Hole spectrum and optical conductivity in high-T_c superconductors

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The spectral function of a hole moving in antiferromagnetic background is evaluated in the framework of the Emery model within the spin-wave approximation. It is shown that in the vicinity of quasiparticle peaks the self-energy is not diagonal. The mixture of the singlet and triplet is found to depend on the momentum **k**. The optical conductivity is estimated. The results of the calculations are in good agreement with experiment and numerical simulations.

In order to understand properly the nature of a superconducting state, it is important to choose a microscopic Hamiltonian that can describe low-energy excitations in high-temperature superconductors in an adequate manner. Anderson[1] suggested that the physical properties of CuO_2 planes can be described with a single-band two-dimensional Hubbard Hamiltonian. However, experiments[2] give evidence in support of a different picture, which is describable with the generalized Hubbard model proposed by Emery.[3] Upon doping La_2CuO_4 with two-valent Sr or Ba ions, holes occurred, occupying O_{2p} orbitals in the CuO_2 planes. Zhang and Rice[4] argued on the formation of a rather localized singlet that consisted of a O_{2p} hole and Cu d spin spread over the crystal, independent of the high-energy triplet. Such a renormalization procedure brings the effective Hamiltonian for CuO_2 planes to be a single-band Hubbard Hamiltonian.

By an analogous procedure, Zhang[5] showed that the Emery Hamiltonian could be reduced to a single-band Hubbard Hamiltonian, as ε_p, $U_d \to \infty$ and $U_d - \varepsilon_p$ is a finite value (U_d is the Hubbard repulsion on the Cu site; ε_p is the spacing between atomic O and Cu levels). However, numerical calculations[6] on finite clusters show that in the limit $U_d \to \infty$ both Hamiltonians[3,4] have different ground states. The authors[6] assume that the reason for this discrepancy is connected with the fact that Zhang and Rice[4,5] have not considered virtual fluctuations of Cu_{3d} states correctly. The analogous results were obtained in Ref. 7, where the quasiparticle spectrum of the Emery model was analyzed within the spin-wave approximation.

It is worth mentioning that in papers[8,9] the authors pointed out that a singlet is a rather localized state which can be described in terms of the Wannier representation without mixing with a high-energy triplet. However, calculations[8,9] were performed within the local approximation and did not take into account long-wavelength fluctuations, but only short-wavelength renormalization. In our opinion such long-wavelength excitations can change the structure of the ground state efficiently and lead to a strong mixing of a singlet and triplet, especially at $\mathbf{k}=(0,0)$.

The spectrum of a hole moving in an antiferromagnetic (AF) ground state of the t-J model was studied in a number of papers using the exact diagonalization technique on finite clusters[10] and within the spin-wave approximation.[11–15] The main peculiar feature of the spectrum is a large incoherent background with a quasiparticle pole located in the vicinity of the bottom of the spectrum. The width of the coherent polaron band is $W \sim J$ and the pole strength is a function of the ratio J/t.[11–15]

The Schwinger-boson–slave-fermion approach to the t-J model was discussed in Ref. 16 beyond the mean-field approximation. It was shown that antiferromagnetic and ferromagnetic correlations coexist for the small doping. These fluctuations lead to a strong renormalization of the fermion propagator as in the single-hole case. For finite hole concentration additional sidebands appear in spectral density coming from multiple scattering on spin excitation.

In this connection a recent series of experiments on the measurement of optical conductivity seems of great importance.[17–19] In the insulating state the $\sigma(\omega)$ shows no absorption in the region $\omega < 1.5-2$ eV. For $\omega > 2$ eV, the $\sigma(\omega)$ has a large step that corresponds to a "charge-transfer gap" in the excitation spectrum. When some carriers are introduced into the CuO_2 plane by doping, a Drude-like peak appears and its weight grows with the carriers concentration. Two peaks in $\sigma(\omega)$ occur for ω lying inside the charge-transfer gap, at $\omega = 0.07-0.1$ eV and $\omega = 0.8-1$ eV. The effective carrier concentration N_{eff}, defined as the integration of $\sigma(\omega)$ over the charge-transfer gap, increases faster than one could expect from the doped concentration. The qualitative interpretation of the experiments within the t-J model was proposed in Ref. 12. The conductivity calculated on finite clusters within the single-band Hubbard model is in good agreement with the experimental data.[20]

In the present paper we have calculated the spectrum of a hole moving in the AF background in the framework of the Emery model within the spin-wave approximation. We have shown that the spectral function consists of two broad incoherent regions. In the lower part of each there are two quasiparticle peaks arising due to a coherent motion of a hole surrounded by magnons. The self-energy turns out not to be diagonal and is strongly dependent on the momentum **k**. It means that mixing of a singlet and triplet is essential. The optical conductivity

$\sigma(\omega)$ is estimated. Our results are in good agreement with experiments.[17–19]

Following Refs. 3, 6, and 21, we adopt the Hamiltonian, as a starting point,

$$H=H_t+H_J=t\sum_{ll'i}p^{\dagger}_{l\sigma}(1+2\mathbf{S}_i\cdot\boldsymbol{\sigma})p_{l'\sigma}+J\sum_{ll'}\mathbf{S}_l\cdot\mathbf{S}_{l'}\ , \qquad (1)$$

where $\mathbf{S}_i=1/2d^{\dagger}_{i\sigma}\boldsymbol{\sigma}d_{i\sigma}$, σ_α are the Pauli matrices, and $p^{\dagger}_{i\sigma},d^{\dagger}_{i\sigma}$ are the creation operators of O_{2p} and Cu_{3d} states, respectively.

Assuming that in the absence of holes the ground state of the system in question is of antiferromagnetic order, it is quite convenient to transform the Hamiltonian (1) by taking the sum over only one sublattice of Cu spins. In addition, we distribute the $p_{i\sigma}$ hole states over O sites using their linear combinations, which are transformed as basic functions of irreducible representations of the group D_4. It can be performed by means of the matrix

$$B=\frac{1}{2}\begin{bmatrix}1 & 1 & -\sqrt{2} & 0\\ 1 & -1 & 0 & \sqrt{2}\\ 1 & 1 & \sqrt{2} & 0\\ 1 & -1 & 0 & \sqrt{2}\end{bmatrix}.$$

However, unlike Ref. 23 we classify the initial $p_{i\sigma}$ orbitals as dependent on their spins. For this purpose we construct the new orbitals $\Psi^{(\alpha)}_{jA}$ ($\Psi^{(\alpha)}_{jB}$) to correspond to the linear combinations of $p_{i\uparrow}$ ($p_{i\downarrow}$) and centered on Cu sites of the A (B) sublattice. In these notations the Hamiltonian takes the following form:

$$\begin{aligned}H_t=&2t\sum_{jA}[\Psi^{(1)\dagger}_{jA}(1+2S^z_i)\Psi^{(1)}_{jA}+\Psi^{(1)\dagger}_{j+2xB}(1-2S^z_{j+2x})\Psi^{(1)}_{j+2xB}]\\&+t/2\sum_{j\in A,\gamma\gamma',\alpha\alpha'}B_{\gamma\alpha}B_{\gamma'\alpha'}[\Psi^{(\alpha)\dagger}_{jA}(1+2S^z_{j+2x-\tau_\gamma})\Psi^{(\alpha)\dagger}_{j+\tau_{\gamma'}-\tau_\gamma}+\Psi^{(\alpha)\dagger}_{j+2xB}(1-2S^z_{j+\tau_\gamma})\Psi^{(\alpha')}_{j+2x+\tau_\gamma-\tau_{\gamma'}B}]\\&+2t\sum_{j\in A,\alpha\gamma}B_{\alpha\gamma}(\Psi^{(1)}_{jA}S^{+}_{j}\Psi^{(\alpha)}_{j+2x-\tau_\gamma B}+\Psi^{(1)}_{j+2xB}S^{-}_{j+2x}\Psi^{(\alpha)}_{j+\tau_\gamma A}+\text{H.c.})\ , \qquad (2)\end{aligned}$$

where

$$\Psi^{(\beta)}_{jA}=\sum_\alpha B_{\alpha\beta}p^{(\alpha)}_{j\uparrow},\quad \Psi^{(\beta)}_{j+2xB}=\sum_\alpha B_{\alpha\beta}p^{(\alpha)}_{j+2x\downarrow}\ ,$$

$$p^{(\alpha)}_{j\sigma}=p_{j+y\sigma}p_{j-x\sigma}p_{j-y\sigma}p_{j+x\sigma}\ ,$$

$$\tau_1=2x-2y,\quad \tau_2=4x,\quad \tau_3=2x+2y,\quad \tau_4=0\ .$$

The translations τ are expressed in units of a, the distance between Cu and O sites. The representation of the Hamiltonian in this form is rather convenient because the summation is taken only over the A sublattice and the $\Psi^{(\alpha)}_{iA,B}$ operators obey the anticommutational relations. If antiferromagnetic order of copper spins is accepted, then Hamiltonian (2) has a symmetrical form. By expressing the spin operators in terms of Schwinger bosons $b_{j\sigma}$ (Refs. 12 and 22) and evaluating the functional integral within the saddle-point approximation, we obtain[12]

$$b_{i\uparrow}=b_{i+2x\downarrow}=0,\quad b_{i\downarrow}=b_{i+2x\uparrow}=\sqrt{2S}\ , \qquad (3)$$

$$\begin{aligned}H=&tSz\sum_k\tilde{\Psi}^{\dagger}_k\begin{bmatrix}\hat{\varepsilon}_k & 0\\ 0 & \hat{\varepsilon}_k\end{bmatrix}\tilde{\Psi}_k\\&+2t\sqrt{2Sz}\sum_{kq}\left[\tilde{\Psi}^{\dagger}_{k+q}\begin{bmatrix}\hat{A}_{kq} & 0\\ 0 & -\hat{A}_{kq}\end{bmatrix}\tilde{\Psi}_k\beta^{\dagger}_{-q}+\text{H.c.}\right]+\sum_q\omega_q\beta^{\dagger}_q\beta_q\ , \qquad (4)\end{aligned}$$

where

$$\hat{\varepsilon}_k=\begin{bmatrix}-\varepsilon_k & 0\\ 0 & \varepsilon_k\end{bmatrix},\quad \varepsilon_k=\sqrt{1-\gamma^2_k}\ ,$$

$$A_{kq}=\begin{bmatrix}u_q\gamma_k\sqrt{(1+\varepsilon_{k+q})/(1+\varepsilon_k)}+v_q\gamma_{k+q}\sqrt{(1+\varepsilon_k)(1+\varepsilon_{k+q})} & u_q\sqrt{(1+\varepsilon_{k+q})+(1+\varepsilon_k)}+v_q\gamma_{k+q}\gamma_k\\ u_q\dfrac{\gamma_{k+q}\gamma_k}{\sqrt{1+\varepsilon_k}\sqrt{1+\varepsilon_{k+q}}}+v_q\sqrt{(1+\varepsilon_{k+q})(1+\varepsilon_k)} & u_q\gamma_{k+q}\sqrt{(1+\varepsilon_k)(1+\varepsilon_{k+q})}+v_q\gamma_k\sqrt{(1+\varepsilon_{k+q})(1+\varepsilon_k)}\end{bmatrix},$$

$$\omega_k=JSz\sqrt{1-\gamma^2_k},\quad \gamma_k=1/z\sum_\delta\exp(i\mathbf{k}\cdot\boldsymbol{\delta}),\quad u_k=\{1/2[(1-\gamma^2_k)^{-1/2}+1]\}^{1/2}\ ,$$

$$v_k=-\text{sgn}(\gamma_k)\{1/2[(1-\gamma^2_k)^{-1/2}-1]\}^{1/2}\ ,$$

$\beta_{\mathbf{k}}^{\dagger}$ is the creation operator of a spin wave with the vector $\mathbf{k}$, $\tilde{\Psi}_{\mathbf{k}}^{\dagger}=(\tilde{\Psi}_{\mathbf{k}}^{(1)\dagger},\tilde{\Psi}_{\mathbf{k}}^{(2)\dagger})$, and $\tilde{\Psi}_{\mathbf{k}}^{(\alpha)\dagger}$ is the hole creation operator in a singletlike (tripletlike) state.[21,7] The singletlike state corresponding to the lowest-energy state is not a straight Zhang-Rice singlet. This state corresponds to a state with the oxygen spin opposed to a copper one in the Néel background.

It should be noted that the approximation (5) is good for describing long-wavelength excitations in a quantum AF, but it violates the hard-core constraint connected with a finite S value which is essential for short-wavelength excitation.[11] We used (5) without consideration of short-wavelength corrections to the spectrum of carriers in a quantum AF. According to Refs. 11 and 12 we can write the equation for the self-energy of a single hole in the noncrossing approximation as

$$\hat{\Sigma}(\mathbf{k},\omega)=t^2z^2\sum_{\mathbf{q}}\hat{A}_{\mathbf{kq}}^{\dagger}\hat{G}(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}})\hat{A}_{\mathbf{kq}}\ , \tag{5}$$

where $\hat{G}(\mathbf{k},\omega)=[\omega-\hat{\varepsilon}_{\mathbf{k}}-\hat{\Sigma}(\mathbf{k},\omega)+i0]^{-1}$ is the Green's function and $\hat{\Sigma}(\mathbf{k},\omega)$ is the self-energy. Vertex corrections are neglected here. For $J\gg t$ these corrections are small.[11] Moreover, the equation for the self-energy within the noncrossing approximation describes the hole spectrum of the t-J model quite adequately.[11,13,14] Therefore, we think that the vertex corrections to (5) cannot change the results qualitatively and Eq. (5) is adequate to describe the hole spectrum of the Emery model.

Note that, for $\mathbf{k}=0$, $\det\hat{A}_{\mathbf{kq}}=0$, and one can easily see that

$$\hat{\Sigma}(\mathbf{k},\omega)=\Sigma\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}.$$

This leads to the appearance of two poles in the Green's function at $\omega=2\Sigma$ and $\omega=0$ having self-vectors of $1/\sqrt{2}(1,\mp1)$. Therefore, the coherent spectrum for the $\mathbf{k}=\mathbf{0}$ point of the Brillouin zone corresponds to a mixture of a singletlike and a tripletlike state taken with equal weights.[7] Otherwise, for $\mathbf{k}=(\mp\pi/2,\mp\pi/2)$ and $\mathbf{k}=(\mp\pi,0)$ and all the points lying on the line between them, the self-energy is a diagonal matrix. It means that quasiparticle excitations correspond to a pure singletlike or a tripletlike ones.[7,21] The self-energy in the incoherent part of the spectrum is not diagonal and the mixed states are responsible for high-energy excitations.[21]

Equation (5) was solved numerically by an iteration procedure. The integral on the right-hand side of the equation was calculated with the Monte Carlo technique. This method saves computer time for the whole procedure, while the accuracy of the calculations remain rather satisfactory. To make the procedure stable a damping constant $\omega\rightarrow\omega+i\delta$ is introduced. We chose the number of points for ω to be 200 and divided the irreducible part of the Brillouin zone into 15 points. The dumping constant was 0.01. Usually we need 8–10 iterations, and the complete time of calculation was estimated to be 3–4 h of an IBM386-like computer per one J/t value.

To check the validity of this method the analogous self-consistent equation for the t-J model was solved and the solution was compared with results published elsewhere.[11,13] Good agreement with previous solutions of the equation and, moreover, with the exact diagonalization on finite clusters was observed. In Fig. 1 our spectral density function is shown (see also the results of Marsiglio *et al.*[11]).

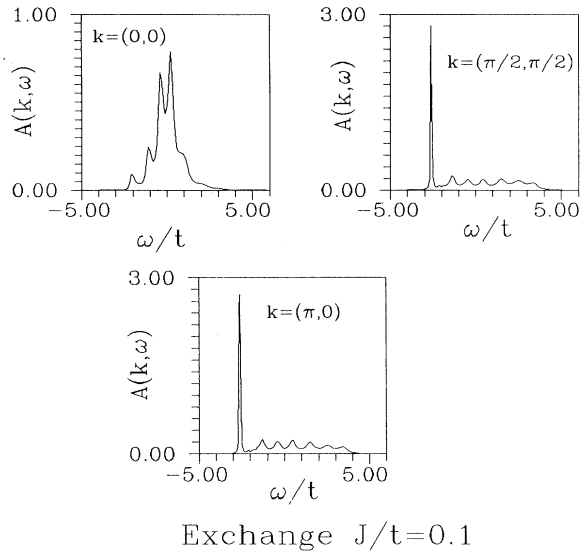

FIG. 1. Spectral density $A(\mathbf{k},\omega)$ of the t-J model ($J/t=0.1$).

Equation (5) was solved in the same way. The spectral density $A(\mathbf{k},\omega)=(1/\pi)\,\mathrm{Im}[\mathrm{Tr}\hat{G}(\mathbf{k},\omega)]$ is shown in Fig. 2. In the bottom of two wide incoherent branches, where $\mathrm{Im}\hat{\Sigma}(\mathbf{k},\omega)\neq0$, two quasiparticle peaks appear [$\mathrm{Im}\hat{\Sigma}(\mathbf{k},\omega)=0$]. Dispersion of the lowest peak $\varepsilon(\mathbf{k})$ can be well approximated by the following expression:

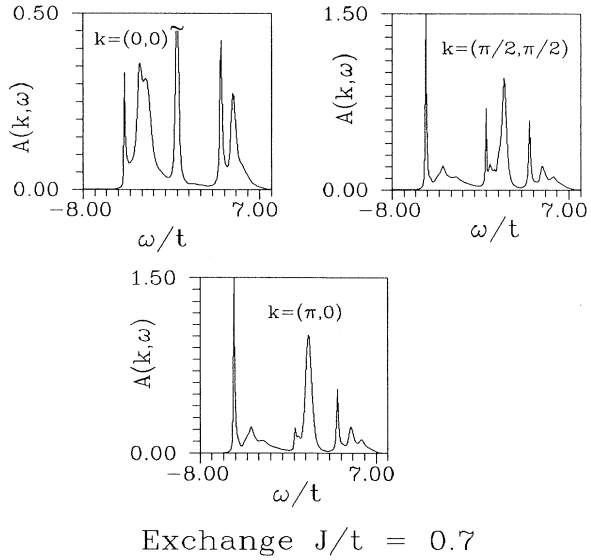

FIG. 2. Spectral density $A(\mathbf{k},\omega)$ of the Emery model ($J/t=0.7$).

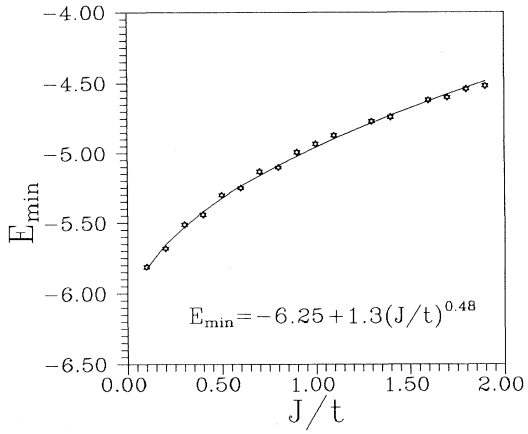

FIG. 3. $\varepsilon_{\min}$ as a function of J/t.

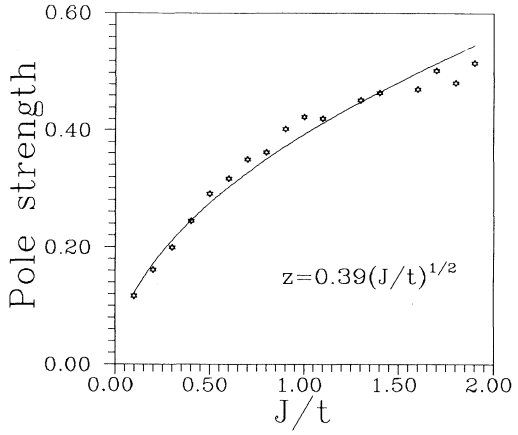

FIG. 5. Pole strength $z(\pi/2,\pi/2)$ as a function of J/t.

$$\varepsilon(\mathbf{k})=\varepsilon_{\min}+\frac{W}{4}[\cos(k_x)+\cos(k_y)]^2 , \tag{6}$$

where

$$\varepsilon_{\min}=-6.25+1.3(J/t)^{0.48} . \tag{7}$$

$\varepsilon_{\min}$, the bandwidth W and the pole strength $z(\pi/2,\pi/2)$ as functions of J/t are presented in Figs. 3, 4, and 5, respectively. The bandwidth is proportional to J/t for $J/t<1$. The pole strength is an increasing function of J over the entire interval tested. Note that our results coincide with the previous analogous calculations.[7,24,25] As can be seen from Fig. 2, for $\mathbf{k}=0$ two coherent peaks arise in $A(\mathbf{k},\omega)$ corresponding to the mixed singlet-triplet states. The lowest peak has a smaller pole strength. The second one at $\omega=0$ is very large, and it is very difficult to estimate the energy of the lowest peak. The wave function at the lowest pole at $\mathbf{k}=\mathbf{0}$ is $1/\sqrt{2}(\Psi^{\dagger}_{\mathbf{k}\uparrow}-\Psi^{\dagger}_{\mathbf{k}\downarrow})|0\rangle$, and there is no coupling of the fermion with the spin background.[7] At $\mathbf{k}=(\mp\pi/2,\mp\pi/2)$ the singletlike excitation is at the lowest energy of the system. Therefore, the Zhang-Rice singlet is not a good approximation for the Emery model. The mixture of a singletlike and a tripletlike excitation in the AF background depends on the momentum $\mathbf{k}$.

To estimate optical conductivity we used the following expression for $\sigma(\omega)$:[12]

$$\sigma(\omega)=\sum_{\mathbf{k}}\int d\Omega\frac{n(\Omega)-n(\Omega+\omega)}{\omega}C(\mathbf{k},\Omega,\omega)^2 \times A(\mathbf{k},\Omega)A(\mathbf{k},\Omega+\omega) , \tag{8}$$

where $n(\omega)$ is the Fermi function and $C(\mathbf{k},\Omega,\omega)$ is the irreducible current vertex with two external hole lines. Equation (8) is good for the description of the optical conductivity in the low-density limit when holes are noninteracting and their spectrum is a single-particle one. For $\omega=0$ we can apply Ward identity to estimate current vertex $C(\mathbf{k},\Omega,\omega)\approx v_{\mathbf{k}}m^*/m$ (see Ref. 12). The Drude weight can be estimated as

$$\sigma_D(\omega)=D\delta(\omega),\quad D=e^2\sum_{\mathbf{k}}\frac{\partial n(\varepsilon(\mathbf{k}))}{\partial\varepsilon(\mathbf{k})}|\mathbf{v}_{\mathbf{k}}|^2 , \tag{9}$$

where $\mathbf{v}_{\mathbf{k}}=\partial\varepsilon(\mathbf{k})/\partial\mathbf{k}$.

The weight's dependence on the Fermi energy (the carriers concentration) is shown in Fig. 6. We found out that D grows rapidly at small doping of CuO_2 planes with

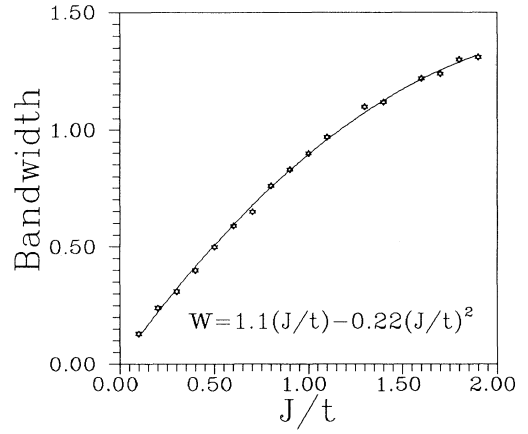

FIG. 4. Bandwidth W as a function of J/t.

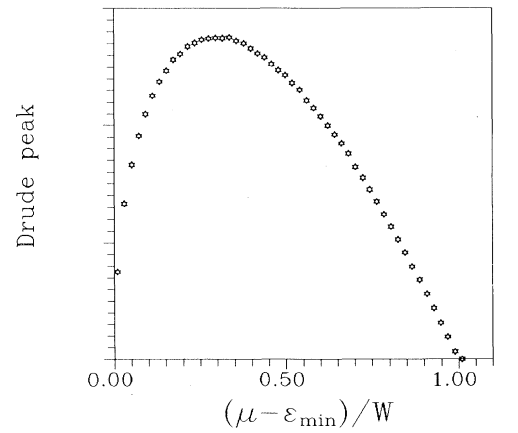

FIG. 6. Dependence of Drude weight D on Fermi energy.

carriers and goes through the maximum for the carrier concentration $n \approx \bar{z}/2$, where $\bar{z}$ is the averaged over Brillouin-zone pole strength. The further increasing of n leads to the decreasing of D due to decreasing average kinetic energy of quasiparticles.

To estimate the optical conductivity for $\omega \geq J$ we have used the approximation, for $\sigma(\omega)$,[26]

$$\sigma(\omega) \sim \frac{1}{\omega} \int d\Omega \rho(\Omega)\rho(\Omega+\omega)[n(\Omega)-n(\Omega+\omega)] , \quad (10)$$

where $\rho(\Omega)=\Sigma_{\mathbf{k}} A(\mathbf{k},\Omega)$ is density of state.

This approximation is good for describing $\sigma(\omega)$ in disordered semiconductors. This approximation contains all essential physical features of mid-infrared optical conductivity due to the fact for $\omega > J$ magnetic excitation can be considered as a static impurity. Note that the current vertex in (10) does not contain momentum dependence in contrast with the approximation of Ref. 16. To estimate $\sigma(\omega)$ for finite ω the authors[16] insert into (8) the current vertex for $\omega=0$. This procedure is not perfectly correct due to the appearance of frequency dependence in the current vertex. This dependence is essential and follows from the Ward identity for a finite ω value.[26]

The results of the calculation of $\sigma(\omega)$ with the aid of (8) are plotted in Fig. 7. The peak in the infrared branch of $\sigma(\omega)$ ($\omega \approx J$) grows fast with increasing carrier concentration n. The second peak, corresponding to excitation of the magnetic polaron to the incoherent part of the spectrum, grows slowly. This fact is connected with the small density of states in the incoherent part of the spectrum. The further increasing of n leads to the decrease of the first peak due to the decreasing number of unoccupied states in the coherent part of the spectrum. The second peak grows with further increasing of n. The third peak, corresponding to interband absorption, grows in the whole region of concentrations. Note that in the present spin-wave approximation absorption due to charge fluctuation (for large ω) does not appear.

Such behavior of the optical conductivity is in qualitative agreement with the experiments on high-T_c superconductors.[18,19,17] The first peak $\omega \approx 1000$ K corresponds to excitation of the magnetic polaron into the first excited

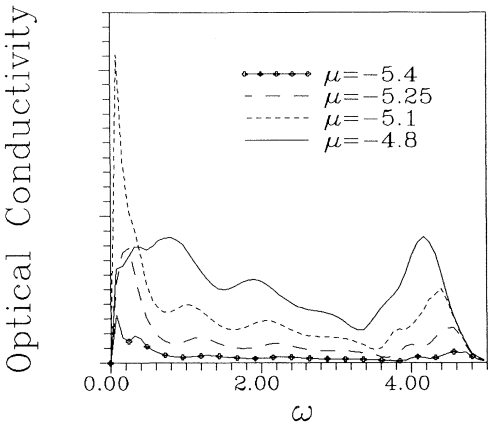

FIG. 7. Optical conductivity $\sigma(\omega)$ for different Fermi energies.

p state.[27] The second peak at $\omega \approx 0.8-1$ eV appears due to incoherent high-energy excitation of polarons. The third peak appears in the branch of $\omega > 1.5-2$ eV, which corresponds to charge fluctuations and must be mixed with absorption due to charge fluctuations.

In conclusion, we would like to summarize the results of the calculation. We have solved the self-consistent equation for self-energy of a hole moving in AF background in the framework of the Emery model within the spin-wave approximation. We have shown that the hole spectrum consist of two incoherent regions in the lowest parts of which two quasiparticle bands appear corresponding to mixed singlet-triplet states. It leads us to the conclusion that the singlet-triplet basis is a rather poor approximation for the Emery model. The optical conductivity estimated within this approximation is in good agreement with experiment[18,19,17] and numerical simulations.[20]

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