Neutron peak in the extended-saddle-point model of high-temperature superconductors

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An explanation is proposed of the maximum at 41 meV in the inelastic spin-flip neutron scattering from $YBa_2Cu_3O_{7-\delta}$, based on the extended-saddle-point model developed by the author in his previous works. It is shown that for appearance of the maximum in the imaginary part of the spin susceptibility a close proximity of the Fermi energy to the extended saddle point is necessary. The energy of the maximum is then close to $2\Delta_{\max}$ in agreement with experiment. Theoretical and experimental evidence concerning the energy of the extended saddle point (flat region) is discussed. Different limiting cases are calculated. A proof is given within the present model that interaction in the final state is small, and hence, no collective modes are formed. A general discussion of the experimental situation is presented.
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I. INTRODUCTION

The famous peak observed in inelastic neutron scattering from single crystals of $YBa_2Cu_3O_{7-\delta}$ (YBCO) (Ref. 1–3) has several characteristic features: (a) It is observed only in spin-flip scattering; (b) until now it was observed only in optimally doped, underdoped, and slightly overdoped YBCO, and in no other material of this kind; (c) it exists only below T_c in optimally doped samples; in underdoped samples a broad peak is observed also above T_c; (d) the momentum transfer is approximately $\mathbf{q}=(\pi,\pi)$ in the ab plane; (e) the dependence on q_z is in favor of a transition with the change of parity of the double-plane electron wave function, e. The energy transfer at the peak is close to 41 meV in optimally doped YBCO and smaller in underdoped samples, at temperatures below T_c; above T_c the position of the peak remains approximately independent on underdoping. The experimental situation is described in detail in two latest review papers.[4,5]

There are principally two different types of explanations of this peak. One was proposed by Zhang:[6,7] it is a collective two-electron mode, which can exist in the normal state, but it is connected to the spin-flip neutron scattering only in the superconducting state. The role of superconductivity is that it can transform an electron into a hole, and therefore, instead of looking for a collective mode in an electron-hole channel, of the type of the ''second sound,'' or spin wave, we have to consider the electron-electron, or hole-hole channel.

Another type of explanation was proposed first in Ref. 3 and then developed in more detail by representatives of the same group[8] and Levin's group[9] in a somewhat different version. The main idea of this approach is that the maximum results from the singular density of states for a two-particle excitation, the interaction of quasiparticles in the final state, which could lead to a collective mode, is relatively small and can be neglected.

In this paper the maximum will be addressed from the viewpoint of our theory that is based on the dominant role of extended saddle-point singularities in the electron spectrum (see Ref. 10 and references therein). Our explanation is close ideologically to the type described in Refs. 8 and 9, despite considerable differences of underlying models. According to it, the maximum is close to $2\Delta_{\max}$ and results from the favorable situation with the densities of the initial and final states in case, if the Fermi level is sufficiently close to the extended saddle point.

The importance of this proximity can be understood from the following reasoning. The process contributing to the scattering cross section is similar to the tunneling current between equal superconductors. It is well known that the tunneling characteristic $I(V)$ at $T=0$ starts with a jump at 2Δ and continues to grow; there is no maximum at this point. Therefore the neutron maximum can appear only as a result of some unusual feature in the electron spectrum, or from their interaction. This situation was mentioned in Ref. 8, where the enhancement in the density of states was due to pair tunneling, and in Ref. 9, where it was ascribed to spin fluctuations.

We will show (Sec. IV) that within the framework of our model the interaction of quasiparticles in the final state is too weak and does not lead to a formation of a collective mode.

II. GENERAL FORMULA

We will first consider a one-layer model, which is sufficient for description of the momentum dependence in the plane, and comment on the q_z dependence later. The magnetic neutron-scattering cross section is proportional to the imaginary part of the spin susceptibility, and the latter is described by two diagrams presented in Fig. 1. The maxi-

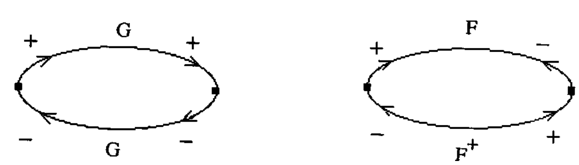

FIG. 1. First-order diagrams for the spin susceptibility.

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mum can be expected for the momentum component $\chi(\mathbf{q})$ with $\mathbf{q}$ in the plane connecting points with the maximal values of the superconducting energy gap that correspond to the vicinities of the extended saddle points, denoted in Ref. 10 as ''a'' and ''b''; this momentum is close to $\mathbf{Q}=(\pi,\pi)$.

We will see that opposite signs of the order parameter at these points are extremely important. This was already mentioned in Ref. 3, and it was stressed there that it provides an independent argument in favor of d-type symmetry of the order parameter, which is free from many objections to other determinations.

In the temperature technique the diagrams of Fig. 1 correspond to

$$\chi(i\Omega,Q)=-T\sum_{\omega}\int dp_x dp_y(2\pi)^{-2}d^{-1}[G_a(\omega,p_x)G_b(\omega-\Omega,p_y)+F_a^{+}(\omega,p_x)F_b(\omega-\Omega,p_y)]$$
$$=-T\sum_{\omega}\int dp_x dp_y(2\pi)^{-2}d^{-1}\times\frac{(i\omega+\xi_a)(i\omega-i\Omega+\xi_b)+\Delta_a\Delta_b}{[\omega^2+\varepsilon_a^2][(\omega-\Omega)^2+\varepsilon_b^2]}. \quad (1)$$

We defined here χ without the factor μ_B^2 (it has the dimensionality of the density of states) and used the fact that in the singular regions ''a'' and ''b'' the spectrum is quasi-one dimensional (see Ref. 10): namely, $\xi_a\approx p_x^2/2m_a-\mu_{1a}$, $\xi_b\approx p_y^2/2m_b-\mu_{1b}$, $\mu_{1a,b}$ being the chemical potential with respect to the corresponding extended saddle-point singularity; d is the period along the c axis. As usual, $\varepsilon_{a,b}^2=\xi_{a,b}^2+\Delta_{a,b}^2$. For simplicity we will consider a tetragonal metal, i.e., the masses and chemical potentials we will assume to be equal, and the Δ's differing only by sign.

Performing the summation over $\omega=2\pi T(n+\frac{1}{2})$, and an analytical continuation to real frequencies, $i\Omega\rightarrow\Omega+i\delta$, we obtain

$$\chi=\int dp_x dp_y(2\pi)^{-2}d^{-1}\Bigg[\frac{\tanh(\varepsilon_a/2T)}{4\varepsilon_a}\times\Bigg(\frac{(\varepsilon_a+\xi_a)(\varepsilon_a-\Omega+\xi_b)-\Delta^2}{(\varepsilon_a-\Omega-i\delta)^2-\varepsilon_b^2}+\frac{(\varepsilon_a-\xi_a)(\varepsilon_a+\Omega-\xi_b)-\Delta^2}{(\varepsilon_a+\Omega+i\delta)^2-\varepsilon_b^2}\Bigg)$$
$$+\frac{\tanh(\varepsilon_b/2T)}{4\varepsilon_b}\Bigg(\frac{(\varepsilon_b+\Omega+\xi_a)(\varepsilon_b+\xi_b)-\Delta^2}{(\varepsilon_b+\Omega+i\delta)^2-\varepsilon_a^2}+\frac{(\varepsilon_b-\Omega-\xi_a)(\varepsilon_b-\xi_b)-\Delta^2}{(\varepsilon_b-\Omega-i\delta)^2-\varepsilon_a^2}\Bigg)\Bigg]. \quad (2)$$

Since the integrals over dp_x and dp_y are symmetric, we can make a substitution $\xi_a\rightleftarrows\xi_b$ in the second term and write both terms as $F(\Omega+i\delta)+F(-\Omega-i\delta)$. If the chemical potential μ_1 were large compared to other energy scales ($\sim\Delta$), we could simply cancel out the odd terms containing $\xi_{a,b}$.

However, as we will see below, the maximum in χ'' appears as a result of the proximity to the singularity, i.e., $\mu_1\lesssim 5\Delta$. The justification of this assumption is a delicate matter. Band-structure calculations based on the local-density approximation (LDA) method for $TlBa_2CaCu_2O_7$,[11] $HgBa_2CuO_4$, $HgBa_2CaCu_2O_6$, and $HgBa_2Ca_2Cu_3O_8$,[12] show that the Fermi energy is close to the extended-saddle-point singularity but not necessarily so close that $\mu_1\lesssim\Delta$. However, these calculations do not take into account the interaction of quasiparticles. This interaction can be of principle importance, as seen from the observed metal-insulator transition in cuprates not predicted by the LDA calculations. There is also a possibility of the so-called ''fermion condensation'' due to interaction of quasiparticles, predicted by V. Khodel *et al.* (see Ref. 13 and references therein), which leads to the appearance of flat regions of the spectrum at the Fermi level. Under such circumstances it is better to rely on experimental data. However, even this is not always the safest thing to do. For high-T_c materials the only existing method is angle resolved photoemission (ARPES). This is a surface probe, and in order to reflect correctly the properties of the bulk material, the surface of the sample must be ideal, i.e., contain no structural defects and no charge. That this is not always the case was shown recently, when the ARPES data for Sr_2RuO_4 were compared with the results of de Haas-van Alphen measurements (see Ref. 14). A great discrepancy for the Fermi surface was found, which is most probably due to the charge on the surface of the sample, which displaces the chemical potential. The only reliable substance is $Bi_2Sr_2CaCu_2O_8$, which can be cleaved along a plane between two BiO planes connected by weak Van-der-Waals forces. For this material the value obtained for μ_1 was indistinguishable from zero.[15]

If $\mu_1\lesssim\Delta$, integrations over positive and negative values of ξ are not symmetric, and the integrals in Eq. (2) can be transformed in the following way:

$$\int_{-\infty}^{\infty}\frac{dp_y}{2\pi}F(\xi_b)\rightarrow\int_{-\mu_1}^{\infty}\frac{(2m)^{1/2}F(\xi_b)d\xi_b}{2\pi(\xi_b+\mu_1)^{1/2}}=\int_0^{\infty}\frac{(2m)^{1/2}F(\xi_b)d\xi_b}{2\pi(\xi_b+\mu_1)^{1/2}}+\int_0^{\mu_1}\frac{(2m)^{1/2}F(-\xi_b)d\xi_b}{2\pi(\mu_1-\xi_b)^{1/2}}. \quad (3)$$

We are actually interested only in the imaginary part of χ, namely, χ''. This part can be obtained from Eq. (2) as resulting from semiresidues of the integral over ξ_b after the substitution $\xi_a\rightleftarrows\xi_b$ in the second term. We get

$$\chi''=(2m)^{1/2}\int_{-\infty}^{\infty}\frac{dp}{2\pi d}\frac{\tanh(\varepsilon/2T)}{4\varepsilon}\left[\frac{\operatorname{sgn}(\varepsilon-\Omega)\,\theta[(\varepsilon-\Omega)^2-\Delta^2]}{|\xi(\varepsilon-\Omega)|}\left(\frac{\varepsilon(\varepsilon-\Omega)+\xi|\xi(\varepsilon-\Omega)|-\Delta^2}{[\mu_1+|\xi(\varepsilon-\Omega)|]^{1/2}}\right.\right.$$
$$\left.+\frac{\varepsilon(\varepsilon-\Omega)-\xi|\xi(\varepsilon-\Omega)|-\Delta^2}{[\mu_1-|\xi(\varepsilon-\Omega)|]^{1/2}}\,\theta(\mu_1-|\xi(\varepsilon-\Omega)|)\right)-\frac{1}{|\xi(\varepsilon+\Omega)|}\left(\frac{\varepsilon(\varepsilon+\Omega)+\xi|\xi(\varepsilon+\Omega)|-\Delta^2}{[\mu_1+|\xi(\varepsilon+\Omega)|]^{1/2}}\right.$$
$$\left.\left.+\frac{\varepsilon(\varepsilon+\Omega)-\xi|\xi(\varepsilon+\Omega)|-\Delta^2}{[\mu_1-|\xi(\varepsilon+\Omega)|]^{1/2}}\,\theta(\mu_1-|\xi(\varepsilon+\Omega)|)\right)\right]. \tag{4}$$

Here $p\equiv p_x$, and all ξ and ε are functions of p; $|\xi(\varepsilon-\Omega)|=[(\varepsilon-\Omega)^2-\Delta^2]^{1/2}$. The integral over dp we transform according to Eq. (3) and pass from the integration over positive ξ to integration over ε:

$$\int_0^a d\xi=\int_\Delta^{[a^2+\Delta^2]^{1/2}}\frac{\varepsilon\,d\varepsilon}{[\varepsilon^2-\Delta^2]^{1/2}}. \tag{5}$$

Since we consider positive Ω, and $\varepsilon>\Delta$, $\varepsilon+\Omega$ will always be larger than Δ. What concerns $\varepsilon-\Omega$, there are two options: either $\varepsilon-\Omega>\Delta$, or $\varepsilon-\Omega<-\Delta$, i.e., $\Delta<\varepsilon<\Omega-\Delta$, and this means $\Omega>2\Delta$. Only the latter integrals are responsible for the maximum of χ'', since the others depend smoothly on Ω around $\Omega=2\Delta$. We can, therefore, significantly reduce the calculations considering only these terms that we denote χ''_m. For simplicity we will put $T=0$. After that, using the symmetry of the integrand with respect to the transformation $\varepsilon\to\Omega-\varepsilon$, we obtain

$$\chi''_m=\frac{m}{2\pi d}\int_0^{\Omega/2-\Delta}d\rho\left[\frac{(\Omega/2)^2-\rho^2+\Delta^2}{|\xi(\Omega/2-\rho)||\xi(\Omega/2+\rho)|}\left(\frac{1}{[\mu_1+|\xi(\Omega/2-\rho)|]^{1/2}}+\frac{\theta(\mu_1-|\xi(\Omega/2-\rho)|)}{[\mu_1-|\xi(\Omega/2-\rho)|]^{1/2}}\right)\left(\frac{1}{[\mu_1+|\xi(\Omega/2+\rho)|]^{1/2}}\right.\right.$$
$$\left.+\frac{\theta(\mu_1-|\xi(\Omega/2+\rho)|)}{[\mu_1-|\xi(\Omega/2+\rho)|]^{1/2}}\right)-\left(\frac{1}{[\mu_1+|\xi(\Omega/2-\rho)|]^{1/2}}-\frac{\theta(\mu_1-|\xi(\Omega/2-\rho)|)}{[\mu_1-|\xi(\Omega/2-\rho)|]^{1/2}}\right)\left(\frac{1}{[\mu_1+|\xi(\Omega/2+\rho)|]^{1/2}}\right.$$
$$\left.\left.-\frac{\theta(\mu_1-|\xi(\Omega/2+\rho)|)}{[\mu_1-|\xi(\Omega/2+\rho)|]^{1/2}}\right)\right]. \tag{6}$$

This part of the susceptibility is zero at $\Omega<2\Delta$ and starts from a finite value at $\Omega=2\Delta+0$.

III. LIMITING CASES

In the case $\mu_1\gg\Omega$ and Δ, all denominators in the square brackets of Eq. (6) become equal to $\mu_1^{1/2}$, the first product becomes equal to $4/\mu_1$ and the second vanishes. We are left with an integral, which starts with a jump at $\Omega=2\Delta$ and then continues to grow with Ω; there is no trace of a maximum. In the opposite limit, $\mu_1=0$, the terms with the θ's vanish, and we come to an integral

$$\chi''_m=\frac{m}{2\pi d}\int_0^{\Omega/2-\Delta}d\rho\left(\frac{(\Omega/2)^2-\rho^2+\Delta^2}{[(\Omega/2-\rho)^2-\Delta^2]^{3/4}[(\Omega/2+\rho)^2-\Delta^2]^{3/4}}-[(\Omega/2-\rho)^2-\Delta^2]^{-1/4}[(\Omega/2+\rho)^2-\Delta^2]^{-1/4}\right). \tag{7}$$

The limiting values are

$$\chi''_m=\frac{m}{4\pi d}\begin{cases}\dfrac{[\Gamma(1/4)]^2}{(2\pi)^{1/2}}\left(\dfrac{\Delta}{\Omega-2\Delta}\right)^{1/2}, & 0<\Omega-2\Delta\ll\Delta\\[2ex] \dfrac{(2\pi)^{3/2}}{[\Gamma(1/4)]^2}\left(\dfrac{\Delta}{\Omega}\right)^{1/2}, & \Omega\gg\Delta,\end{cases} \tag{8}$$

and the full dependence is presented in Fig. 2 (we remind that $\chi''_m=0$ at $\Omega<2\Delta$).

The infinity at $\Omega=2\Delta$ disappears, if μ_1 is finite. There appears, however, another singularity. It is associated with the simultaneous vanishing of the denominators in Eq. (6): $|\xi(\Omega/2-\rho)|^{-1}$ and $[\mu_1-|\xi(\Omega/2+\rho)|]^{-1/2}$. This happens for $\rho=\Omega/2-\Delta$, and $\Omega=\Delta+[\mu_1^2+\Delta^2]^{1/2}$. After some calculations we obtain χ''_m in this vicinity;

$$\chi''_m\approx\frac{m}{\sqrt{2}\pi d}\frac{[\Delta+(\Delta^2+\mu_1^2)^{1/2}]\Delta^{1/2}}{\mu_1(\Delta^2+\mu_1^2)^{1/4}}\times\ln\left(\frac{2[(\Delta^2+\mu_1^2)^{1/2}-\Delta]}{|\Omega-[(\Delta^2+\mu_1^2)^{1/2}+\Delta]|}\right). \tag{9}$$

If one takes into account that the quasiparticle energy is

$$\varepsilon=[(p_x^2/2m-\mu_1)^2+\Delta^2]^{1/2}, \tag{10}$$

or the same with p_y, one sees that it has a minimal value Δ at $p_x=\pm(2m\mu_1)^{1/2}$ and also a maximum $(\mu_1^2+\Delta^2)^{1/2}$ at $p_x=0$. At these values there are maxima in the 1-particle density of states. The excitation energy $\Omega=\Delta+[\mu_1^2+\Delta^2]^{1/2}$ means that the transition occurs with excitation of an electron near the minimum in the vicinity of one extended saddle point and a hole near the maximum in the vicinity of

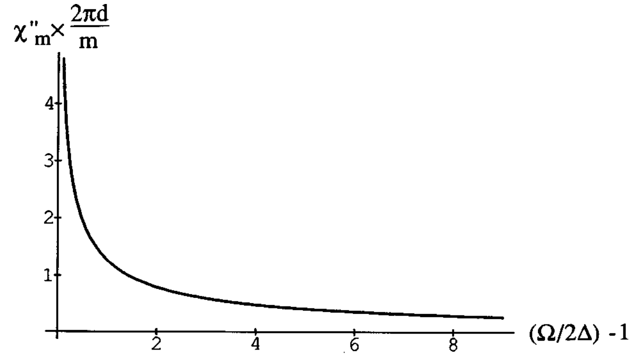

FIG. 2. Plot of $\chi''_m \times 2\pi d/m$, as function of $(\Omega/2\Delta)-1$ in the case $\mu_1=0$.

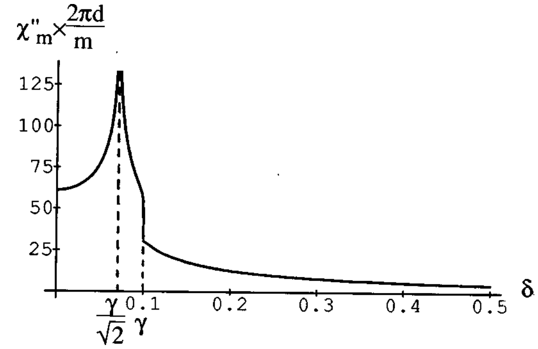

FIG. 3. Plot of $\chi''_m \times 2\pi d/m$, as function of $\delta \equiv (\Omega/\Delta-2)^{1/2}$ in the case $\gamma \equiv \mu_1/\Delta = 0.1$.

the other saddle point. One can easily see that this Ω is not a threshold. Such a singularity makes sense, if μ_1 is comparable with Δ. Otherwise it is moved far away from the interesting region. Since it is logarithmic, it can be rounded by a finite temperature, disorder, or simply by the deviation of the real band from the idealized flat behavior.

In the case $\Omega/\Delta - 2 \ll 1$, $\mu_1/\Delta \ll 1$, Eq. (6) transforms into

$$\chi''_m = \frac{m}{2\pi d\delta} \int_0^1 \frac{dz}{(1-z^2)^{1/2}} \{[\gamma/\delta + (1-z)^{1/2}]^{-1/2} + [\gamma/\delta - (1-z)^{1/2}]^{-1/2}\}\{[\gamma/\delta + (1+z)^{1/2}]^{-1/2} + [\gamma/\delta - (1+z)^{1/2}]^{-1/2}\}, \tag{11a}$$

if $\delta \equiv (\Omega/\Delta-2)^{1/2} < \gamma/\sqrt{2}$, where $\gamma \equiv \mu_1/\Delta$, $z=\rho/(\Omega/2-\Delta)$;

$$\chi''_m = \frac{m}{2\pi d\delta} \left(\int_0^1 \frac{dz}{(1-z^2)^{1/2}} \{[\gamma/\delta + (1-z)^{1/2}]^{-1/2} + [\gamma/\delta - (1-z)^{1/2}]^{-1/2}\}[\gamma/\delta + (1+z)^{1/2}]^{-1/2} + \int_0^{(\gamma/\delta)^2-1} \frac{dz}{(1-z^2)^{1/2}} \{[\gamma/\delta + (1-z)^{1/2}]^{-1/2} + [\gamma/\delta - (1-z)^{1/2}]^{-1/2}\}[\gamma/\delta - (1+z)^{1/2}]^{-1/2} \right), \tag{11b}$$

if $\gamma > \delta > \gamma/\sqrt{2}$;

$$\chi''_m = \frac{m}{2\pi d\delta} \left(\int_0^1 \frac{dz}{(1-z^2)^{1/2}} [\gamma/\delta + (1-z)^{1/2}]^{-1/2} \times [\gamma/\delta + (1+z)^{1/2}]^{-1/2} + \int_{1-(\gamma/\delta)^2}^1 \frac{dz}{(1-z^2)^{1/2}} \times [\gamma/\delta - (1-z)^{1/2}]^{-1/2} [\gamma/\delta + (1+z)^{1/2}]^{-1/2} \right), \tag{11c}$$

if $\delta > \gamma$.

According to (9), χ''_m has a logarithmic singularity at $\delta = \gamma/\sqrt{2}$:

$$\chi''_m \approx \frac{m\sqrt{2}}{\pi d\gamma} \ln\left(\frac{\gamma/\sqrt{2}}{|\gamma/\sqrt{2} - \delta|} \right). \tag{9$'$}$$

In the limit $\delta \to \gamma - 0$ the second integral in Eq. (11b) is equal to π, and hence, at this point χ''_m has a discontinuity. The plot of $\chi''_m(\delta)$ for $\gamma=0.1$ is presented in Fig. 3. Similar results were obtained in Refs. 16 and 17 for a somewhat different model.

The complicated form presented in Fig. 3 differs from a simple maximum, since it contains a threshold at 2Δ and a subsequent maximum, Exactly such a form was observed in recent detailed measurements[5] for optimally doped and underdoped samples. As far as I know, this form appeared only in Refs. 16 and 17 and in the present calculation.

Now we turn to the dependence on q_z. The experimental results[18] indicate that if the dependence of the cross section is represented as a superposition of terms, proportional to $\sin^2(\pi q_z c)$ and $\cos^2(\pi q_z c)$, where c is the distance between the two layers forming a CuO_2 bilayer, the maximum appears only in the term, proportional to $\sin^2(\pi q_z c)$. This is evidence that the tunneling between these layers is important, and the transition takes place between electron states of different parity with respect to permutation of the planes. The only paper, where this issue was addressed theoretically, is Ref. 9, and the explanation is rather complicated.

Actually, the same can be described in different terms, namely, that the maximum appears only when the neutron interacts with the electron spin fluctuation that is odd with respect to permutation of spins in both layers. Indeed, if we introduce odd and even operators

$$\psi_e = 2^{-1/2}(\psi_1 + \psi_2), \quad \psi_0 = 2^{-1/2}(\psi_1 - \psi_2),$$

then

$$\psi_1^+ \sigma \psi_1 - \psi_2^+ \sigma \psi_2 = \psi_e^+ \sigma \psi_0 + \psi_0^+ \sigma \psi_e .$$

The odd fluctuation corresponds to the odd spin wave in the antiferromagnetic phase. Contrary to the even spin wave, it has no gap, and this is quite natural, since the exchange interaction between spins is invariant with respect to rotation, and in the ground state the spins of the nearest Cu atoms in the bilayer have opposite directions. In the metallic phase there is no antiferromagnetic order, and hence, no spin waves. That means that a spin wave decays rapidly into other excitations. The only exception is the odd fluctuation with zero exchange energy, and this is the one which corresponds

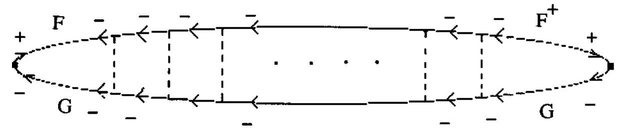

FIG. 4. Diagram for the spin susceptibility with interaction of electrons in the final state.

to the neutron maximum. Although this argument is rather qualitative, it is sufficient to demonstrate that the $\sin^2(\pi q_z c)$ dependence has nothing to do with superconductivity and cannot serve as an argument for selection of the proper microscopic concept.

IV. ABSENCE OF A COLLECTIVE MODE

Let us check the existence of a collective mode. Consider the diagram of Fig. 4. The inner part is a Bethe-Salpeter type chain, and its pole could lead to collective mode. The repeated element is

$$\Pi = gT \sum_{|\omega_1| < \omega_0} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left(\frac{\kappa^2}{k^2+\kappa^2}\right)^n G_a(-\omega+\omega_1, -p_x + k_x) G_b(\omega-\omega_1 - xQ, p_y - k_y), \tag{12}$$

where we inserted the interaction used in our previous papers (see, e.g., Ref. 19):

$$V(\mathbf{k},\omega_1) = -g\left(\frac{\kappa^2}{k^2+\kappa^2}\right)^n \theta(\omega_0 - |\omega_1|); \tag{13}$$

here $n \geqslant 1$, and ω_0 is the characteristic phonon frequency. It was assumed that the main part of the sum and integral corresponds to energies much larger than Δ (this will be confirmed below), and therefore, only the Green functions of the normal metal were left in Eq. (12). After substitution of these Green functions

$$G_{a,b} = [i\omega - (p_{x,y}^2/2m) - \mu_1]^{-1}, \tag{14}$$

summation over ω_1, continuation to real Ω, and taking into account that due to the presence in the diagram of Fig. 4 of two F functions, only values of $p_{x,y} \sim (2m\mu_1)^{1/2}$, $(2m\Delta)^{1/2} \ll k$ are important, we obtain

$$\Pi = g \int_0^\infty \frac{dk_z}{2\pi} \left(\frac{\kappa^2}{k_z^2+\kappa^2}\right)^n \int \frac{dk_x dk_y 2m(2\pi)^{-2}}{k_x^2+k_y^2+2m(\Omega-2\mu_1)+i\delta}. \tag{15}$$

The second integral is logarithmic in the region

$$k_z^2 \sim \kappa^2 \gg k_x^2 + k_y^2 \gg \max(\Omega, \mu_1, \Delta).$$

Therefore, by order of magnitude

$$\Pi \sim gm\kappa \ln\left[\frac{\kappa^2/m}{\max\ (\Omega,\mu_1,\Delta)}\right]. \tag{16}$$

After summation of all diagrams of the type presented in Fig. 4 we get a geometric progression, and the pole will be at $\Pi = 1$. On the other hand, the interaction constant g in Eq. (16) can be expressed in terms of Δ. In the case $\mu_1 \ll \Delta$, we obtain (see Ref. 20) $g \sim (\Delta/m)^{1/2}\kappa^{-2}$. Substituting into the expression (16) we get

$$\Pi \sim \frac{(\Delta m)^{1/2}}{\kappa} \ln\left(\frac{\kappa^2/m}{\max\ (\Omega,\mu_1,\Delta)}\right). \tag{16a}$$

The first factor in this expression is very small—this is the basis of our model—and the log cannot be so large, as to make $\Pi \sim 1$. Therefore, in this case $\Pi \ll 1$. In the opposite limiting case, $\mu_1 \gg \Delta$ (see Ref. 20) $g \sim (\mu_1/m)^{1/2}\kappa^{-2}/\ln(\mu_1/\Delta)$. Hence, in this case

$$\Pi \sim \frac{(\mu_1 m)^{1/2}}{\kappa} \frac{\ln\{\kappa^2/[m \times \max\ (\Omega,\mu_1,\Delta)]\}}{\ln(\mu_1/\Delta)}. \tag{16b}$$

The first factor here is small, and again, the other factor cannot compensate it. Therefore, in this case Π is also small. So we see that in both cases the equation $\Pi = 1$ cannot be satisfied. Therefore, the interaction of quasiparticles in the final state is insufficient for formation of a collective mode.

V. DISCUSSION

The parameter Δ in all our formulas corresponds to the maximal gap. It can be found as the voltage at the maximum in the tunneling conductance. For optimally doped YBCO it corresponds to 19–25 meV.[21] The value is somewhat sample dependent but, anyhow, 2Δ fits the generally accepted energy of the neutron maximum, 41 meV. If we use our interpretation of Fig. 3 for the initial rise of χ'', observed in Ref. 5, then 2Δ will be somewhat smaller, but for $\mu_1 \lesssim \Delta$ the interpretation of tunneling data is not so straightforward.

In order to have a further check it would be fine to have the same data for other substances. Such measurements were performed by Fong *et al.*[22] on underdoped YBCO, and the energy of the maximum varied proportional to T_c. Unfortunately, no reliable data on Δ exist for such samples. It is important, however, to remind that our calculations were based on the ideas of the BCS theory. If this theory describes correctly the high-T_c cuprates, and this is likely for optimally doped and overdoped samples, then Δ varies proportional to T_c and can be defined from the maximum of the tunneling conductance vs voltage curve. For underdoped samples the validity of the BCS-type approach is doubtful. This is most clearly seen from the data on underdoped $Bi_2Sr_2CaCu_2O_{8-\delta}$ (BSCCO) where the ARPES experiments demonstrated the existence of a pseudogap. Recently it was shown[23] that for such samples the voltage corresponding to the maximum of the tunneling conductance first increases with underdoping, contrary to T_c, and then starts to fall. For overdoped samples both quantities decrease monotonically with overdoping. One has to take into account that the neutron maximum was found only in YBCO, whereas the above mentioned pseudogap measurements were performed on BSCCO. Nevertheless, there are indications of a pseudogap in YBCO in the form of a ‘‘spin gap.’’[24]

Since the neutron maximum disappears above T_c (we are not speaking here about the broad maximum in underdoped samples above T_c) it is definitely connected with the existence of superconductivity, and the location of the maximum does not correspond to the binding energy of ‘‘preformed pairs,'' if this concept for the pseudogap is correct. Then what is it, and could there be any other possible measurements of this energy? A possible interpretation is that the spin fluctuation corresponding to zero exchange energy and $q=0$ (with q defined with respect to the antiferromagnetic wave vector) has a long correlation length, and it is measuring not the local pseudogap but the averaged quantity characterizing the supercurrent. A definite answer can be given only by a theory incorporating the pseudogap. Therefore, the complete solution of the problem requires further work, both experimental and theoretical.

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