RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 42, NUMBER 13 1 NOVEMBER 1990

Optical properties of one- and two-dimensional Hubbard and t-J models

W. Stephan and P. Horsch

Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 6 June 1990)

The optical conductivity for the Hubbard and t-J models is calculated numerically by use of a Lanczos algorithm. One- and two-dimensional systems of up to 16 sites with periodic and open boundary conditions are examined for the t-J model, as well as Hubbard-model systems of up to 9 sites. In the one-dimensional (1D) case, the low-frequency part of the conductivity away from half filling is shown to consist almost entirely of a single δ function (Drude peak) even for J of the order of t. This is a direct consequence of the decoupling of charge and spin in 1D. In two dimensions there is an additional broad absorption band above the Drude peak, consistent with the experimentally observed midinfrared band in the copper oxide superconductors. The importance of vertex corrections is demonstrated by comparing the exact conductivity with the convolution integral of the exact single-particle Green's function.

The discovery of superconductivity in the copper oxides[1] in the vicinity of the Mott-Hubbard metal-insulator transition has intensified interest in the electronic properties of strongly correlated electronic systems.[2] One very detailed probe of the electronic structure of these high-temperature superconducting (HTSC) compounds is given by their optical properties. In particular, with either electron or hole doping an anomalous midinfrared (mid-IR) band emerges in the charge-transfer gap of these compounds.[3,4] We show in this Rapid Communication that the optical conductivity of the 2D Hubbard model is indeed in good agreement with these and other experimental observations, and discuss further tests for the applicability of this model.

As originally emphasized by Anderson,[5] the essential aspects of the electronic structure of the CuO_2 planes may be described by the two-dimensional (one-band) Hubbard model, with the Hamiltonian given by

$$H=-t\sum_{\langle i,j\rangle\sigma}(c_{i,\sigma}^{\dagger}c_{j,\sigma}+\text{H.c.})+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow} \tag{1}$$

in standard notation. In Eq. (1), $\langle i,j\rangle$ represents a nearest-neighbor pair. For large on-site repulsion U, the Hubbard-model Hamiltonian can be transformed into the t-J-model Hamiltonian acting on the space with no doubly occupied sites,[6]

$$H=-t\sum_{\langle i,j\rangle\sigma}(\tilde{c}_{i,\sigma}^{\dagger}\tilde{c}_{j,\sigma}+\text{H.c.})+J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right). \tag{2}$$

This effective Hamiltonian consists of the Heisenberg Hamiltonian plus a restricted hopping term for the holes, where $\tilde{c}_{i,\sigma}=c_{i,\sigma}(1-n_{i,-\sigma})$. We choose $t=1$ as our unit of energy. The Heisenberg exchange is $J=4t^2/U$, when derived from the one-band Hubbard model.

The Kubo formula for the real (absorptive) part of the optical conductivity at zero temperature may be written in the form

$$\mathrm{Re}\sigma_{\alpha\beta}(\omega)=-\frac{1}{\pi\omega}\mathrm{Im}\langle\psi_0|j_\alpha\frac{1}{\omega+E_0-H+i\delta}j_\beta|\psi_0\rangle, \tag{3}$$

where the current operator is[7]

$$j_\alpha=ieat\sum_{\mathbf{l},\sigma}(\hat{c}_{\mathbf{l}+\boldsymbol{\alpha},\sigma}^{\dagger}\hat{c}_{\mathbf{l},\sigma}-\text{H.c.})e^{i\mathbf{q}\cdot\mathbf{x}_\mathbf{l}}. \tag{4}$$

In this work we will always use the restriction $\alpha=\beta=x$, so the tensor indices of the conductivity will henceforth be suppressed. In accordance with this convention, the vector α is a unit vector in the x direction. The operators $\hat{c}_{\mathbf{l},\sigma}$ appearing in (4) are normal Fermionic annihilation operators for the Hubbard model, but must be replaced by the restricted operators $\tilde{c}_{\mathbf{l},\sigma}$ for the t-J model. The calculation of such dynamical correlation functions by means of the Lanczos algorithm is straightforward.[8]

The analog of the f-sum rule for both models is[7,9-11]

$$\int_0^\infty d\omega\,\sigma(\omega)=\tfrac{1}{2}(ea)^2\langle H_t\rangle_x, \tag{5}$$

where on the right-hand side the subscript x indicates the contribution to the expectation value of kinetic energy from hopping in the x direction. This sum rule is valid for systems with open boundary conditions (OBC) with $\mathbf{q}=0$, and with periodic boundary conditions (PBC) for $\mathbf{q}\neq0$.[10,11] The nonexistence[12] of such a sum rule with PBC for $\mathbf{q}=0$ is consistent with the conventional recipe that the thermodynamic limit should be taken before the limit $\mathbf{q}\to0$, and corresponds to the physically reasonable requirement of a nonzero momentum transfer in order to generate real absorption for a finite noninteracting single-band system for example.

The Hubbard model has three energy scales on which interesting optical effects may be expected: U, t, and $J=4t^2/U$ in decreasing order for the parameter range of interest here. Let us first consider the two larger energy scales, U and t. In the half-filled case ($n_h=0$), a Mott-Hubbard gap for charge excitations Δ_{MH} is expected, perhaps for U above some critical value for spatial dimensionality larger than 1. Within the present context this may be described simply with the following argument: The half-filled ground state has essentially no doubly occupied sites for U large compared to t. The application of the current operator (4) to this state then necessarily

creates a state with one doubly occupied site and one empty site, that is a state belonging to the upper Hubbard band (UHB). This then immediately leads to an absorption band centered near U. It is obvious from the above argument that the spectral intensity of this interband transition will decrease upon hole doping, reflecting the decreased probability of generating a doubly occupied site upon application of the current operator. Additional absorption will also appear at low energy due to the possibility of intraband transition within the lower Hubbard band (LHB). The results of numerical calculations on 3×3 Hubbard-model clusters with OBC shown in Fig. 1(a) support the simple picture outlined above. In the absense of holes (solid line) there is a gap $\Delta_{MH}\approx U-3t$. With hole doping, spectral weight is transferred to the low-energy region $\omega\approx t$, and the lower edge of the UHB shifts to higher energy. This upward shift is a direct consequence of the narrowing of the UHB upon doping. These trends are in good agreement with experiment,[4] and imply effective parameters $t\approx0.2$–0.3 eV and $U\approx2.0$ eV for Nd_2CuO_4, for example. The integrated conductivity

$$Z(\omega)=\int_0^{\omega}d\omega'\,\sigma(\omega') \tag{6}$$

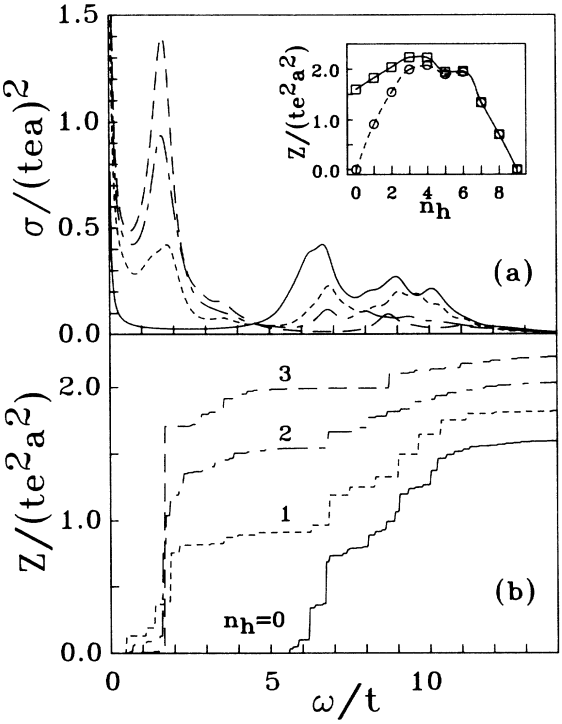

FIG. 1. (a) Frequency-dependent optical conductivity and (b) integrated conductivity for a 3×3 Hubbard model with open boundary conditions and $U=8(t=1)$. A relatively large broadening $\delta=0.4$ has been used in (a) in order to display $\sigma(\omega)$ for several fillings, resulting in a finite conductivity for $\omega<\Delta_{MH}$ at zero doping for example. The actual thresholds may be seen in (b), where $Z(\omega)$ has been calculated with $\delta\to0$. Curves are labeled by the number of holes away from half filling, as specified in (b). Inset: Doping dependence of integrated conductivity $Z(\infty)$ (squares) indicating the total sum rule, and the absorption in the lower Hubbard band $Z(\Delta_{MH}\approx5.5)$ (circles). The lines are merely guides to the eye.

for the same data is displayed in Fig. 1(b) in order to illustrate a further interesting point: Not only does intensity shift from the energy region of the UHB to the LHB with hole doping, also the total sum rule $Z(\infty)$ increases, at least up to doping levels $\approx30\%$. This point is important because the observation of such dependence would be a clear indication of the dominance of correlation effects even in the range of doping where metallic behavior exists. This information is summarized for a larger range of doping concentration in the inset of Fig. 1(a). In a weakly correlated semiconductor model with rigid band behavior the integrated conductivity decreases monotonically upon hole doping, as opposed to the initial increase starting from a value $O(t^2/U)$ in the Hubbard model. Note also that the doping dependence of the full sum rule $Z(\infty)$ for the t-J model is similar to the integrated conductivity of the LHB $Z(\Delta_{MH})$, and that there is negligible spectral intensity in the UHB for hole concentrations beyond quarter filling.

In order to examine the physics on the scale J, and at the same time to look more carefully on the scale t, it is useful to move on to the t-J model, where it is practical to diagonalize larger clusters. As a prelude to the examination of numerical results for this model let us first briefly recall some insights gained regarding the single-particle excitations.[8] Near half filling, coherent quasiparticle (QP) excitations with a bandwidth $\approx2J$ are observed, separated by a gap $\propto J$ from a continuum of width $7t$. In the most naive picture for the optical conductivity at small doping one might expect the emergence of a Drude-like peak associated with intraband absorption within the QP band. In a finite system this must appear at a finite energy, which should, however, be a fraction of the total coherent bandwidth $\sim2J$. Further, an additional absorption band due to interband transitions involving the QP band and the continuum should appear. While this picture cannot be entirely correct for finite doping, it does at least provide a scheme for interpreting the results of the numerical calculations. The J dependence of the frequency-dependent conductivity for a single hole of 4×4 clusters with OBC is shown in Fig. 2. The tendency for the conductivity to take the form of a low-energy peak ($\omega<0.5$) separated by a gap or pseudogap $\approx J$ from a broad absorption band is clearly evident here. The low-energy peak (or peaks due to the use of OBC) move toward $\omega=0$ with increasing system size, and may be called the Drude peak.

This interpretation of the low-energy part of $\sigma(\omega)$ of the Hubbard or t-J models at low doping as being describable in terms of a Drude peak separated from a mid-IR band by a gap or pseudogap $\approx J$ is further supported by the results for 4×4 clusters with PBC shown in Fig. 3. Figure 3(a) shows $\sigma(\omega)$ for momentum transfer $\mathbf{q}=(\pi/2,0)$ in a system with two holes. The separation of the low-energy Drude peak from the mid-IR band ($\omega\geq1$) is clearly visible, with a gap $\approx J$ for both one (not shown) and two holes in this cluster size.

With PBC there is the previously mentioned technical difficulty that the quantity of physical interest is actually $\lim_{q\to0}$ of the momentum- and frequency-dependent conductivity. For a small finite system this implies the re-

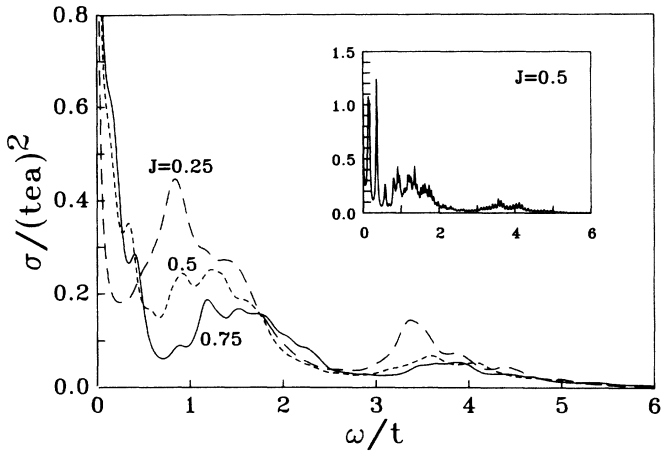

FIG. 2. Frequency-dependent optical conductivity for 4×4 t-J model cluster with open boundary conditions and a single doped hole. The curves are labeled by J, and have been broadened with $\delta=0.1$ for clarity of presentation. The inset shows one example ($J=0.5$) plotted with a higher resolution $\delta=0.02$.

striction to rather large momenta. One can calculate using $q=0$, but no sum rule of the form (5) exists. The problem manifests itself in the form of unphysical behavior at least at low frequencies. For example, for one hole there is a pole at $\omega=0$, whose very existence shows the nonexistence of a sum rule similar to (5), plus a mid-IR band starting at approximately the same frequency as for $\mathbf{q}=(\pi/2,0)$. The two-hole case has similar mid-IR behavior, but has no peak at all below this band. This momentum dependence is shown for two holes in Fig. 3(b). From the above discussion it should be clear that the large peak near $\omega=1$ for the $\mathbf{q}=(0,0)$ curve should *not* be connected with the Drude contribution, but is rather at the lower edge of the mid-IR band. At higher energy the trends for the shifting of intensity from low to high energy with increasing q are physically reasonable, including the $\mathbf{q}=(0,0)$ results. This continuous evolution of the distribution of spectral intensity with momentum transfer, together with the results with OBC, make it plausible that the "interband" part of the conductivity is given correctly for $\mathbf{q}=0$ with PBC. Thus, as a whole, the numerical results for $\mathbf{q}=0$ are not inconsistent with the near $1/\omega$ dependence for large ω found by Rice and Zhang.[9]

In Fig. 3(c) the conductivity for a system with three doped holes is shown. The mid-IR band begins at lower frequency than with one or two holes, as indicated by the position of the shoulder of the $\mathbf{q}=(0,0)$ curve (solid line) below $\omega=1$. A further difference between these results and those for lower doping is the vanishing of the gap between the Drude peak and the mid-IR band for $\mathbf{q}=(\pi/2,0)$. This tendency for the spectral intensity to shift to lower frequency is at least in qualitative agreement with experimental observations of the doping dependence of HTSC materials, where the center of gravity of the mid-IR band moves to lower frequency with increased doping.[4]

It is amusing to contrast the above described behavior for the 2D t-J model with that of the 1D case. In 1D, as has been pointed out by Anderson,[13] there is clearly decoupling of charge and spin excitations, at least within the context of the Bethe-ansatz (BA) description. What appears to be a nontrivial problem, however, is the con-

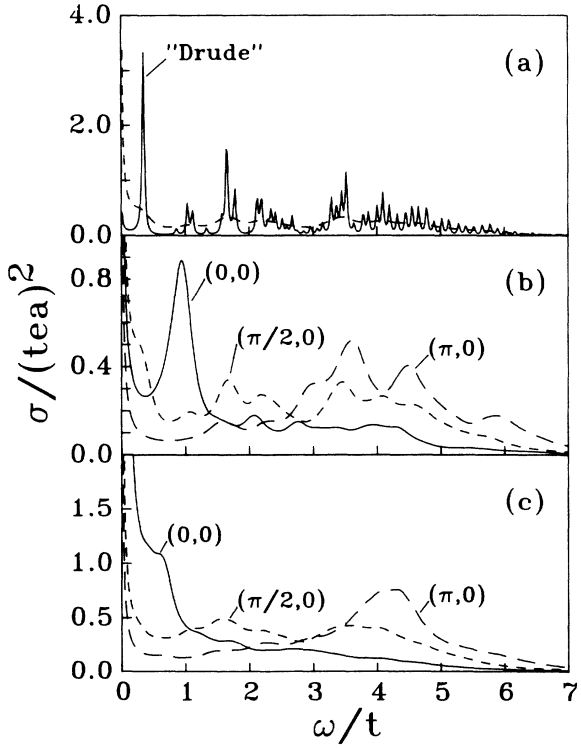

FIG. 3. Frequency-dependent optical conductivity for a 4×4 t-J-model cluster with periodic boundary conditions and $J=0.5$. (a) Two holes, momentum transfer $\mathbf{q}=(\pi/2,0)$ with broadening $\delta=0.02$ (solid line) and 0.2 (dashed line). In (b) the conductivity is shown for different momentum transfers for two holes with a broadening $\delta=0.2$ for clarity. (c) As in (b), but measured in the three-hole ground state.

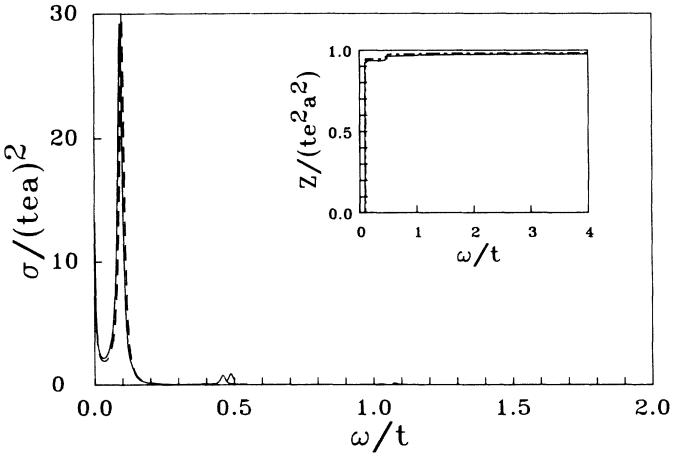

FIG. 4. Frequency-dependent optical conductivity for one hole in a 16-site 1D t-J-model cluster with open boundary conditions and $J=0.5$, plotted with broadening $\delta=0.01$. The solid line is the result measured in the spin-$\frac{1}{2}$ ground state, and the dashed line is the result in the spin-$\frac{15}{2}$ ferromagnetic state, which is identical to the spinless-fermion result. The inset shows the integrated conductivity for the same cases.

nection between the QP excitations of the BA solution and the physical electrons, which must be determined in order to calculate the coupling to an external electromagnetic field for example. There is no such difficulty with diagonalization. Some results are shown in Fig. 4, and may be summarized succinctly by stating that they reflect simple free-electron or spinless-fermion behavior. Similar results are also found at higher doping levels. With increasing chain length the low-energy Drude peak shifts to lower energy $\sim 1/N$, and the small higher-energy structures ($\omega \approx 0.5t$ in Fig. 4) decrease in intensity. This behavior is trivial for the case $J=0$, but the small influence of even rather large J is a remarkable manifestation of charge-spin separation. The simplicity of this result is all the more remarkable when we recall that the single-particle Green's function at half filling for the 1D case is entirely incoherent, and consists only of a continuum.[8] Any attempt to calculate the conductivity from a convolution of single-particle Green's functions is destined to fail in 1D. In 2D the situation is not quite so hopeless, as the convolution of exact single-particle Green's functions for the one- or two-hole ground state does tend to produce a conductivity which falls off roughly as $1/\omega$. The characteristic shift of weight to higher energy with increasing $|\mathbf{q}|$ is not properly given by such an approach, however. This indicates that vertex corrections are also essential for a proper estimate of $\sigma(\omega)$ in 2D, as is obviously the case in 1D.

Calculations for the 1D Hubbard model with $U \geq 8t$ give similar behavior below the gap to that shown for the t-J model in Fig. 4. Furthermore, the doping and U dependence of the fraction of spectral intensity below the gap (ratio of Drude weight to the total sum rule) is in good agreement with the calculation performed in the thermodynamic limit by Schulz[14] even for very short chains of $N=8$ sites with OBC in this parameter range.

Let us now briefly summarize the main points of this paper. First, the charge-spin separation in the 1D Hubbard model is clearly seen in the optical properties, which are free-electron-like at low energy for large U. Second, in the 2D case the shift of spectral intensity from the region of the charge-transfer gap Δ_{MH} to low energy with doping would by itself not suffice to rule out a weakly correlated single-particle semiconductor model for HTSC. However, the existence of the mid-IR band in both the Hubbard model and in experiments on HTSC is solid evidence for a strong correlation picture. Furthermore, the fact that the sum rule $Z(\infty)$ within the Hubbard model clearly increases with initial hole doping as compared to the monotonic decrease expected in the weakly correlated picture suggests that optical experiments be analyzed to search for this behavior.

Note added in proof. Related work for the single hole case was recently reported by Sega and Prelovšek,[15] Moreo and Dagotto,[16] and based on a variational approach by Inoue and Maekawa.[17]

We would like to acknowledge useful discussions with P. Fulde, W. Hanke, T. Timusk, and M. Ziegler.

[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

[2] See, e.g., *Proceedings of the Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors II, Stanford, 1989* [Physica C **162-164** (1989)].

[3] T. Timusk, M. Reedyk, R. Hughes, D. A. Bonn, J. D. Garret, J. E. Greedan, C. V. Stager, D. B. Tanner, Feng Gao, S. L. Herr, K. Kamarás, G. A. Thomas, S. L. Cooper, J. Orenstein, L. F. Schneemeyer, and A. J. Millis, Physica C **162-164**, 841 (1989).

[4] S. Uchida, Mod. Phys. Lett. B **4**, 513 (1990); Y. Tokura, T. Arima, S. Koshihara, T. Ido, S. Ishibashi, H. Takagi, and S. Uchida, in *Proceedings of the Second International Symposium on Superconductivity, Tsukuba, Japan* (Springer-Verlag, Berlin, 1990); S. Tajima, S. Tanaka, and T. Ido, and S. Uchida, *ibid.*

[5] P. W. Anderson, Science **235**, 1196 (1987).

[6] L. N. Bulaevskii, E. L. Nagaev, and D. L. Khomskii, Zh. Eksp. Teor. Fiz. **54**, 1562 (1968) [Sov. Phys. JETP **27**, 836 (1968)]; J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985).

[7] P. F. Maldague, Phys. Rev. B **16**, 2437 (1977); D. Baeriswyl, C. Gros, and T. M. Rice, Phys. Rev. B **35**, 8391 (1987).

[8] P. Horsch, W. H. Stephan, K.v. Szczepanski, M. Ziegler, and W. von der Linden, Physica C **162-164**, 783 (1989); K. J. von Szczepanski, P. Horsch, W. Stephan, and M. Ziegler, Phys. Rev. B **41**, 2017 (1990).

[9] T. M. Rice and F. C. Zhang, Phys. Rev. B **39**, 815 (1989).

[10] E. Y. Loh Jr., T. Martin, P. Prelovšek, and D. K. Campbell, Phys. Rev. B **38**, 2494 (1988).

[11] X. Zotos, P. Prelovšek, and I. Sega, this issue, Phys. Rev. B **42**, 8445 (1990).

[12] An extension of the optical conductivity sum rule to the case $\mathbf{q}=0$ has been discussed recently in Ref. 11 and by B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).

[13] P. W. Anderson, Int. J. Mod. Phys. B **4**, 181 (1990).

[14] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).

[15] I. Sega and P. Prelovšek, Phys. Rev. B **42**, 892 (1990).

[16] A. Moreo and E. Dagotto, Phys. Rev. B **42**, 4786 (1990).

[17] J. Inoue and S. Maekawa, J. Phys. Soc. Jpn. **59**, 2110 (1990).