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2002 J. Phys.: Condens. Matter 14 9651

(http://iopscience.iop.org/0953-8984/14/41/320)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 9651–9658 PII: S0953-8984(02)37116-9

In-plane optical conductivity due to scattering from spin fluctuations in d-wave superconductors

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Received 17 May 2002, in final form 3 September 2002
Published 4 October 2002
Online at stacks.iop.org/JPhysCM/14/9651

Abstract

The in-plane optical conductivity of high-T_c cuprates in the superconducting (SC) and normal states is studied on the basis of the slave-boson mean-field approach to the 2D t–t'–J model and the antiferromagnetic spin fluctuation correction in the framework of the renormalized random-phase approximation. The mid-infrared contribution to the conductivity in the normal state and the peak/dip/hump feature of the spectra in the SC state are reproduced, and are shown to be caused by coupling to spin fluctuations, in particular by coupling to the resonance mode of the spin fluctuations.

1. Introduction

Far-infrared spectroscopy of high-T_c superconductors has provided much valuable information about low-energy electronic excitations [1–7]. The in-plane optical conductivity $\sigma_1(\omega, T)$ is believed to provide a sensitive probe for detecting the dynamic properties of the carriers in the CuO_2 plane. It has been shown [3, 4] that the spectra in the normal state have a Drude-like contribution at very low frequencies which is followed by an anomalous strong mid-infrared (MIR) contribution. In the superconducting (SC) state, the spectrum around 500 cm^{-1} is lower than for the normal state, but when the frequency exceeds about 1000 cm^{-1} it recovers and almost coincides with that for the normal state [7]. In the early days, this unusual behaviour was explained on the basis of a phenomenological two-component model which consists of a 'free-carrier' Drude-like contribution at low frequencies and the MIR one associated with 'bound carriers' [9]. An alternative one-component model in which the quasi-particle scattering rate has the so-called 'marginal-Fermi-liquid' form has also been proposed [10]. Recently, theoretical calculations based on the scattering by spin fluctuations have been carried out, in which a d-wave BCS model incorporating the spin fluctuations within a weak-coupling Hubbard model picture [11] or in a phenomenological form has been adopted [12, 13].

On the other hand, many anomalous features of high-T_c cuprates observed in other measurements such as ARPES (angle-resolved photoemission spectroscopy) [14, 15] and SIN (superconductor–insulator–normal) and SIS (superconductor–insulator–superconductor) tunnelling spectroscopy [16] have suggested that conducting electrons in the SC state are strongly coupled to collective excitations centred at $\boldsymbol{Q} = (\pi, \pi)$. It has been speculated that these collective excitations may be the resonance mode observed in the inelastic neutron scattering (INS) experiments [17–19]. Recently, Carbotte *et al* [8] have analysed the optical properties of the copper oxides in detail. They found that the strength of coupling of the charged quasiparticles to the spin resonance mode, which can be inferred from experiments, is sufficient to account for the high SC transition temperatures, therefore providing strong support for this suggestion.

The slave-boson mean-field approach to the two-dimensional (2D) t–t'–J model and the treatment of the antiferromagnetic (AF) fluctuations in the renormalized random-phase-approximation (RPA) form have been able to reproduce many important features of the resonance peak observed in INS experiments [21–23], and have been successfully used to explain the peak/dip/hump structure observed in ARPES [22] and to account for the condensation energy [24]. In this approach the dispersion of quasiparticles and the SC gap for different hole doping concentrations are determined self-consistently; therefore a semi-quantitative comparison with experiments is possible. In this paper we shall examine the in-plane optical conductivity on the basis of this approach. Our results show that in the normal state there is a MIR contribution that is very weakly dependent on frequency and temperature, while a peak/dip/hump feature is found in the spectra of the SC state. We attribute the anomalous structure of the latter to scattering off the spin resonance. To avoid the complication arising from the pseudogap, which appears in the normal state of the underdoped cuprates below a certain temperature T^* above T_c, we will confine our discussion about the normal state to the optimally doped case. The pseudogap is beyond the scope of this paper.

The paper is organized as follows. Section 2 contains a detailed account of the model and the computational approach. Results are presented and discussed in section 3. A short summary is given in section 4.

2. Model and computation

We start with the 2D t–t'–J model which reads

$$H = -\sum_{\langle ij\rangle,\sigma} t c^{\dagger}_{i\sigma} c_{j\sigma} - \text{h.c.} - \sum_{\langle ij\rangle',\sigma} t' c^{\dagger}_{i\sigma} c_{j\sigma} - \text{h.c.} + J \sum_{\langle ij\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

where $\langle ij\rangle$ denotes the summation over nearest-neighbour (nn) bonds and $\langle ij\rangle'$ the next-nearest-neighbour (nnn) bonds, $\boldsymbol{S}_i = \frac{1}{2}\sum_{\alpha,\beta} c^{\dagger}_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}$, where $\sigma_{\alpha\beta}$ is the Pauli spin matrix and $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the electron creation (annihilation) operator at the ith site, which implicitly excludes double occupancy on the same lattice site. In the slave-boson method, c_i is expressed as the combination of slave bosons b_i carrying the charge and fermions $f_{i\sigma}$ representing the spin, so we rewrite as follows: $c_{i\sigma} = b^{\dagger}_i f_{i\sigma}$. The local single-occupancy constraint leads to $b^{\dagger}_i b_i + \sum_\sigma f^{\dagger}_{i\sigma} f_{i\sigma} = 1$, which will be satisfied at the mean-field level on average. In the SC state, we consider the order parameters $\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow}\rangle = \pm\Delta_0$ with d-wave symmetry and $\chi_{ij} = \langle f^{\dagger}_{i\uparrow} f_{j\uparrow} + f^{\dagger}_{i\downarrow} f_{j\downarrow}\rangle = \chi_0$, while bosons condense: $b_i \to \langle b_i\rangle = \sqrt{\delta}$ (δ is the hole concentration). Using the Hartree–Fock–Bogoliubov decomposition [25], we obtain the mean-field Hamiltonian H_m of equation (1):

$$H_m = \sum_{k\sigma} \epsilon_k f^{\dagger}_{k\sigma} f_{k\sigma} - \sum_k \Delta_k (f^{\dagger}_{k\uparrow} f^{\dagger}_{-k\downarrow} + \text{h.c.}) + 2NJ'(\chi_0^2 + \Delta_0^2) \tag{2}$$

where $\epsilon_k = -2(\delta t + J'\chi_0)[\cos(k_x) + \cos(k_y)] - 4\delta t' \cos(k_x)\cos(k_y) - \mu$, $\Delta_k = 2J'\Delta_0[\cos(k_x) - \cos(k_y)]$, with $J' = 3J/8$. The values of the parameters in the t–t'–J model are given by $t = 2J$, $t' = -0.45J$, and $J \approx 130$ meV, as used previously [21, 22]. The mean-field parameters χ_0, Δ_0, and chemical potential μ for different doping (δ) and temperature values are obtained from the following self-consistent equations derived by minimizing the total free energy:

$$\begin{aligned}
\chi_0 &= -\frac{1}{2N}\sum_k \frac{\gamma_k \varepsilon_k}{E_k}\tanh\left(\frac{\beta E_k}{2}\right) \\
1 &= \frac{1}{N}\sum_k \frac{J'\varphi_k^2}{E_k}\tanh\left(\frac{\beta E_k}{2}\right) \\
\delta &= \frac{1}{N}\sum_k \frac{\varepsilon_k}{E_k}\tanh\left(\frac{\beta E_k}{2}\right)
\end{aligned} \tag{3}$$

where $\gamma_k = \cos(k_x) + \cos(k_y)$, $\varphi_k = \cos(k_x) - \cos(k_y)$, and $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$ is the quasiparticle excitation energy in the SC state. In the optimally doped region, the parameters in the mean-field Hamiltonian for the normal state are obtained similarly, by simply enforcing the SC gap $\Delta_0 = 0$ during the calculation. This extrapolation has been proved successful in a previous work that calculated the SC condensation energy [24].

The inclusion of the AF spin fluctuations can be done by perturbing around the mean-field Hamiltonian; i.e., we write the Hamiltonian as $H = H_m + H'$, and treat H' as a perturbation. In principle, all fluctuations should be included. However, different selections of subset diagrams may result in different kinds of fluctuation. We calculate the AF spin fluctuations in the RPA form which includes a series of ring diagrams, as done previously [21, 22]. The resulting spin susceptibility is given by

$$\chi(\boldsymbol{q}, \omega) = \frac{\chi^0(\boldsymbol{q}, \omega)}{1 + \alpha J(\boldsymbol{q})\chi^0(\boldsymbol{q}, \omega)} \tag{4}$$

in which $J(\boldsymbol{q}) = J[\cos(k_x) + \cos(k_y)]$ and $\chi^0(\boldsymbol{q}, \omega)$ is the bare spin susceptibility which is calculated from the fermionic bubbles representing particle–hole (p–h) excitations and can be obtained by the analytic continuation ($\mathrm{i}\omega \to \omega + \mathrm{i}\eta$; η is a positive infinitesimal) of the Matsubara Green function $\chi^0(\boldsymbol{q}, \mathrm{i}\omega)$:

$$\begin{aligned}
\chi^0(\boldsymbol{q}, \mathrm{i}\omega) = -\frac{1}{4N}\sum_k \Bigg\{ & \left(1 - \frac{\epsilon_k\epsilon_{k+q} + \Delta_k\Delta_{k+q}}{E_k E_{k+q}}\right) \\
& \times \left[\frac{1 - f(E_k) - f(E_{k+q})}{\mathrm{i}\omega - E_k - E_{k+q}} - \frac{1 - f(E_k) - f(E_{k+q})}{\mathrm{i}\omega + E_k + E_{k+q}}\right] \\
& - \left(1 + \frac{\epsilon_k\epsilon_{k+q} + \Delta_k\Delta_{k+q}}{E_k E_{k+q}}\right) \\
& \times \left[\frac{f(E_k) - f(E_{k+q})}{\mathrm{i}\omega - E_k + E_{k+q}} - \frac{f(E_k) - f(E_{k+q})}{\mathrm{i}\omega + E_k - E_{k+q}}\right]\Bigg\}
\end{aligned} \tag{5}$$

where $f(E_k)$ is the Fermi distribution function.

In the usual RPA approach, the parameter α in equation (4) should be 1. However, $\alpha = 1$ will give rise to an AF instability at doping $\delta \approx 0.22$, which is much larger than $\delta_c \approx 0.02$ as observed in experiments. In the renormalized RPA approach that Brinckmann and Lee discussed clearly in [21], α is taken as a phenomenological parameter which is determined by reducing the AF instability to be at $\delta = 0.02$. This gives $\alpha = 0.34$, which is the only adjusted parameter in our paper.

The fermionic self-energy is obtained from the lowest-order contribution of the scattering of fermions by spin fluctuations. In the Matsubara–Nambu representation [26], the self-energy is in the form of a 2×2 matrix which is expressed as follows:

$$\hat{\Sigma}(\boldsymbol{k}, \mathrm{i}\omega_n) = -\frac{3}{2}\frac{1}{\beta N}\sum_{\boldsymbol{q}}\sum_{\mathrm{i}\omega_m} J^2(\boldsymbol{q})\chi(\boldsymbol{q}, \mathrm{i}\omega_m)\hat{\sigma}_3\hat{G}(\boldsymbol{k}-\boldsymbol{q}, \mathrm{i}\omega_n - \mathrm{i}\omega_m)\hat{\sigma}_3. \tag{6}$$

The fermionic Green function is calculated via usual Dyson equations, $\hat{G}^{-1}(\boldsymbol{k}, \omega) = \hat{G}_0^{-1}(\boldsymbol{k}, \omega) - \hat{\Sigma}(\boldsymbol{k}, \omega)$, where $\hat{G}_0(\boldsymbol{k}, \omega)$ is the unperturbed Green function and is given by

$$\hat{G}_0(\boldsymbol{k}, \omega) = \frac{\mathrm{i}\omega\hat{\sigma}_0 + \epsilon_{\boldsymbol{k}}\hat{\sigma}_3 + \Delta_k\hat{\sigma}_1}{(\mathrm{i}\omega)^2 - \epsilon_{\boldsymbol{k}}^2 - \Delta_k^2} \tag{7}$$

with $\hat{\sigma}_i$ being the Pauli matrices. The Kubo formula is used to calculate the in-plane optical conductivity within the BCS framework. The real part of the conductivity, labelled as $\sigma_1(\omega)$, is given by [27]

$$\sigma_1(\omega) = -\frac{\mathrm{Im}\,\Pi_{xx}(\omega)}{\omega}, \tag{8}$$

with

$$\mathrm{Im}\,\Pi_{xx}(\omega) = \sum_{\boldsymbol{k}}\frac{\pi e^2}{N}\int \mathrm{d}\omega'\,[v_x(\boldsymbol{k})]^2\,\mathrm{Tr}[\hat{A}(\boldsymbol{k}, \omega+\omega')\hat{A}(\boldsymbol{k}, \omega')][f(\omega+\omega') - f(\omega')] \tag{9}$$

where the spectral function $\hat{A}(\boldsymbol{k}, \omega) = -(1/\pi)\,\mathrm{Im}\,\hat{G}(\boldsymbol{k}, \omega)$ and v_x is the x-component of the fermionic quasiparticle group velocity.

In the following numerical calculations, the summation of k over the 2D Brillouin zone (BZ) is performed by dividing the BZ into a conventional rectangular mesh containing 256×256 k-points. One can see that the computational task is huge if we directly calculate the self-energy from equation (6). Fortunately, equation (6) is in the form of a discrete convolution where the convolution theorem is valid, so we can adopt a fast Fourier transform algorithm [28] to calculate the self-energy, which saves a lot of time and improves the efficiency greatly.

3. Results and discussion

The ω-dependence of the in-plane optical conductivity $\sigma_1(\omega)$ at optimal doping $\delta = 0.16$ is shown in figure 1 for different temperatures. We first discuss the conductivity in the normal state, which is shown as the short-dashed line ($T = 0.2\ J \approx 300$ K), the dashed–dotted line ($T = 0.133\ J \approx 200$ K), and the dotted line ($T = 0.066\ J \approx 100$ K). The spectra have a prominent Drude-like component at low frequencies followed by a MIR component. As temperature decreases (still higher than T_c), the width of the low-frequency part shrinks and the corresponding intensity goes up sharply. However, almost no change is found in the MIR part of the spectra. This is in agreement with the spectra observed in experiments [3, 4, 7], where the MIR contribution exhibits a weak temperature dependence. The most remarkable difference between the spectra presented here and those of conventional metals is the existence of the MIR component, which can be attributed to the coupling to spin fluctuations that show up as a broad hump in the normal state around $\boldsymbol{q} \approx (\pi, \pi)$ in INS experiments [17, 20].

When temperature is decreased to below T_c, a narrower residual Drude-like response remains, but the spectra around $0.7\ J$ are heavily suppressed compared to the normal-state counterpart, as shown in figure 1. However, the spectra of the two states almost coincide when the frequency exceeds $1.5\ J$. Thus, a dip forms between the Drude-like component and the MIR component, and the whole spectrum has a peak/dip/hump structure which shares some kind of similarity with the single-particle spectrum observed in ARPES [14, 15].

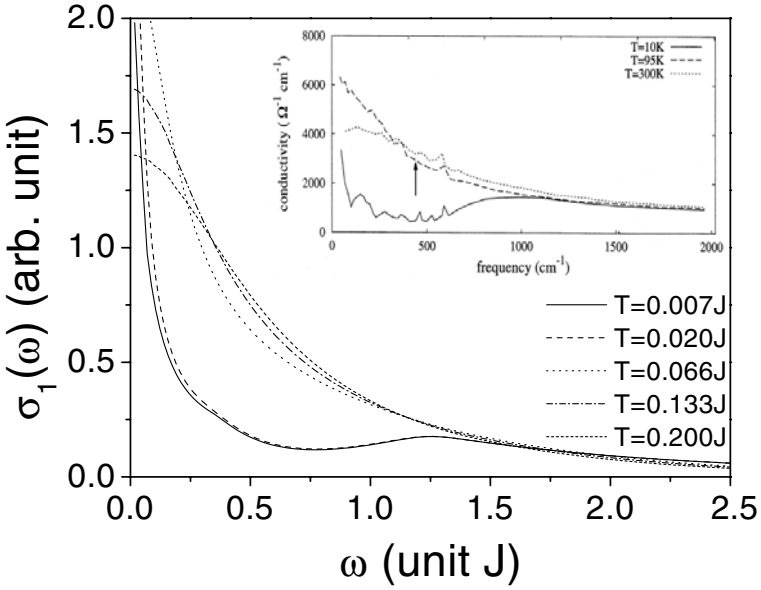

Figure 1. The ω-dependence of the in-plane optical conductivity $\sigma_1(\omega)$ at optimal doping $\delta = 0.16$ for different temperatures. For comparison, we show in the inset the experimental results for an optimally doped YBCO sample given by Puchkov *et al* [4].

To compare with experiments, we present one typical result of Puchkov *et al* for YBCO single crystals [4] as shown in the inset of figure 1. Considering the shape of the spectra, the agreement of our results with experimental data is quite good. We note that the YBCO materials contain a CuO_2 bilayer and a special CuO chain structure, which are not considered here. However, the coincidence with corresponding experiments can also be found in other families of high-T_c superconductors including the single-layered compound Tl2201 and bilayer Bi2212 [4, 7], neither of which contains a CuO chain. Therefore, the rough shape of the spectra may be an intrinsic property of the CuO_2 plane. In addition, the maximum of the broad hump in our results appears at about $1.25\ J \approx 1300\ \mathrm{cm}^{-1}$, which is also in reasonable agreement with the experimental value $\sim 1000\ \mathrm{cm}^{-1}$. But the spectra (both in the normal and the SC states) descend more rapidly than the experimental data. It is important to note that we do not introduce more adjustable parameters and an empirical formula to fit the experimental data. The values of the mean-field parameters χ_0, Δ_0, and μ are all determined self-consistently. The only adjustable parameter is α which is chosen to be $\alpha = 0.34$ based on the agreement of the theoretical and experimental results on the AF instability [21]. The values of t, t' and J in the t–t'–J model have been used in previous calculations and have given good results for the spin and charge responses [21–24].

For comparison, in the practical computation we have adopted three different damping rates for the quasiparticles Γ (used during the procedure of analytic continuation), namely 0.02, 0.01, and 0.003 J. Our numerical results are found to be robust and reliable, since no obvious difference in the spectra is found.

Now we turn to the origin of the peak/dip/hump structure in the in-plane optical conductivity. The spin excitation resonance mode is the prominent feature of the spin fluctuation spectrum in the SC state observed by means of neutron scattering, and can be reproduced theoretically via the renormalized RPA form of the spin susceptibility equation (4) [21–23].

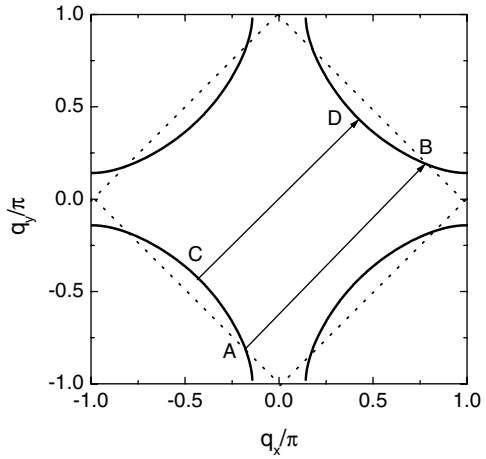

Figure 2. Schematic topological structure of the Fermi surface, represented by the thick solid curve. The thin solid and dashed lines denote the threshold p–h excitations for different wavevectors (see the text).

Because it appears around the AF wavevector $\boldsymbol{Q} = (\pi, \pi)$, the quasiparticle excitations with transition momentum $\boldsymbol{q} \approx \boldsymbol{Q}$ will be most effectively affected by the spin resonance. These involve the excitations from A to B, as shown schematically in figure 2, with the transition energy Ω_0 (the spin excitation resonance mode energy) which is determined from the peak position of the spin susceptibility, as calculated using equation (4) [22, 23], and is found to be smaller than the maximum of the d-wave gap. On the other hand, those excitations near the diagonal direction fail to feel the effect of the spin resonance, due to the requirement of momentum conservation. In this case the transition energy approaches zero, because the SC gap $\Delta_{\boldsymbol{k}}$ vanishes in this direction due to the $d_{x^2-y^2}$-wave symmetry. Thus the conductivity at very low frequencies involves only those excitations from C to D, i.e., along the diagonal direction, and these nodal quasiparticle excitations contribute to the low-energy Drude-like component in the optical conductivity. When the frequency increases to the spin resonance frequency Ω_0 or so, the coupling of quasiparticles to the spin resonance mode comes into effect and this furnishes an additional scattering channel. Therefore, the spectra are suppressed. This is in analogy with the case of the dip formation in the single-particle spectrum [22] and suggests that the dip in the in-plane conductivity comes from the coupling to the spin resonance.

The ω-dependence of the in-plane optical conductivity $\sigma_1(\omega)$ at $T = 0.007\ J \approx 10$ K for different doping levels ($\delta = 0.065$, 0.10, 0.16, and 0.20) is shown in figure 3. Though the dip in the spectra is shallow, we can still see that it shifts to low frequencies when the hole concentration is decreased. From both the experimental data [17] and the theoretical calculations [22], we know that Ω_0 also decreases with the decrease in hole concentration. This doping dependence of the dip position is therefore consistent with the above explanation of its formation. Finally, we note that the MIR spectra at high frequencies are almost independent of the variation of hole concentration.

Though the agreement of the spectral lineshape with many experiments is quite good as shown above, our calculations deviate much from the experimental data for single-layer LSCO families [29]. The spin excitation resonant mode observed by means of neutron scattering in other cuprates is, thus far, still unidentified in the LSCO family. However, it has just been discovered that this resonant mode is present in $Tl_2Ba_2CuO_{6+\delta}$ [30]. $Tl_2Ba_2CuO_{6+\delta}$ is also a single-layer compound and the lineshape of its optical conductivity [4, 7] agrees well with

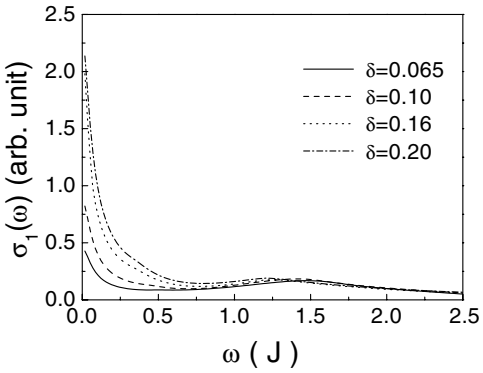

Figure 3. The ω-dependence of the in-plane optical conductivity $\sigma_1(\omega)$ at temperature $T = 0.007\ J$ (10 K) for different doping levels $\delta = 0.065$, 0.10, 0.16, and 0.20.

our above results. This is consistent with our above analysis based on the spin resonant mode. Therefore there may be some peculiar factor in the LSCO family which determines this anomaly and has not been considered in our calculation. Further experimental and theoretical work is necessary.

Finally, we note that our calculation does not incorporate the scattering of quasiparticles by impurities, which has been considered by other researchers [11, 13]. This is because optical measurements are usually carried out on untwinned single-crystal samples of high quality and the impurity scattering is small relative to the strong inelastic scattering from AF spin fluctuations, and gives only a minor correction to the spectral lineshape. In addition, more phenomenological parameters must be introduced during the theoretical treatment of impurity scattering.

4. Summary

On the basis of the slave-boson mean-field approach to the 2D t–t'–J model and taking into consideration the AF spin fluctuations via the renormalized RPA approximation, we have calculated the in-plane optical conductivity of high-T_c copper oxides in both the SC and the normal states. For the normal state, our results exhibit a prominent MIR contribution that is weakly dependent on frequency and temperature. For the SC state we reproduce the peak/dip/hump structure in the spectra of the conductivity. These results are consistent with experiments. It is shown that the dip in the conductivity in the SC state is caused by the scattering of the charge quasiparticles off the spin resonance mode, which shares a common origin with the dip in the single-particle spectrum observed by ARPES [22]. In the light of the recent studies of the effect of the spin resonance on the condensation energy [24] and on the spectra of angle-resolved photoemission and tunnelling in high-T_c cuprates [31], we think that our results give additional support to the importance of the resonant spin excitation mode in determining many physical properties of the SC state of high-T_c cuprates.

Acknowledgments

This work is partially supported by the National Natural Science Foundation of China under Grant No 10074077. We thank Professor X G Qiu and Dr P S Luo for illuminating discussions about relevant optical experiments.

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