Spin Fluctuations of *d*-Wave Superconductors

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(Received 22 November 1993)

The dynamic spin correlation function near the commensurate point $\mathbf{Q}=(\pi,\pi)$ in the superconducting state is calculated within mean field theory. We take the generalized t-J model as used by Tanamoto *et al.* For d-wave superconductor at $T=0$ K, we find that there will be no energy gap at incommensurate point, while the energy gap $E_g=2\mu$ develops at commensurate point in the particle-hole channel. On the other hand for s-wave superconductor a large energy gap develops irrespective of the nature of antiferromagnetic fluctuations. Therefore the d-wave model describes the neutron scattering data from both $La_{1.86}Sr_{0.14}CuO_4$ by Mason *et al.* and $YBa_2Cu_3O_{6+x}$ by Rossat-Mignod *et al.* quite well, while the s-wave model is incompatible with these results.

PACS numbers: 74.72.–h, 74.25.Ha

Recently a number of people [1–5] proposed that the d-wave superconductor is a good candidate for high T_c copper oxide superconductors. The linear T dependence of the superfluid density observed [6] in YBaCuO, the angle resolved photoemission experiment [7] in BiSrCaCuO, and the π shift in the Josephson interference experiment [8,9] favor the d-wave model.

In this Letter we report our theoretical results on the dynamical spin correlation function in the superconducting state in the vicinity of the commensurate point $\mathbf{Q}=(\pi,\pi)$ within the generalized t-J model [10]. However, unlike Tanomoto, Kohno, and Fukuyama [10], we interpret the fermion loop in terms of ordinary hole [11] rather than spinon. In this scheme the superconducting correlation is easily incorporated. Further, the spin exchange term provides the necessary attractive interaction for the d-wave model [1], while for the s-wave model we have to introduce an additional pairing interaction. Within the mean field theory the spin correlation function is given by [10,11]

$$\chi(\mathbf{q},\omega)=\chi_0(\mathbf{q},\omega)[1+J(\mathbf{Q}+\mathbf{q})\chi_0(\mathbf{q},\omega)]^{-1}, \tag{1}$$

where

$$J(\mathbf{Q}+\mathbf{q})=J(\cos(\pi+q_x)+\cos(\pi+q_y)) = -J(\cos q_x+\cos q_y), \tag{2}$$

and $\chi_0(\mathbf{q},\omega)$ is obtained from

$$\chi_0(\mathbf{q},i\omega_\nu)=2T\sum_n\int\frac{d^2k}{(2\pi)^2}\frac{-\omega_n\omega_{n+\nu}+\xi_k\xi_{k'}+\Delta_k\Delta_{k'}}{(\omega_n^2+\xi_k^2+\Delta_k^2)(\omega_{n+\nu}^2+\xi_{k'}^2+\Delta_{k'}^2)} \tag{3}$$

by analytical continuation [12], $\mathbf{k}'=\mathbf{k}+\mathbf{Q}+\mathbf{q}$, and $\mathbf{q}$ is the momentum measured from the commensurate point. Within the t-J model we have

$$\xi_k=-2t(\cos k_x+\cos k_y)-\mu, \tag{4}$$

where t is the renormalized transfer integral due to the electron-electron interaction and μ is the chemical potential. In the following analysis we take $t=50$ meV both for $La_{1.86}Sr_{0.14}CuO_4$ and for $YBa_2Cu_3O_{6+x}$, consistent with recent specific heat data [13].

The $\mathbf{k}$ integrals in Eq. (3) are easily done for small $\mathbf{q}$ and not too small μ [12],

$$\chi_0(\mathbf{q},\omega)=2N_0[\Lambda_s-F(\mathbf{q},\omega)], \tag{5}$$

where

$$\Lambda_s=\begin{cases}\ln\left(\dfrac{8\gamma|t|}{\pi T}\right) & \text{for } T>T_c,\\[2ex] \ln\left(\dfrac{8\gamma|t|}{\pi T_c}\right) & \text{for } T<T_c \text{ and } s \text{ wave},\end{cases} \tag{6}$$

$$\Lambda_s=\int_0^{4|t|}dE\left\langle\mathrm{Re}\frac{1}{\sqrt{E^2-\Delta^2|f|^2}}\right\rangle\tanh\left(\frac{\beta}{2}E\right) \quad \text{for } T<T_c \text{ and } d \text{ wave}, \tag{7}$$

$$F=\begin{cases}\left\langle\dfrac{\eta^2-\frac{1}{4}\omega^2}{\Delta^2|f|^2}f(\eta,\omega)\right\rangle & \text{for } d \text{ wave}, & (8)\\[2ex] \Delta^{-2}\langle(\eta^2+\Delta^2-\frac{1}{4}\omega^2)f(\eta,\omega)\rangle & \text{for } s \text{ wave}, & (9)\end{cases}$$

and η is the parameter describing the imperfect nesting

$$\eta=2t[\sin(\tfrac{1}{2}q_x)\pm\sin(\tfrac{1}{2}q_y)]\sin(2\phi)-\mu \tag{10}$$

and

$$\Delta_k=\Delta f=\begin{cases}\Delta\cos(2\phi) & \text{for } d \text{ wave},\\ \Delta & \text{for } s \text{ wave},\end{cases} \tag{11}$$

and $\langle\,\rangle$ means the average over ϕ. The + sign in Eq. (10) has to be taken in the first and third quadrants while the − sign in the second and fourth in the k_x-k_y plane. Finally $f(\eta,\omega)$ is the generalized superfluid density [14].

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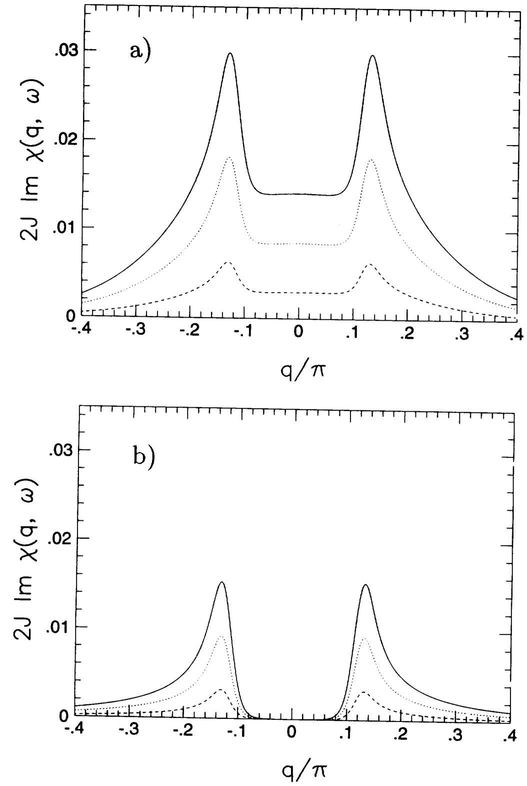


FIG. 1. $2J\,\mathrm{Im}\chi(\mathbf{q},\omega)$ for two q scans at $T=T_c$ (=33 K) and for $\omega=6$ meV (——), 3.5 meV (· · ·), and 1.2 meV (---). (a) Q_δ scan and (b) Q_γ scan.

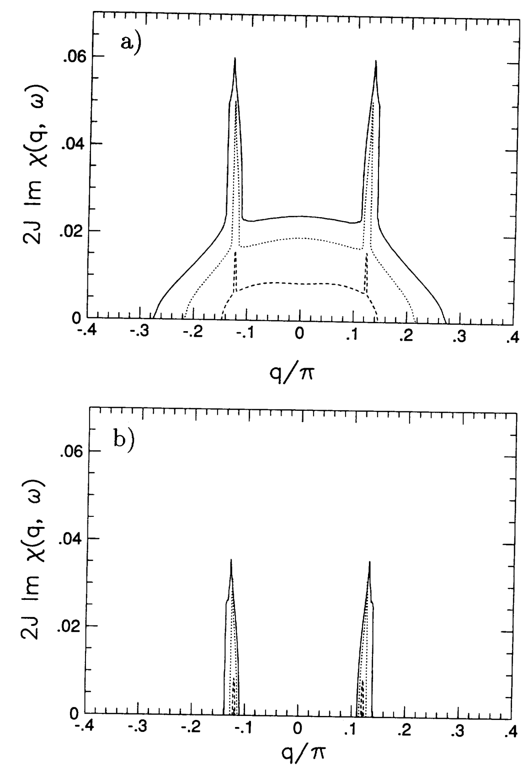


FIG. 2. $2J\,\mathrm{Im}\chi(\mathbf{q},\omega)$ for two q scans at $T=0$ K and for $\omega=6$ meV (——), 3.5 meV (· · ·), and 1.2 meV (---). (a) Q_δ scan and (b) Q_γ scan. Note the change in the vertical scale.

When $T>T_c$, the F function in Eq. (8) is simplified as [14]

$$F=\frac{1}{2}\left\langle \psi\left(\frac{1}{2}+\frac{i(\eta+\frac{1}{2}\omega)}{2\pi T}\right)+\psi\left(\frac{1}{2}-\frac{i(\eta-\frac{1}{2}\omega)}{2\pi T}\right)\right\rangle -\psi(\tfrac{1}{2}), \tag{12}$$

where $\psi(z)$ is the digamma function. If we substitute $\chi_0(q,\omega)$ in Eq. (1), our $\chi(\mathbf{q},\omega)$ reproduces in essence the numerical result by Tanomoto, Kohno, and Fukuyama [10]. In Figs. 1(a) and 1(b) we show $2J\,\mathrm{Im}\chi(\mathbf{q},\omega)$ at $T=T_c(=33$ K) and for $\omega=6$, 3.5, and 1.2 meV for two q scans: $\mathbf{Q}_\delta$ scan; $\mathbf{q}=(q+\frac{1}{2}q_0,q-\frac{1}{2}q_0)$ and $q_0=0.245\pi$ and $\mathbf{Q}_\gamma$ scan; $\mathbf{q}=(q,q)$ which may be compared with the neutron scattering data from $La_{1.86}Sr_{0.14}$–CuO_4 by Mason *et al.* [15]. As easily seen $\mathrm{Im}\chi(\mathbf{q},\omega)$ in the first scan has rather extended plateaus between two peaks corresponding to the incommensurate points; otherwise the theory reproduces the neutron scattering data quite well [15]. We took $\mu=435.5$ K, so that the incommensurate peak appears at $\mathbf{q}=(\pm q_0,0)$ and $(0,\pm q_0)$. We have chosen here $4JN_0=0.25$ where N_0 is the density of states at the Fermi surface per spin. When $T=0$ K, on the other hand, we obtain

$$\Lambda_s=\ln(8\gamma|t|/\pi T_c)+\tfrac{1}{2} \tag{13}$$

and

$$F=\left\langle \left(\frac{\eta^2-\frac{1}{4}\omega^2}{\Delta^2|f|^2+\eta^2-\frac{1}{4}\omega^2}\right)^{1/2} \operatorname{arcsinh}\left(\frac{\eta^2-\frac{1}{4}\omega^2}{\Delta|f|}\right)\right\rangle \tag{14}$$

for the d-wave superconductor. The real part of $\chi_0(q,0)$ [or equivalently $F(\omega=0)$] has already been evaluated numerically by Konno [16]. Indeed our analytical result [12] reproduces his numerical result quite well . Since $\mathrm{Im}F$ is given by

$$\mathrm{Im}F=\frac{\pi}{2}\left\langle \left(\frac{\frac{1}{4}\omega^2-\eta^2}{\frac{1}{4}\omega^2-\eta^2-\Delta^2|f|^2}\theta\right)^{1/2}(\tfrac{1}{4}\omega^2-\eta^2-\Delta^2|f|^2)\right\rangle, \tag{15}$$

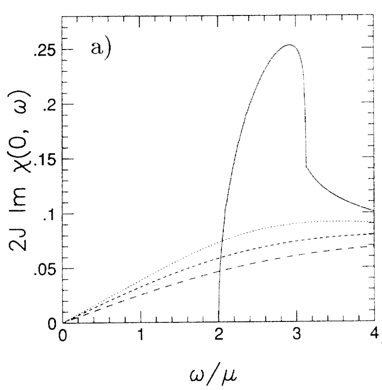
$\mathrm{Im}\chi(\mathbf{q},\omega)$ is gapless at the incommensurate points $(\mathbf{q}_0,0)$, $(0,\mathbf{q}_0)$, etc. In Figs. 2(a) and 2(b), $2J\,\mathrm{Im}\chi(\mathbf{q},\omega)$ at $T=0$ K for the same $\mathbf{q}$ scans as in Figs. 1(a) and 1(b). Except for the fact that the theoretical curves have more structures, the theory reproduces fairly well the experimental data at $T=4.5$ K by Mason *et al.* [15]. We have repeated a similar analysis for s-wave superconductors. Contrary to the d-wave superconductor, the scattering intensity at $T=4.5$ K for the s-wave superconductor should be less than 10^{-5} for both q scans, since the energy gap is larger than 2Δ for all $\mathbf{q}$ values and $|\omega|<2\Delta$ with Δ the energy gap at $T=0$ K, $\mathrm{Im}\chi(q,\omega)\propto e^{-\Delta}/T$. Therefore we conclude that the neutron scattering data [16] from $La_{1.86}Sr_{0.14}CuO_4$ definitely favor the d-wave model.

For the $YBa_2Cu_3O_{6+x}$ system $\mathrm{Im}\chi(\mathbf{q},\omega)$ has a clear peak [17] at $\mathbf{q}=0$ (the commensurate point). Then it is immediately clear that the observed spin gap E_g is in conflict with the s-wave model. For the d-wave model the energy gap in the particle-hole channel is given by 2μ just as in the normal state [10]. In particular at $T=0$ K, $\mathrm{Im}F(0,\omega)$ for the d-wave model is given by

$$\mathrm{Im}F(0,\omega)=\begin{cases}\dfrac{\sqrt{\frac{1}{4}\omega^2-\mu^2}}{\Delta}K\left(\dfrac{\sqrt{\frac{1}{4}\omega^2-\mu^2}}{\Delta}\right) & \text{for } 2\mu<\omega<2\sqrt{\mu^2+\Delta^2},\\ K\left(\dfrac{\Delta}{\sqrt{\frac{1}{4}\omega^2-\mu^2}}\right) & \text{for } \omega>2\sqrt{\mu^2+\Delta^2},\end{cases} \tag{16}$$

where $K(z)$ is the complete elliptic integral.

In Figs. 3(a) and 3(b) we show $2J\,\mathrm{Im}\chi(0,\omega)$ for $T=2T_c$, $1.5T_c$, T_c, and 0 K for $YBa_2Cu_3O_{6.92}$ and $YBa_2Cu_3O_{6.51}$, respectively, as functions of ω. Here we took $\mu=14$ and 2 meV and $T_c=91$ and 47 K, respectively. The theoretical curves reproduce qualitatively the neutron scattering data, especially the peak at 41 meV in $YBa_2Cu_3O_{6.91}$ at low temperatures, though a shoulder near 30 meV is missing [18]. Therefore we conclude again that the d-wave model gives a qualitative description of the neutron scattering data by Rossat-Mignod *et al.* [17]. Further, since the energy gap E_g at the commensurate point scales with 2μ, we expect the second plateaux in the E_g-T_c diagram [16] between $T_c=59$ and 90 K. On the other hand in the s-wave model, the corresponding energy gap is $E_g=2(\mu^2+\Delta^2)^{1/2}$, and again it is incompatible with the neutron scattering data by Rossat-Mignod *et al.*



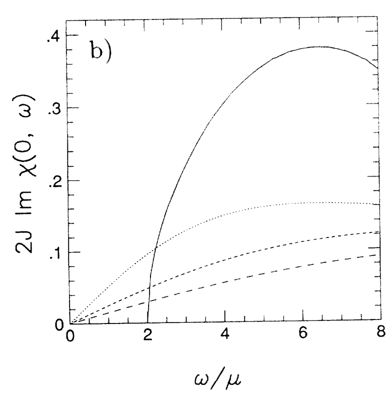


FIG. 3. $2J\,\mathrm{Im}\chi(0,\omega)$ for $T=2T_c$ (— —), $1.5T_c$ (------), T_c (···), and 0 K (——) are shown for (a) $\mu=14$ meV and $T_c=91$ K and (b) $\mu=2$ meV and $T_c=47$ K.

In summary we have incorporated the superconducting correlation in spin fluctuation within mean field theory. We show that the d-wave model describes the neutron scattering data from both $La_{1.86}Sr_{0.14}CuO_4$ and $YBa_2Cu_3O_{6+x}$ reasonably well, while the s-wave model is incompatible with these data in the absence of substantial pair breaking. More details of this work will be published elsewhere. After completing this work we learned that Tanomoto, Kohno, and Fukuyama [19] have done work parallel to ours within the RVB scheme. Their result is similar to ours in general but different in details. For example, they predict a nonvanishing spin gap even at the incommensurate points in contrast to the present result.

We are grateful to Thom Mason and Jean Rossat-Mignod for enlightening discussions on their neutron scattering data from $La_{1.86}Sr_{0.14}CuO_4$ and $YBa_2Cu_3O_{6+x}$, respectively. We also benefited from the insight and suggestions of Fusayoshi Ohkawa. K.M. gratefully acknowledges a Japan Society of Promotion of Science Fellowship while H. W. gratefully acknowledges a Korean Science and Engineering Foundation travel grant, which made our stay in Japan enjoyable. We are also grateful for the hospitality of Yukawa Institute for Theoretical Physics. The present work is in part supported by National Science Foundation under Grant No. DMR92-18317.

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