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Dispersion of the π resonance in the superconducting state of the cuprates

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We study the dispersion of π resonance in the superconducting state within the projected SO(5) model [S.C. Zhang *et al.*, Phys. Rev. B **60**, 13 070 (1999)]. Away from the commensurate momentum, the propagation of the π resonance creates phase flips in the superconducting order parameter. This frustration effect leads to a strong dressing of the π resonance and a downward dispersion away from the commensurate wave vector. Based on these results, we argue that the commensurate resonance and incommensurate magnetic fluctuations in the cuprates are continuously connected.

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The emergence of a commensurate neutron resonance peak below T_c is one of the most striking properties of the cuprates. There are many different theoretical approaches to the problem. Within the SO(5) theory,[1] this resonance peak is interpreted as a collective mode describing a rotation from the superconducting (SC) state to the commensurate antiferromagnetic (AF) state. Since the rotation operator is a triplet particle-particle operator, which can only couple to neutrons in a SC state, this theory predicts that the intensity of the π resonance mode is proportional to the square of the SC order parameter.[2] This fact naturally explains the temperature dependence of the resonance intensity observed in experiments,[3] and anticipated[4,5] the recently observed dependence of the resonance intensity on the magnetic field.[6] A c-axis magnetic field creates non-SC vortex cores, therefore it reduces the SC order parameter on the average. On the other hand, a magnetic field aligned in the ab plane has little effect in reducing the SC order parameter. From the dependence of the resonance intensity on the SC order parameter within the SO(5) theory, one would therefore naturally expect a reduction of the resonance intensity in the presence of a c-axis magnetic field.

More recently, incommensurate magnetic fluctuations have also been observed in the Y-Ba-Cu-O superconductors.[7,8] Unlike their counterparts in the La-Sr-Cu-O superconductors, these incommensurate magnetic fluctuations are energy dependent, and seem to merge continuously into the π resonance mode. In fact, this behavior is predicted by Furusaki and one of us,[9] who applied the SO(5) theory to the ladder systems. Using an asymptotically exact renormalization-group method, they found that the π resonance mode in the ladder system has a downward dispersion away from the commensurate wave vector. In fact, in an earlier work, Poilblanc, Scalapino, and Hanke[10] found similar behavior in an exact diagonalization study of the ladder systems. The purpose of this work is to identify the physical origin of this downward dispersion relation and construct a unified theory of the commensurate and incommensurate magnetic fluctuations in the cuprates.

To understand the basic physics of the competition between the commensurate and incommensurate magnetic fluctuations, let us first consider a very simple system of the doped t-$J_{||}$-$J_\perp$ ladder. In the $J_\perp \gg J_{||}$ limit, the SC state of the doped ladder system can be viewed as a coherent linear superposition of a hole pair and a singlet pair on each rung. In this picture, the π resonance is simply a linear superposition of a spin triplet excitation on each rung. Because the SC state is a broken symmetry state, such an excitation can be either created by a spin triplet operator or a triplet particle-particle operator, the so-called π operator. Simple second-order perturbation theory shows that the exchange parameter between the triplet and a hole pair is $-4t^2/J_\perp$, which has a negative sign, while the exchange parameter between the triplet and the singlet pair is $J_{||}/2$, which has a positive sign. The positive exchange sign prefers a minimal energy wave vector at $q_{min}=\pi$, while the negative sign prefers a minimal energy wave vector at $q_{min}=0$. Since the SC ground state is a linear superposition of both the hole pair and the singlet pair, this effect leads to a competition between these two band minima. In one dimension, this competition always leads to an incommensurate band minimum.

In this paper, we shall generalize this physics to two dimensions and study the propagation of the π resonance in the SC state, within the projected SO(5) model [pSO(5) model]. Just like the physical picture outlined above, the propagation of the π resonance leads to a sign reversal of the SC order parameter behind it. Therefore, the problem is similar to the problem of the propagation of a single hole in the antiferromagnetic background, which has been studied extensively in the literature.[12–15] In fact, using basically the same approximations, we shall show that the quantum fluctuations erase the string of sign reversals, but lead to a nontrivial correction to the dispersion of the π resonance. Depending on parameters of the model, the correction can give rise to a downward dispersion of the π mode, reaching a minimum at the incommensurate wave vector. Current experiments only show a downward dispersion of the π resonance. The main prediction of our theory is that there will be an upward turn in the dispersion after the minimum is reached.

We begin with the projected SO(5) model defined on a lattice (using the notations of Ref. 11)

$$H=\Delta_s\sum_x t_\alpha^\dagger(x)t_\alpha(x)+\tilde{\Delta}_c\sum_x n_i(x)n_i(x)$$
$$-J_s\sum_{\langle xx'\rangle} n_\alpha(x)n_\alpha(x')-J_c\sum_{\langle xx'\rangle} n_i(x)n_i(x')$$
$$+V\sum_{\langle xx'\rangle} L_{ab}(x)L_{ab}(x'), \tag{1}$$

where $i=1,5$, $\alpha=2,3,4$, and $\tilde{\Delta}_c=\Delta_c-\mu$ where μ is the chemical potential. In SO(5) superspin notation, the superspin is defined as

$$n_1=\frac{1}{2}(t_h+t_h^\dagger),\quad n_5=\frac{1}{2i}(t_h-t_h^\dagger), \tag{2}$$

$$n_\alpha=\frac{1}{\sqrt{2}}(t_\alpha+t_\alpha^+), \tag{3}$$

where t_h and t_α are hard-core boson annihilation operators for the hole pair and the magnon. Here one lattice site of this effective model corresponds to a plaquette in the original C_uO_2 plane, and we have made a shift of the momentum vector for t_α bosons by (π,π). The pSO(5) model[11] is constructed by projecting out the doubly occupied configuration from the local SO(5) multiplets. Even though some members of the SO(5) multiplets are projected out, at $\Delta_s=\tilde{\Delta}_c$ and $J_c=2J_s$, the mean-field ground-state manifold is still SO(5) symmetric, and AF can be smoothly rotated into SC with no energy cost. In Ref. 11, we have shown this model gives a realistic description of the global phase diagram of the cuprates and many of their physical properties. In that paper, the V term in the above Hamiltonian was simply ignored because it does not impact the mean-field phase diagram if only the pure AF phase and SC phase are concerned. However, one important observation in this paper is that this term plays an important role on the dispersion of the π mode. If we limit our discussion to one single magnon in Hilbert space, the V term simply describes the hopping exchange between a hole pair and a magnon. The hopping between a magnon and a singlet is described in the term $-J_s n_\alpha(x)n_\alpha(x')$. Since we only discuss the motion of a single magnon, all other matrix elements for these two terms vanish except

$$VL_{ab}(x)L_{ab}(x')[t_h^+(x)t_\alpha^+(x')|0\rangle]=Vt_h^+(x')t_\alpha^+(x)|0\rangle,$$

$$-J_s n_\alpha(x)n_\alpha(x')[b^+(x)t_\alpha^+(x')|0\rangle]$$
$$=-J_s b^+(x')t_\alpha^+(x)|0\rangle, \tag{4}$$

where $b^+(x)$ creates a singlet at site x. Since both J_s and V are positive in this model, we see that these two hopping processes have opposite signs. Therefore, in a pure SC state, which is a coherent state of singlet and hole pair on each site, the hopping of magnon flips the phase of the local SC order. More precisely, let us take a mean-field pure SC state, Φ,

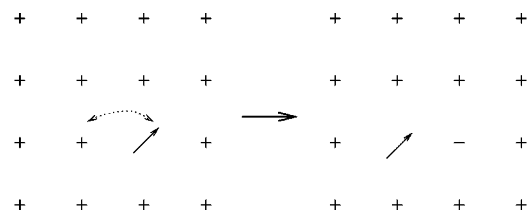

FIG. 1. Schematic diagram of the hopping of a magnon in the SC state. The arrow represents a magnon while the signs represent the phase of SC order.

$$\Phi=\prod_x \phi_+(x),\quad \phi_\pm(x)=[\cos\theta b^+(x)\pm\sin\theta t_h^+(x)]|0\rangle, \tag{5}$$

which has SC order, $\langle n_1(x)\rangle=\frac{1}{2}\sin(2\theta)$, on each site. Taking the hopping term of a magnon between sites x,x' we obtain for $V=J_s$,

$$[L_{ab}(x)L_{ab}(x')-n_\alpha(x)n_\alpha(x')]t_\alpha^+(x')\phi_+(x)$$
$$=t_\alpha^+(x)\phi_-(x'), \tag{6}$$

in which the SC order at site x', $n_1(x')$, takes value $\langle n_1(x')\rangle=-\frac{1}{2}\sin(2\theta)$. A schematic diagram is shown in Fig. 1 to reflect the hopping of a magnon in the SC state. The motion of the magnon creates the phase mismatch similar to the spin mismatch caused by the motion of a single hole in an AF state.

Similar to a single hole problem, quantum phase fluctuations in the SC state can erase the string effect and modify the dispersion relation. We employ the same method in Refs. 14 and 15 to solve the problem.

Taking the variational wave function in Eq. (5), a simple mean-field calculation gives the hole-pair density $\rho=\sin^2(\theta)=(J_cz-\tilde{\Delta}_c)/2J_cz$, where z is the coordination number on the lattice. We introduce a Lagrangian multiplier field λ to enforce the hard-core boson constraint on average. To obtain the collective phase mode, we define two new boson operators,

$$\alpha_1(x)=\sin\theta b(x)-\cos\theta t_h(x),$$
$$\alpha_2(x)=\cos\theta b(x)+\sin\theta t_h(x), \tag{7}$$

which satisfy $\alpha_1(x)|\Phi\rangle=0, \langle\alpha_2(x)\rangle=1$. The quadratic Hamiltonian describing the phase fluctuation above the mean-field state is therefore given by

$$H'=H-\langle H\rangle$$
$$=-J_cz\sum_q\left\{\left[1-\gamma(q)+\frac{\sin^2(2\theta)}{2}\gamma(q)\right]\alpha_1^+(q)\alpha_1(q)\right.$$
$$\left.+\frac{\sin^2(2\theta)}{4}\gamma(q)[\alpha_1(-q)\alpha_1(q)+\text{H.c.}]\right\}, \tag{8}$$

where $\gamma(q)=[\cos(q_x)+\cos(q_y)]/2$. In the following part of paper, we normalize all of the energy scale by taking $(J_s+V)z/2=1$ and define two additional dimensionless parameters,

$$x=\frac{V-J_s}{J_s+V},\quad y=\frac{2J_c}{(J_s+V)}. \tag{9}$$

By standard diagonalization,

$$H'=\sum_q \epsilon(q)\beta^+(q)\beta(q), \tag{10}$$

where

$$\beta(q)=u(q)\alpha_1(q)-v(q)\alpha_1^+(-q), \tag{11}$$

$$\epsilon(q)=y\sqrt{[1-\gamma(q)]^2+\sin^2(2\theta)\gamma(q)[1-\gamma(q)]}, \tag{12}$$

$$u(q)=\sqrt{\frac{1}{2}+y\frac{1-\gamma(q)+\frac{\sin^2(2\theta)}{2}\gamma(q)}{2\epsilon(q)}}, \tag{13}$$

$$v(q)=-\mathrm{sgn}[\gamma(q)]\sqrt{-\frac{1}{2}+y\frac{1-\gamma(q)+\frac{\sin^2(2\theta)}{2}\gamma(q)}{2\epsilon(q)}}. \tag{14}$$

The hopping of a single magnon can be described by the following Hamiltonian:

$$H_m=-J_s\sum_{xx'}[t_\alpha^+(x)t_\alpha(x')b^+(x')b(x)+\mathrm{H.c.}]$$
$$+V\sum_{xx'}[t_\alpha^+(x)t_\alpha(x')t_h^+(x')t_h(x)+\mathrm{H.c.}]. \tag{15}$$

Taking the mean-field expectations and using the relations of Eq. (5), we get

$$H_m=\sum_q [E_b(q,\theta)t_\alpha^+(q)t_\alpha(q)+\mathrm{H.c.}]$$
$$+\sum_{kq} f(k,q)t_\alpha^+(k)t_\alpha(k-q), \tag{16}$$

where

$$E_b(q,\theta)=[x-\cos(2\theta)]\gamma(q), \tag{17}$$

$$f(k,q)=\sin(2\theta)\{[\gamma(k-q)u(q)+\gamma(k)v(q)]\beta(q)$$
$$+[\gamma(k)u(q)+\gamma(k-q)v(q)]\beta^+(-q)\}. \tag{18}$$

Given the Hamiltonian composed of Eq. (10) and Eq. (16), we can calculate the dynamic spin correlation function,

$$G(x,t)=-i\langle\Phi|T[t_\alpha(x,t)b^+(x,t)t_\alpha^+(0,0)b(0,0)]|\Phi\rangle. \tag{19}$$

Taking the mean-field value on b and using the self-consistent perturbation which sums only noncrossing diagrams, we obtain the following Dyson's equation:

$$G(k,\omega)=\frac{\cos^2(\theta)}{\omega-E_0(k,\theta)-\sum_q F(k,q,\theta)G(k-q,\omega-\epsilon(q))}, \tag{20}$$

where

$$F(k,q,\theta)=\sin^2(2\theta)|\gamma(k-q)u(q)+\gamma(k)v(q)|^2. \tag{21}$$

In this approximation, the vertex is neglected, which is small according to the calculation in Ref. 15 for the single-hole problem. We numerically solve the above integral equations to obtain the spectrum, $A(k,\omega)=-(1/\pi)G(k,\omega)$, and in particular the minimum position of the dispersion in the broad range of parameters. We first observe that the bare dispersion of magnon, $E_b(k)$, can be removed in Eq. (20) by shifting ω. Moreover, if y is large, it is better to rescale $\epsilon(q)$ in numerical calculation, which can narrow the energy range required to find a solution. Combining these two observations, the numerical convergence is rather fast.

Throughout the numerical calculation, a sharp coherent peak is found in all momentum space. The spectral function can be generally written as

$$A(k,\omega,\theta,y)=\cos^2(\theta)Z(k,\theta,y)\delta(\omega-\Omega(k,\theta,y))+A' \tag{22}$$

where A' is the incoherent part and $\Omega(k,\theta,y)$ defines the energy dispersion. From our numerical result, we find that the energy dispersion, Ω, can be written as

$$\Omega(x,k,\theta,y)=\Omega_0(x,0,\theta,y)+[E_b(k,\theta)-E_b(0,\theta)]$$
$$-\delta\Omega(k,\theta,y), \tag{23}$$

where the first term is the energy at $k=(0,0)$, the second one is the bare dispersion, and the third is the relative energy shift contributed by fluctuation correction. Based on the symmetry of our model, $\delta\Omega(k,\rho,y)=\delta\Omega(k,1-\rho,y)$. We find that $\delta\Omega(k,\theta)$ fits very well a product of two separated functions, $h(\theta,y)$ and $g(k)$, where $h(\theta,y)$ is independent of k. Considering the symmetry of the lattice, we find the function $g(k)$ can be well fitted to the following form:

$$g(k_x,k_y)=0.128[\sin^2(k_x)+\sin^2(k_y)]$$
$$+0.054[\cos(k_x)-\cos(k_y)]^2. \tag{24}$$

Thus, the minimum of Ω can be analytically determined by plugging Eq. (24) into Eq. (23). The global minimum always occurs along the diagonal (π,π) direction. However, along the $(\pi,0)$ direction, there is a local minimum. The global and local minimum positions start to shift from (0,0) at a common critical density ρ_I which is approximately determined by the equation

$$\cos(2\theta_I)-0.512h(\theta_I,y)-x=0. \tag{25}$$

In Fig. 2, we show the global minimum position, (k_m,k_m), and local minimum, $(k_m,0)$, as the function of the density. In Fig. 3, we also show the full dispersion of the π mode at the density $\rho=0.4$.

There is another important density in the problem. Within the pSO(5) model, the uniform SC state can only exist for densities exceeding ρ_c. Ignoring small quantum corrections, ρ_c is given by

$$\rho_c=\frac{r-\delta_s+0.5(1-x)}{0.5y+r+1}, \tag{26}$$

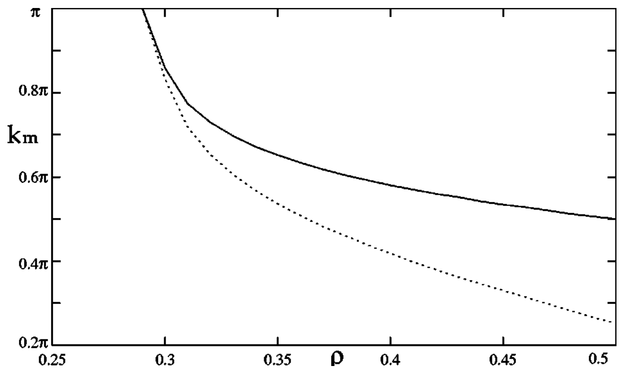

FIG. 2. The minimum momentum position k_m as the function of density ρ at parameters $x=0$, $y=0.5$. The solid line reflects (π,π) direction and dashed line represents $(\pi,0)$ direction [we have made a shift back (0,0) to (π,π) in all figures in this paper].

where $r=J_s/(J_s+V)$ and $\delta_s=\Delta_s/(J_s z+Vz)$. Therefore, depending on the parameters, ρ_I could be larger or smaller than ρ_c. For example, at $x=0$, $y=0.5$, and $r=0.25$, $\rho_c>\rho_I$ for $\delta_s<0.3$ and $\rho_c<\rho_I$ for $\delta_s>0.3$. At $\rho=0$, we have a pure AF state, while for $\rho>\rho_c$, we have a pure SC state. In the intermediate density regime where $0<\rho<\rho_c$, a mixed state between the AF and SC state is obtained. If the transition from the pure SC state to the mixed state is of second order, our theory can actually predict the nature of the mixed state. The second-order transition usually occurs through a ''mode softening'' mechanism. If $\rho_I>\rho_c$, the lowest energy magnetic fluctuations are commensurate at the transition, therefore, a uniform mixed state between commensurate AF and SC is obtained. On the other hand, if $\rho_I<\rho_c$, the lowest magnetic excitations are incommensurate at the transition, a mixed state of incommensurate AF and SC is obtained. Such a state can alternatively be interpreted as a stripe state. Phenomenologically, the Y-Ba-Cu-O materials of high T_c superconductors seem to fall into the first class, while the La-Sr-Cu-O materials seem to fall into the second class.

Finally we would like to compare our results with two classes of theory of the π resonance, one based on the particle-particle picture[2,1] and the other based on the particle-hole picture.[16] Since all calculations are carried out in the SC state, where these two channels mix, distinctions can only be made meaningfully by comparing the final physical predictions. In this work, the intensity of the peak is determined as $\cos^2(\theta)Z(k,\theta)$, where $Z(k,\theta)$ is basically independent of the density parameter θ. Therefore, the intensity of the magnetic collective mode is $\cos^2(\theta)=1-\rho=|\langle n_1\rangle|^2/\rho$, where $\langle n_1\rangle$ is the SC order parameter. This result agrees exactly with the prediction of the particle-particle picture.[2,17] The energy of the collective mode is independent of the SC energy gap, and is expected to be temperature independent. Both these properties are in contrast with the predictions based on the particle-hole picture, where the mode intensity is insensitive to the SC order, and the mode energy is always less than the SC pairing gap. The particle-hole based pictures[16] can also explain the downward dispersion, however, the mode terminates at a certain wave vector due to Landau damping. On the other hand, our current work predicts a minimum in the dispersion. The energy at the minimum is the spin gap in the system. Our present theory does not predict a sharp variation of the intensity with respect to momentum. This is because we restricted ourselves to the single mode approximation. Scattering between these collective excitations is expected to change the momentum dependence of the intensity. However, a proper treatment of this effect is beyond the scope of the current paper.

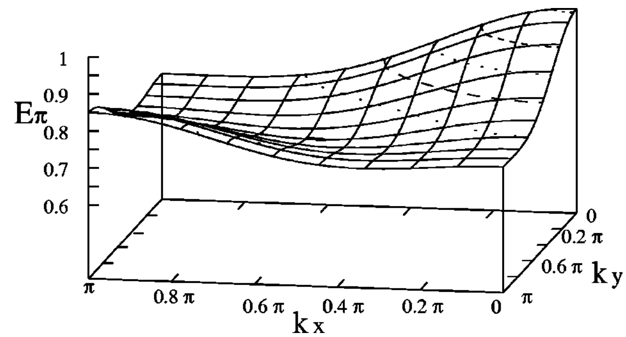

FIG. 3. The full dispersion of π mode, E_π, as a function of k_x, k_y at density $\rho=0.4$ with the parameters $x=0$, $y=0.5$, $z=0.5$, $\delta_s=1$.

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