Collective modes in high-temperature superconductors

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The role of collective modes in various experiments on the cuprates is investigated. We calculate the neutron scattering, photoemission [angle-resolved photoemission spectroscopy (ARPES)], and Raman-scattering intensities below T_c within the fluctuation-exchange approximation for the two-dimensional Hubbard model. It is shown that the large peak in the dynamical spin susceptibility arises from a weakly damped spin-density-wave collective mode. This gives rise to a dip between the sharp low-energy peak and the higher binding energy hump in the ARPES spectrum. Furthermore, we show that the collective mode of the amplitude fluctuation of the d-wave gap yields a broad peak above the pair-breaking threshold in the B_{1g} Raman spectrum. [S0163-1829(98)00142-8]

A wide variety of collective modes has been observed in the three phases of superfluid ^{3}He.[1] These fluctuations of the spin-triplet p-wave gap have been calculated from coupled Bethe-Salpeter equations for the T matrices in the particle-particle and particle-hole channels.[2,3] This method has also been used to investigate the collective modes in hypothetical p-wave pairing superconductors like heavy fermion superconductors.[4] A detailed study of the collective modes for three-dimensional (3D) d-wave superconductors, including different order-parameter symmetries, has been made in Ref. 5. Recently, pair fluctuations and the associated Raman scattering intensity have been calculated for a two-dimensional (2D) d-wave weak-coupling superconductor.[6]

In this note we investigate the collective modes within the fluctuation-exchange (FLEX) approximation for the 2D one-band Hubbard model and their relevance to neutron-scattering, photoemission, and Raman-scattering experiments in high-T_c cuprates. The FLEX approximation for the particle-hole channel[7-9] yields the dynamical spin susceptibility, $\chi_s = \chi_{s0}(1 - U\chi_{s0})^{-1}$, and the charge susceptibility, $\chi_c = \chi_{c0}(1 + U\chi_{c0})^{-1}$. Here, U is the on-site Coulomb repulsion, and $\chi_{s0}(\mathbf{q},\omega)$ and $\chi_{c0}(\mathbf{q},\omega)$ are the irreducible susceptibilities. The latter are calculated from the *dressed* normal and anomalous Green's functions G and F. The corresponding normal self-energies, $\omega[1 - Z(\mathbf{k},\omega)]$ and $\xi(\mathbf{k},\omega)$, and the d-wave gap function, $\phi(\mathbf{k},\omega)$, are determined self-consistently by the Eliashberg equations with interactions given by $(3/2)U^2\text{Im}\,\chi_s(\mathbf{q},\omega) \pm (1/2)U^2\text{Im}\,\chi_c(\mathbf{q},\omega)$ [plus (minus) sign for normal (anomalous) self-energy].

Below T_c large peaks evolve in the spectral density Im $\chi_s(\mathbf{q},\omega)$, i.e., four distinct peaks at wave vectors $\mathbf{q}$ near $\mathbf{Q} = (\pi,\pi)$ for next-nearest neighbor hopping $t' = 0$,[8] and a broad peak centered at $\mathbf{Q}$ for $t' = -0.45t$ (t is the near-neighbor hopping energy).[9] These results are in qualitative agreement with neutron-scattering experiments on La$_{2-x}$Sr$_x$CuO$_4$ and YBa$_2$Cu$_3$O$_{7-\delta}$, respectively.[10] Similar results have been obtained within the $t-J$ model.[11] In Fig. 1

we show Im $\chi_s(\mathbf{Q},\omega)$ for $U = 3.6t$, $t' = -0.45t$, and band filling $n = 0.90$. One sees that a large peak evolves at about $\omega_0 = 0.08t$ as T decreases below $T_c = 0.022t$. The amplitude Δ_0 of the $d_{x^2-y^2}$-wave gap rises much more rapidly below T_c than the BCS d-wave gap and reaches at our lowest temperature $T = 0.017t$ ($T/T_c = 0.77$) a value of about $\Delta_0 = 0.1t$ (see Fig. 3). We find that the peak in Fig. 1 is due to a slightly damped collective mode because the susceptibility has a pole at ω_0, more exactly, Re $\chi_{s0}(\mathbf{Q},\omega_0) - U^{-1} = 0$, and the height of the peak is large of the order of the quasiparticle lifetime $1/\Gamma(\omega_0)$. Here, $\Gamma(\mathbf{k},\omega) = \omega$ Im $Z(\mathbf{k},\omega)/$Re $Z(\mathbf{k},\omega)$ is the quasiparticle scattering rate. Since this is decisive for the observability of the collective modes in the cuprates we show in Fig. 2 the functions ω Im $Z(\mathbf{k},\omega)$ and Re $Z(\mathbf{k},\omega)$ at the antinode $\mathbf{k}_a$ and the node $\mathbf{k}_b$ of the gap on the Fermi line. One sees from Fig. 2 that for T below T_c the scattering rate decreases dramatically for frequencies ω below the pair-breaking threshold $2\Delta_0 \simeq 0.2t$.
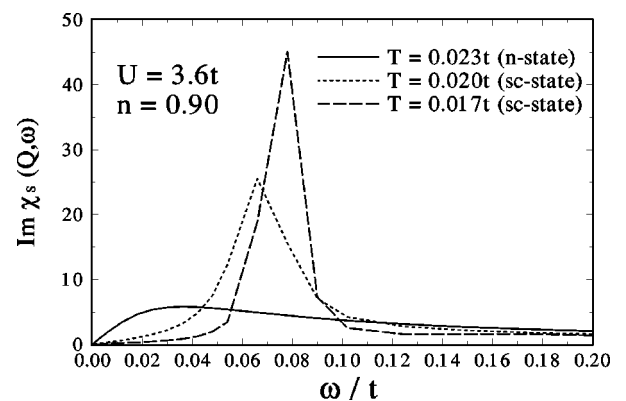
In order to understand somewhat better the origin of this

FIG. 1. Spectral density of spin susceptibility at wave vector $\mathbf{Q} = (\pi,\pi)$, Im $\chi_s(\mathbf{Q},\omega)$, for temperatures $T = 0.023t$, $0.020t$, and $0.017t$ ($T_c = 0.022t$). Here, $U = 3.6t$ is the on-site Coulomb repulsion, t is the near-neighbor hopping energy, $t' = -0.45t$ is the next-nearest-neighbor-hopping, and $n = 0.90$ is the renormalized band filling.
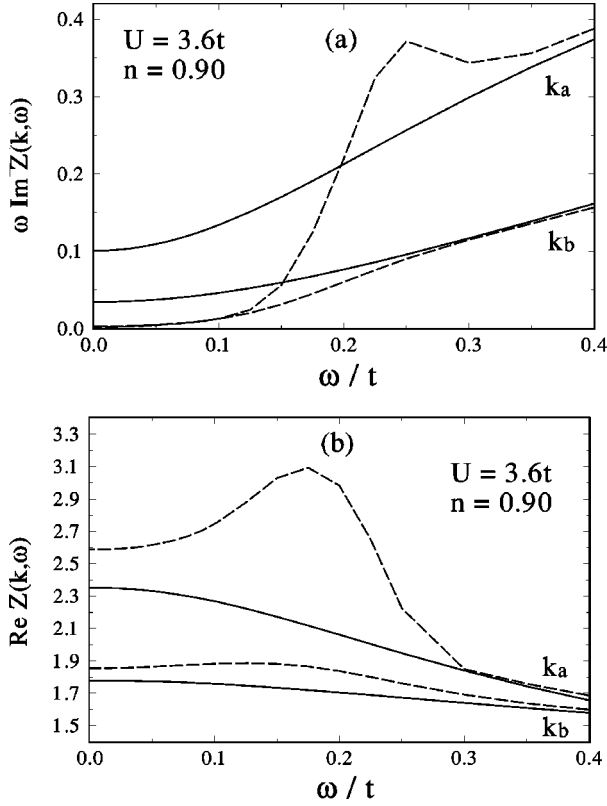
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FIG. 2. Quasiparticle scattering rate, $\Gamma(\mathbf{k},\omega)$ $= \omega\,\mathrm{Im}\,Z(\mathbf{k},\omega)/\mathrm{Re}\,Z(\mathbf{k},\omega)$, at antinode $\mathbf{k}_a$ and node $\mathbf{k}_b$ of the d-wave gap, in the normal state at $T=0.023t$ (solid lines), and in the superconducting state at $T=0.017t$ ($T/T_c=0.77$) (dashed lines). (a) $\omega\,\mathrm{Im}\,Z(\mathbf{k},\omega)$; (b) mass enhancement $\mathrm{Re}\,Z(\mathbf{k},\omega)$.

spin-density-wave collective mode we have calculated $\chi_{s0}(\mathbf{Q},\omega)$ in the weak-coupling limit. The sums over Matsubara frequencies have been carried out with the help of the methods developed for superfluid $^3\mathrm{He}$.[3] The effect of quasiparticle damping is taken into account by carrying out the analytical continuation of this result from $i\omega_m$ to $\omega+i\Gamma$. For a gap $\Delta(\mathbf{k})=(\Delta_0/2)(\cos k_x-\cos k_y)$ and a band $\epsilon(\mathbf{k})$ with $t'=0$ and chemical potential μ the summation over $\mathbf{k}$ in the square Brillouin zone has been carried out numerically in the following expression for $T=0$:

$$\chi_{s0}(\mathbf{Q},\omega)=\sum_k \frac{E_kE_{k+Q}-\epsilon_k\epsilon_{k+Q}-\Delta_k\Delta_{k+Q}}{(E_k+E_{k+Q})^2-(\omega+i\Gamma)^2}\frac{E_k+E_{k+Q}}{2E_kE_{k+Q}}.$$
(1)

Here, $E_k^2=\epsilon^2(\mathbf{k})+\Delta^2(\mathbf{k})$. Then we obtain a peak in the ω function $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega)$ at the kinematical gap $\omega=2|\mu|$,[13] whose height decreases with increasing Γ. The approximate analytic result for $T=0$ is given by

$$\chi_{s0}(\mathbf{Q},\omega)=V_0^{-1}-N_F(z/1+z)^{1/2}\ln[4(1+z)^{1/2}],$$

$$z=[4\mu^2-(\omega+i\Gamma)^2]/(2\Delta_0)^2,$$
(2)

$$V_0^{-1}=N_F\ln(2W/\Delta_0).$$

Here, $W=4t$ is the half bandwidth. The function $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega)$ in Eq. (2) rises first with ω^2 and then exhibits a peak at the kinematical gap $2|\mu|$ whose height is about $V_0^{-1}-(\pi/2)N_F(\Gamma/2\Delta_0)$. A low-frequency mode, i.e., a zero of equation $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega)=1/U$, is obtained only for a finite range of U values which decreases with increasing Γ. For $t'=-0.45t$ a kinematical gap no longer exists and the effective $|\mu|$ is nearly zero. Then the approximate analytical result for the expression in Eq. (2) becomes equal to

$$\chi_{s0}(\mathbf{Q},\omega)=V_0^{-1}+\frac{1}{2}N_Fi\,\frac{\bar\omega^2}{(\bar\omega+i\gamma)}K(\bar\omega+i\gamma),$$

$$\bar\omega=\omega/2\Delta_0,\quad \gamma=\Gamma/2\Delta_0.$$
(3)

Here, K is the first elliptic integral. Now the peak of $\mathrm{Re}\,\chi_{s0}$ as a function of ω occurs approximately at $\omega\simeq2\Delta_0$. This result has been checked by carrying out numerically the sum over $\mathbf{k}$ in Eq. (1) for $t'=-0.45t$ and for different amplitudes Δ_0 and chemical potentials μ. In fact, we find that the function $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega)$ exhibits a peak at about $\omega\simeq2\Delta_0$ whose height decreases as μ increases, for example, from -1.3 (unrenormalized band filling $n_0=0.84$) to -0.8 ($n_0=1.03$). A solution $\omega_0<2\Delta_0$ of the equation $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega_0)=1/U$ exists only for a small range of U values near $U\simeq3t$. The strong-coupling calculation yields a smaller resonance energy. Another difference in comparison to the weak-coupling result is the fact that the self-consistent strong-coupling calculations yield a collective mode for much higher values of U, for example, $U=6.8t$ in Ref. 9. This shows how important it is to take into account the feedback effect of the self-energy on the dynamical spin susceptibility χ_s. These strong renormalization effects might also be responsible for the observed broadening and decrease of the resonance energy of the neutron-scattering peak in underdoped $\mathrm{YBa_2Cu_3O_{6+x}}$ which goes in proportion to the decrease of T_c or doping level.[12] In fact, for decreasing doping $x=n-1$, or increasing chemical potential μ, the position and height of the function $\mathrm{Re}\,\chi_{s0}(\mathbf{Q},\omega)$ decrease which means that the position of the peak of $\mathrm{Im}\,\chi_s$ is decreased and its width is increased.

We show now that the spin-density-wave collective mode has a large effect on the angle-resolved photoemission intensity (ARPES) below T_c. In Fig. 3(a) we have plotted our results for $N(\mathbf{k},\omega)f(\omega)$ [where $N(\mathbf{k},\omega)$ is the quasiparticle spectral function and $f(\omega)$ is the Fermi function] for several $\mathbf{k}$ vectors ranging from $\mathbf{k}=(\pi,0),(7\pi/8,0),(13\pi/16,0),\ldots$, down to $(0,0)$. The parameter values are the same as in Figs. 1 and 2. For $\mathbf{k}$ vectors near $(\pi,0)$ we have a sharp low-energy peak followed by a dip and then a hump at higher energy. For $\mathbf{k}$ moving from $(\pi,0)$ to $(0,0)$, the sharp peak remains first at about the same position while the broad hump moves to higher binding energy. In Fig. 3(b) we show the corresponding normal-state spectra at $T=0.023t$. One notices that the broad hump at higher binding energy remains at the same position upon entering the normal state, while the sharp peak and the dip feature disappear. In the superconducting state along the nodal direction of the d-wave order parameter we do not observe the dip feature as we have shown previously.[9] These
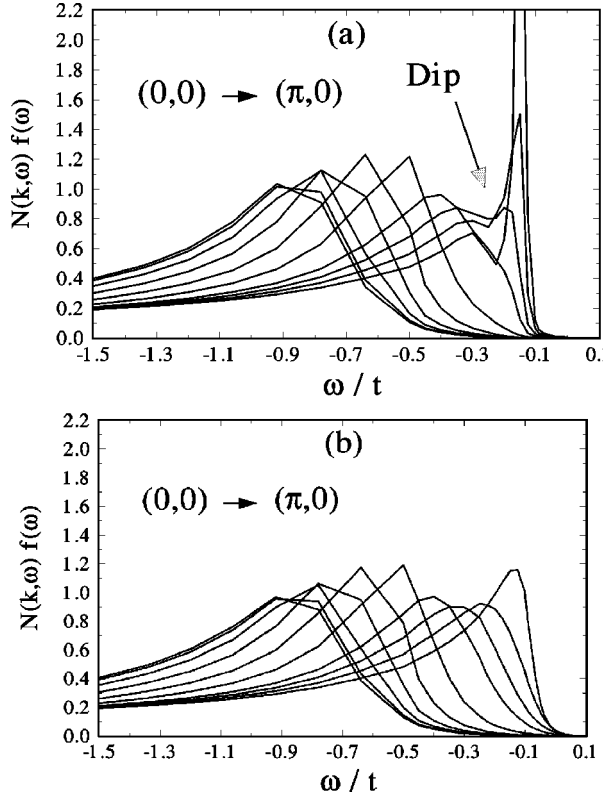
FIG. 3. Photoemission intensity, $N(\mathbf{k},\omega)f(\omega)$ (here N is the quasiparticle spectral function and f the Fermi function) for $\mathbf{k} = (k\pi,0)$ where $k = 1, 7/8, 13/16, 3/4, 5/8, 1/2, 3/8, 1/4, 1/8$, and 0. (a) in the superconducting state at $T/T_c = 0.77$. The narrow peaks at low binding energy decrease and vanish, and the binding energies of the broad humps increase in the sequence of k values. (b) in the normal state at $T = 0.023t$. Note, that the broad humps are at the same position as in the superconducting state.

results are in qualitative agreement with the photoemission spectra of $Bi_2Sr_2CaCu_3O_{8+\delta}$ (Bi 2212).[14] In this paper it was argued that the dip in the spectrum stems from a steplike edge in the quasiparticle scattering rate which arises from the interaction with a collective mode. This scenario is confirmed by our results for the collective mode shown in Fig. 1 and by the scattering rate shown in Fig. 2. We estimate from the edge of the peak in Fig. 3 a gap amplitude $\Delta_0 \simeq 0.1t$ at $T/T_c = 0.77$ and a spectral dip at binding energy of about $2.3\Delta_0$ corresponding to a mode frequency $\omega_0 \simeq 1.3\Delta_0$ according to the estimates of Ref. 14. However, here we have a discrepancy with regard to the latter estimates because our mode frequency shown in Fig. 1 is much lower, i.e., $\omega_0 \simeq 0.8\Delta_0$. We note that we obtain also a dip in the density of states $N(\omega)$ below the gap peak at negative ω values which agrees qualitatively with scanning tunneling microscopy measurements on Bi 2212.[15]

We want to mention that higher-order peaks in the photoemission spectra due to the collective mode as have been observed for example in solid hydrogen[16] are not visible here. This is due to the fact that in our case the spin-density-wave collective mode is a damped mode and the strong quasiparticle damping rate washes out higher-order peaks. In addition, the self-energy contains an average over momentum, further reducing this effect. This is documented by the fact that the normal-state spectrum in Fig. 3(b), where there

is no collective mode present, is not much different from the spectrum in the superconducting state in Fig. 3(a) at higher binding energy.

We come now to the discussion of order-parameter collective modes in d-wave superconductors which can be calculated in analogy to those in p-wave pairing superconductors.[4] In general it can be said that the $d_{x^2-y^2}$-wave pairing component in weak-coupling theory gives rise to the phase-fluctuation mode which is renormalized into a 2D plasmon,[6] and to the amplitude fluctuation mode of the d-wave gap. For each additional (weaker) pairing component, like an extended s-wave component, one obtains an amplitude (real) and a phase (imaginary) fluctuation mode. Let us first consider the amplitude fluctuation mode of the $d_{x^2-y^2}$-wave gap. We have calculated the mode frequency ω_0 from the weak-coupling expression in Ref. 3 for $\mathbf{q}=0$:

$$\mathrm{Re}\left[\sum_k (\omega^2 - 4\Delta_k^2)[\cos(k_x) - \cos(k_y)]^2 \right.$$

$$\left. \times [4E_k^2 - (\omega + i\Gamma)^2]^{-1} \frac{\tanh(E_k/2T)}{E_k} \right] = 0. \qquad (4)$$

By summing numerically over $\mathbf{k}$ in the square Brillouin zone we obtain for $t' = 0$ in $\epsilon(\mathbf{k})$ and $T = 0$ two solutions with frequencies $\omega_0 \simeq \sqrt{3}\Delta_0$ provided that the damping Γ is sufficiently large, namely, $\omega_0 < 3.5\Gamma$. For $t' = -0.45t$ and $T = 0$ we obtain two solutions whose frequencies are somewhat larger, $\omega_0 \simeq 2\Delta_0$, where again the condition $\omega_0 < 3.5\Gamma$ has to be satisfied. For a mode frequency $\omega_0 = 2\Delta_0 \simeq 0.2t$ at $T/T_c = 0.77$ (see Fig. 3) one finds from Fig. 2 a damping $\Gamma(\omega_0) \simeq 0.1t$ at the antinode $\mathbf{k}_a$ which means that the condition $\omega_0 < 3.5\Gamma$ is satisfied. In Ref. 6 a frequency $\omega_0 = \sqrt{3}\Delta_0$ was obtained for the amplitude collective mode, however, the coupling of this mode to the charge fluctuations was neglected. We find that the coupling of this fluctuation in the particle-particle channel to the charge fluctuation in the particle-hole channel yields approximately the following contribution χ_{fl} to the charge susceptibility χ_{c0} at $T = 0$ (see Refs. 3 and 4):

$$\chi_{fl}(\mathbf{q}=0,\omega) = 2\left(\frac{N_F'}{N_F} \frac{1}{V_0} \right)^2 \Delta_0^2 \frac{1}{g(\omega)}, \qquad (5)$$

$$g(\omega) = N_F \left[\frac{2}{3}\bar{\omega}^2 + \frac{4}{3}\gamma^2 - 1 - \frac{8}{3}i\bar{\omega}\gamma \right.$$

$$\left. + \gamma(4\bar{\omega}^2 - 2\gamma^2 + 6i\bar{\omega}\gamma)\ln(4[1 - (\bar{\omega} + i\gamma)^2]^{-1/2}) \right],$$

$$\bar{\omega} = \omega/2\Delta_0, \qquad \gamma = \Gamma/2\Delta_0. \qquad (6)$$

Here, N_F and $N_F' = dN_F/d\omega$ are the density of states and its derivative at the Fermi energy $\omega = 0$. One notices from Eq. (6) that in the limit $\gamma \to 0$ one obtains no valid solution of the equation $\mathrm{Re}\, g(\omega_0) = 0$ because the solution $\overline{\omega_0} = \sqrt{3/2}$ violates the condition that $\overline{\omega_0} \leq 1$. However, for suffiently large val-

ues of Γ ($\gamma \gtrsim \bar{\omega}/2$) one obtains a solution of the equation Re $g(\omega_0)=0$ which satisfies the condition $\overline{\omega_0} \lesssim 1$. One sees from Fig. 2 that this condition is approximately satisfied for $\omega_0 = 2\Delta_0 \simeq 0.2t$ because then one enters the pair-breaking continuum where $\Gamma \sim \omega/2$ near the antinode $\mathbf{k}_a$. Thus the mode frequency is about $\omega_0 = 2\Delta_0$ for damping $\Gamma = \Delta_0$ in agreement with the numerical results.

We have calculated the resonance frequency of the exciton-like s-wave mode of the order parameter which is caused by an additional s-wave pairing component $|g_0|$ which is smaller than the main d-wave pairing component $|\bar{g}_2|$ (see Ref. 6). The method of Refs. 3 and 4 yields the following contribution χ_{exc} of this order-parameter fluctuation mode to the charge susceptibility χ_{c0} at $T=0$:

$$\chi_{\text{exc}}(\mathbf{q}=0,\omega) = -(N_F \omega)^2 [g_{\text{exc}}(\omega)]^{-1}, \quad (7)$$

$$g_{\text{exc}}(\omega) = \left(1 - \frac{\bar{g}_2}{g_0}\right) \sum_k \frac{1}{2E_k}$$
$$+ \frac{1}{2}\omega^2 \sum_k \frac{\tanh(E_k/2T)}{E_k[4E_k^2 - (\omega+i\Gamma)^2]}. \quad (8)$$

From Eq. (8) we obtain the following approximate result:

$$g_{\text{exc}}(\omega) = \left(1 - \frac{\bar{g}_2}{g_0}\right) \frac{1}{V_0} + N_F i \frac{\bar{\omega}^2}{(\bar{\omega}+i\gamma)} K(\bar{\omega}+i\gamma), \quad (9)$$

where V_0^{-1} is given by Eq. (2) and $\bar{\omega}$ and γ by Eq. (3). We have carried out the summation over $\mathbf{k}$ in Eq. (8) numerically and find in agreement with Ref. 6 that a solution of the equation in Re $g_{\text{exc}}(\omega_0)=0$ at given Δ_0 and Γ exists only for very small values of the parameter $(\bar{g}_2/g_0) - 1 (\lesssim 0.1)$. This means that the s-wave pairing coupling has to be almost as strong as the d-wave pairing component which is quite unrealistic. However, for increasing Γ the resonance frequency ω_0 decreases and becomes much smaller than the pair-breaking threshold $2\Delta_0$ for reasonably large scattering rates ($\Gamma/2\Delta_0 \sim 1/2$). This means that the contribution Im $\chi_{\text{exc}}(\omega)$ of the excitonlike mode to Raman-scattering intensity with B_{1g} polarization shows up as a small peak below the pair-breaking threshold. Since the damping Γ in the direction of the momentum of the antinode of the order parameter rises rapidly with ω [see Fig. 2(a)] it may be that this peak becomes observable for smaller values of the ratio $g_0/\bar{g}_2$ of s-wave and d-wave pairing couplings than those which have been obtained from weak-coupling theory.[6]

In the weak-coupling limit it has been shown that vertex corrections due to the d-wave pairing interaction together with electron-electron scattering lead to good agreement with the B_{1g} Raman data on YBCO.[17] In Fig. 4 we show our strong-coupling results for the Raman response functions Im $\chi_\gamma(\mathbf{q}=0,\omega)$ where γ are the vertices $\gamma = t[\cos(k_x) - \cos(k_y)]$ and $\gamma = -4t'\sin(k_x)\sin(k_y)$ for B_{1g} and B_{2g} symmetry. One sees that for B_{1g} symmetry a gap and a pair-breaking threshold develop below T_c with a threshold at about $0.15t \simeq (3/2)\Delta_0$ at $T/T_c = 0.77$ (see Fig. 3). This means that the peak of the order-parameter collective mode at $\omega_0 \simeq 2\Delta_0$ and width Δ_0 lies in the pair-breaking continuum.
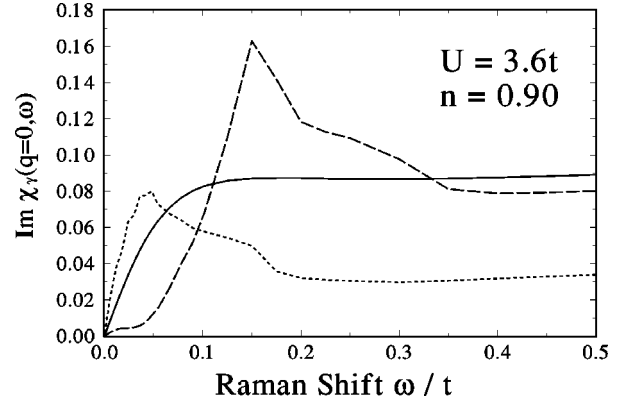

FIG. 4. Raman spectra Im $\chi_\gamma(\mathbf{q}=0,\omega)$ for B_{1g} symmetry at $T=0.023t$ (solid line) and $T/T_c=0.77$ (dashed line), and Raman spectrum for B_{2g} symmetry at $T/T_c=0.77$ (dotted line). $T_c=0.022t$.

The question arises whether or not the contribution Im χ_{fl} to the B_{1g} Raman spectrum is sizeable because the coupling strength proportional to N_F'/N_F in Eq. (5) arising from particle-hole asymmetry is rather small. However, in the strong-coupling calculation the coupling strength of this mode to charge density given by $T\Sigma_k \Sigma_n G(\mathbf{k},i\omega_{n+m})F(\mathbf{k},i\omega_n)$ is much larger. The reason is that beside the term proportional to $\epsilon(\mathbf{k})$ yielding N_F'/N_F, one obtains additional terms proportional to the self-energy components Re $\xi(\mathbf{k},\omega)$ and Im $\xi(\mathbf{k},\omega)$ which give relatively large contributions. In addition, one obtains a contribution from the imaginary part of the gap function, i.e., Im $\phi(\mathbf{k},\omega)$.

In conclusion, we can say that the spin-density-wave collective mode below T_c gives rise to large effects in the magnetic neutron scattering and photoemission intensities and the tunneling density of states. In order to explain the physical basis of our strong-coupling results we have compared them with analytical expressions derived from weak-coupling theory. This shows that the gap in the scattering rate and the strong mass enhancement of the quasiparticles below T_c are decisive for the observability of this mode. On the other hand, the amplitude fluctuation mode of the d-wave gap couples only weakly to the charge fluctuations and yields a broad peak above the pair-breaking threshold in the B_{1g} Raman spectrum. This peak may be, at least partially, responsible for the observed broadening above the pair-breaking peak because the coupling strength due to particle-hole asymmetry is enhanced by strong-coupling self-energy effects.

Previous work on collective modes in high-T_c superconductors[6,18-21] has been restricted to weak-coupling and mean-field calculations. The FLEX approach we use here, is a self-consistent and conserving approximation scheme, which goes well beyond mean-field approximation. Especially the feedback effect of the one-particle properties on the collective modes in the superconducting state is included self-consistently and the importance of the quasiparticle damping becomes clear. It is therefore a highly nontrivial and satisfactory result, that the resonance in the spin susceptibility, the steplike edge in the quasiparticle scattering rate, and the dip features in the ARPES and tunneling spectra can all be understood within one theory in a self-consistent

fashion. The self-consistent calculation also yields a larger coupling strength of the d-wave amplitude mode to the charge density and a lower resonance frequency of the s-wave exciton-like mode of the order parameter which makes it more likely that these modes show up in the B_{1g} Raman-scattering channel.

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