Origin of peak-dip-hump structure in the in-plane optical conductivity of the high-T_C cuprates: Role of antiferromagnetic spin fluctuations of short-range order

Sung-Sik Lee,[1] Jae-Hyeon Eom,[1] Ki-Seok Kim,[1] and Sung-Ho Suck Salk[1,2]
[1]*Department of Physics, Pohang University of Science and Technology, Pohang, Kyoungbuk, Korea 790-784*
[2]*Korea Institute of Advanced Study, Seoul, 130-012 Korea*
(Received 4 June 2002; published 23 August 2002)

An improved U(1) slave-boson approach is applied to study the optical conductivity of the two-dimensional systems of antiferromagnetically correlated electrons over a wide range of hole doping and temperature. Interplay between the spin and charge degrees of freedom is discussed to explain the origin of the peak-dip-hump structure in the in-plane conductivity of high-T_C cuprates. The role of spin fluctuations of short-range order (spin singlet pair) is investigated. It is shown that the spin fluctuations of the short-range order can cause the midinfrared hump, by exhibiting a linear increase of the hump frequency with the antiferromagnetic Heisenberg coupling strength.

DOI: 10.1103/PhysRevB.66.064520 PACS number(s): 74.20.Mn, 74.25.Fy, 74.25.Gz

High-T_C superconductors are the systems of strongly correlated electrons which show two dimensionality in charge transport. Various levels of the gauge theoretic slave-boson approach to the t-J Hamiltonian have been proposed to study high-T_C superconductivity.[1–7] Recently we proposed an SU(2) slave-boson theory[6] which incorporated coupling between the charge and spin degrees of freedom into the Heisenberg term. The predicted phase diagram showed an arch-shaped bose condensation line in agreement with observation. Using an improved U(1) slave-boson theory over our earlier one,[7] in this paper we study the cause of peak-dip-hump structures of observed optical conductivity.[8–12] Various theories have been proposed to explain the cause of the peak-dip-hump structure in the optical conductivity.[13–15] However, most studies have been made to a limited range of hole doping and temperature, based on empirical parameters deduced from measurements such as the inelastic neutron scattering (INS) and the angle-resolved photoemission spectroscopy (ARPES) data.

Using the nearly antiferromagnetic Fermi-liquid theory, Stojković and Pines[13] reported a study of normal-state optical conductivity for optimally doped and overdoped systems. They showed that the highly anisotropic scattering rate in different regions of the Brillouin zone leads to an average relaxation rate of the marginal Fermi-liquid form. Their computed optical conductivity agreed well with experimental data for the normal state of an optimally doped sample. Using the spin-fermion model[16,17] and spin susceptibility parameters obtained from INS and nuclear magnetic resonance, Munzar, Bernhard, and Cardona[14] calculated the in-plane optical conductivity of optimally doped $YBa_2Cu_3O_{7-\delta}$. Their study showed a good agreement with the observed peak-dip-hump structure at optimal doping. From the computed self-energy they showed that the hump originates from the hot quasiparticles and the Drude peak originates from the cold quasiparticles. Haslinger, Chubukov, and Abanov[15] reported optical conductivities $\sigma(\omega)$ of optimally doped cuprates in the normal state by allowing coupling between the spin fermions and the bosonic spin fluctuations. They found that the width of the peak in the spectral function $A_{\mathbf{k}}(\omega)$ scales linearly with ω in both hot and cold spots in the Brillouin zone and $\sigma(\omega)$ is inversely linear in ω up to very high frequencies.

Various studies have been limited to a restricted range of hole doping and temperature, relying on empirical parameters deduced from INS and ARPES. It is thus of great interest to resort to a theory that depends least on empirical parameters, and fits for a wide range both of hole doping (including the important region of underdoping) and temperature (encompassing the pseudogap phase and the superconducting phase). For this cause we use an improved slave-boson theory of the t-J Hamiltonian[6] that we developed recently.

Here we briefly discuss the slave-boson theory to discuss the coupling between the spin and charge degrees of freedom.[6] The t-J Hamiltonian in the presence of the external electromagnetic field $\mathbf{A}$ is written as

$$H=-t\sum_{\langle i,j\rangle}(e^{iA_{ij}}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.})+J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_in_j\right)-\mu\sum_{i,\sigma}c^{\dagger}_{i\sigma}c_{i\sigma},\qquad(1)$$

with $\mathbf{S}_i=\frac{1}{2}\Sigma_{\alpha\beta}c^{\dagger}_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}$. Here A_{ij} is the external electromagnetic vector potential, $\tilde{c}_{i\sigma}$ ($\tilde{c}^{\dagger}_{i\sigma}$) is the electron annihilation (creation) operator at each site, and $\sigma_{\alpha\beta}$ is the Pauli spin matrix. Rewriting the electron operator as a composite of spinon (f) and holon (b) operators, $c_{i\sigma}=f_{i\sigma}b^{\dagger}_i$ with the single occupancy constraint, $b^{\dagger}_ib_i+\Sigma_{\sigma}f^{\dagger}_{i\sigma}f_{i\sigma}=1$, we obtain the partition function

$$Z=\int \mathcal{D}f\mathcal{D}b\mathcal{D}\lambda\exp\left(-\int_0^{\beta}d\tau\mathcal{L}\right),\qquad(2)$$

with $\mathcal{L}=\Sigma_{i,\sigma}f^{*}_{i\sigma}\partial_{\tau}f_{i\sigma}+\Sigma_ib^{*}_i\partial_{\tau}b_i+H_{t\text{-}J}$ where $H_{t\text{-}J}$ is the U(1) slave-boson representation of the above t-J Hamiltonian [Eq. (1)],

$$H_{t\text{-}J}=-t\sum_{\langle i,j\rangle}(e^{iA_{ij}}f_{i\sigma}^{\dagger}f_{j\sigma}b_j^{\dagger}b_i+\text{c.c.})-\frac{J}{2}\sum_{\langle i,j\rangle}b_ib_jb_j^{\dagger}b_i^{\dagger}(f_{i\downarrow}^{\dagger}f_{j\uparrow}^{\dagger}-f_{i\uparrow}^{\dagger}f_{j\downarrow}^{\dagger})(f_{j\uparrow}f_{i\downarrow}-f_{j\downarrow}f_{i\uparrow})-\mu\sum_{i,\sigma}f_{i\sigma}^{\dagger}f_{i\sigma}+i\sum_i\lambda_i(f_{i\sigma}^{\dagger}f_{i\sigma}+b_i^{\dagger}b_i-1). \quad (3)$$

This Hamiltonian can readily be derived from the SU(2) theory.[6]

From the Hubbard-Stratonovich transformations involving hopping, spinon pairing and holon pairing orders we obtain the partition function

$$Z=\int\mathcal{D}f\mathcal{D}b\mathcal{D}\chi\mathcal{D}\Delta^f\mathcal{D}\Delta^b\mathcal{D}\lambda\exp\left(-\int_0^{\beta}d\tau\mathcal{L}_{eff}\right), \quad (4)$$

with $\mathcal{L}_{eff}=\mathcal{L}^f+\mathcal{L}^b+\mathcal{L}_0$ being the Lagrangian, where

$$\mathcal{L}^f=\sum_{i,\sigma}f_{i,\sigma}^{\dagger}\partial_{\tau}f_{i,\sigma}-\frac{J(1-\delta)^2}{4}\sum_{\langle i,j\rangle}\{\chi_{ij}f_{i,\sigma}^{\dagger}f_{j,\sigma}+\text{H.c.}\}-\frac{J(1-\delta)^2}{2}\sum_{\langle i,j\rangle}\{\Delta_{ij}^f(f_{i,\downarrow}f_{j,\uparrow}-f_{i,\uparrow}f_{j,\downarrow})+\text{H.c.}\}$$

for the spinon sector,

$$\mathcal{L}^b=\sum_i b_i^{\dagger}\partial_{\tau}b_i-t\sum_{\langle i,j\rangle}\{e^{iA_{ij}}\chi_{ij}b_i^{\dagger}b_j+\text{H.c.}\}-\frac{J}{2}\sum_{\langle i,j\rangle}|\Delta_{ij}^f|^2\{\Delta_{ij}^b b_i^{\dagger}b_j^{\dagger}+\text{H.c.}\}$$

for the holon sector, and

$$\mathcal{L}_0=J(1-\delta)^2\sum_{\langle i,j\rangle}\left\{\left|\Delta_{ij}^f\right|^2+\frac{1}{4}\left|\chi_{ij}\right|^2+\frac{1}{4}n_i\right\}+\frac{J}{2}\sum_{\langle i,j\rangle}|\Delta_{ij}^f|^2|\Delta_{ij}^b|^2.$$

Here χ, Δ^f, and Δ^b are the hopping, spinon pairing, and holon pairing order parameters, respectively.

We obtain the optical conductivity $\sigma(\omega)$ and the current response function $\Pi(\omega)$ of an isotropic two-dimensional mediun in the external electric field $\mathbf{E}(\omega)$ by evaluating the second derivative of the free energy with respect to the external vector potential $\mathbf{A}$,

$$\sigma(\omega)=\left.\frac{\partial J_x(\omega)}{\partial E_x(\omega)}\right|_{E_x=0}=-\frac{1}{i\omega}\left.\frac{\partial^2F}{\partial A_x^2}\right|_{A_x=0}=\frac{\Pi_{xx}(\omega)}{i\omega}, \quad (5)$$

where J_x is the induced current in the x direction, $F=-k_BT\ln Z$ is the free energy, and $\Pi_{xx}=-\partial^2F/\partial A_x^2|_{A_x=0}$ is the current response function in the x direction. The total response function $\Pi=\Pi^P+\Pi^D$ is the sum of the paramagnetic response function given by the current-current correlation function $\Pi^P(r'-r,t'-t)=\langle j_x(r',t')j_x(r,t)\rangle-\langle j_x(r',t')\rangle\langle j_x(r,t)\rangle$, with the current operator $j_x(r,t)=it[c_{r+x,\sigma}^{\dagger}(t)c_{r,\sigma}(t)-c_{r,\sigma}^{\dagger}(t)c_{r+x,\sigma}(t)]$ and the diamagnetic response function associated with the average kinetic energy, $\Pi^D=\langle K_{xx}\rangle=\langle -t\Sigma_{i,\sigma}(c_{i,\sigma}^{\dagger}c_{i+x,\sigma}+\text{H.c.})\rangle$.[18]

The phase difference per unit lattice spacing associated with the hopping order parameter $\chi_{ij}=|\chi_{ij}|e^{a_{ij}}$ defines the gauge field, $a_{ij}=\partial_{ij}\theta=\theta_i-\theta_j$. The gauge fluctuations allow the back-flow condition in association with an interplay between the charge and spin degrees of freedom originated from the effective kinetic-energy term of the t-J Hamiltonian. The effects of spin degrees of freedom are manifested through the antiferromagnetic spin fluctuations which appear in the Heisenberg exchange-coupling term. The antiferromagnetic spin fluctuations of short-range order (spin singlet pair) occur through the presence of correlations between adjacent electron spins. We consider both the amplitude fluctuations of the spinon pairing (spin singlet) order parameter $|\Delta^f|$ and the gauge-field fluctuations. We first integrate out the spinon and holon fields and take the saddle-point value with respect to the holon pairing order parameter, spinon pairing order parameter phase, the amplitude of hopping order parameter, and the Lagrangian multiplier fields in Eq. (4). We then obtain

$$F[\mathbf{A}]=-k_BT\ln\int\mathcal{D}f\mathcal{D}b\mathcal{D}\chi\mathcal{D}\Delta^f\mathcal{D}\Delta^b\mathcal{D}\lambda\times\exp\left(-\int_0^{\beta}d\tau(\mathcal{L}^f+\mathcal{L}^b+\mathcal{L}_0)\right)\approx-k_BT\ln\int\mathcal{D}\mathbf{a}\mathcal{D}|\Delta^f|(e^{-\beta(F^f[\mathbf{a},|\Delta^f|]+F^b[\mathbf{A},\mathbf{a},|\Delta^f|]}\times e^{F_0[|\Delta^f|]}), \quad (6)$$

where $F^f=-k_BT\ln\int\mathcal{D}f\exp(-\int_0^{\beta}d\tau\mathcal{L}^f)$ is the spinon free energy, $F^b=-k_BT\ln\int\mathcal{D}b\exp(-\int_0^{\beta}d\tau\mathcal{L}^b)$ is the holon free energy, and $F_0=-k_BT\ln\exp(-\int_0^{\beta}d\tau\mathcal{L}_0)$. The external electromagnetic field couples only to the holon field but not to the spinon field.

Considering the gauge and antiferromagnetic spin fluctuations up to second order we obtain the current response function

$$\Pi=\frac{\Pi^f\Pi^b}{\Pi^f+\Pi^b}+\frac{\left(\Pi_{a\Delta}^b-\dfrac{\Pi_{a\Delta}^b+\Pi_{a\Delta}^f}{\Pi^b+\Pi^f}\Pi^b\right)^2}{2\dfrac{(\Pi_{a\Delta}^b+\Pi_{a\Delta}^f)^2}{\Pi^b+\Pi^f}-(\Pi_{\Delta\Delta}^0+\Pi_{\Delta\Delta}^b+\Pi_{\Delta\Delta}^f)}, \quad (7)$$

where Π^f (Π^b) is the spinon (holon) response function associated with the gauge field $\mathbf{a}$ ($\mathbf{a}$ and $\mathbf{A}$), $\Pi_{XY}^f=-\partial^2F^f/\partial X\partial Y$ ($\Pi_{XY}^b=-\partial^2F^b/\partial X\partial Y$) is the spinon (holon) response function associated with both the gauge fields and the spinon pairing field, and $\Pi_{\Delta\Delta}^0$ is the response function associated with the spinon pairing field. It is shown that the first term represents the Ioffe-Larkin rule[19] for the current response function contributed only from the gauge field fluctuations, and the second term represents that from the spin fluctuations. Each contribution comes from the coupling between the charge and spin degrees of freedom, as manifested by Eq. (7). Because of the allowance of the gauge fluctuations in Eq. (6), the back-flow condition is automatically satisfied in Eq. (7), that is, the sum of the spinon and holon current vanishes. This can be easily seen from

$$\begin{aligned}\langle \mathbf{j}^f+\mathbf{j}^b\rangle &= -\frac{\beta}{Z}\int \mathcal{D}\mathbf{a}\mathcal{D}|\Delta^f|e^{-\beta(F^f[\mathbf{a},|\Delta^f|]+F^b[\mathbf{A},\mathbf{a},|\Delta^f|]+F_0[|\Delta^f|])}\\ &\quad\times\left(\frac{\delta F^f[\mathbf{a},|\Delta^f|]}{\delta\mathbf{a}}+\frac{\delta F^b[\mathbf{A},\mathbf{a},|\Delta^f|]}{\delta\mathbf{a}}\right)\\ &=\frac{1}{Z}\int \mathcal{D}\mathbf{a}\mathcal{D}|\Delta^f|\frac{\delta}{\delta\mathbf{a}}e^{-\beta(F^f[\mathbf{a},|\Delta^f|]+F^b[\mathbf{A},\mathbf{a},|\Delta^f|]+F_0[|\Delta^f|])}\\ &=0. \qquad (8)\end{aligned}$$

It is noted that the amplitude fluctuation of the spinon pairing order parameter does not interfere with the back-flow condition.

The response function Π^f (Π^b) is contributed to from both the paramagnetic and diamagnetic parts. The paramagnetic response function is obtained from the current-current correlation functions $\Pi^f_{xx}(P)=\langle j^f_x(r',t')j^f_x(r,t)\rangle-\langle j^f_x(r',t')\rangle\langle j^f_x(r,t)\rangle$ for the spinon and $\Pi^b_{xx}(P)=\langle j^b_x(r',t')j^b_x(r,t)\rangle-\langle j^b_x(r',t')\rangle\langle j^b_x(r,t)\rangle$ for the holon, and the diamagnetic response function involves the average kinetic energy of the spinon (holon). $\Pi^f_{a\Delta}$ ($\Pi^b_{a\Delta}$) is given by the correlations between the spinon (holon) current and the anomalous spinon (holon) pairing, $\Pi^f_{a\Delta}=\langle j^f_x(r',t')D^f(r,t)\rangle-\langle j^f_x(r',t')\rangle\langle D^f(r,t)\rangle$ [$\Pi^b_{a\Delta}=\langle j^b_x(r',t')D^b(r,t)\rangle-\langle j^b_x(r',t')\rangle\langle D^b(r,t)\rangle$] with $D^f(r,t)\sim\Sigma_l[e^{-i\tau}f_{r,\downarrow}(t)f_{r+l,\uparrow}(t)+\text{H.c.}]$ and $D^b(r,t)\sim\Sigma_l[b_r(t)b_{r+l}(t)+\text{H.c.}]$. Here l represents nearest-neighbor sites around location r and $\tau=\pm\pi/2$ [$+(-)$ for x (y) direction] is a phase to represent the spinon pairing of d-wave symmetry. $\Pi_{\Delta\Delta}$ represents correlations between pairing currents; $\Pi^f_{\Delta\Delta}=\langle D^f(r',t')D^f(r,t)\rangle-\langle D^f(r',t')\rangle\times\langle D^f(r,t)\rangle$ for the spinon pairs and $\Pi^b_{\Delta\Delta}=\langle D^b(r',t')D^b(r,t)\rangle-\langle D^b(r',t')\rangle\langle D^b(r,t)\rangle$ for the holon pairs.

Figure 1 shows computed optical conductivities from the U(1) slave-boson t-J Hamiltonian [Eq. (3)] with $J=0.3t$ for the underdoped ($\delta=0.05$), optimally doped ($\delta=0.07$) and overdoped ($\delta=0.1$) regions. T_c and T^* represent the superconducting temperature and the pseudogap temperature, respectively. Compared to the present U(1) result of optimal doping, the SU(2) slave-boson theory[6] predicted a more realistic value of optimal doping close to $\delta\approx0.15$, by yielding a phase diagram showing an arch-shaped bose condensation temperature, in better agreement with observation. To avoid complexity, we resort to the simpler case of U(1), as our prime interest lies in the investigations of the role of spin fluctuations and the coupling between the charge and spin degrees of freedom on the formation of peak-dip-hump structures. The accurate SU(2) theory will not alter the physics of the peak-dip-hump structure formation. Although not shown here for other values of J we find qualitative agreements with experiments, in that the peak-dip-hump structures are well predicted below T^* and T_C. In Fig. 2 the hump peak position is seen to remain nearly constant with the variation of hole doping and temperature below T^* but not so above T_C. In general, the predicted hump position tends to shift to a lower frequency with increasing hole concentra-

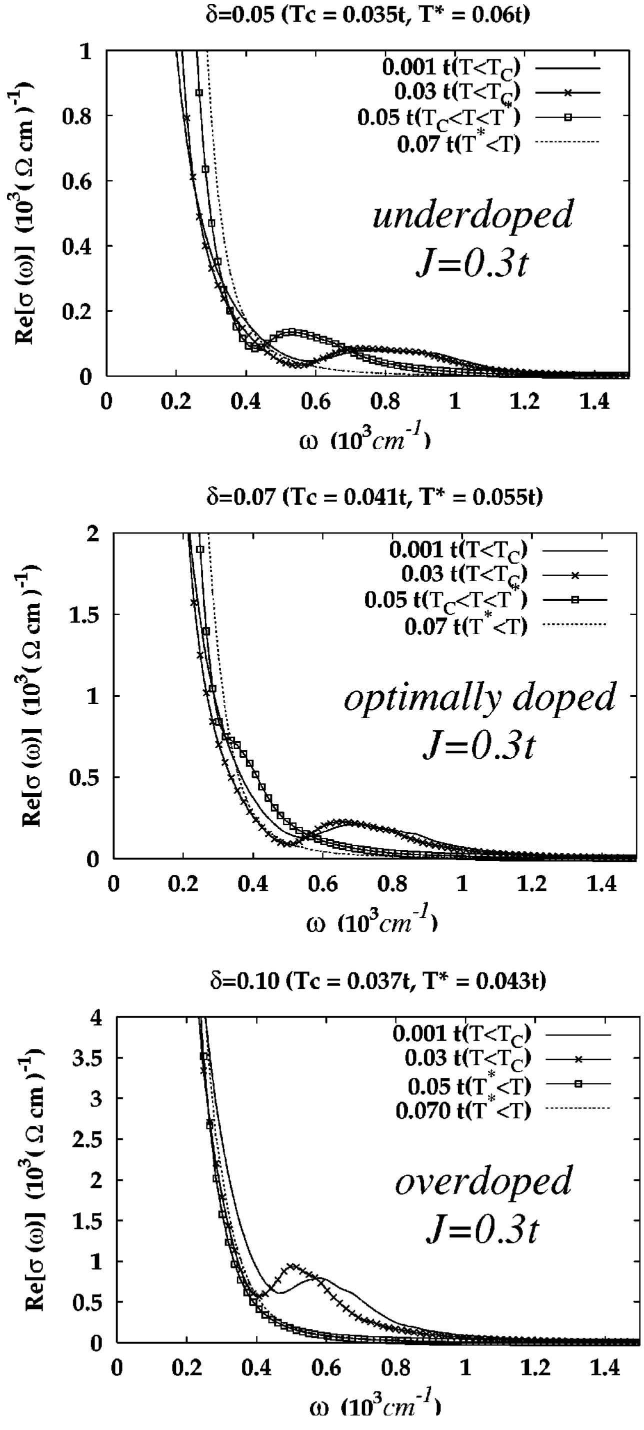

FIG. 1. Computed optical conductivities as a function of temperature for $\delta=0.05$ (under doped), $\delta=0.07$ (optimally doped), and $\delta=0.1$ (over doped) cases with the antiferromagnetic Heinsenberg coupling strength of $J=0.3$ for all cases.

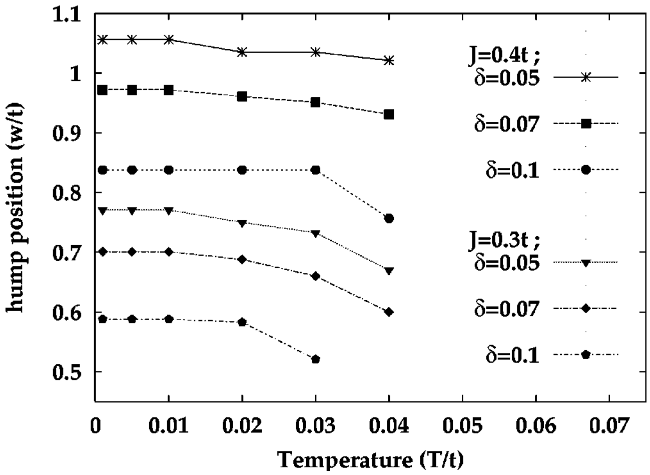

FIG. 2. Temperature dependence of hump position as a function of antiferromagnetic coupling J and hole concentration.

tion and with temperature, showing a gradual disappearance of the hump. A trend of rapid drop in a high-frequency region is seen to be unrealistic. In order to find the role of spin fluctuations, we neglected the second term in Eq. (7). The hump structure (dotted line in Fig. 3) completely disappeared, clearly indicating that spin-spin correlations or spin fluctuations associated with the spin singlet excitations are responsible for the hump formation in the optical conductivity (Fig. 3). For an additional analysis of spin fluctuation, we computed the optical conductivity using the Lanczos exact diagonalization method for a two-hole doped 4×4 lattice by introducing various Heisenberg antiferromagnetic coupling strengths J. Despite the finite-size effects, an irregular but gross feature of the peak-dip-hump structure is still predicted, indicating that the hump is originated from the spin-spin correlations. A linear increase in the hump position with J is predicted. From both the slave-boson and Lanczos calculations we note that the peak locations of the hump are sensitive to the variation of the antiferromagnetic coupling strength J, by showing a linear increase. Further, as mentioned above, the neglect of the spin fluctuations [the second term in Eq. (7)] led to a sudden disappearance of the hump structure.

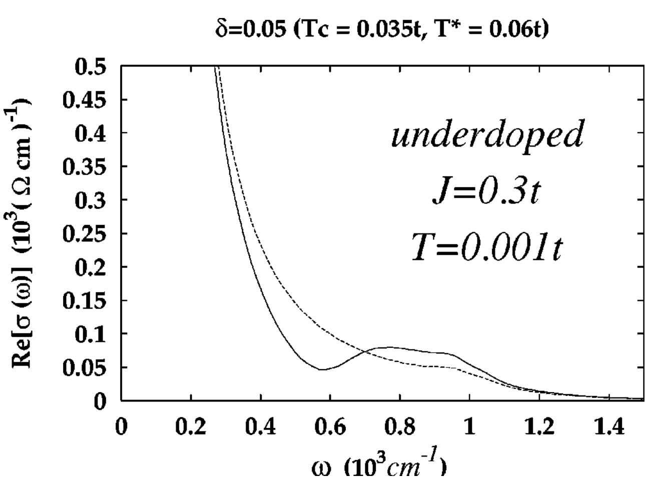

FIG. 3. The total optical conductivity (solid line) vs a partial one (dotted line) contributed only from the first term and thus from the neglect of the spin fluctuation (second) term in Eq. (7).

Although not shown here, using the present U(1) slave-boson theory the predicted spectral functions around the $(\pi,0)$ point in the momentum space also showed the peak-dip-hump structure consistent with the ARPES data. This incoherent background or the hump around the $(\pi,0)$ point was found to occur as a result of the antiferromagnetic spin fluctuations, having a feature common with the hump structure of the optical conductivity. Thus we conclude from these multifaceted studies that the spin-spin correlations or the spin fluctuations involved with electrons around the $(\pi,0)$ point in the momentum space are definitely the prime cause of the hump structures below T^* and T_C.

In our earlier slave-boson approach[6] of the t-J Hamiltonian not only the spin degree of freedom but also the charge degree of freedom is introduced into the slave-boson representaion of the Heisenberg term, $J\Sigma_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-1/4n_in_j)$. This is obvious from the expression of the n_in_j term here, which represents the charge degree of freedom. Thus the spin and charge degrees of freedom are well manifested in both the hopping and Heisenberg terms in the t-J Hamiltonian. This resulted in the arch-shaped T_c curve in the phase diagram,[6] the trend of which is consistent with observation. We would like to note that using one of the Ginzburg-Landau theories[20–22] of spin-charge separated superconductivity, Rodriguez[22] reported an arch-shaped T_c line. However there exists no further report on the test of this theory to predict observations such as optical conductivity, inelastic neutron scattering, and angle-resolved photemission spectroscopy. One of our main objective here was to test the validity of our recently proposed theory[6] by making a comparison with observations. In this study we computed the optical conductivity for high-T_c cuprates based on the slave-boson representation of the t-J Hamiltonian with the on-site slave-boson constraint $\Sigma_\sigma f_{i\sigma}^\dagger f_{i\sigma}+b_i^\dagger b_i=1$ in a mean-field level. The d-wave symmetry and the back-flow condition are satisfied in the U(1) slave-boson representation [Eq. (7)] of the optical conductivity. Falck *et al.*[23] reported measurements of the polarized midinfrared-reflectivity spectrum and its temperature dependence for lightly oxygen-doped La_2CuO_{4+x} single crystals. They conjectured that the 0.13-eV absorption band is attributed to the photoionization of polaronic impurities (photoexcitation of localized holes from impurities). On the other hand, we find from a rigorous study of the t-J Hamiltonian that the antiferromagnetic fluctuations of short range cause the hump structure (midinfrared band) in high-T_c cuprates.

In the present study, by paying attention to a wide range of both hole doping (underdoping, optimal doping, and overdoping) and temperature ($T<T_C$, $T_C<T<T^*$, and $T^*<T$) with no empirical parameters obtained from measurements, we examined the optical conductivity as a function of frequency for the two-dimensional systems of strongly correlated electrons. Allowing the coupling between the spin and charge degrees of freedom as manifested in Eq. (7), the peak-dip-hump structures are predicted in agreement with observations. It is shown that the antiferromagnetic spin

fluctuations of short range associated with the spin singlet pair excitations are important in yielding the observed hump structure, and that the hump position linearly increases with the antiferromagnetic Heisenberg coupling strength. Although not plotted, the peak-dip-hump structure was predicted to persist in the region of $J/t=0.1$–0.4, by showing a propensity of hump height increment with increasing J/t. This again indicates that the effects of spin-spin correlations (fluctuations) of short range are important for the formation of the hump structure. In general, the predicted peak-dip-hump structures are in qualitative agreement with observations, particularly in the temperature ranges of $T<T_C$ and $T_C<T<T^*$ for the underdoped case. It is shown that the spin fluctuations of the shortest possible antiferromagnetic correlation length (that is, the spin singlet pair) alone can cause the formation of the hump structure. However, considerations of both the antiferromagnetic spin fluctuations of correlation lengths larger than the spin singlet pair and the direct-channel single-spin fluctuations at high energies may be needed to remedy quantitative discrepancies in the rapid drops of optical conductivity at temperatures above T^* and at frequencies beyond the peak location of the hump.

One of us (S.H.S.S.) acknowledges the generous support of the Korea Ministry of Education (Hakjin Excellence Leadership Program 2001) and the POSRIP Project at Pohang Unversity of Science and Technology.

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