative phase between Δ_k' and Δ_k is another important issue. In the absence of the interlayer hopping, Δ_k' can be either real or purely imaginary to meet the requirement of the time-reversal symmetry. However, a real Δ_k' will lead to different energy gap at momentums (k_x,k_y) and (k_y,k_x), since Δ_k' and Δ_k have different momentum dependence in the CuO_2 plane. Therefore Δ_k' must be purely imaginary.

To discuss the *c*-axis modulation of the CuO_2 bilayer system, it is convenient to use the bonding band and the antibonding band representation[6,11,16]

$$c_k^{(b)}=\frac{1}{\sqrt{2}}\left(c_k^{(1)}+c_k^{(2)}\right),$$

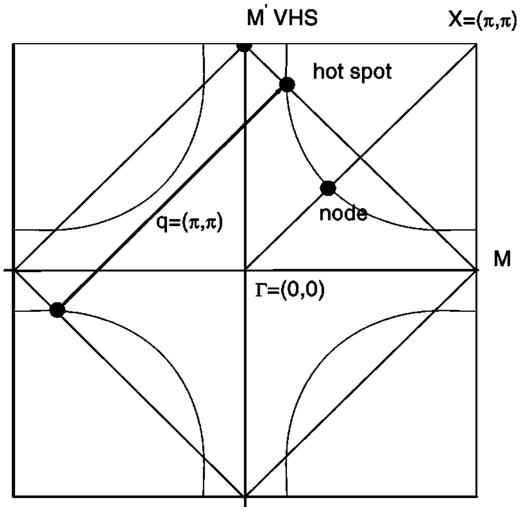

FIG. 1. The Fermi surface and the important momentum in our discussion. VHS denotes the Van Hove singularity.

$$c_k^{(a)}=\frac{1}{\sqrt{2}}(c_k^{(1)}-c_k^{(2)}). \tag{2}$$

Here b and a represent the bonding and the antibonding band, respectively. In this representation, the mean-field Hamiltonian reads

$$H_{MF}=\sum_{k,\alpha,\sigma}\xi_k c_{k\sigma}^{(\alpha)\dagger}c_{k\sigma}^{(\alpha)}+\sum_{k,\alpha}(\Delta_k^{(\alpha)}c_{k\uparrow}^{(\alpha)\dagger}c_{-k\downarrow}^{(\alpha)\dagger}+\text{H.c.}), \tag{3}$$

$\alpha=a,b$ is the band index and $\Delta_k^{(\alpha)}=\Delta_k+f(\alpha)\Delta_k'$, where

$$f(\alpha)=\begin{cases}+1, & \text{for } \alpha=\text{b},\\ -1, & \text{for } \alpha=\text{a}.\end{cases}$$

In the bonding and the antibonding band representation, the even- and the odd-channel magnetic response come from the intraband and the interband electronic transition, respectively,[6,11,16]

$$\begin{aligned}\chi_0^{(even)}(q,\omega)&=\chi_0^{(aa)}(q,\omega)+\chi_0^{(bb)}(q,\omega),\\ \chi_0^{(odd)}(q,\omega)&=\chi_0^{(ab)}(q,\omega)+\chi_0^{(ba)}(q,\omega),\end{aligned} \tag{4}$$

in which the mean field susceptibility $\chi_0^{(aa)}(q,\omega)$, $\chi_0^{(bb)}(q,\omega)$, $\chi_0^{(ab)}(q,\omega)$, and $\chi_0^{(ba)}(q,\omega)$ are given by (for simplicity we discuss the zero-temperature case)[11,22]

$$\chi_0^{(ij)}(q,\omega)=\frac{1}{4}\sum_k\left(1-\frac{\xi_k\xi_{k+q}+\Delta_k^{(i)}\Delta_{k+q}^{(j)*}}{E_k^{(i)}E_{k+q}^{(j)}}\right)\times\left(\frac{1}{\omega+E_k^{(i)}+E_{k+q}^{(j)}+i\delta}-\frac{1}{\omega-E_k^{(i)}-E_{k+q}^{(j)}+i\delta}\right). \tag{5}$$

Here i, $j=a$, b, and $E_k^{(i)}=\sqrt{(\xi_k)^2+|\Delta_k^{(i)}|^2}$ is the quasiparticle energy.

To see the effect of the interlayer pairing on the momentum dependence of the magnetic response, let us look at the BCS coherence factor $[1-(\xi_k\xi_{k+q}+\Delta_k^{(i)}\Delta_{k+q}^{(j)*})/(E_k^{(i)}E_{k+q}^{(j)})]$, which contains the information about the internal structure of the Cooper pair. In the absence of the interlayer pairing, the even and the odd channels have the same coherence factor $[1-(\xi_k\xi_{k+q}+\Delta_k\Delta_{k+q})/(E_kE_{k+q})]$ and both channels are fully enhanced at momentum transfer $q=(\pi,\pi)$ since $\Delta_k\Delta_{k+q}<0$. That is, the system does not distinguish the even and the odd channels at the mean-field level. As we have mentioned at the beginning of this paper, the RPA correction from the interlayer exchange is far too small to make this mean-field result agree with the observed large difference between the even and the odd channels.

In the presence of the interlayer pairing, the even and the odd channels behave differently. For the odd channel, since $\Delta_k^{(a)}\Delta_{k+q}^{(b)*}=\Delta_k^{(b)}\Delta_{k+q}^{(a)*}=-(\Delta_k^2+|\Delta_k'|^2)$ (using the properties $\Delta_{k+q}=-\Delta_k$, $\Delta_{k+q}'=\Delta_k'$), the coherence factor can still reach its maximum value of 2 on the Fermi surface. That is, the odd-channel magnetic response is still fully enhanced. While for the even channel, since $\Delta_k^{(a)}\Delta_{k+q}^{(a)*}=-(\Delta_k^2-|\Delta_k'|^2-2i\Delta_k\Delta_k')=-(\Delta_k^2-|\Delta_k'|^2)=\Delta_k^{(b)}\Delta_{k+q}^{(b)*}$ (the cross term of Δ_k and Δ_k' vanishes upon summing over k since Δ_k and Δ_k' have different symmetry), the coherence factor can take any value ranging from 0 (totally suppressed) to 2 (fully enhanced) on the Fermi surface depending on the ratio $|\Delta_k'|/\Delta_0$. As a result, the even-channel magnetic response is suppressed with the increase of the interlayer pairing. Fig. 2 shows the calculated susceptibility for $|\Delta_k'|/\Delta_0=1$ (the magnitude of the interlayer pairing will be discussed later). We see the interlayer pairing suppresses the even-channel magnetic response very effectively.

So far, we have discussed the bare susceptibility χ_0. To obtain the fully renormalized susceptibility, we still have to include the RPA correction from the antiferromagnetic exchange coupling. In the presence of the interlayer exchange coupling, the even and odd channel magnetic responses are renormalized differently,[10,11,16]

$$\begin{aligned}\chi^{(even)}(q,\omega)&=\frac{\chi_0^{(even)}(q,\omega)}{1+(J_q+J_p)\chi_0^{(even)}(q,\omega)/2},\\ \chi^{(odd)}(q,\omega)&=\frac{\chi_0^{(odd)}(q,\omega)}{1+(J_q-J_p)\chi_0^{(odd)}(q,\omega)/2},\end{aligned} \tag{6}$$

in which $J_q=J(\cos q_x+\cos q_y)$ is the intralayer exchange, and J_p is the interlayer exchange coupling. Experimentally, $J\sim0.15$ eV, $J_p/J\sim 0.1$.[23] Figure 3 shows the renormalized susceptibility. After the RPA correction, a sharp resonance appears well below the gap edge in the odd channel,[18] while in the even channel, there is only a small peak very close to the gap edge. This result can be understood by examining the resonance condition for both channels. As can be seen from

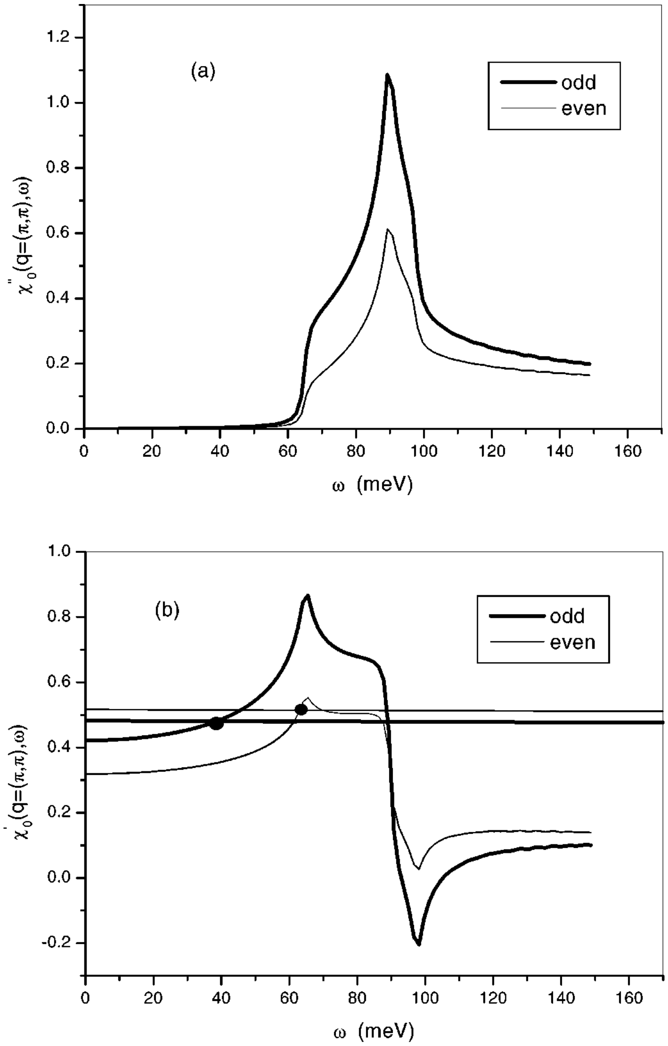

FIG. 2. The imaginary (a) and the real (b) parts of the bare susceptibility for $|\Delta'_k|/\Delta_0=1$, $\sqrt{\Delta_0^2+|\Delta'_k|^2}=35$ meV. The Fermi surface is 34 meV above the VHS. Note that both the maximal gap and the chemical potential are the same as those used in Ref. 18. The intersections of the straight lines and the curves in (b) give the resonance energies in the odd and the even channel for $J=150$ meV, $J_p=0.1$ J.

Fig. 2, the resonance condition is fulfilled well below the gap edge in the odd channel, while in the even channel, this condition is only fulfilled very close to the gap edge because of the reduced magnitude of the bare susceptibility in the even channel (J_p alone is too small to produce the observed even-odd difference). Here we find the magnetic response starts at different energies in the odd and even channels. This agrees very well with experimental observations.[24] According to our theory, the resonance energy of the odd channel is unrelated to the superconducting gap while the energy threshold for even-channel magnetic response is about twice the superconducting gap.

In the foregoing discussion, we have neglected the momentum dependence of the interlayer pairing. This is reasonable for the discussion of the (π,π) resonance that mainly concerns the hot spots on the Fermi surface. However, a

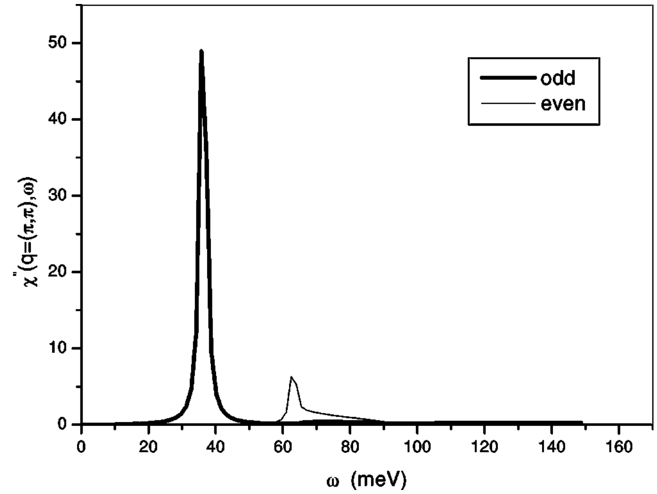

FIG. 3. The susceptibility after the RPA correction for $J=150$ meV, $J_p=0.1$ J.

momentum-independent interlayer pairing is inconsistent with experimental observation of the gap nodes along the $(0,0)-(\pi,\pi)$ direction since the total-energy gap equals $\sqrt{\Delta_k^2+|\Delta'_k|^2}$. To be consistent with the existence of the gap nodes, Δ'_k must be negligibly small along the node direction. Thus, the interlayer pairing must be strongly momentum dependent in the CuO_2 plane. Here, a closely related problem is the magnitude of the interlayer pairing. In our calculation, we have assumed $|\Delta'_k|/\Delta_0=1$. This may seem arbitrary at first. However, if we assume that the superconducting pairing originates from the exchange of the antiferromagnetic spin fluctuation,[25,26] especially the (π,π) resonance,[27] then both the magnitude and the momentum dependence of the interlayer pairing can be easily understood. Since the resonance occurs only in the odd channel, the spin fluctuations mediating the intralayer and the interlayer pairings have the same propagator except for an overall sign (note that $\chi^{(even)}=\chi^{(intra)}+\chi^{(inter)}$; $\chi^{(odd)}=\chi^{(intra)}-\chi^{(inter)}$). Hence it is quite reasonable that the intralayer and the interlayer pairings have comparable magnitudes (but different symmetry). At the same time, since the (π,π) resonance is sharply peaked at (π,π),[4,5] only momentum close to the hot spots is significantly affected by the interlayer pairing. Hence the interlayer pairing must be strongly momentum dependent.

Interestingly, this pairing mechanism also naturally explains the different symmetry of the intralayer and the interlayer pairings. This difference comes from the overall sign change between the intralayer and the interlayer spin-fluctuation propagators. Since the exchange of intralayer antiferromagnetic spin fluctuation favors *d*-wave intralayer pairing,[25,26] or $\Delta_{k+(\pi,\pi)}=-\Delta_k$, the interlayer pairing mediated by the interlayer spin fluctuation must have *s*-wave symmetry, or $\Delta'_{k+(\pi,\pi)}=\Delta'_k$. When Δ'_k is transformed into the real space, we will see that the interlayer pairing exists only between sites of the same magnetic sublattice on the two CuO_2 planes. According to our discussion concerning the relation between the momentum dependence of the magnetic response and the internal structure of the Cooper pair, such interlayer pairing will enhance the odd-channel response and suppress the even-channel response, as we have observed.

In conclusion, we find the sinusoidal modulation of the (π,π) resonance observed in experiments can be explained with the inclusion of the interlayer pairing in the theory. We find the interlayer pairing has *s*-wave symmetry in the CuO_2 plane and has comparable magnitude with the *d*-wave intralayer pairing. We also find the interlayer pairing has strong momentum dependence and mainly affects momentum close to the hot spots on the Fermi surface. We find these characteristics of the interlayer pairing can be understood in a model in which the superconducting pairing comes from the exchange of the antiferromagnetic spin fluctuation, especially the (π,π) resonance.

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