Neutron scattering in a $d_{x^2-y^2}$-wave superconductor

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(Received 14 October 1993)

Recent neutron-scattering experiments on $La_{1.86}Sr_{0.14}CuO_4$ find an isotropic but incomplete suppression of the scattering intensity below T_c. Here we show that for a $d_{x^2-y^2}$-wave superconductor with a strong enhancement of the spin-fluctuation scattering and a proper choice of the model parameters, this is the type of behavior that is expected.

Recent neutron-scattering measurements[1–4] provide detailed information on the wave vector, frequency, and temperature dependence of the spin fluctuations in $La_{1.86}Sr_{0.14}CuO_4$. At temperatures below T_c and frequencies ω less than 2Δ the scattering is suppressed but even at low temperatures and frequencies, spin-fluctuation excitations were found to persist. In these experiments the momentum structure of the scattering intensity, while suppressed, remains similar to that observed in the normal state.

Some theories[5,6] had predicted an anisotropy in this suppression, and its absence in the experimental data was interpreted[4,7] as evidence against $d_{x^2-y^2}$ pairing. However, we find that these experimental results are consistent with previous work[8,9] in which the nuclear relaxation rates T_1^{-1} and T_2^{-1} were calculated for the superconducting state of the cuprates. The model parameters that we will use here in calculating neutron-scattering intensities are similar to those used in the previous analysis of NMR experiments, and small variations in them do not affect the results. A key feature of this model is the large enhancement of the incommensurate spin-fluctuation scattering over that obtained from the bare, band-structure, BCS magnetic susceptibility. This enhancement is also clearly seen in the large magnitude of the experimental scattering intensity reported by Mason *et al.*[7]

In order to understand this, we consider a simple one-band Hubbard model with a near-neighbor hopping t and an on-site Coulomb interaction U:

$$H=-t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}-\sum_i\mu(n_{i\uparrow}+n_{i\downarrow})\ . \qquad (1)$$

Here $c_{i\sigma}^{\dagger}$ creates an electron of spin σ on site i of a two-dimensional square lattice, and μ is a chemical potential used to adjust the band filling $\langle n\rangle=\langle n_{i\uparrow}+n_{i\downarrow}\rangle$.

Monte Carlo calculations[10] have shown that at higher temperatures ($T\gtrsim 8t/50$) the magnetic susceptibility

$$\chi(\mathbf{q},i\omega_m)=\int_0^\beta d\tau\, e^{i\omega_m\tau}\langle Tm_{\mathbf{q}}^{-}(\tau)m_{\mathbf{q}}^{+}(0)\rangle \qquad (2)$$

with $m_{\mathbf{q}}^{+}=\sum_{\mathbf{p}}c_{\mathbf{p}+\mathbf{q}\uparrow}^{\dagger}c_{\mathbf{p}\downarrow}$ and $m_{\mathbf{q}}^{+}(\tau)=\exp(-H\tau)m_{\mathbf{q}}^{+}\exp(H\tau)$ is well approximated by the random-phase-approximation (RPA) form

$$\chi(\mathbf{q},i\omega_m)=\frac{\chi_0(\mathbf{q},i\omega_m)}{1-\bar{U}\chi_0(\mathbf{q},i\omega_m)}\ . \qquad (3)$$

Here $\bar{U}$ is a renormalized interaction strength (e.g., $\bar{U}\simeq 2t$ for $U=4t$ at a filling $\langle n\rangle=0.85$), and χ_0 is the bare band-structure susceptibility.[11] Based on this, we suggested[8,9] that both the NMR relaxation rates and neutron scattering in a $d_{x^2-y^2}$ superconducting state could be analyzed using the RPA form, Eq. (3), with $\chi_0(\mathbf{q},i\omega_m\to\omega+i\delta)$ replaced by the BCS expression,

$$\chi_0(\mathbf{q},\omega)=\frac{1}{N}\sum_p\left\{\frac{1}{2}\left[1+\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_p+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}}\right]\frac{f(E_{\mathbf{p}+\mathbf{q}})-f(E_{\mathbf{p}})}{\omega-(E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}})+i\delta}+\frac{1}{4}\left[1-\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_{\mathbf{p}}+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}}\right]\frac{1-f(E_{\mathbf{p}+\mathbf{q}})-f(E_{\mathbf{p}})}{\omega+(E_{\mathbf{p}+\mathbf{q}}+E_{\mathbf{p}})+i\delta}\right.$$
$$\left.+\frac{1}{4}\left[1-\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_{\mathbf{p}}+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}}\right]\frac{f(E_{\mathbf{p}+\mathbf{q}})+f(E_{\mathbf{p}})-1}{\omega-(E_{\mathbf{p}+\mathbf{q}}+E_{\mathbf{p}})+i\delta}\right\}\ . \qquad (4)$$

Here $E_{\mathbf{p}}=(\varepsilon_{\mathbf{p}}^2+\Delta_{\mathbf{p}}^2)^{1/2}$ with $\varepsilon_{\mathbf{p}}=-2t(\cos p_x+\cos p_y)-\mu$ and $\Delta_{\mathbf{p}}=[\Delta(T)/2](\cos p_x-\cos p_y)$. The terms in the brackets in Eq. (4) are the usual BCS coherence factors.

We have evaluated $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ for a filling $\langle n\rangle=0.85$ at $T=T_c$, where $\Delta_{\mathbf{p}}$ vanishes, and at $T=0.1T_c$, where the $d_{x^2-y^2}$-wave gap is well developed. Figures 1(a) and 1(b) show $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ versus $\mathbf{q}$ for $\omega=0.4T_c$ at these two temperatures. We have taken $T_c=0.05t$ and $2\Delta(0)/kT_c\sim 6$ so that $\omega=0.4T_c$ is small compared to $2\Delta(0)$. These results were obtained from the numerical evaluation of the imaginary part of Eq. (4) on a 512×512 lattice with a finite broadening $\Gamma=0.03t$ for $T=T_c$ and $\Gamma=0.005t$ for $T=0.1T_c$. At $T=T_c$, $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ peaks at an incommensurate edge wave vector $\mathbf{Q}_\delta$ [see the inset in Fig. 3(a)] but at $T=0.1T_c$, where the $d_{x^2-y^2}$ gap is well formed, the dominant structure in $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ is associated with the nodal contributions along the diagonal at $\mathbf{Q}_\gamma$. When Figs. 1(a) and 1(b) are extended to form a repeating zone, the change in the pattern of intensity between $T=T_c$ and $T=0.1T_c$ has been described as a "45° rotation of the peak structure." This is the type of $d_{x^2-y^2}$ anisotropy predicted in models that either neglect[5] or have a relatively small spin-fluctuation enhancement.[6]

From Eq. (3), we have

$$\mathrm{Im}\chi(\mathbf{q},\omega)=\frac{\mathrm{Im}\chi_0(\mathbf{q},\omega)}{[1-\bar{U}\,\mathrm{Re}\chi_0(\mathbf{q},\omega)]^2+[\bar{U}\,\mathrm{Im}\chi_0(\mathbf{q},\omega)]^2}\,. \tag{5}$$

This is plotted in Fig. 2 versus $\mathbf{q}$ for $T=T_c$ and $0.1T_c$ with $\omega=0.4T_c$ and should be compared with Fig. 1. With the enhancement factor $[1-\bar{U}\,\mathrm{Re}\chi_0(\mathbf{q},\omega)]^{-2}$, which peaks at the incommensurate momentum transfer $\mathbf{Q}_\delta$, the peaks remain at $\mathbf{Q}_\delta$ even down to temperatures of $0.1T_c$.

In order to obtain a clearer comparison with experiment, we have averaged $\mathrm{Im}\chi(\mathbf{q},\omega)$ over a resolution ellipse similar to the resolution function of Ref. 4, and plotted the results for $\mathbf{q}$ varying along the solid and dashed lines shown in the inset to Fig. 3(a). The response shown in Fig. 3(a) corresponds to $\mathbf{q}$ varying along the solid line and passing through the incommensurate peak at $\mathbf{Q}_\delta$. As the temperature is lowered, $\langle\mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ averaged around $\mathbf{Q}_\delta$ decreases by approximately 50% for $\omega=0.4T_c$. Figure 3(b) shows that the peak at $\mathbf{Q}_\gamma$ also decreases and furthermore, the ratio of the $\mathbf{Q}_\gamma$ to $\mathbf{Q}_\delta$ peak heights remains essentially unchanged.

The temperature dependence of $\langle\mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ is summarized in Fig. 4. The dependence of $\langle\mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ on

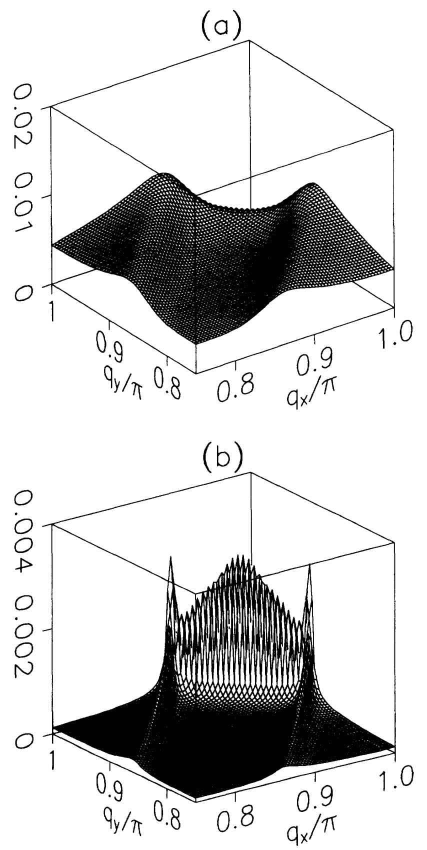

FIG. 1. Imaginary part of the bare magnetic susceptibility $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ vs $\mathbf{q}$ for (a) $T=T_c$ and (b) $T=0.1T_c$. Here $\omega=0.4T_c$ and $2\Delta(0)/kT_c=6$, corresponding to an $\omega/2\Delta(0)=0.067$, and the results are plotted in units of t^{-1}.

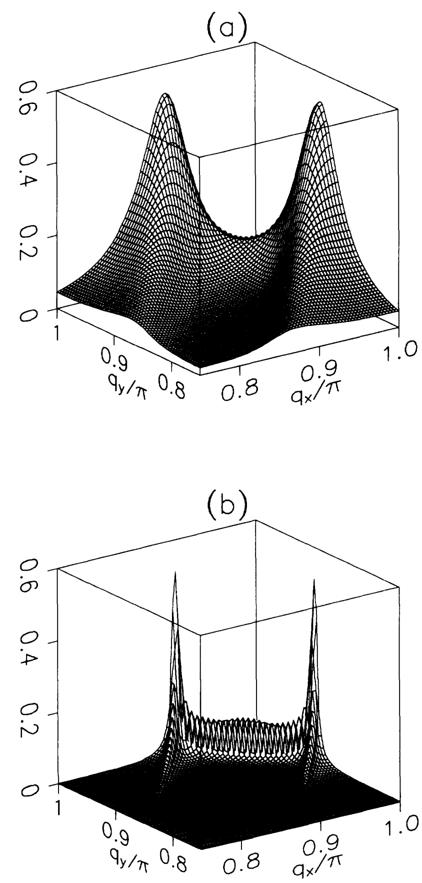

FIG. 2. Imaginary part of the RPA susceptibility $\mathrm{Im}\chi(\mathbf{q},\omega)$ vs $\mathbf{q}$ for (a) $T=T_c$ and (b) $T=0.1T_c$ with $\omega=0.4T_c$.

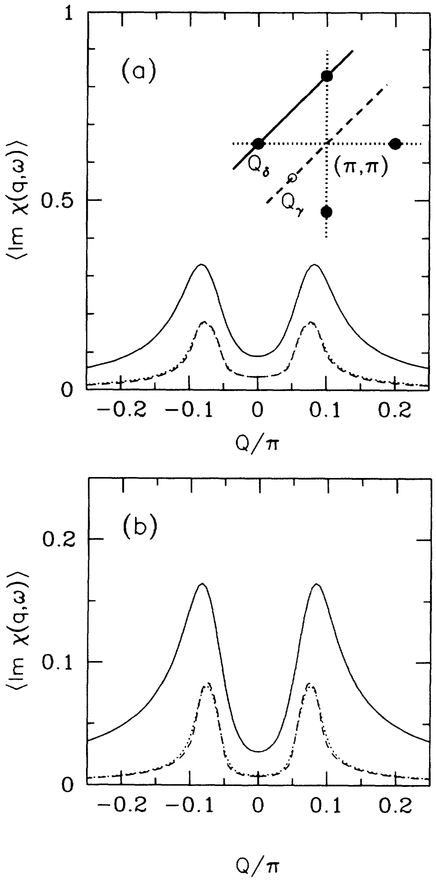

FIG. 3. Momentum dependence of $\langle \mathrm{Im}\chi(\mathbf{q},\omega)\rangle$, averaged over an ellipse centered at $\mathbf{q}$, for $\omega=0.4T_c$. (a) For $\mathbf{q}$ varying along the solid line passing through $\mathbf{Q}_\delta$ shown in the inset. (b) For $\mathbf{q}$ varying along the dashed line passing through $\mathbf{Q}_\gamma$ shown in the inset. Here results are given for $T=T_c$ (solid lines), $0.4T_c$ (dotted lines), and $0.1T_c$ (dashed lines).

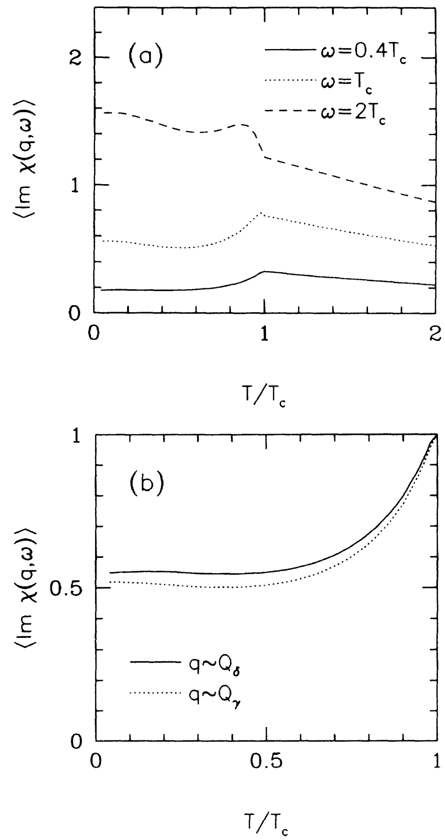

FIG. 4. (a) Temperature dependence of $\langle \mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ averaged around $\mathbf{Q}_\delta$ at various frequencies. (b) Response $\langle \mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ vs T/T_c, normalized to its value at T_c, for $\omega=0.4T_c$ and $\mathbf{q}$ averaged around $\mathbf{Q}_\delta$ (solid line) and $\mathbf{Q}_\gamma$ (dotted line).

T/T_c is shown in Fig. 4(a) for $\mathbf{q}$ averaged around $\mathbf{Q}_\delta$ at various frequencies. Figure 4(b) shows $\langle \mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ for $\omega=0.4T_c$, normalized to its value at T_c, versus T/T_c for $\mathbf{q}$ averaged around $\mathbf{Q}_\delta$ and $\mathbf{Q}_\gamma$. The relatively isotropic suppression of $\langle \mathrm{Im}\chi(\mathbf{q},\omega)\rangle$ below T_c, calculated from Eqs. (4) and (5) with a $d_{x^2-y^2}$-wave gap, is consistent with the experimental observations.

To summarize, we believe that the strength of the scattering, characterized by the size of $\mathrm{Im}\chi(\mathbf{q},\omega)/\omega$, implies that there is a large enhancement of the spin fluctuations and that this must be taken into account in the description of the superconducting state. When this is done, within the approximate RPA-BCS framework previously proposed[8,9] one obtains results, which are consistent with recent neutron-scattering measurements.

Further work, which treats the band structure within the three-band Hubbard model so as to obtain the correct splitting of the incommensurate peak is of interest. Furthermore, at low reduced temperatures and low frequencies, the quasiparticle lifetime is dominated by impurity scattering. Preliminary calculations[12] of the effect of unitary scattering on $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ show that it acts to maintain the peaks at $\mathbf{Q}_\delta$. The resulting RPA form is similar to that reported here.

The authors wish to acknowledge useful conversations with E. Abrahams, G. Aeppli, R. J. Birgeneau, T. Mason, D. Pines, and S. Quinlan. N.B. would like to acknowledge support by the National Science Foundation Grant No. (DMR 91-20000) through the Science and Technology Center for Superconductivity, and D.J.S. would like to acknowledge support for this work from the National Science Foundation under Grant No. DMR-92-25027. The numerical calculations reported in this paper were performed at the San Diego Supercomputer Center.

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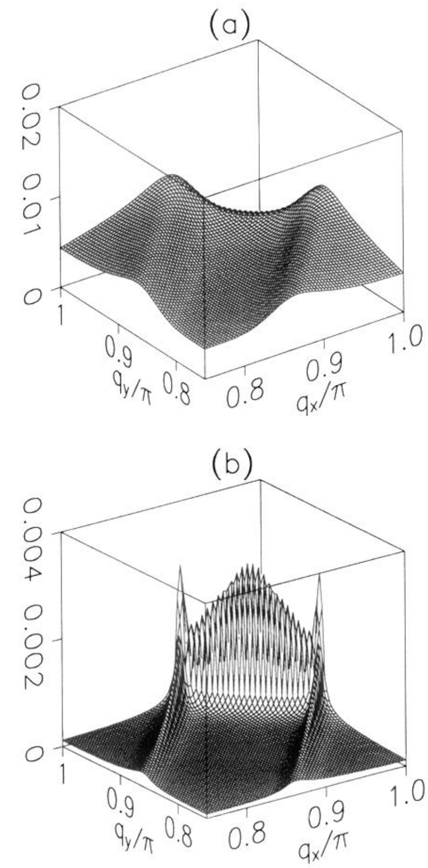

FIG. 1. Imaginary part of the bare magnetic susceptibility $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ vs $\mathbf{q}$ for (a) $T=T_c$ and (b) $T=0.1T_c$. Here $\omega=0.4T_c$ and $2\Delta(0)/kT_c=6$, corresponding to an $\omega/2\Delta(0)=0.067$, and the results are plotted in units of t^{-1}.

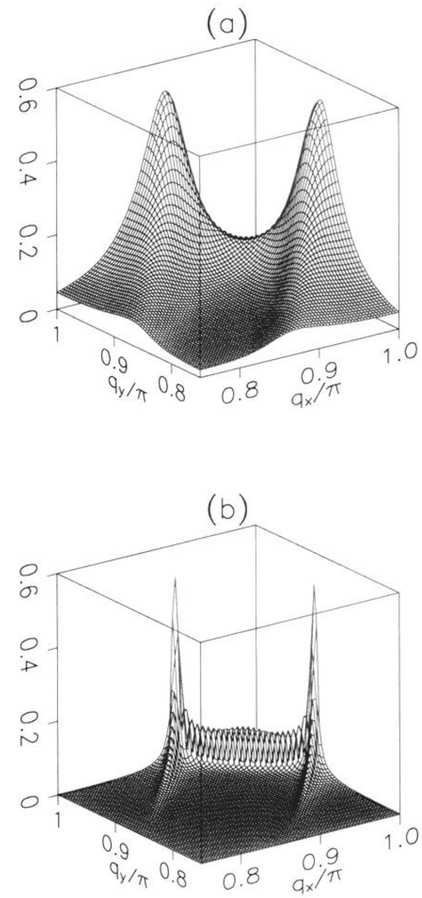

FIG. 2. Imaginary part of the RPA susceptibility Im$\chi(\mathbf{q},\omega)$ vs $\mathbf{q}$ for (a) $T=T_c$ and (b) $T=0.1T_c$ with $\omega=0.4T_c$.