π excitation of the t-J model

Eugene Demler
Department of Physics, Stanford University, Stanford, California 94305

Hiroshi Kohno
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

Shou-Cheng Zhang
Department of Physics, Stanford University, Stanford, California 94305
(Received 14 October 1997; revised manuscript received 5 March 1998)

In this paper, we present analytical and numerical calculations of the π resonance in the t-J model. We show in detail how the π resonance in the particle-particle channel couples to the dynamical spin correlation function in a superconducting state. The contribution of the π resonance to the spin excitation spectrum can be estimated from general model-independent sum rules, and it agrees with our detailed calculations. The results are in overall agreement with the exact diagonalization studies of the t-J model. Earlier calculations predicted the correct doping dependence of the neutron resonance peak in the $YBa_2Cu_3O_{6+x}$ superconductor, and in this paper detailed energy and momentum dependence of the spin correlation function is presented. The microscopic equations of motion obtained within current formalism agree with that of the SO(5) nonlinear σ model, where the π resonance is interpreted as a pseudo-Goldstone mode of the spontaneous SO(5) symmetry breaking. [S0163-1829(98)02933-6]

I. INTRODUCTION

Of many fascinating experiments on high-T_c superconductors, the resonant neutron-scattering peak observed in the $YBa_2Cu_3O_{6+x}$ family is an extremely striking one.[1–5] It was first observed in the optimally doped $YBa_2Cu_3O_7$ materials. The mode exists only in a narrow region in reciprocal space near $(\pi/a,\pi/b,\pi/c)$, where a and b are the lattice constants in the CuO_2 plane and c is the distance between two neighboring CuO_2 planes in a unit cell. (In the following, we will set these lattice constants to unity to simplify notations). The energy of the resonance is 41 meV and it disperses weakly in reciprocal space. Perhaps the most striking property of this mode is its disappearance above T_c. More recently, this type of collective mode has also been observed in the underdoped families of the $YBa_2Cu_3O_7$ superconductors. Here the energy of this mode is 33 and 25 meV, for materials with T_c values of 62 and 52 K, respectively. While the mode energy decreases monotonically with T_c, the mode intensity increases as T_c decreases. Compared with the 41 meV peak, these modes also have a broader spectral distribution below T_c. In these underdoped materials the resonance is also observed above T_c where it becomes significantly broader. All the modes have been observed in the neutron spin-flip channel, and more recently, the 41 meV mode was seen to broaden under a uniform magnetic field,[6] both indicating that the modes are spin triplets.

These striking resonances have generated wide theoretical interests and a number of theoretical ideas have been suggested in order to explain their properties.[7–16] We believe that one key ingredient is the coupling of the neutron to the particle-particle $(p$-$p)$ channel which occurs in the superconducting (SC) state via the condensate. In particular for a $d_{x^2-y^2}$ gap, the coherence factor $[1-\Delta_{k+q}\Delta_k/E_kE_{k+q}]/2$ for $q=(\pi,\pi,\pi)$ goes to unity at threshold rather than vanishing as it would for an s-wave superconductor.[1,17] Furthermore, two of us argued that the p-p interactions in this channel leads to a sharp resonance which was called the π mode.[7] In the normal state, the resonance is decoupled from the neutron scattering, but can in principle be observed in pair tunneling experiments.[18] This theory predicted the doping dependence of the mode energy and intensity which was subsequently verified experimentally.[19] This picture was also later verified in detailed numerical calculations of the Hubbard and the t-J models by Meixnet *et al.*[20] and by Eder, Hanke, and one of us.[21]

In this paper, we study the π resonance using a self-consistent linear response (SCLR) theory which formally takes into account the mixing of the particle-hole $(p$-$h)$ with the p-p channels in the SC state. This formalism is explained in Sec. II. In Sec. III, we present numerical results based on this formalism and show the overall structure of the spin correlation function. We then give an approximate but analytic expression for the resonance in Sec. IV. In Sec. V, we compare our formalism with the results obtained by using equations of motion for the t-J model and with the SO(5) quantum nonlinear σ model. In Sec. VI, we summarize the results and conclude the paper with some general remarks. Before going into these details, we give here some general features of the π resonance.

The central object of the theory of the π resonance is the so-called π operator,[7] defined by

$$\pi_\alpha^\dagger=\frac{1}{2}\sum_p g_p c_{p+Q}^\dagger \sigma^\alpha \sigma^y c_{-p}^\dagger \tag{1}$$

with σ^α being Pauli matrices, $c_p^\dagger=(c_{p\uparrow}^\dagger,c_{p\downarrow}^\dagger)$, and

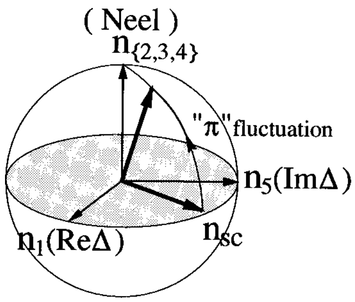

FIG. 1. Geometric interpretation of the π resonance in the superspin phase.

$$g_p=\frac{1}{\sqrt{2}}(\cos p_x-\cos p_y). \tag{2}$$

This operator is a spin triplet and carries charge 2. This operator inspired one of us (S.C.Z.) to formulate the SO(5) theory of high-T_c superconductivity.[22] Together with the total spin and total charge operators, the six π operators form an SO(5) Lie algebra. A natural vector representation of this SO(5) Lie algebra is the superspin

$$\vec{n}=(n_1,n_2,n_3,n_4,n_5)=\left(\frac{\Delta+\Delta^\dagger}{2},N_x,N_y,N_z,\frac{\Delta-\Delta^\dagger}{2i}\right) \tag{3}$$

formed out of the antiferromagnetic (AF) order parameter

$$N_\alpha=\frac{1}{2}\sum_p c^\dagger_{p+Q}\sigma^\alpha c_p \tag{4}$$

and the real and imaginary components of the d-wave superconducting (dSC) order parameter

$$\Delta=\sum_p g_p c_{-p\downarrow}c_{p\uparrow}. \tag{5}$$

Here g_p, Eq.(2), is the d-wave form factor. The π operator rotates N_α and Δ into each other

$$[\pi_\alpha,N_\beta]=i\Delta\,\delta_{\alpha\beta}, \tag{6}$$

therefore within the SO(5) theory, AF and dSC are unified into a common object, called superspin, which can be pictured as a unit vector on an SO(5) sphere, see Fig. 1. A direct first-order transition between these two phases can be induced by a chemical potential μ, and the superspin flops from the AF direction into the dSC direction. However, inside the dSC phase, there are four collective modes, which can be viewed as Goldstone modes of the spontaneous SO(5) symmetry breaking. The usual SC phase mode corresponds to the rotation inside the dSC plane, while there are three extra π modes, corresponding to rotations towards the AF directions, see Fig. 1. Because μ breaks the SO(5) symmetry explicitly and constrains the superspin to lie at the equator, the π fluctuations are massive. From this general consideration, we expect its mass, or the resonance energy, to decrease with decreasing doping.

The SO(5) theory therefore provides a simple picture of the π modes as collective rotations in the SO(5) sphere. Without going into the microscopic details, this picture immediately provides us with some useful quantitative information. Inside the dSC phase, the right-hand side of the operator equation (6) can be replaced by the expectation value of the dSC order parameter, giving

$$[\pi_\alpha,N_\beta]=i\langle\Delta\rangle\,\delta_{\alpha\beta}. \tag{7}$$

This equation can be simply interpreted as the commutation relation between a set of canonically conjugate variables, just like p and q in elementary quantum mechanics. Therefore, we see that a new set of collective quantum degrees of freedom emerges in the broken symmetry state characterized by a dSC order Δ. This simple consideration explains why the π resonance mode is only observed below T_c. However, in the regime where a fluctuating Δ order parameter exists, the π resonance can also appear as a broad feature.

In the dSC state, the π mode couples directly to the spin operator $\vec{S}_Q=\vec{N}$. What is the dynamics associated with the π operator? This is a model-dependent microscopic question. If one is dealing with an SO(5) symmetric microscopic model,[23–25] the dynamics of the π operator is determined by the equation

$$[\mathcal{H},\pi^\dagger_\alpha]=\omega_0\pi^\dagger_\alpha, \tag{8}$$

where $\omega_0=-2\mu$. Therefore, SO(5) symmetric models predict a sharp π resonance whose energy scales with doping. The dynamics associated with the coupled π and spin operator in the t-J model is the central question studied in our current paper. However, even without detailed microscopic calculations, we can give general arguments to estimate the contribution from the π operator to the spin correlation function. Equation (7) leads to an important sum rule for the mixed correlation function between the spin and the π operators. Defining the mixed correlation function as

$$m_{\alpha\beta}(\omega)=-\left\langle 0\left|\pi_\alpha\frac{1}{\omega-\mathcal{H}+E_0+i0}N_\beta - N_\beta\frac{1}{\omega-\mathcal{H}+E_0+i0}\pi_\alpha\right|0\right\rangle \tag{9}$$

and making use of Eq. (7), we have

$$\int\frac{d\omega}{2\pi}m_{\alpha\beta}(\omega)=-\delta_{\alpha\beta}\langle 0|\Delta|0\rangle. \tag{10}$$

In addition, we also have another sum rule for the π correlation function, which follows from the commutation relation

$$[\pi_\alpha,\pi^\dagger_\beta]=(1-n)\,\delta_{\alpha\beta}, \tag{11}$$

where n is a filling factor (half filling corresponds to $n=1$). From these two sum rules, we can put a lower bound on the π contribution to the spin excitation spectrum as

$$I_\pi \equiv \frac{1}{\pi}\int_{\pi\ \mathrm{peak}} d\omega \operatorname{Im}\chi^{+-}(Q,\omega) \gtrsim \frac{2|\Delta|^2}{1-n} \qquad (12)$$

as shown in the Appendix. Therefore, one would expect the π contribution to the dynamic spin correlation function to scale as the square of the dSC order parameter and inversely with the doping $x=1-n$. Both of these conclusions are consistent with the experimental finding in the optimally doped $YBa_2Cu_3O_7$ that the neutron resonance mode disappears above T_c as a sharp excitation, and with the doping dependence of its intensity. We can use typical values of $\Delta_{(\pi,0)}=40$ meV (see Appendix for converting the order parameter to the quasiparticle energy gap), $J=120$ meV, and doping $x=15\%$ to estimate the lower bound for I_π as 0.32. This is close to and consistent with the experimentally measured value 0.51 ± 0.1.[2] In a realistic model, the π operator is not an exact eigenoperator of the Hamiltonian, and Eq. (8) is only approximately fulfilled with other contributions to the energy ω_0. However, as long as the π operator remains as an approximate eigenoperator, it will make a sharp contribution to the spin correlation function, and the energy of the mode will have a leading contribution of -2μ.

II. SELF-CONSISTENT FORMALISM

In this paper, we shall study the π mode of the t-J model with nearest-neighbor (NN) hopping. Before presenting the details of the formalism, we would like to answer some general questions regarding the use of this model and the approximations.

The first question concerns the effect of the NN Coulomb interaction $V\Sigma_{i,j}n_i n_j$.[26] Even if we did not include a bare V term, the reduction from the on-site Hubbard model to the t-J model would generate such a term with $V=-J/4$. Actually, at this particular value of V, the interaction between the quasiparticles making up a spin triplet is zero. One might be concerned that without the multiple scattering in the triplet channel, there would not be any π resonance. However, this is not the case. Even in the absence of a triplet interaction, there is a sharp π mode given by

$$\int dt e^{i\omega t}\theta(t)\langle 0|\pi_\alpha(t)\pi^\dagger_\beta(0)|0\rangle = \frac{1-n}{\omega+2\mu+i0}\delta_{\alpha\beta}. \qquad (13)$$

This occurs because the p-p continuum collapses to a point at total momentum $q=Q$. Interaction in the triplet channel simply shifts the resonance energy from -2μ. In this paper, we shall only calculate the π and spin correlation function with $V=0$. The effect of V is twofold, it changes *both* the interaction in the π triplet channel and the energy to destroy a d-wave pair in the ground state, thereby changing the chemical potential μ. Since the V interaction does not distinguish between the singlet Cooper pair and the triplet π pair, these two contributions will essentially cancel each other. This cancellation is indeed observed rather accurately in the numerical calculations in both the Hubbard and the t-J model.[20,21] Because the J interaction is different in the singlet and triplet channels, this cancellation does not occur. Therefore, in this paper, we shall only study the effect of the J interaction.

The second question concerns the effect of the next-nearest-neighbor hopping term t'.[20,21,26,27] In the presence of this term, the p-p continuum no longer collapses at total momentum Q, and it is not clear if the π mode can remain sharp in the presence of t'. This question depends on the bandwidth around the $(\pi,0)$ and $(0,\pi)$ points in reciprocal space. While the bare bandwidth might be large, it is known from both photoemission and numerical experiments that many-body corrections reduce the bandwidth at these points significantly. Assuming the reduced band structure, the π mode remains sharp in the normal state. Direct numerical calculations on the π resonance also show that the π mode remains sharp for a wide range of t'.[20,21] Because the many-body reduction of the bandwidth is hard to obtain from direct perturbation theory, we shall not address the t' issue in this paper.

In this work, we shall mainly discuss the two-dimensional case where the π operator carries momentum (π,π). Generalizations to bilayer system is straightforward. In this case, the π operator rotates the three-dimensional (3D) AF state into the 3D dSC state, and carries momentum (π,π,π), i.e., it is odd under bilayer interchange. If the 3D π operator is an approximate eigenoperator of the interlayer Hamiltonian, analysis presented in this paper will carry through in the bilayer case as well.

Finally we would like to address the issue of the large Hubbard U repulsion or the no double occupancy constraint in the t-J model.[28,29] In this paper, we shall only treat the Hubbard U within the Hartree approximation. In this case, its effect can be captured by a renormalization of the chemical potential[29] and the hopping t. Alternatively, we can treat the t-J model within the slave boson mean field theory. Here one replaces the electron operator $c_{i\sigma}$ by a product of $b_i f_{i\sigma}$. Within the dSC state, the holons b_i are condensed and can be replaced by its c-number expectation value. The resulting Hamiltonian for the spinons $f_{i\sigma}$ is just a t-J model with renormalized parameters, where the constraint is only treated on the average, again by adjusting the chemical potential and renormalizing the hopping parameter.[30] These two formalisms therefore lead to the same perturbation series in the interaction J.

We now review the self-consistent formalism for computing the spin correlation function in the SC state. This self-consistent approach has been pioneered by Anderson[31] and Rickayzen[32] in treating the problem of the response of a superconductor to an electromagnetic field and later used by Bardasis and Schrieffer to study collective excitations in a superconductor.[33] The basic idea of this method is the same as that of any linear response calculation. We perturb a system by a small external field and then compute the corresponding induced response. It is, however, important to remember that when the system has SC order, any fluctuation in the p-h channel immediately mixes with fluctuations in the p-p and hole-hole channels. This mixing is responsible for restoration of the transversality of the electromagnetic response of a superconductor[32] and preserving the Ward identities.[34] Microscopically it corresponds to taking into account the response of the superconductor due to the backflow of the condensate as well as the creation of the quasiparticle excitations. We have applied this formalism to the η resonance in the negative-U Hubbard model[34] (see also Ref. 35), and shown that it constitutes a conserving approximation, which gives excellent agreement with the exact theorems on the η resonance of the $U<0$ Hubbard model.[36,37] A similar formalism has been used recently by Kohno, Normand, and Fukuyama,[38] Salkola and Schrieffer,[39] and Brinckmann and Lee[40] to study collective excitations.

In this paper we emphasize that the origin of the neutron resonance peak is coupling to the p-p channel below T_c. The SCLR formalism is a complete framework which takes this effect into account, and has been shown to agree with exact theorems where they are available.[34] However, the naive random-phase approximation (RPA) formula $\chi_{\mathrm{RPA}}=\chi_{\mathrm{BCS}}/(1+V_Q\chi_{\mathrm{BCS}})$ also contains partial information about mixing into the noninteracting p-p channel due to the anomalous $F^\dagger F$ term in χ_{BCS}. Therefore the peak observed at -2μ in the RPA treatment may also have its origin due to p-p mixing. This argument is further strengthened by the findings in our present work that the RPA peak at -2μ moves to the energy of the interacting triplet pair within SCLR formalism.

We start by considering the t-J Hamiltonian

$$\mathcal{H}=-t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^\dagger c_{j\sigma}+\mathrm{H.c.})+J\sum_{\langle ij\rangle}\mathbf{S}_i\mathbf{S}_j+U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}n_{i\sigma}. \tag{14}$$

Within the Hartree-Fock approximation that we use here, the Hubbard U only renormalizes the band structure, but it does not affect the collective excitations of the order of J (see discussion above). Therefore in the rest of the paper we disregard the U term in Hamiltonian (14), and assume that the appropriate renormalization of parameters has been performed.[41]

In this paper, we also restrict ourselves to a dSC state at zero temperature, and assume that the equilibrium state may be described by the BCS mean-field Hamiltonian

$$\mathcal{H}_0=\sum_{p\sigma}\epsilon_p c_{p\sigma}^\dagger c_{p\sigma}+\sum_p \Delta_p c_{p\uparrow}^\dagger c_{-p\downarrow}^\dagger+\sum_p \Delta_p^* c_{-p\downarrow}c_{p\uparrow}, \tag{15}$$

where $\Delta_p=\Delta_0 g_p$ is the d-wave pairing gap[42] and $\epsilon_p=-2t(\cos p_x+\cos p_y)-\mu$. The magnitude of Δ_0 is determined by the self-consistent equation

$$1=V_{\mathrm{BCS}}\sum_p \frac{g_p^2}{2E_p}\tanh\left(\frac{E_p}{2T}\right) \tag{16}$$

(with $T=0$), where $V_{\mathrm{BCS}}=3J/2$ and $E_p=\sqrt{\epsilon_p^2+\Delta_p^2}$.

If we now apply the magnetic field $h_{q\omega}e^{-i\omega t}$ that couples to the spin operator $S_q^-=\Sigma_p c_{p\downarrow}^\dagger c_{q+p\uparrow}$ (only the Zeeman effect of the applied field is of interest to us), the system will respond in the spin channel as well as in the π channels in such a way that the operators

$$S_q=\sum_p c_{q+p\uparrow}^\dagger c_{p\downarrow}, \tag{17}$$

$$\pi_q^+=\sum_p g_p c_{q+p\uparrow}^\dagger c_{-p\uparrow}^\dagger, \tag{18}$$

$$\pi_q^-=\sum_p g_p c_{-q-p\downarrow}c_{p\downarrow} \tag{19}$$

get nonvanishing time-dependent expectation values. Their Fourier transform will be denoted as $S_{q\omega}=\int dt e^{i\omega t}\langle S_q(t)\rangle$ and $\pi_{q\omega}^\pm=\int dt e^{i\omega t}\langle\pi_q^\pm(t)\rangle$. The weight function g_p [Eq. (2)] of the $\pi_q^\pm$ operators arises from the assumed d-wave symmetry of the SC order parameter.[43] The perturbed Hamiltonian (14) is then linearized around the unperturbed one $\mathcal{H}_0$ by factoring out the quantities $S_{q\omega}$ and $\pi_{q\omega}^\pm$:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \tag{20}$$

$$\begin{aligned}\mathcal{H}_1=&(V_qS_{q\omega}-h_{q\omega})e^{-i\omega t}\sum_p c_{p\downarrow}^\dagger c_{q+p\uparrow}\\&+\frac{J}{4}\pi_{q\omega}^+e^{-i\omega t}\sum_p g_p c_{-p\uparrow}c_{q+p\uparrow}\\&+\frac{J}{4}\pi_{q\omega}^-e^{-i\omega t}\sum_p g_p c_{p\downarrow}^\dagger c_{-q-p\downarrow}^\dagger,\end{aligned} \tag{21}$$

where $V_q=J(\cos q_x+\cos q_y)$. Taking $\mathcal{H}_1$ as the perturbation, we then use Kubo formulas

$$\langle\hat f(t)\rangle=-i\int_{-\infty}^t dt'\langle[\hat f(t),\mathcal{H}_1(t')]\rangle_{\mathcal{H}_0} \tag{22}$$

to determine expectation values $S_{q\omega}$ and $\pi_{q\omega}^\pm$ (and hence their responses to the original perturbation $h_{q\omega}$) in a self-consistent manner. This procedure of SCLR is described in detail in our earlier paper on the η excitation of the negative-U Hubbard model.[34]

It is convenient to introduce the amplitude and phase oscillations as $b_{q\omega}^+=\pi_{q\omega}^++\pi_{q\omega}^-$ and $b_{q\omega}^-=\pi_{q\omega}^+-\pi_{q\omega}^-$. After some simple calculations, we arrive at the coupled equations for $b_{q\omega}^+$, $b_{q\omega}^-$ and $S_{q\omega}$

$$\begin{aligned}b_{q\omega}^+&=\frac{J}{4}t_{++}b_{q\omega}^++\frac{J}{4}t_{+-}b_{q\omega}^--2V_qm_+(S_{q\omega}-h_{q\omega}/V_q),\\b_{q\omega}^-&=\frac{J}{4}t_{+-}b_{q\omega}^++\frac{J}{4}t_{--}b_{q\omega}^--2V_qm_-(S_{q\omega}-h_{q\omega}/V_q),\end{aligned} \tag{23}$$

$$S_{q\omega}=-\frac{J}{4}m_+b_{q\omega}^+-\frac{J}{4}m_-b_{q\omega}^--V_q\chi_0(S_{q\omega}-h_{q\omega}/V_q), \tag{24}$$

where

$$t_{++}=i\sum_p g_p^2\int\frac{d\nu}{2\pi}\{G_{-p}(\nu-\omega)G_{p+q}(-\nu)+G_{-p}(\nu)G_{p+q}(\omega-\nu)+2F_{-p}(\nu-\omega)F_{p+q}(-\nu)\}$$
$$=2\sum_p g_p^2(u_{-p}u_{p+q}+v_{-p}v_{p+q})^2\frac{\nu_{pq}}{\omega^2-\nu_{pq}^2},$$

$$t_{+-}=i\sum_p g_p^2\int\frac{d\nu}{2\pi}\{G_{-p}(\nu-\omega)G_{p+q}(-\nu)-G_{-p}(\nu)G_{p+q}(\omega-\nu)\}=2\sum_p g_p^2(v_{-p}^2v_{p+q}^2-u_{-p}^2u_{p+q}^2)\frac{\omega}{\omega^2-\nu_{pq}^2},$$

$$t_{--}=i\sum_p g_p^2\int\frac{d\nu}{2\pi}\{G_{-p}(\nu-\omega)G_{p+q}(-\nu)+G_{-p}(\nu)G_{p+q}(\omega-\nu)-2F_{-p}(\nu-\omega)F_{p+q}(-\nu)\}$$
$$=2\sum_p g_p^2(u_{-p}u_{p+q}-v_{-p}v_{p+q})^2\frac{\nu_{pq}}{\omega^2-\nu_{pq}^2}, \tag{25}$$

$$m_+=i\sum_p g_p\int\frac{d\nu}{2\pi}\{F_{p+q}(\nu)G_{-p}(\nu+\omega)-F_{-p}(-\nu-\omega)G_{p+q}(\nu)\}=2\sum_p g_pu_{p+q}v_{p+q}(u_{-p}^2-v_{-p}^2)\frac{\nu_{pq}}{\omega^2-\nu_{pq}^2},$$

$$m_-=-i\sum_p g_p\int\frac{d\nu}{2\pi}\{F_{p+q}(\nu)G_{-p}(\nu+\omega)+F_{-p}(-\nu-\omega)G_{p+q}(\nu)\}=-2\sum_p g_pu_{p+q}v_{p+q}\frac{\omega}{\omega^2-\nu_{pq}^2},$$

$$\chi_0=i\sum_p \int\frac{d\nu}{2\pi}\{G_{-p}(\nu)G_{p+q}(\nu+\omega)+F_{-p}(-\nu)F_{p+q}(\nu-\omega)\}=-\sum_p (u_{p+q}v_{-p}-u_{-p}v_{p+q})^2\frac{\nu_{pq}}{\omega^2-\nu_{pq}^2}.$$

In the equations above, $\nu_{pq}=E_{p+q}+E_{-p}$, $u_pv_p=\Delta_p/2E_p$, $u_p^2=\frac{1}{2}(1+\epsilon_p/E_p)$, and $v_p^2=\frac{1}{2}(1-\epsilon_p/E_p)$. The Green's functions have been defined as

$$G_p(\omega)=\int dte^{i\omega t}(-i)\langle Tc_{p\sigma}(t)c_{p\sigma}^\dagger(0)\rangle,$$

$$F_p(\omega)=\int dte^{i\omega t}(-i)\langle Tc_{p\uparrow}(t)c_{-p\downarrow}(0)\rangle, \tag{26}$$

$$F_p^\dagger(\omega)=\int dte^{i\omega t}(-i)\langle Tc_{-p\downarrow}^\dagger(t)c_{p\uparrow}^\dagger(0)\rangle.$$

In Eq. (25), ω should be taken to have an infinitesimal imaginary part, $\Gamma=0^+$, coming from causality.

Solution of Eqs. (24) gives the dynamical spin susceptibility in the present SCLR formalism:

$$\chi_{\rm SCLR}(q,\omega)=i\int dte^{i\omega t}\theta(t)\langle[S_q^+(t),S_{-q}^-(0)]\rangle=\frac{S_{q\omega}}{h_{q\omega}}. \tag{27}$$

It can be written in the form

$$\chi_{\rm SCLR}(q,\omega)=\frac{\chi_{\rm irr}}{1+V_q\chi_{\rm irr}}, \tag{28}$$

$$\chi_{\rm irr}=\chi_0+\Delta\chi, \tag{29}$$

$$\Delta\chi=-\frac{J}{2}\frac{m_+^2+m_-^2-\frac{J}{4}m_+^2t_{--}-\frac{J}{4}m_-^2t_{++}+\frac{J}{2}m_-m_+t_{+-}}{1-\frac{J}{4}t_{++}-\frac{J}{4}t_{--}+\frac{J^2}{16}t_{++}t_{--}-\frac{J^2}{16}t_{+-}^2}, \tag{30}$$

and may be understood as a modified random-phase approximation where the bare bubble χ_0 has been modified by including the ladder diagrams. Figure 2 gives the diagrammatic interpretation of formulas (29) and (30).

The procedure for finding the p-p correlation function

$$P(q,t)=-i\theta(t)\langle[\pi_q^+(t),\pi_q^-(0)]\rangle \tag{31}$$

is similar to the one shown above for the spin channel. We only need to add an external field in the $\pi_Q^\dagger$ channel and compute the response in the same channel. Skipping the laborious but straightforward calculations we present the final expression for its Fourier transform

$$P(q,\omega)=\frac{t_{++}+t_{--}+\frac{J}{2}t_{+-}^2-\frac{J}{2}t_{++}t_{--}-2t_{+-}-\frac{J}{4}\,\frac{m_+^2\left(1-\frac{J}{2}t_{--}\right)+m_-^2\left(1-\frac{J}{2}t_{++}\right)-2m_+m_-\left(1-\frac{J}{2}t_{+-}\right)}{1+V_q\chi_0}}{1-\frac{J}{4}t_{++}-\frac{J}{4}t_{--}-\frac{J^2}{16}t_{+-}^2+\frac{J^2}{16}t_{++}t_{--}+J^2\,\frac{m_+^2\left(1-\frac{J}{4}t_{--}\right)+m_-\left(1-\frac{J}{4}t_{++}\right)+\frac{J}{2}m_+m_-t_{+-}}{1+V_q\chi_0}}. \tag{32}$$

In the normal state this reduces to a simple T-matrix expression that was studied in Ref. 7. There it was shown that, in the normal state, the p-p spectrum at $q=Q$ is dominated by the collective π-mode resonance that appears due to the collapse of the p-p continuum ($\epsilon_{p+Q}+\epsilon_{-p}=-2\mu$) and the repulsive interaction of two particles in a triplet state sitting on NN sites. We suggested that this collective mode may contribute to the spin-fluctuation spectrum when the system becomes superconducting. However, such an argument raises an immediate concern that superconductivity could in principle lead to another effect—a significant broadening of the π resonance due to possible scattering into the p-h excitations. The goal of the next part is to show that this does not happen. The π resonance survives as a collective mode and affects strongly the dynamic spin-spin correlation function in the SC state. The important point here is that unlike χ_0, $\Delta\chi$ in $\chi_{\rm irr}$ contains information about the π resonance. As we shall see in the next section, $\mathrm{Im}\chi_{\rm irr}$ nearly vanishes at the π resonance energy, where $\mathrm{Re}\chi_{\rm irr}$ is sharply peaked. The combination of these two effects gives rise to a sharp π resonance in $\chi_{\rm SCLR}$.

III. NUMERICAL RESULTS

It is well known that the RPA form of the spin correlation function overestimates the antiferromagnetic instability. Therefore, if we see a peak in the dynamic spin correlation function, it is important to check if it is an artifact due to the RPA type of overestimate or due to a genuine collective mode. Moreover, the size of the dSC gap relative to T_c is significantly larger than the BCS estimate. Namely, the BCS gap equation (16) with the bare pairing interaction $V_{\rm BCS}=3J/2$ gives a ratio $2\Delta_{(\pi,0)}/k_BT_c$ of about 4 which is small compared to the typically observed value of 6 to 8. Therefore, in what follows, we take two approaches to these problems. We introduce an effective reduction of the antiferromagnetic vertex $V_{\mathbf{Q}}=\alpha V_{\mathbf{Q}}^{\rm bare}$ with $\alpha<1$, as a way to model vertex corrections, or we take the dSC gap Δ_0 to be bigger than its mean-field value.[44] Both of these approaches have the effect of removing the RPA type of AF instability. We shall see that the π resonance is robust against these variations.

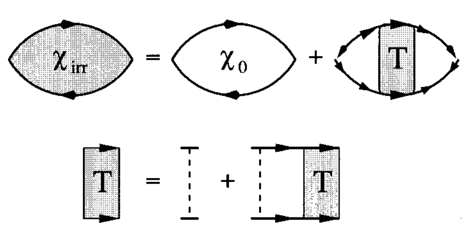

FIG. 2. Modification of $\chi_{\rm irr}$ due to ladder diagrams.

A. π resonance and its robustness against vertex corrections

In this section we take $J=0.6t$ and $\mu=-0.3t$. We choose the mean-field value of $\Delta_0=0.0094t$ and the reduction of V_Q is set by $\alpha=0.82$. We assume a finite value $\Gamma=10^{-4}t$ for the imaginary infinitesimal in the energy denominator and perform integration by dividing the Brillouin zone into a 32 000 $\times$32 000 lattice.

Figure 3 shows the ''mechanics'' of the resonance in $\chi_{\rm SCLR}$. In the normal state the p-p channel has a sharp peak at $\omega_0\approx-2\mu+(J/2)(1-n)=0.655t$. Notice that there is no visible shift of the energy of this resonance in the SC state, but only a small broadening. This resonance in the p-p channel $P(Q,\omega)$ then leads to a peak in $\mathrm{Re}\chi_{\rm irr}$. Consequently at a frequency where $\mathrm{Re}\chi_{\rm irr}=|1/V_Q|$ the real part of the denominator in the SCLR expression (28) vanishes leading to a peak in $\mathrm{Im}\chi_{\rm SCLR}$. At these frequencies, the imaginary part of the denominator ($\mathrm{Im}\chi_{\rm irr}$) is also small, and the resonance appears to be quite sharp.

In Fig. 4, we compare the real part of $\chi_{\rm irr}$ with that of χ_0. As discussed above, we have resonance peaks in $\mathrm{Im}\chi_{\rm SCLR}$ when $\mathrm{Re}\chi_{\rm irr}=|1/V_Q|$. We can see that taking $\chi_{\rm irr}$ instead of χ_0 considerably suppresses the divergence around -2μ (this divergence comes from the dynamic nesting of the Fermi surface; it gives rise to the RPA peak, the only resonance one gets from a naive RPA calculation) and leads to the development of a peak at the energy of the π excitation. It is easily noticeable that if we do not take into account reduction of V_Q, but exploit the bare value of $V_Q^{\rm bare}=-2J$, then

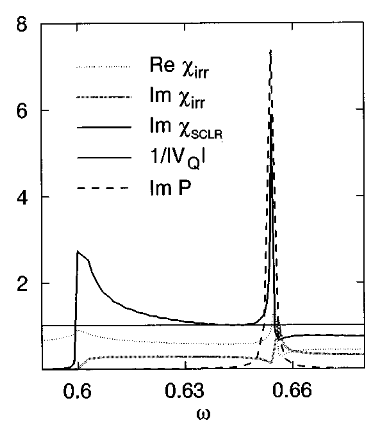

FIG. 3. $\mathrm{Re}\chi_{\rm irr}$, $\mathrm{Im}\chi_{\rm irr}$, $\mathrm{Im}\chi_{\rm SCLR}$, and $\mathrm{Im}P$ vs ω.

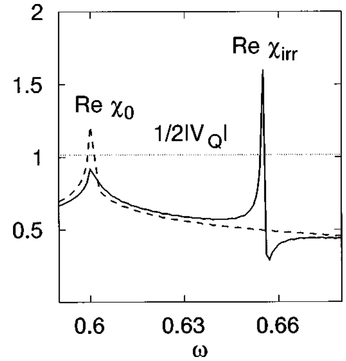

FIG. 4. $\mathrm{Re}\chi_{\mathrm{irr}}$ and $\mathrm{Re}\chi_0$ vs ω. The dotted line represents the line of $1/2J$.

$\mathrm{Re}\chi_{\mathrm{irr}}$ will cross it at two points ($\omega\sim-2\mu$ and ω_0), giving rise to both—RPA and π peaks (see Fig. 7). However, the divergence of $\mathrm{Re}\chi_{\mathrm{irr}}$ around ω_0 is much stronger, making the π peak more robust against variations in V_Q.

In Fig. 5, we show the imaginary part of χ_{irr} and χ_0. Note that a dip develops in $\mathrm{Im}\chi_{\mathrm{irr}}$ at the energy of the π excitation. This means that the π resonance is much less damped than one might have expected. In the normal state, the stability of the π resonance is guaranteed by the absence of the phase space available for decay (p-p continuum collapses to a point). In the dSC state, this argument no longer works. Mixing of the p-h and p-p channels could provide a mechanism for the decay of the π excitation. However, we see that the system accommodates the π excitation by suppressing $\mathrm{Im}\chi_{\mathrm{irr}}$ at its energy. In Sec. IV, we shall give an approximate analytical derivation of this important feature.

In Fig. 6, we compare the self-consistent spin-spin correlation function χ_{SCLR} with the one obtained from the RPA calculation χ_{RPA}. The latter one has an RPA peak that comes from the dynamic nesting of the tight-binding Hamiltonian at momentum Q. In $\mathrm{Im}\chi_{\mathrm{SCLR}}$, this peak disappears almost completely, and the spectral weight is transferred into the π excitation.

In Fig. 7, we show the comparison of different choices of α in V_Q. Notice the coexistence of the RPA peak with the π peak for the choice of bare parameter ($\alpha=1$). Reducing α has no effect on the π resonance but completely destroys the RPA peak. From the analysis carried out in this subsection, we conclude that the RPA peak might be the result of overestimating the AF instability, while the π peak is robust against vertex corrections.

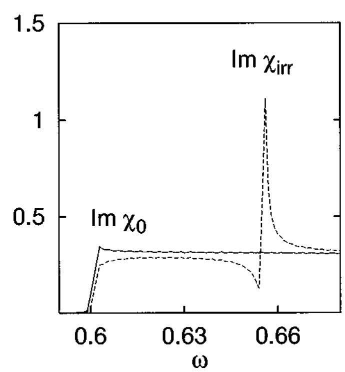

FIG. 5. $\mathrm{Im}\chi_{\mathrm{irr}}$ and $\mathrm{Im}\chi_0$ vs ω.

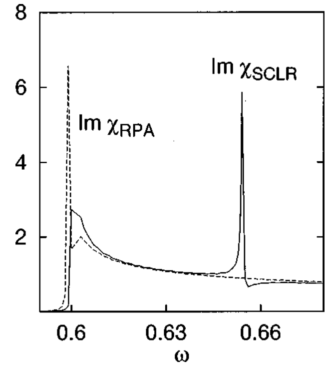

FIG. 6. $\mathrm{Im}\chi_{\mathrm{SCLR}}$ and $\mathrm{Im}\chi_{\mathrm{RPA}}$ vs ω

B. Robustness of the π peak against variations of the superconducting gap

Another way of suppressing AF instability within RPA or SCLR formalism is to choose a larger dSC energy gap. In Fig. 8, we compare the results of SCLR calculations for the spin correlation function for two choices of Δ_0. The smaller one $\Delta_0=0.0094t$ corresponds to the self-consistent (mean-field) value, and the bigger one was taken as $\Delta_0=0.05t$. In these calculations, we take $J=0.6t$ and $\mu=-0.3t$ as before, but with $V_Q=-2J$, the bare value ($\alpha=1$).

We observed in the previous subsection that two peaks (RPA and π) coexist with the choice of the mean-field value for Δ_0 and a bare value for V_Q. Figure 8 shows that taking a larger dSC gap removes the RPA peak and increases the spectral weight of the π peak. This has an even stronger effect than we saw in the previous section by reducing the AF exchange constant. The latter one, as we found, only removes the RPA peak without affecting the π resonance. It is also interesting to find that for the larger gap there is an increase in the energy of the resonance.

A tenacious effect of the large dSC gap is explained in Fig. 9. Here the choice of parameters is the same as in the previous figure with $\Delta_0=0.05t$. By looking at χ_{irr} in this case of large Δ_0, we find that the RPA peak in the real part ($\omega\approx-2\mu$) has completely disappeared. For the mean-field value of Δ_0, there was only a suppression of this peak. In contrast to that, the only effect of taking a larger Δ_0 on the π peak in $\mathrm{Re}\chi_{\mathrm{irr}}$ was to make it broader. This broadening explains the increase in the total weight of the π peak in χ_{SCLR} (the slope of $\mathrm{Re}\chi_{\mathrm{irr}}$ at the crossing point with $1/2J$ deter-

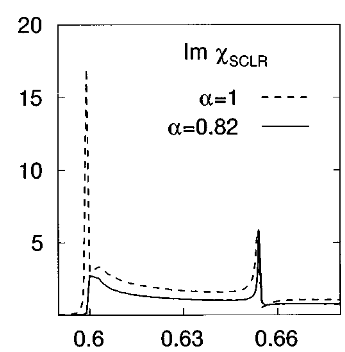

FIG. 7. $\mathrm{Im}\chi_{\mathrm{SCLR}}$ vs ω for two different values of vertex correction parameter α.

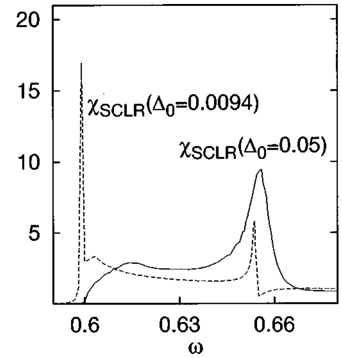

FIG. 8. Imχ_{SCLR} vs ω for different values of Δ_0.

mines the total weight of the π resonance in χ_{SCLR}; see more on that in Sec. IV). Also note an enormous suppression of imaginary part of χ_{irr} for energies below ω_0 in this case of large Δ_0.

In Fig. 10, we show the $\mathbf{q}$ and ω dependence of Im$\chi_{\mathrm{SCLR}}(\mathbf{q},\omega)$. This plot has been done for $\Delta_0 = 0.05t$, $\alpha = 1$ and for computational reasons we took a larger $\Gamma = 10^{-2}t$, which leads to considerable smearing. However, the general picture of the $\mathbf{q}$ dependence of Im$\chi_{\mathrm{SCLR}}(\mathbf{q},\omega)$ may be seen quite clearly. We have an incommensurate structure at low frequencies, which is followed by a commensurate π peak. Right after the peak, there is a missing spectral weight at the commensurate wavevector. Qualitatively this picture is similar to what is seen in inelastic neutron scattering in $YBa_2Cu_3O_{6+x}$.[5] (The incommensurate peaks in that case will be rotated by 45° due to a different band structure. Calculations for the $YBa_2Cu_3O_{6+x}$ band structure will be published elsewhere.[51])

IV. ANALYTICAL DERIVATION OF THE π RESONANCE

In the previous section, we showed numerically that at the energy of the π excitation, χ_{irr} possesses a sharp peak in the real part and a dip in the imaginary part. In this section, we study the origin of these properties analytically.[45] When looking at the structure of the expressions in Eq. (24), one encounters very often analogous integrals that only differ by a factor g_p^2 in the p summation. To simplify the following analysis, we make an approximation that this factor may be replaced by its average value of 1. A similar assumption has

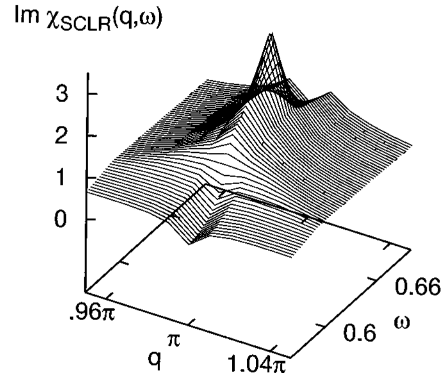

FIG. 10. Im$\chi_{\mathrm{SCLR}}(\mathbf{q},\omega)$ for $\mathbf{q}=(q,q)$.

been used in Ref. 22 to obtain approximate SO(5) algebra. It is important to realize that one should take the average of g_p^2 not over the whole Brillouin zone but over a narrow band around the Fermi surface, since in most of these expressions the other factors in the integrals restrict the important domain of integration to this region.

We introduce

$$I_1(\omega) = \sum_p g_p^2 \frac{1 - v_{-p}^2 - v_{p+Q}^2}{\omega^2 - \nu_{pQ}^2},$$

$$I_2(\omega) = \sum_p g_p \frac{u_{p+Q}v_{p+Q} - u_{-p}v_{-p}}{\omega^2 - \nu_{pQ}^2}, \tag{33}$$

and use some identities for the BCS coherence factors and the approximation $g_p^2 \sim 1$ to express all the factors in Eq. (24) as

$$\begin{aligned} t_{++} &= -4\mu I_1(\omega), \\ t_{+-} &= -2\omega I_1(\omega), \\ t_{--} &= \frac{1-n}{\mu} - \frac{\omega^2}{\mu} I_1(\omega), \\ m_{+} &= -2\mu I_2(\omega), \\ m_{-} &= -\omega I_2(\omega), \\ \chi_0 &= \frac{2}{3J} + \frac{\omega^2 - 4\mu^2}{2\Delta_0} I_2(\omega). \end{aligned} \tag{34}$$

Substituting these expressions into Eq. (30) and using the identity $-4\mu\Delta_0 I_2(\omega) = (1-n) + (4\mu^2 - \omega^2)I_1(\omega)$ which holds within the approximation described above, we get

$$\chi_{\mathrm{irr}} = \frac{1}{V_{\mathrm{BCS}}} + \frac{I_2(\omega)}{2\Delta_0} \frac{(\omega^2 - \omega_0^2)(\omega^2 - 4\mu^2)}{\omega^2 - \omega_0^2 + \Delta_0 J I_2(\omega)(\omega^2 - 2\mu\omega_0)}, \tag{35}$$

where V_{BCS} comes from the gap equation $\Sigma_p g_p u_p v_p = \Delta_0 / V_{\mathrm{BCS}}$ [Eq. (16)], and $\omega_0 = -2\mu + (J/2)(1-n)$. In the mean field analysis of the t-J model, $V_{\mathrm{BCS}} = 3J/2$. Since $I_2(\omega) < 0$ for $\omega \sim \omega_0$, the denominator of the expression (35) vanishes when the frequency is larger than ω_0 but very close

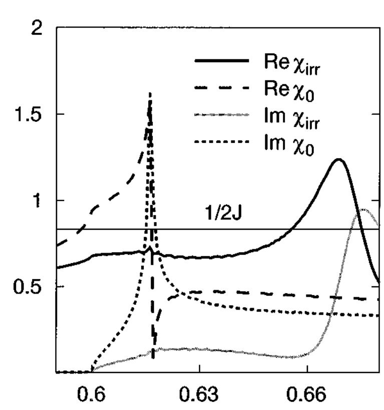

FIG. 9. χ_{irr} and χ_0 vs ω for the case when Δ_0 is larger than its BCS value.

to it (the energy separation is proportional to Δ_0^2). This explains the peak in $\mathrm{Re}\chi_{\mathrm{irr}}$, and the factor $\omega^2-\omega_0^2$ in the numerator explains the dip in the imaginary part.

Expression (35) allows us to estimate the integrated spectral weight of the π excitation in the spin-spin correlation function. For simplicity, we neglect a small imaginary part of χ_{irr} near ω_0. Then a pole in χ_{SCLR} occurs when

$$\mathrm{Re}\chi_{\mathrm{irr}}=-\frac{1}{V_Q}. \tag{36}$$

Expanding χ_{SCLR} around this frequency ω_* we find that

$$\chi_{\mathrm{SCLR}}=\frac{\chi_{\mathrm{irr}}}{V_Q(\partial\chi_{\mathrm{irr}}/\partial\omega)}\bigg|_{\omega_*}\frac{1}{\omega-\omega_*+i0}$$
$$=\frac{1}{V_Q^2(\partial\chi_{\mathrm{irr}}/\partial\omega)|_{\omega_*}}\frac{-1}{\omega-\omega_*+i0}. \tag{37}$$

Earlier we introduced two distinct energies in our system. The BCS coupling V_{BCS} and the AF coupling $V_Q=-2J$. If we consider a *hypothetical* situation when $V_Q=-V_{\mathrm{BCS}}$, we can see that the condition (36) is satisfied exactly at ω_0 and a simple calculation gives $\chi_{\mathrm{SCLR}}(\omega)=2\Delta_0^2/V_Q^2(1-n)[-1/(\omega-\omega_0+i0)]$. If we take here V_Q to be $V_{\mathrm{BCS}}=3J/2$, we have for the intensity of the π resonance

$$I_\pi=\frac{1}{\pi}\int_{\omega_0-\nu}^{\omega_0+\nu'}d\omega\chi''_{\mathrm{SCLR}}=\frac{8\Delta_0^2}{9J^2(1-n)}. \tag{38}$$

The right-hand side is equal to the expression derived in the Appendix as a lower bound. In Eq. (38), ν and ν' characterize the width of the π resonance around ω_0, and we introduced a factor $1/\pi$ since the Lehmann representation of Eq. (27) is given by $\mathrm{Im}\chi(Q,\omega)=\pi\Sigma_n|\langle n|S_Q^+|0\rangle|^2\delta(\omega-\omega_{n0})$. This definition of I_π is the same as $A(T)$ of Refs. 2 and 46. Expression (38) is also what we obtained for the intensity of the π resonance in Ref. 7 using a T-matrix analysis.[47]

If we take realistic values of $J=120$ meV, $\Delta_{(\pi,0)}=40$ meV (this corresponds to $\Delta_0=28.3$ meV) and $1-n=15\%$ and substitute them into Eq. (38), we get $I_\pi=0.32$. For the t-J model, $|V_Q|>V_{\mathrm{BCS}}$, and the energy satisfying the condition (36) is lower than ω_0 and the slope $\partial\chi_{\mathrm{irr}}/\partial\omega$ is smaller than the above estimate (see Fig. 4). This will be partly cancelled with the increse of V_Q, and we expect Eq. (38) gives a semiquantitative estimate for I_π.

V. COMPARISON WITH THE SO(5) EQUATIONS OF MOTION

We now study the Heisenberg equations of motion (EOM) for the π and spin operators

$$\pi_{pQ}^+=c_{p+Q\uparrow}^\dagger c_{-p\uparrow}^\dagger,$$
$$\pi_{pQ}^-=c_{-p-Q\downarrow}c_{p\downarrow}, \tag{39}$$
$$S_{pQ}^+=c_{p+Q\uparrow}^\dagger c_{p\downarrow},$$

using Eq. (14) as a Hamiltonian. A closed set of equations may be obtained by taking commutators of the operators (39) with the Hamiltonian and then factorizing the results in terms of the occupation numbers for the electrons $v_p^2=\langle c_{p\sigma}^\dagger c_{p\sigma}\rangle$ and BCS anomalous averages $u_pv_p=\langle c_{-p\uparrow}c_{p\downarrow}\rangle$. As shown by Anderson and others,[31] this procedure recovers the modified random phase and T-matrix approximations.

$$\begin{aligned}[\mathcal{H},\pi_{pQ}^+]=&(\tilde{\epsilon}_{p+Q}+\tilde{\epsilon}_{-p})\pi_{pQ}^+\\&+\frac{J}{2}(1-v_p^2-v_{p+Q}^2)\sum_k \pi_{kQ}^+\eta(p-k)\\&-\frac{3J}{2}(S_{pQ}^++S_{-p-QQ}^+)\sum_p u_kv_k\eta(p-k)\\&+4Ju_pv_p\sum_k S_{kQ}^+,\end{aligned} \tag{40}$$

$$\begin{aligned}[\mathcal{H},S_{pQ}^+]=&(\tilde{\epsilon}_{p+Q}-\tilde{\epsilon}_p)S_{pQ}^++2J(v_{p+Q}^2-v_p^2)\sum_k S_{kQ}^+\\&-\frac{3J}{2}(\pi_{pQ}^+-\pi_{pQ}^-)\sum_k u_kv_k\eta(p-k)\\&-\frac{J}{2}u_pv_p\sum_k(\pi_{kQ}^+-\pi_{kQ}^-)\eta(p-k),\end{aligned} \tag{41}$$

$$\begin{aligned}[\mathcal{H},\pi_{pQ}^-]=&-(\tilde{\epsilon}_{p+Q}+\tilde{\epsilon}_{-p})\pi_{pQ}^-\\&-\frac{J}{2}(1-v_p^2-v_{p+Q}^2)\sum_k \pi_{kQ}^-\eta(p-k)\\&+\frac{3J}{2}(S_{pQ}^+-S_{-p-QQ}^+)\sum_p u_kv_k\eta(p-k)\\&-4Ju_pv_p\sum_k S_{kQ}^+.\end{aligned} \tag{42}$$

Here $\eta(p)=\cos p_x+\cos p_y$ and the bare dispersion is renormalized into $\tilde{\epsilon}_p=\epsilon_p-(3J/2)\Sigma_kv_k^2\eta(p-k)$. The latter corresponds to a trivial rescaling of t which we will disregard.

The operator of the collective excitation in the π^+ channel is $\pi_Q^+=\Sigma_pg(p)\pi_{pQ}^\dagger$. Then from Eq. (40) we have

$$[\mathcal{H},\pi_Q^+]=\omega_0\pi_Q^++\frac{J\Delta_0}{V_{\mathrm{BCS}}}S_Q^+, \tag{43}$$

where $S_Q^+=\Sigma_pS_{pQ}^+$ and V_{BCS} has been defined earlier. Analogously,

$$[\mathcal{H},\pi_Q^-]=-\omega_0\pi_Q^--\frac{J\Delta_0}{V_{\mathrm{BCS}}}S_Q^+. \tag{44}$$

We can see that in the SC state the EOM for $\pi_Q^\pm$ no longer close on themselves. The third and the fourth terms in Eqs. (40) and (42), that come from anomalous self-energy and scattering correspondingly, do not cancel each other exactly. This may be contrasted to the η excitation in the negative-U Hubbard model,[34] where exact cancelation of such terms occurs.

The collective mode in the S channel may be obtained by summing Eq. (41) over different p's.

$$[\mathcal{H},S_Q^+]=-\frac{2J\Delta_0}{V_{\rm BCS}}(\pi_Q^+-\pi_Q^-). \tag{45}$$

In order to derive this result, we had to disregarded the first term of Eq. (41). In the language of our earlier SCLR approach, this means neglecting χ_0 in comparison with $\Delta\chi$. In the close vicinity of ω_0, this is a justifiable assumption, because at these frequencies $\Delta\chi$ is strongly peaked and is the dominant part of $\chi_{\rm irr}$. However, it is less so at other frequencies, where the incoherent continuum is more important. Thus the meaning of going from Eq. (41) to Eq. (45) is a single mode approximation, which captures collective degrees of freedom only. How good is this approximation? One can see from the numerical results of Sec. III that for Δ_0 around $0.1J$ the π peak already became a dominant feature of the S_Q^+ spectrum. Some estimates of the realistic value of Δ_0 find it to be close to $0.2J$. In this case, such a single mode approximation will truly be a good one.[48]

It is instructive to compare our microscopic EOM's with the SO(5) EOM's in the SC state.[22] We have

$$-i\dot{\pi}_\alpha^\pm=\pm(B_{15}\pi_\alpha^\pm+g\langle n_5\rangle n_\alpha), \tag{46}$$

$$-i\dot{n}_\alpha=-\frac{1}{2\chi_{1\alpha}}\langle n_5\rangle(\pi_\alpha^\dagger-\pi_\alpha), \tag{47}$$

with $\pi_\alpha^\pm=L_{1\alpha}\pm iL_{5\alpha}$ and we assumed dSC ordering along n_5. Equation (46) is the analog of Eqs. (43) and (44), and Eq. (47) corresponds to Eq. (45). This comparison of Eqs. (43), (45)–(47) is very revealing in that it gives a deeper understanding of the nature of the π excitation. Usually the existence of the sharp resonance is not coincidental but is related to some symmetry present in the system. In our case it is an approximate SO(5) symmetry of the t-J model that gives rise to such pronounced π resonance. The agreement between the equations of motion derived from the SO(5) quantum nonlinear σ model[22] and the microscopic t-J model is a key result of this section. It demonstrates that the SO(5) quantum nonlinear σ model can be used as an effective low-energy Hamiltonian to describe the π resonance.

VI. SUMMARY

We have presented detailed analytical and numerical calculations for the contribution from the π resonance to the spin correlation function in the dSC state. The results of these calculations support our earlier interpretation of the resonant neutron-scattering peak in terms of the p-p collective mode in the π channel. Various approximations were used in the calculations presented in this work, some of them are model dependent and may not be well controlled. Therefore, it is important to summarize here the main points leading to our conclusion.

(1) From general model-independent sum rules on various correlation functions, one can conclude that the contribution from the π correlation function to the dynamic spin correlation function is of the order of $|\Delta|^2/(1-n)$, in excellent agreement with the two key experimental observations, namely, the vanishing of the sharp mode above T_c and the doping dependence of its intensity.

(2) Within model-dependent calculations, there is a well-defined π mode in the p-p channel in the normal state, and this mode couples to the p-h spin channel in the dSC state, where it remains as a sharp excitation. The energy of this mode is not directly related to the dSC gap, but is directly related to the doping x. In the underdoped materials, the dSC gap increases slightly as doping is reduced, while the neutron resonance peak energy decreases with x. This important experimental finding shows that the neutron resonance peak is not simply a ''2Δ'' phenomenon, and our interpretation in terms of the π resonance naturally resolves this apparent paradox. The doping dependence of both energy and intensity of the neutron resonance peak were predicted[7,22] before the experiments in the underdoped superconductors were carried out.[4,3]

(3) Many approximations within our current calculations are not completely controlled. However, the main behavior can be verified in the case where exact knowledge is available. First of all, detailed exact diagonalization studies have been carried out both for the t-J and the Hubbard models.[21,20] It is clearly seen that the π mode in the p-p channel exists in all doping range, and it has a low-energy peak where both the energy and intensity scale with x, in agreement with our T-matrix calculation. In contrast to the π correlation function, the spin correlation function does not have sharp peaks in the high doping range. In the doping range where there are dSC fluctuations, the π peak coincides with the spin peak. From these results, one can conclude that the π mode is a genuine collective mode. We can also compare our approximations with the exact SO(5) models,[23] where the π operators are exact eigenoperators of the Hamiltonian. The manipulations presented in this work lead to results consistent with the exact SO(5) Ward identities. The π resonance is an exact excitation of the SO(5) models, and it has exactly the same doping dependence of the mode energy and intensity as obtained here.

(4) The distinction between the ''RPA peak'' and the ''π peak'' in the dSC state will be a model-dependent one. In the dSC state, they share the same quantum numbers, and both are based on approximate calculations. The origin of the RPA peak may be related to the overestimate of the magnetic instability and we see that it may not be robust against variations of the vertex corrections or variations of the gap, both of which diminish AF instability. On the other hand, the SCLR treatment of the π peak is more robust against these variations. One can test these two approximate schemes within the exact SO(5) models. Only SCLR treatment including the ''π'' process agree with the exact answer in this case. Therefore, calculations including the π process is a better approximation than the simple RPA calculation.

(5) Within our approximations, the spin spectrum consists of an incommensurate structure at low frequencies, a sharp commensurate peak arising from the triplet excitation in the p-p channel (the π peak), and a missing spectral weight at commensurate wave vector at higher frequencies. These features are in overall agreement with experiments. The predicted weight of the π resonance agrees quantitatively with experiments.

Therefore, while each of the above arguments are not complete on their own, the combination of them makes a strong overall case. From the interpretation of the neutron resonance peak in terms of the π mode, we hope to learn a general principle, rather than a specific model for fitting a specific experiment. In strongly correlated systems, most degrees of freedoms are strongly coupled, and most spectra are incoherent. Usually, only a symmetry principle can forbid the decay of a collective excitation. In the case of the resonant neutron-scattering peak, we believe that it is the SO(5) symmetry principle at work, and the π mode is the pseudo-Goldstone boson associated with this spontaneous symmetry breaking. In this paper, we have shown that such an interpretation is consistent with the key experimental facts, but it may not be the only possible interpretation. Its utility lies in the simplicity and generality of the principle, which can be applied to other related experiments and lead to new experimental predictions.

ACKNOWLEDGMENTS

We would like to express our deep gratitude to Dr. R. Eder and W. Hanke for extensive discussions on the numerical results on the t-J model in connection with our present work, and Dr. D. J. Scalapino for his numerous suggestions and constant support during the course of this work. We would also like to gratefully acknowledge useful conversations with Dr. J. Brinckmann, H. F. Fong, H. Fukuyama, B. Keimer, P. Lee, S. Meixner, H. Mook, and B. Normand. This work was supported by the NSF under Grant Nos. DMR-9400372 and DMR-9522915.

APPENDIX: MODEL-INDEPENDENT ESTIMATE OF THE π CONTRIBUTION TO THE SPIN SUSCEPTIBILITY

A spectral function for any two operators A and B is defined as

$$\rho_{A,B}(\omega)\equiv\frac{1}{2\pi i}[D^{\rm ret}_{A,B}(\omega)-D^{\rm adv}_{A,B}(\omega)]$$

$$=\sum_n [\langle 0|A|n\rangle\langle n|B|0\rangle\delta(\omega+E_0-E_n)$$

$$-\langle 0|B|n\rangle\langle n|A|0\rangle\delta(\omega-E_0+E_n)], \quad (A1)$$

where $D^{\rm ret}_{A,B}(\omega)$ and $D^{\rm adv}_{A,B}(\omega)$ are retarded and advanced response functions, respectively, $|n\rangle$'s are eigenstates of the system Hamiltonian with energy E_n, and $|0\rangle$ is the ground state with energy E_0. If we restrict the above summation only to intermediate states that have nonzero overlap with $\pi^\dagger_\alpha|0\rangle$, then such a quantity

$$\rho^{\pi_\alpha}_{A,B}(\omega)=\sum_{n:\langle 0|\pi_\alpha|n\rangle\neq 0}[\langle 0|A|n\rangle\langle n|B|0\rangle\delta(\omega+E_0-E_n)$$

$$-\langle 0|B|n\rangle\langle n|A|0\rangle\delta(\omega-E_0+E_n)] \quad (A2)$$

may be regarded as the contribution of the π excitation to the full spectrum $\rho_{A,B}(\omega)$. We can introduce ω-integrated spectral weight as

$$[\rho^{\pi_\alpha}_{A,B}]^{\omega_2}_{\omega_1}=\int_{\omega_1}^{\omega_2}d\omega\rho^{\pi_\alpha}_{A,B}(\omega). \quad (A3)$$

All of the above spectral functions (or spectral weight) are bilinear with respect to A and B, and have the property $\rho_{A,A^\dagger}\geqslant 0$ for $\omega\geqslant 0$ or $\omega_2\geqslant\omega_1\geqslant 0$. Therefore, the Cauchy-Schwarz inequality holds provided that the same frequency condition is satisfied:[49]

$$\rho_{A,A^\dagger}\rho_{B,B^\dagger}\geqslant|\rho_{A,B^\dagger}|^2. \quad (A4)$$

Here $\rho_{A,B^\dagger}$ can be either of $\rho_{A,B^\dagger}(\omega)$, $\rho^{\pi_\alpha}_{A,B^\dagger}(\omega)$ or $[\rho^{\pi_\alpha}_{A,B^\dagger}]^{\omega_2}_{\omega_1}$.

In Sec. I we derived two sum rules $\int d\omega\rho^{\pi_\alpha}_{\pi_\alpha,\pi^\dagger_\alpha}(\omega)=1-n$ and $\int d\omega\rho^{\pi_\alpha}_{\pi_\alpha,N^\dagger_\alpha}(\omega)=i\Delta$. If most of the π spectrum is accommodated in an interval $(\omega_0-\nu,\omega_0+\nu')$ on the positive real axis and around the π-resonance energy ω_0, we can write

$$[\rho^{\pi_\alpha}_{\pi_\alpha,\pi^\dagger_\alpha}]^{\omega_0+\nu'}_{\omega_0-\nu}\sim 1-n, \quad [\rho^{\pi_\alpha}_{\pi_\alpha,N^\dagger_\alpha}]^{\omega_0+\nu'}_{\omega_0-\nu}\sim i\Delta. \quad (A5)$$

Equation (A4) then immediately gives us

$$[\rho^{\pi_\alpha}_{N_\alpha,N^\dagger_\alpha}]^{\omega_0+\nu'}_{\omega_0-\nu}\gtrsim\frac{|\Delta|^2}{1-n}. \quad (A6)$$

The left-hand side of this equation represents the contribution of the π mode to the spin excitation spectrum (e.g., $\mathrm{Im}\chi^{zz}/\pi$) and the right-hand side gives its lower bound.[50] This is a model-independent result.

Noting that $\mathrm{Im}\chi^{+-}=2\,\mathrm{Im}\chi^{zz}$, we obtain Eq. (12). When applying this result to the present analysis of the t-J model, where $\Delta_0=V_{\rm BCS}\Delta=(3J/2)\Delta$, we have $I_\pi\gtrsim(8/9J^2)[|\Delta_0|^2/(1-n)]$. The analysis in this appendix can be generalized to finite temperatures by considering the spectral function

$$\rho_{A,B}(\omega)=\frac{1}{Z}\sum_{n,m}(e^{-\beta E_n}-e^{-\beta E_m})\langle n|A|m\rangle\langle m|B|n\rangle$$

$$\times\delta(\omega+E_n-E_m). \quad (A7)$$

[1] H. F. Fong, B. Keimer, P. W. Anderson, D. Reznik, F. Dogan, and I. A. Aksay, Phys. Rev. Lett. **75**, 316 (1995).

[2] H. F. Fong, B. Keimer, D. Reznik, D. L. Milius, and I. A. Aksay, Phys. Rev. B **54**, 6708 (1996).

[3] P. Dai, M. Yethiraj, H. A. Mook, T. B. Lindemer, and F. Dogan, Phys. Rev. Lett. **77**, 5425 (1996).

[4] H. F. Fong, B. Keimer, D. L. Milius, and I. A. Aksay, Phys. Rev. Lett. **78**, 713 (1997).

[5] P. Dai, H. A. Mook, and F. Dogan, Phys. Rev. Lett. **80**, 1738 (1998).

[6] P. Bourges, H. Casalta, L. P. Regnault, J. Bossy, P. Burlet, C. Vettier, E. Beaugnon, P. Goutier-Picard, and R. Tournier (unpublished).

[7] E. Demler and S. C. Zhang, Phys. Rev. Lett. **75**, 4126 (1995).

[8] N. Bulut and D. Scalapino, Phys. Rev. B **53**, 5149 (1996).

[9] I. Mazin and V. Yakovenko, Phys. Rev. Lett. **75**, 4134 (1995).

[10] D. Z. Liu, Y. Zha, and K. Levin, Phys. Rev. Lett. **75**, 4130 (1995).

[11] F. Onufrieva, Physica C **251**, 348 (1995).

[12] G. Blumberg, B. P. Stojkovic, and M. V. Klein, Phys. Rev. B **52**, 15 741 (1995).

[13] Y. Zha, V. Barzykin, and D. Pines, Phys. Rev. B **54**, 7561 (1996).

[14] A. J. Millis and H. Monien, Phys. Rev. B **54**, 16 172 (1996).

[15] L. Yin, S. Chakravarty, and P. W. Anderson, Phys. Rev. Lett. **78**, 3559 (1997); P. W. Anderson, J. Phys.: Condens. Matter **8**, 10 083 (1996).

[16] A. Abrikosov (unpublished).

[17] D. J. Scalapino, Phys. Rep. **250**, 329 (1995).

[18] Y. Bazaliy, E. Demler, and S. C. Zhang, Phys. Rev. Lett. **79**, 1921 (1997).

[19] B. Keimer, H. F. Fong, S. H. Lee, D. L. Milius, and I. A. Aksay, Physica C **282-287**, 232 (1997).

[20] S. Meixner, W. Hanke, E. Demler, and S. C. Zhang, Phys. Rev. Lett. **79**, 4902 (1997).

[21] R. Eder, W. Hanke, and S. C. Zhang, cond-mat/9707233 (unpublished).

[22] S. C. Zhang, Science **275**, 1089 (1997).

[23] S. Rabello, H. Kohno, E. Demler, and S. C. Zhang, Phys. Rev. Lett. **80**, 3586 (1998).

[24] C. Henley, Phys. Rev. Lett. **80**, 3590 (1998).

[25] C. Burgess, J. M. Cline, R. MacKenzie, and R. Ray, Phys. Rev. B **57**, 8549 (1998).

[26] G. Baskaran and P. W. Anderson, cond-mat/9706076 (unpublished).

[27] S. C. Zhang, cond-mat/9709289.

[28] M. Greiter, Phys. Rev. Lett. **79**, 4898 (1997).

[29] E. Demler, S. C. Zhang, S. Meixner, and W. Hanke, cond-mat/9705191 (unpublished).

[30] A. Tsvelik, *Quantum Field Theory in Condensed Matter Physics* (Cambridge University Press, Cambridge, 1995).

[31] P. Anderson, Phys. Rev. **112**, 1900 (1958).

[32] G. Rickayzen, Phys. Rev. **115**, 795 (1959).

[33] A. Bardasis and J. R. Schriffer, Phys. Rev. **121**, 1050 (1961).

[34] E. Demler, S. C. Zhang, N. Bulut, and D. Scalapino, Int. J. Mod. Phys. B **10**, 2137 (1996).

[35] T. Kostyrko and R. Micnas, Phys. Rev. B **46**, 11 025 (1992).

[36] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989); C. N. Yang and S. C. Zhang, Mod. Phys. Lett. B **4**, 759 (1990).

[37] S. C. Zhang, Phys. Rev. Lett. **65**, 120 (1990); S. C. Zhang, Int. J. Mod. Phys. B **5**, 153 (1991).

[38] H. Kohno, B. Normand, and H. Fukuyama, in *Proceedings of the 10th Anniversary HTS Workshop* (World Scientific, Singapore, 1996), p. 521; Physica C **282-287**, 1685 (1997).

[39] M. Salkola and J. R. Schrieffer (unpublished).

[40] J. Brinckmann and P. Lee, cond-mat/9710065 (unpublished).

[41] An exact diagonalization study of the Hubbard model (Ref. 29) supports the idea that the π excitation survives strong Hubbard repulsion.

[42] Δ_0 is the energy gap, which is related to the order parameter Δ defined earlier by the relation $\Delta_0 = V_{\mathrm{BCS}}\Delta$ with $V_{\mathrm{BCS}} = 3J/2$.

[43] In principle, the symmetry of the interaction leads to responses in the p-h channel that differ from Eq. (17) by the possible symmetry factors $S_q^\alpha = \Sigma_p \alpha_p c^\dagger_{p+q\uparrow} c_{p\downarrow}$, where α_p may be $(\sin p_x \pm \sin p_y)$ or $(\cos p_x \pm \cos p_y)$. Such $S^\alpha_{q\omega}$ fields provide intermediate states that the spin fluctuations can be scattered into. In general this can modify the amplitude of the induced $S_{q\omega}$ field. However, it turns out that for the q's of interest near $Q = (\pi,\pi)$, the effect of such $S^\alpha_{q\omega}$ fields is negligible.

[44] To avoid the problem of the system being unstable against order parameter fluctuations when the value of the dSC gap is increased from its mean-field value, one may think of the proposed procedure as preserving the self-consistency condition, but taking a bigger value for the BCS coupling constant V_{BCS}, while keeping all the other constants to have the same value. This may be achieved by adding an appropriate interaction to the original t-J Hamiltonian.

[45] We restrict this analysis to the case $q = Q = (\pi,\pi)$.

[46] For unit convention, see Appendix B of Ref. 2.

[47] Note a factor of $\sqrt{2}$ difference in the definitions of Δ_0 here and in Ref. 7, $\Delta_0(\text{present}) = \sqrt{2}\Delta_0$ (Ref. 7).

[48] However, this approximation seems to overemphasize the importance of the anomalous scattering terms in the energy of the π excitation. The anomalous self-energy tends to increase the energy of the resonance, whereas the anomalous scattering decreases it [see Eqs. (40), (41), and (42), for example]. In Secs. III and IV, we saw that in the complete calculations, the resonance energy in the SC state turns out to be above its value in the normal state. However, from Eqs. (43), (44), and (45), we find that the resonance energy in the SC state is decreased, $\omega_s^2 = \omega_0^2 - (2J\Delta_0/V_{\mathrm{BCS}})^2$.

[49] This may be proved as follows. From bilinearity and (semi) positivity, we have $0 \leqslant \rho_{A+\lambda B, A^\dagger + \lambda^* B^\dagger} = \rho_{A,A^\dagger} + \lambda \rho_{B,A^\dagger} + \lambda^* \rho_{A,B^\dagger} + |\lambda|^2 \rho_{B,B^\dagger}$ for any complex number λ. Defining θ as the phase of the mixed correlation function as $\rho_{A,B^\dagger} = \rho^*_{B,A^\dagger} = |\rho_{A,B^\dagger}| e^{i\theta}$, and choosing $\lambda = x e^{i\theta}$ $(-\infty < x < \infty)$, we have $\rho_{A,A^\dagger} + 2x|\rho_{A,B^\dagger}| + x^2 \rho_{B,B^\dagger} \geqslant 0$. Since this inequality holds for any real number x, the inequality (A4) should hold.

[50] The (near) equality holds if and only if there exists such λ that $\langle 0|\pi_\alpha + \lambda N_\alpha|n\rangle = 0$ for all eigenstates $|n\rangle$ satisfying $\langle 0|\pi_\alpha|n\rangle \neq 0$. For example, exact equality holds when π operator is an exact eigenoperator and hence there is only one energy eigenstate which satisfies $\langle 0|\pi_\alpha|n\rangle \neq 0$.

[51] H. Kohno, E. Demler, and S.C. Zhang (unpublished).