

Spin dynamics in D -wave superconductors

Hyekyung Won* and Kazumi Maki†

Department of Physics, Hokkaido University, Sapporo 060, Japan

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The dynamic spin-correlation function in the superconducting states (i.e., D wave and S wave) in the vicinity of the commensurate point $\mathbf{Q}=(\pi, \pi)$ is obtained within mean-field theory. As a model we take the generalized t - J model as analyzed by Tanamoto, Kohno, and Fukuyama though we interpret the fermion loop as associated with a renormalized hole. For $T \geq T_c$ where T_c is the superconducting transition temperature our result is essentially the same as Tanamoto, Kohno, and Fukuyama, but the superconducting correlation is easily incorporated within the present scheme. We find recent neutron-scattering data from both $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ by Mason *et al.* and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ by Rossat-Mignod *et al.* are consistent with the D -wave model but incompatible with the S -wave model.

I. INTRODUCTION

Recently, a number of people¹⁻⁵ proposed that the D -wave superconductor is a more appropriate candidate for high- T_c superconductors. In particular the linear T dependence of the superfluid density observed⁶ in Y-Ba-Cu-O (YBCO), the angle-resolved photoemission experiment⁷ Bi-Sr-Ca-Cu-O (BSCCO), and π shift in the Josephson interference experiment^{8,9} appear to favor the D -wave model.

The object of this paper is to study the spin fluctuation in the superconducting state (i.e., D wave and S wave) in the vicinity of the commensurate point $\mathbf{Q}=(\pi, \pi)$ within the generalized t - J model.¹⁰ Indeed our result in the normal state in essence reproduces the result by Tanamoto, Kohno, and Fukuyama¹⁰ (TKF). However, unlike TKE, we interpret the fermion loop as due to ordinary holes¹¹ rather than spinons albeit the hole mass has to be renormalized from the original t in parallel to TKF. Then in this scheme it is easy to incorporate the superconducting correlation within mean-field approximation. In particular for D -wave model the spin exchange term in the t - J model provides the necessary pairing interaction,¹ while for S -wave model we have to supplement an additional pairing interaction. We find that $\chi(\mathbf{q}, 0)$ for $T \leq T_c$ is essentially the same as the one at $T = T_c$ for D -wave superconductor while it decreases somewhat for $T < T_c$ for S -wave superconductor where \mathbf{q} is the momentum measured from the commensurate point. More interesting is the presence of the energy gap E_g at $T = 0$ K, which is defined by the minimum value of $2[(\mu - \mathbf{v} \cdot \mathbf{q})^2 + \Delta^2 |f|^2]^{1/2}$ on the Fermi surface where μ is the chemical potential, \mathbf{v} is the Fermi velocity and $f = \cos(2\phi)$ and 1 for D - and S -wave superconductor, respectively, and ϕ is the angle \mathbf{v} makes from the a axis. In particular the presence of the chemical-potential term in the energy gap has been noted already by TKF. This implies first of all that the neutron-scattering data from $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ reported by Mason *et al.*¹² and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ by Rossat-Mignod *et al.*^{13,14} are compatible with the D -wave model but not with the S -wave model. As we shall see our model repro-

duces all the qualitative features of the data by Mason *et al.*¹² as well as by Rossat-Mignod *et al.*,^{13,14} though the peaks we predict are in general much sharper and contain fine structures not revealed by experiment. Therefore we conclude that D -wave model can describe most of the features observed by the neutron-scattering experiment, while the S -wave model cannot in the absence of significant pair breaking.

II. THEORETICAL MODEL

The spin-spin correlation in the t - J model is calculated as^{10,11}

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

where

$$\begin{aligned} J(\mathbf{Q} + \mathbf{q}) &= J[\cos(\pi + q_x) + \cos(\pi + q_x)] \\ &= -J(\cos q_x + \cos q_y) \end{aligned} \quad (2)$$

and $\chi_0(\mathbf{q}, \omega)$ is obtained by analytical continuation from $\chi_0(\mathbf{q}, i\omega_\nu)$;

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

and $\mathbf{k}' = \mathbf{k} + \mathbf{Q} + \mathbf{q}$ and \mathbf{q} is the momentum measured from the commensurate point.

In the t - J model we have

$$\xi_k = -2t^*(\cos k_x + \cos k_y) - \mu, \quad (4)$$

where μ is the chemical potential and t^* is the renormalized t due to the interaction. In the later numerical calculation we choose $t^* = 50$ meV both for $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6.92}$ consistent with recent specific-heat data by Loram *et al.*¹⁵

We can simplify the integrals in Eq. (3) by introducing new variables by

$$\begin{aligned}\xi_k &= \xi + \eta, \\ \xi_{k'} &= -\xi + \eta,\end{aligned}\quad (5)$$

where

$$\begin{aligned}\xi &= -2t^* [\cos(\frac{1}{2}q_x) \cos k_x + \cos(\frac{1}{2}q_y) \cos k_y], \\ \eta &= 2t^* [\sin(\frac{1}{2}q_x) \sin k_x + \sin(\frac{1}{2}q_y) \sin k_y] - \mu.\end{aligned}\quad (6)$$

Then replacing the k integrals by $(2\pi)^{-1} N_0 d\xi d\phi$ for not too small μ , which amounts to ignoring the van Hove singularity, we can simplify the integral for small q ;

$$\begin{aligned}(2N_0)^{-1} \chi_0(\mathbf{q}, \omega) \\ = \int_0^{4|t^*|} dE \operatorname{Re} \left\langle \frac{1}{\sqrt{E^2 - \Delta^2 |f|^2}} \right\rangle \tanh(\frac{1}{2}\beta E) - F(\mathbf{q}, \omega),\end{aligned}\quad (7)$$

where

$$F(\mathbf{q}, \omega) = \frac{1}{2} [F(y_+, \omega) + F(y_-, \omega)], \quad (8)$$

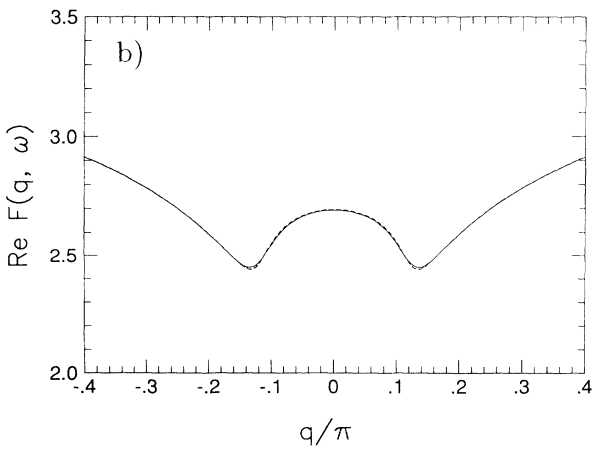
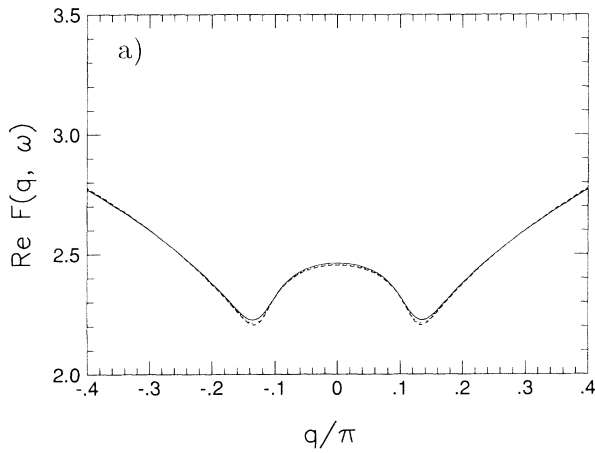


FIG. 1. $\operatorname{Re}F(\mathbf{q}, \omega)$ for two q scans at $T=T_c$ and for $\omega=6$ meV (—), 3.5 meV (⋯), and 1.2 meV (---). (a) Q_δ scan and (b) Q_γ scan.

$$F(y, \omega) = \begin{cases} \left\langle \frac{\eta^2 - \frac{1}{4}\omega^2}{\Delta^2 |f|^2} f(\eta, \omega) \right\rangle & \text{for } D \text{ wave} \\ \left\langle \frac{\eta^2 + \Delta^2 - \frac{1}{4}\omega^2}{\Delta^2} f(\eta, \omega) \right\rangle & \text{for } S \text{ wave}, \end{cases}\quad (9)$$

$$\eta = \mu - y \sin(2\phi),$$

$$f = \begin{cases} \cos(2\phi) & \text{for } D \text{ wave} \\ 1 & \text{for } S \text{ wave}, \end{cases}\quad (10)$$

$$(11)$$

y takes y_+ or y_- , where

$$y = 2t^* [\sin(\frac{1}{2}q_x) \pm \sin(\frac{1}{2}q_y)], \quad (12)$$

N_0 is the density of states at the Fermi surface per spin, $f(\eta, \omega)$ is the generalized superfluid density,¹⁶ and $\langle \rangle$ means average over ϕ . In the following we shall consider some limiting cases.

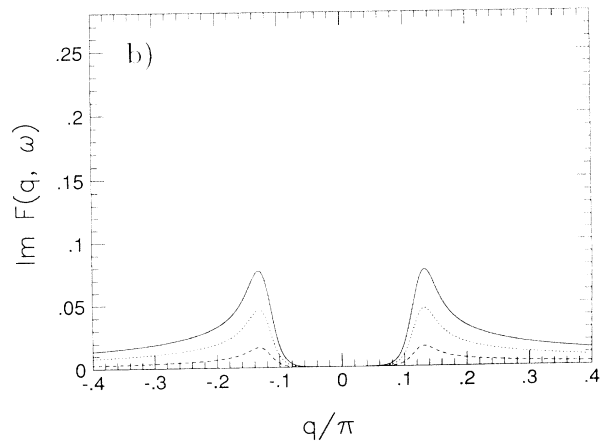
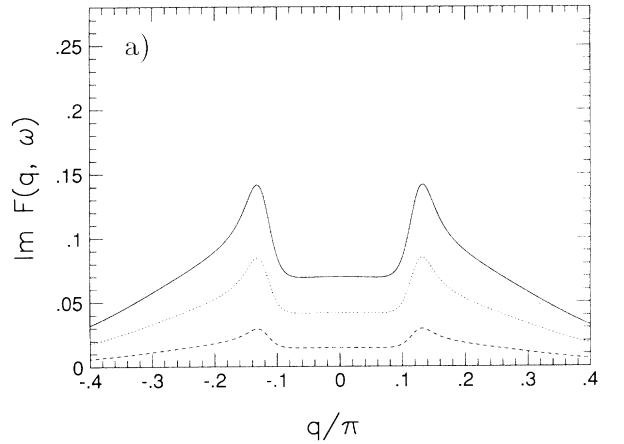


FIG. 2. $\operatorname{Im}F(\mathbf{q}, \omega)$ for two q scans at $T=T_c$ and for ω 's as in Fig. 1. (a) Q_δ scan and (b) Q_γ scan.

A. $T > T_c$ (the normal state)

Although this case is already treated by TKF, we describe our result for completeness. When Δ tends to zero, we obtain

$$\Lambda_s = \int_0^{4|t^*|} dE \frac{1}{E} \tanh \left[\frac{\beta}{2} E \right] = \ln \left[\frac{8\gamma|t^*|}{\pi T} \right], \quad (13)$$

$$F(\mathbf{q}, \omega) = \frac{1}{2} \left\langle \psi \left[\frac{1}{2} + i \frac{(\eta + \omega/2)}{2\pi T} \right] + \psi \left[\frac{1}{2} - i \frac{(\eta - \omega/2)}{2\pi T} \right] \right\rangle - \psi\left(\frac{1}{2}\right), \quad (14)$$

where $\psi(z)$ is the digamma function and $\gamma = 1.7810\dots$ is the Euler constant. Further,

$$\text{Im}F(\mathbf{q}, \omega) = \frac{\pi}{2} \sinh \left[\frac{\omega}{2T} \right] \left\langle \left[\cosh \left[\frac{\eta}{T} \right] + \cosh \left[\frac{\omega}{2T} \right] \right]^{-1} \right\rangle. \quad (15)$$

We show $\text{Re}F(\mathbf{q}, \omega)$ and $\text{Im}F(\mathbf{q}, \omega)$ for the two q scans [Q_δ scan; $\mathbf{q} = (q + \frac{1}{2}q_0, q - \frac{1}{2}q_0)$ and Q_γ scan; $\mathbf{q} = (q, q)$] for $\omega = 6, 3.5,$ and 1.2 meV in Figs. 1(a), 1(b), 2(a), and 2(b) at $T = T_c$. We have chosen parameters corresponding to $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$; $q_0 = 0.245\pi$, $\mu = 435.5$ K, and $T_c = 33$ K. For this choice $\chi(\mathbf{q}, 0)$ has peaks at the incommensurate point $\mathbf{q} = (q_0, 0)$ and $(0, q_0)$ as observed¹² experimentally. In Fig. 3 we show $\chi(\mathbf{q}, 0)$ at $T = T_c$ together with these in *D*- and *S*-wave superconductors at $T = 0$ K. Here we took $4JN_0 = 0.25$, where N_0 is the density of states at the Fermi surface per spin. Finally in Figs. 4(a) and 4(b) we show $\text{Im}\chi(\mathbf{q}, \omega)$ for two q scans and $\omega = 6, 3.5$ and 1.2 meV. These figures reproduce quite well the neutron-scattering data near $T = T_c$, though we

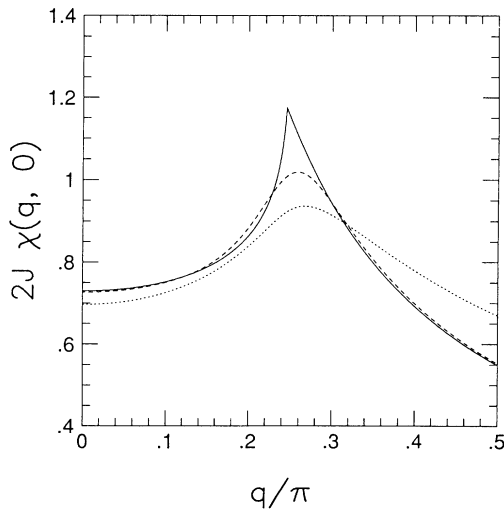


FIG. 3. $2J\chi(\mathbf{q}, 0)$ for $T = T_c$ (---) and for $T = 0$ K for the *D* wave (—) and for the *S* wave (⋯). For the *D* wave at $T = 0$ K, $\chi(\mathbf{q}, 0)$ is almost the same as the one at $T = T_c$ except the sharpness of the peak at $q = q_0$ incommensurate point.

expect rather extended plateau between two peaks for the Q_δ scan. We note also the present result reproduces most of the numerical result in TKF as it should be.

B. $T = 0$ K (*D* wave)

At $T = 0$ K and for the *D* wave, Eq. (7) simplifies as

$$(2N_0)^{-1}\chi_0(\mathbf{q}, \omega) = \Lambda_s + \frac{1}{2} - F(\mathbf{q}, \omega), \quad (16)$$

where

$$\Lambda_s = \ln \left[\frac{8\gamma|t^*|}{\pi T_c} \right] \quad (17)$$

$$F(y, \omega) = \left\langle \left[\frac{\eta^2 - \frac{1}{4}\omega^2}{\eta^2 + \Delta^2|f|^2 - \frac{1}{4}\omega^2} \right]^{1/2} \times \sinh^{-1} \left[\frac{\sqrt{\eta^2 - (1/4)\omega^2}}{\Delta|f|} \right] \right\rangle. \quad (18)$$

More explicitly

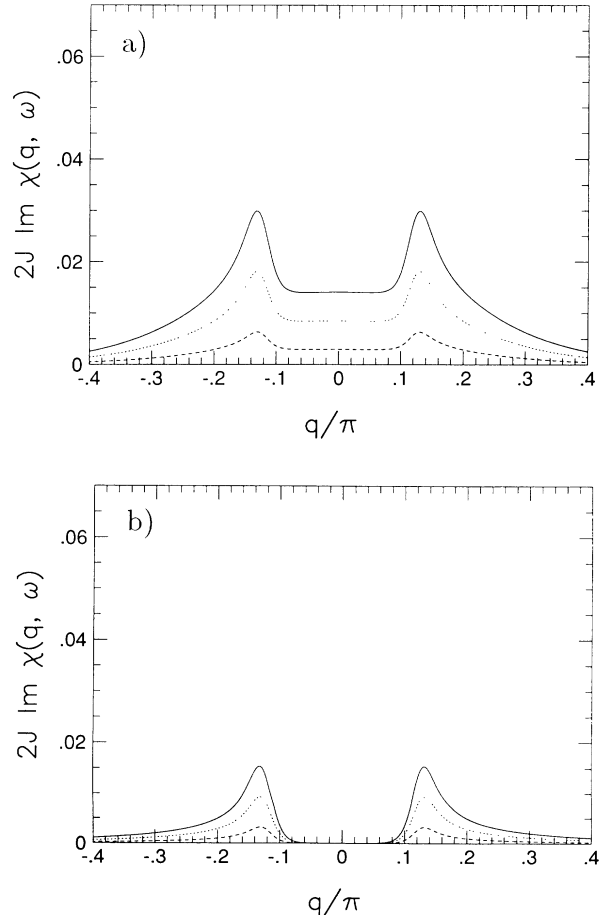


FIG. 4. $2J\text{Im}\chi(\mathbf{q}, \omega)$ for ω 's as in Fig. 1 at $T = T_c$ for two scans (a) Q_δ scan and (b) Q_γ scan.

$$\text{Re}F(y, \omega) = I_1 + I_2 + I_3, \quad (19)$$

$$I_1 = \left\langle \theta(2|\eta| - \omega) \left[\left(\frac{\eta^2 - \frac{1}{4}\omega^2}{\eta^2 + \Delta^2|f|^2 - \frac{1}{4}\omega^2} \right)^{1/2} \sinh^{-1} \left(\frac{\sqrt{\eta^2 - (1/4)\omega^2}}{\Delta|f|} \right) \right] \right\rangle,$$

$$I_2 = - \left\langle \theta(\omega - 2|\eta|) \theta(2\sqrt{\eta^2 + \Delta^2|f|^2} - \omega) \left[\left(\frac{\frac{1}{4}\omega^2 - \eta^2}{\eta^2 + \Delta^2|f|^2 - \frac{1}{4}\omega^2} \right)^{1/2} \sin^{-1} \left(\frac{(1/4)\omega^2 - \eta^2}{\Delta|f|} \right) \right] \right\rangle,$$

$$I_3 = \left\langle \theta(\omega - 2\sqrt{\eta^2 + \Delta^2|f|^2}) \left[\left(\frac{\frac{1}{4}\omega^2 - \eta^2}{\frac{1}{4}\omega^2 - \eta^2 - \Delta^2|f|^2} \right)^{1/2} \cosh^{-1} \left(\frac{\sqrt{(1/4)\omega^2 - \eta^2}}{\Delta|f|} \right) \right] \right\rangle,$$

and

$$\text{Im}F(y, \omega) = \frac{\pi}{2} \left\langle \left(\frac{\frac{1}{4}\omega^2 - \eta^2}{\frac{1}{4}\omega^2 - \eta^2 - \Delta^2|f|^2} \right)^{1/2} \theta(\omega - 2\sqrt{\eta^2 + \Delta^2|f|^2}) \right\rangle. \quad (21)$$

$\text{Re}F(\mathbf{q}, \omega)$ and $\text{Im}F(\mathbf{q}, \omega)$ are evaluated for two q scans for $\omega = 6, 3.5,$ and 1.2 meV and shown in Figs. 5(a)–6(b), respectively. Compared with the result at $T = T_c$, we note that $\text{Re}F(\mathbf{q}, \omega)$'s are almost the same as the one at $T = T_c$ if we subtract $\frac{1}{2}$ from Λ_s at $T = 0$ K, though $\text{Re}F(\mathbf{q}, \omega)$ develops fine structures. As seen from $\chi(\mathbf{q}, 0)$

shown in Fig. 3, $\chi(\mathbf{q}, 0)$ at $T = 0$ K is very similar to the one at $T = T_c$. Finally we show $\text{Im}\chi(\mathbf{q}, \omega)$ for two q scans in Figs. 7(a) and 7(b), which describe quite well the neutron-scattering data by Mason *et al.* at low temperatures,¹² though we predict much sharper peaks at the incommensurate points and the peaks have fine structures. Further the actual peak position is shifted to the larger

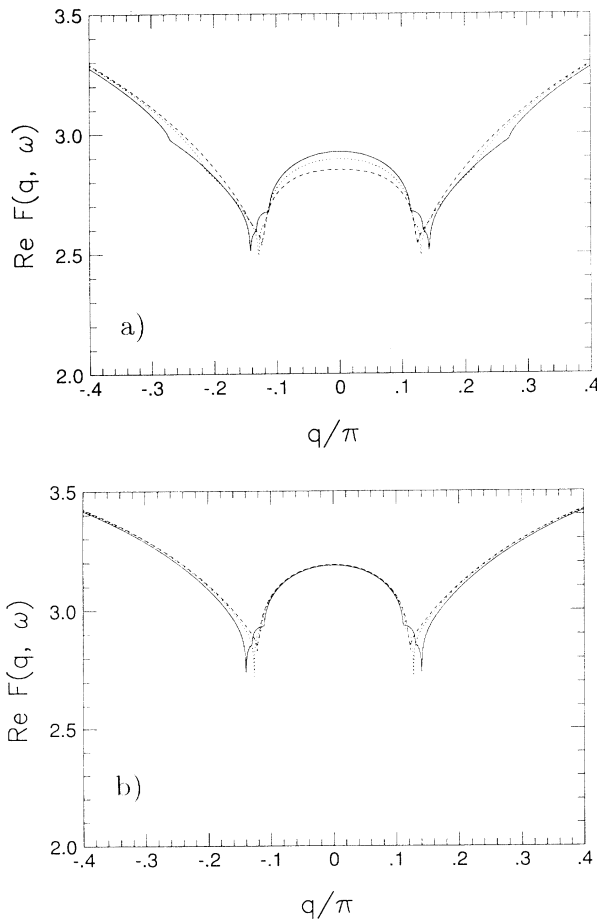


FIG. 5. $\text{Re}F(q, \omega)$ for two q scans at $T = 0$ K for the D -wave superconductor for $\omega = 6$ meV (—), 3.5 meV (\cdots), and 1.2 meV (---). (a) Q_8 scan and (b) Q_γ scan.

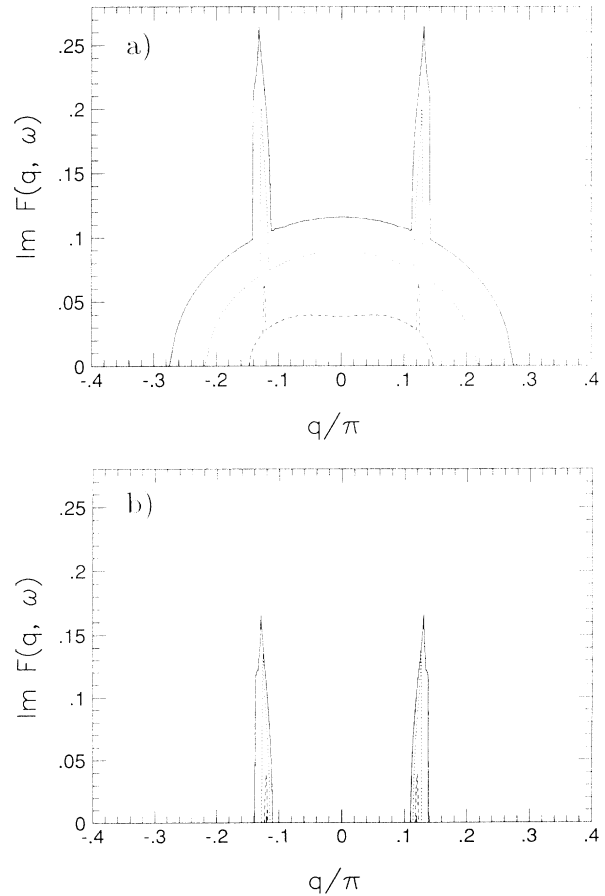


FIG. 6. $\text{Im}F(q, \omega)$ for two q scans at $T = 0$ K for the D -wave superconductor for ω 's as in Fig. 5. (a) Q_8 scan and (b) Q_γ scan.

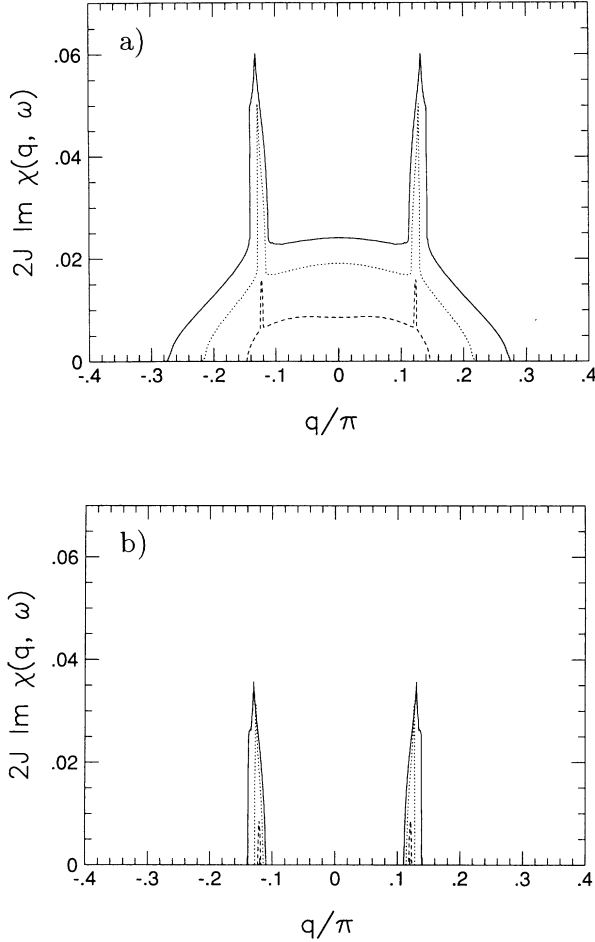


FIG. 7. $2J \text{Im} \chi(q, \omega)$ at $T=0$ K for *D*-wave superconductors for ω 's as in Fig. 5. (a) Q_δ scan and (b) Q_γ scan.

momentum $q_0^* \cong q_0 + 0.3896(\omega/\mu)$. We may conclude that the *D*-wave model describes quite well the neutron-scattering data by Mason *et al.* contrary to their claim.¹² As mentioned in the Introduction, the energy gap is given by

$$E_g = \begin{cases} 2|\mu - y| & \text{for } 0 < y < y_c \\ 2\Delta \left[1 - \frac{\mu^2}{y^2 - \Delta^2} \right]^{1/2} & \text{for } y > y_c, \end{cases} \quad (22)$$

where

$$y_c = \frac{1}{2}(\mu + \sqrt{\mu^2 + 4\Delta^2}). \quad (23)$$

In particular at $y = \mu$ the energy gap vanishes as shown in Fig. 8.

$$\text{Im}F(\mathbf{q}, \omega) = \frac{\pi}{2} \sinh \left[\frac{\omega}{2T} \right] \left\langle \left[\frac{\eta^2 - \frac{1}{4}\omega^2}{\eta^2 + \Delta^2 |f|^2 - \frac{1}{4}\omega^2} \right]^{1/2} \left[\cosh \left[\frac{\eta}{T} \left[\frac{\eta^2 + \Delta^2 |f|^2 - \frac{1}{4}\omega^2}{\eta^2 - \frac{1}{4}\omega^2} \right]^{1/2} \right] + \cosh \left[\frac{\omega}{2T} \right] \right]^{-1} \right\rangle, \quad (28)$$

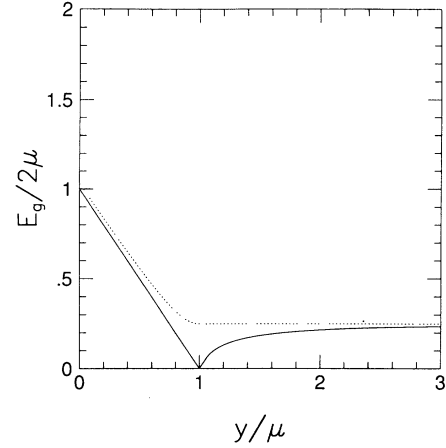


FIG. 8. The energy gap E_g is shown as a function of y for *D*-wave (—) and *S*-wave (---) superconductors. Here we took $\Delta/\mu = 0.25$.

C. $T=0$ K (*S* wave)

For the *S*-wave superconductor, we have

$$(2N_0)^{-1} \chi_0(\mathbf{q}, \omega) = \ln \left[\frac{8\gamma |t|}{\pi T_c} \right] - F(\mathbf{q}, \omega) \quad (24)$$

with

$$F(y, m) = \left\langle \left[\frac{\eta^2 + \Delta^2 - \frac{1}{4}\omega^2}{\eta^2 - \frac{1}{4}\omega^2} \right]^{1/2} \sinh^{-1} \left[\frac{\sqrt{\eta^2 - \frac{1}{4}\omega^2}}{\Delta} \right] \right\rangle. \quad (25)$$

In particular

$$\text{Im}F(y, \omega) = \frac{\pi}{2} \left\langle \theta(\omega - 2\sqrt{\eta^2 + \Delta^2}) \left[\frac{\eta^2 + \Delta^2 - \frac{1}{4}\omega^2}{\eta^2 - \frac{1}{4}\omega^2} \right]^{1/2} \right\rangle. \quad (26)$$

This implies that the *S*-wave model has a large energy gap

$$E_g = \begin{cases} 2\sqrt{(\mu - y)^2 + \Delta^2} & \text{for } (0 < y < \mu) \\ 2\Delta & \text{for } y > \mu, \end{cases} \quad (27)$$

which is also shown in Fig. 8. Therefore at $T=0$ K there should be no scattering intensity for the experiment by Mason *et al.*¹² Even if $T \neq 0$ K, the intensity is of the order of $e^{-\Delta/T} \cong 10^{-6}$ for $T=4$ K in $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$, which is clearly negligible.

D. $T \neq 0$ K (*D* wave)

For $T \neq 0$ K the generalized condensed density is rather a complicated function. However, we have already seen that $\text{Re}F(\mathbf{q}, \omega)$ has little temperature dependence $T < T_c$. Further $\text{Im}F(\mathbf{q}, \omega)$ at an arbitrary temperature is given by

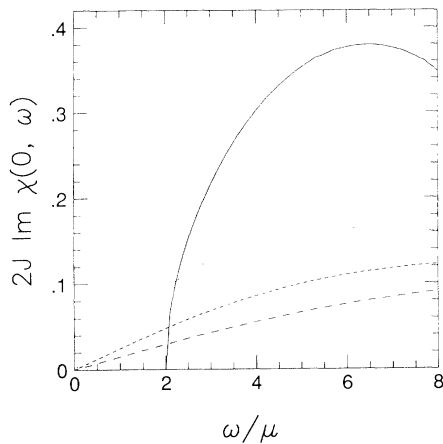


FIG. 9. $2J \text{Im}\chi(0, \omega)$ for $T=2T_c$ (— · — · —), $1.5T_c$ (---), T_c (· · · · ·), and 0 K (—) for D -wave superconductors are shown for $\mu=2$ meV and $T_c=47$ K.

where $\Delta=\Delta(T)$ the temperature-dependent order parameter. But we shall explore the temperature dependence of $\chi(\mathbf{q}, \omega)$ elsewhere.

III. $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ system

So far we have concentrated on the $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ experiment. A similar model applies to YBCO as well with a slight modification.¹⁰ In particular the theoretical analysis is simpler, since most of data are taken at the commensurate point (i.e., $\mathbf{q}=0$). First, at the qualitative level, the spin gap, which we call simply the energy gap, found by Rossat-Mignod *et al.*^{13,14} is incompatible with the S -wave model but is fully consistent with the D -wave model, since for all the concentration observed E_g are smaller than the corresponding 2Δ . Indeed E_g scales with 2μ as already noted by TKF, which is also true for the D wave when $y=0$ (i.e., at the commensurate point). Further since $E_g=2\mu$ and $\mu \propto (x-0.42)^{1.7}$, the E_g - T_c curve should exhibit a plateau for $55 \text{ K} < T_c < 92 \text{ K}$. More quantitative level we analyze $\text{Im}\chi(0, \omega)$ for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ with $x=0.51$ (with $T_c=47$ K) and $x=0.92$ (with $T_c=91$ K). For μ we used one half of the values quoted as the spin gap^{13,14} (i.e., 2 and 14 meV, respectively). The results are shown in Figs. 9 and 10, respectively, where we used $(4JN_o)^{-1}=0.22$. We note that these figures describe qualitatively the experimental data, though $\text{Im}\chi(0, \omega)$ measured is much suppressed when $\omega \geq 4\mu$ than our theory predicts. But we believe that this suppression is due to the quasiparticle damping which we have not considered in the present analysis.

IV. CONCLUDING REMARKS

We obtain a simple expression of the spin-spin correlation function where the superconducting correlation is in-

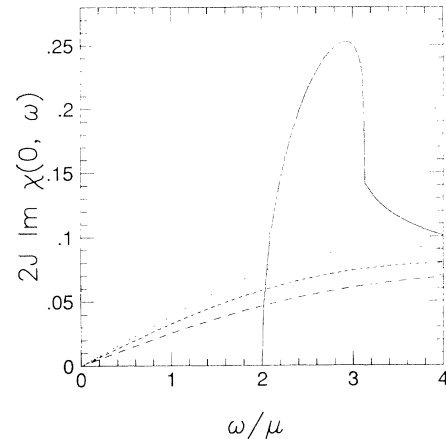


FIG. 10. $2J \text{Im}\chi(0, \omega)$ for $T=2T_c$ (— · — · —), $1.5T_c$ (---), T_c (· · · · ·) and $T=0$ K (—) for D -wave superconductors are shown for $\mu=14$ meV and $T_c=91$ K.

cluded within mean-field approximation. We show that the neutron-scattering data of both Mason *et al.*¹² and Rossat-Mignod *et al.*^{13,14} are consistent with the D -wave model but incompatible with the S -wave model. Also the present theory predicts fine structures in the spin-fluctuation spectrum, which has not been resolved experimentally. In any case we believe that the neutron scattering will provide unique insight on the symmetry of the underlying superconductor. After completing the present work we learned that Tanamoto, Kohno, and Fukuyama¹⁷ had done a similar analysis within the RVB scheme. However, though their result appears to be similar to ours in general, it differs in details. For example we predict the gapless region in the vicinity of the incommensurate antiferromagnetic points, while they predict a nonvanishing energy gap everywhere.

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*On sabbatical leave from Physics Department, Hallym University, Chunchon 200-702, South Korea.

†On sabbatical leave from Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484.

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