PHYSICAL REVIEW B VOLUME 42, NUMBER 7 1 SEPTEMBER 1990

Rapid Communications

Rapid Communications are intended for the accelerated publication of important new results and are therefore given priority treatment both in the editorial office and in production. A Rapid Communication in **Physical Review B** *should be no longer than 4 printed pages and must be accompanied by an abstract. Page proofs are sent to authors.*

Optical conductivity of the Hubbard and t-J models

Adriana Moreo and Elbio Dagotto
Physics Department and Institute for Theoretical Physics, University of California at Santa Barbara, Santa Barbara, California 93106

(Received 28 February 1990; revised manuscript received 11 June 1990)

We calculate the optical conductivity $\sigma(\omega)$ of the Hubbard and t-J models on 10- and 16-site lattices, respectively, using a Lanczos method. Results are presented for various values of the couplings U/t, J/t, and band fillings, using free- and periodic-boundary conditions. We discuss the behavior of the kinetic energy in the ground state, the distribution of spectral weight of $\sigma(\omega)$ between low and high energies, and the sum rule. Indications of a Drude-like peak at low energy in the one-hole subspace are observed in both models. Assuming that holes behave like independent (mass-renormalized) particles in the normal state of the superconductors, our results also suggest that the optical midinfrared broadband observed experimentally can be explained by hole excitations of strongly correlated systems.

The study of the infrared properties of high-T_c superconductors like $YBa_2Cu_3O_{7-\delta}$ gives us information about the normal and superconducting states of these materials. Results for the reflectivity and the optical conductivity $\sigma(\omega)$ produced by different experimental groups are now in reasonable agreement with one another but the theoretical interpretation of the data is controversial. Of particular interest is a distinct knee[1,2] found in the reflectivity at a frequency 435 cm^{-1} in the normal and superconducting states.[2] The normal-state conductivity has a Drude-like peak at zero energy followed by strong absorption in the midinfrared with a broad peak centered[1] near $\omega \sim 1700$ cm^{-1}. There is no clear explanation for the origin of this absorption.[3]

How can we analyze theoretically the optical conductivity $\sigma(\omega)$? Simple Hubbard-like models in the strong-coupling regime may qualitatively describe the physics of the materials, but in that region there are no widely accepted analytic techniques for their study. Then, in order to compare experimental results with Hubbard-model predictions it is useful to perform numerical studies. In this paper we use exact diagonalization techniques of small clusters. The study of the dynamical properties of holes in the t-J and Hubbard models was recently initiated in the subspaces of one and two holes.[4] In this paper we extend those numerical results to the calculation of $\sigma(\omega)$. The Hamiltonian of the one-band Hubbard model has the well-known form

$$H = -t \sum_{\mathbf{i},\hat{\boldsymbol{\delta}},\sigma} (c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{i}+\hat{\boldsymbol{\delta}},\sigma} + \text{H.c.}) + U \sum_{\mathbf{i}} (n_{\mathbf{i},\uparrow} - \tfrac{1}{2})(n_{\mathbf{i},\downarrow} - \tfrac{1}{2}) , \quad (1)$$

where $c^{\dagger}_{\mathbf{i},\sigma}$ creates an electron of spin σ at site $\mathbf{i}$ of a two-dimensional (2D) square lattice, $n_{\mathbf{i},\sigma}$ is the number operator, and $\hat{\boldsymbol{\delta}}$ is a unit vector connecting nearest-neighbor sites. We have also studied the conductivity of the t-J model defined by the Hamiltonian

$$H = J \sum_{\mathbf{i},\hat{\boldsymbol{\delta}}} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}+\hat{\boldsymbol{\delta}}} - t \sum_{\mathbf{i},\hat{\boldsymbol{\delta}},\sigma} (\bar{c}^{\dagger}_{\mathbf{i},\sigma} \bar{c}_{\mathbf{i}+\hat{\boldsymbol{\delta}},\sigma} + \text{H.c.}) , \quad (2)$$

where $\bar{c}^{\dagger}_{\mathbf{i},\sigma}$ is a hole operator acting in the space where there is no double occupancy, and the rest of the notation is standard. For the t-J model we worked on a 4×4 lattice while for the Hubbard model we worked on $\sqrt{8}\times\sqrt{8}$ and $\sqrt{10}\times\sqrt{10}$ site lattices.[4] To study the optical conductivity in the Hubbard model we define the current operator in the x direction at zero momentum as

$$j_x = it \sum_{\mathbf{i},\sigma} (c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{i}+\hat{\mathbf{x}},\sigma} - c^{\dagger}_{\mathbf{i}+\hat{\mathbf{x}},\sigma} c_{\mathbf{i},\sigma}) ,$$

while for the t-J model we simply replace $c_{\mathbf{i},\sigma}$ by $\bar{c}_{\mathbf{i},\sigma}$. Through the usual linear-response theory the optical absorption is now defined as

$$\sigma(\omega) = -\frac{1}{\omega\pi} \text{Im} \left(\langle \psi_{\text{g.s.}} | j_x \frac{1}{\omega + E_{\text{g.s.}} + i\epsilon - H} j_x | \psi_{\text{g.s.}} \rangle \right) , \quad (3)$$

where $|\psi_{\text{g.s.}}\rangle$ is the ground state of the Hubbard or t-J models with a given number of holes and energy $E_{\text{g.s.}}$, which we obtain with a modified Lanczos method.[4] ϵ is a small parameter that moves away from the real axis poles that otherwise would appear in Eq. (3). For a (i) finite lattice with *open* boundaries and (ii) an infinite lattice, it can be shown[5] that the sum rule

$$\int_0^{\infty} d\omega\, \sigma(\omega) = \frac{\langle T_x \rangle}{2} \quad (4)$$

is satisfied where $\langle T_x \rangle$ represents the mean value in the ground state of the hopping term of Eqs. (1) and (2) in the x direction. Using Eq. (3), $\sigma(\omega)$ can be evaluated by a continued fraction expansion using the Lanczos method.[4] We will mainly concentrate on the case of zero and one holes since we are interested in the properties of the Hubbard model at low temperature and small doping where the holes can be treated as independent.[6]

Since $\langle T_x \rangle$ is related with the integrated $\sigma(\omega)$ it is instructive to analyze its behavior as a function of U/t. For a half-filled system $\langle T_x \rangle$ decreases as a function of U/t as expected and it vanishes at $U=\infty$. Thus, in this limit the optical spectral weight goes to zero. In Fig. 1(a) we show $\langle T \rangle_U / \langle T \rangle_0$ vs U/t for the two-dimensional Hubbard model on a 10-site lattice with periodic- (PBC) and free-boundary conditions (FBC) at half filling using a Lanczos technique (exact). $\langle T \rangle_U$ is the total kinetic energy (summed over x and y directions) at coupling U $(t=1)$ (we explicitly checked that for large U we reproduce the results of the Heisenberg model). We also plot results obtained from a mean-field (MF) calculation at half filling and a Monte Carlo (MC) simulation.[7] There is a good agreement among all the different techniques. For completeness, in the same graph we show results for the 1D chain in the bulk limit[8] which are similar to the two-dimensional case. In Fig. 1(b) $\langle T \rangle_U / \langle T \rangle_0$ obtained numerically is plotted as a function of doping for different values of U/t on an 8-site lattice with PBC ($\langle n \rangle = 1$ is half filling). As expected for intermediate and strong coupling, when the system is doped away from half filling the kinetic energy increases and thus there is more spectral weight in $\sigma(\omega)$ through the sum rule [Eq. (4)]. Note that in this region the slope of kinetic energy versus $\langle n \rangle$ curve indicates that the carriers are holes.

In Fig. 2(a) we show $\sigma(\omega)$ at $U=8$ $(t=1)$ in the subspaces of zero and one hole with FBC on a 10-site lattice. We explicitly checked that the sum rule [Eq. (4)] is satisfied. For this and higher values of the coupling and one hole, there is a clear separation between the high energy $(\omega \sim U)$ states having charge excitations and the low-energy excitations which are produced by the distortions of the spin background when the hole moves.[4] At half filling we only observe charge excitations located at roughly the same position as with one hole although having more spectral weight [region III in Fig. 2(a)]. The threshold for charge excitations is in good agreement with previous results for the one-hole spectrum of the Hubbard model.[4] It is very interesting that in the one-hole subspace a large peak at low energies appears [region I in Fig. 2(a)]. It is natural to assume that this peak will become a Drude-like peak at $\omega=0$ for a large system. The FBC used in this lattice simply introduce a small shift in its position to higher energies. This interpretation is supported by solving a one-particle problem on a lattice with FBC of increasing size. A large peak appears accumulating spectral weight at low energy and finally becoming the Drude peak in the bulk limit. Note also that there is addi-

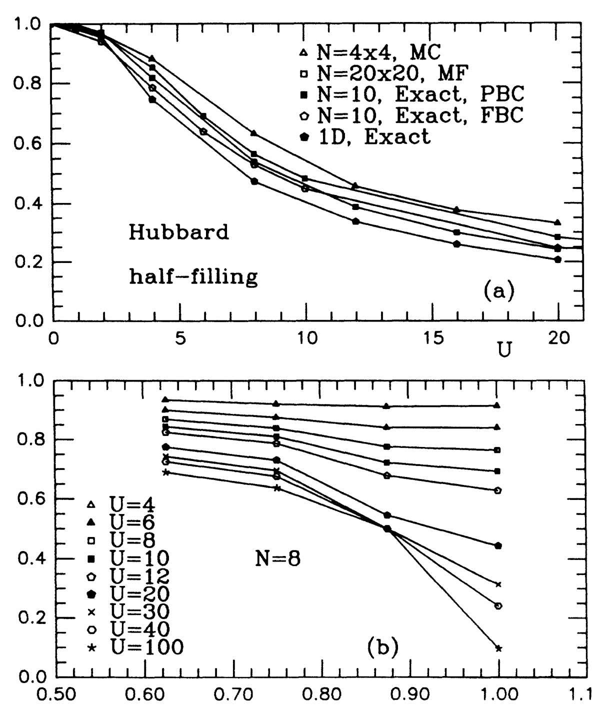

FIG. 1. (a) Ratio of kinetic energies $\langle T \rangle_U / \langle T \rangle_0$ in the ground state of the half-filled Hubbard model as a function of $U(t=1)$ on a 10-site lattice with FBC and PBC (exact results). MC (MF) denotes Monte Carlo (mean-field) results while 1D are exact results for the one-dimensional chain. (b) $\langle T \rangle_U / \langle T \rangle_0$ as a function of doping $\langle n \rangle$ on an 8-site lattice for various values of the coupling $U(t=1)$.

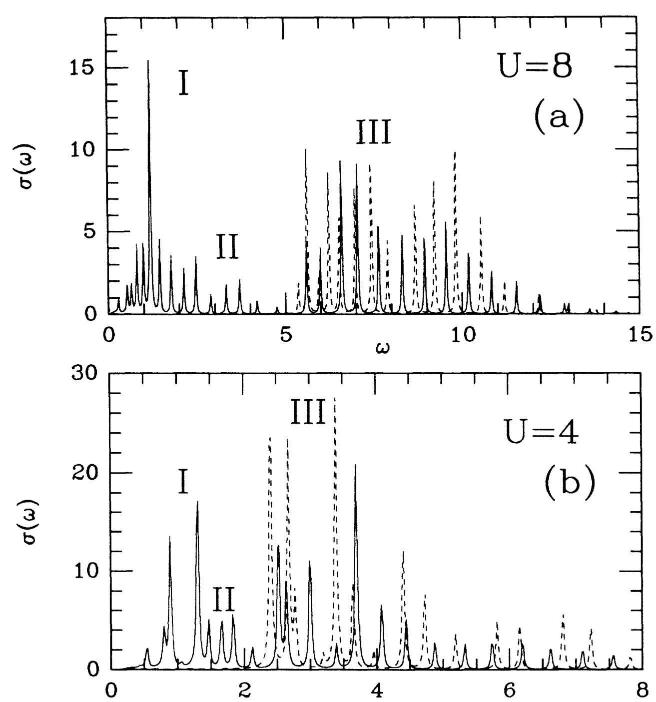

FIG. 2. (a) $\sigma(\omega)$ vs ω for a 10-site lattice at $U=8$. The dashed line corresponds to the half-filled case while the solid line represents results when one particle is removed. We use $\epsilon = 0.02$, $t=1$, and FBC. (b) Same as (a) but at $U=4$.

tional spectral weight [region II in Fig. 2(a)] immediately after that Drude peak. These states correspond to the hole in excited states as described in Ref. 4 using a "string" picture. We believed that it is possible to explain the midinfrared features of the superconductors within the context of the Hubbard model through these hole excited states. In Fig. 2(b) we present similar results but for $U=4$, which is a representative of the weak-coupling region. Here spin and charge excitations cannot be separated easily, although they can still be distinguished from each other.[9] We have also studied two holes in the Hubbard model showing that the results are similar to one hole with more spectral weight accumulating in the Drude peak as expected.

It is important to know how the spectral weight of $\sigma(\omega)$ is distributed between the high- and low-energy states. For this purpose we found it useful to define the quantity[5] $Z(\omega)=\int_0^\omega d\omega' \sigma(\omega')$. The ratio $Z(\omega)/Z(\infty)$ interpolates between 0 ($\omega=0$) and 1 ($\omega=\infty$). Typical results are shown in Fig. 3. At $U=10$ and one hole the plateau observed in this figure shows that the charged states contain only $\sim 50\%$ of the spectral weight (the rest being concentrated at low energies). This percentage decreases when U increases. On the other hand, the result for $U=4$ shows no clear separation between charge and spin excitations.

Now we turn to the t-J model. $\sigma(\omega)$ for this model was analyzed previously in the region $\omega \gg J$ assuming a diffusive motion for the hole and also using a self-consistent perturbation theory.[10] Since in the Hubbard model with 10 sites we found no large differences between FBC and PBC at large U/t (where the t-J model is a good approximation to the Hubbard model) we decided to use PBC which simplifies the numerical work. In Figs. 4(a) and 4(b) we show our numerical results for the t-J model on a 4×4 lattice. From this spectrum we subtracted the trivial divergence at $\omega=0$ due to the finite momentum of the hole.[5] There is a large peak at finite but small energy resembling the results we obtained for the Hubbard model. This feature is present for all values J/t we investigated ($0.2 \le J \le 1.0$) and it is tempting to speculate that it will become the Drude peak in the bulk limit.[5] Note that after the main peak in Figs. 4(a) and 4(b) additional structure is present. In particular, a second peak can be clearly observed above the background. As for the Hubbard model, we believe that this accumulation of spectral weight after the Drude peak may account for the midinfrared absorption observed experimentally. What is the meaning of this broadband? By analyzing the current spectral function we found a strong correspondence with the previously obtained spectral function of one hole.[4] In this case we also found the existence of peaks on top of a featureless structure. These peaks were identified as excited states of a hole self-trapped in a linear potential as it happens in the Ising limit. We believe that if the Hubbard or t-J models are good descriptions of the new materials, then a more careful experimental analysis of $\sigma(\omega)$ should show additional structure beyond the Drude peak at low temperatures.[11]

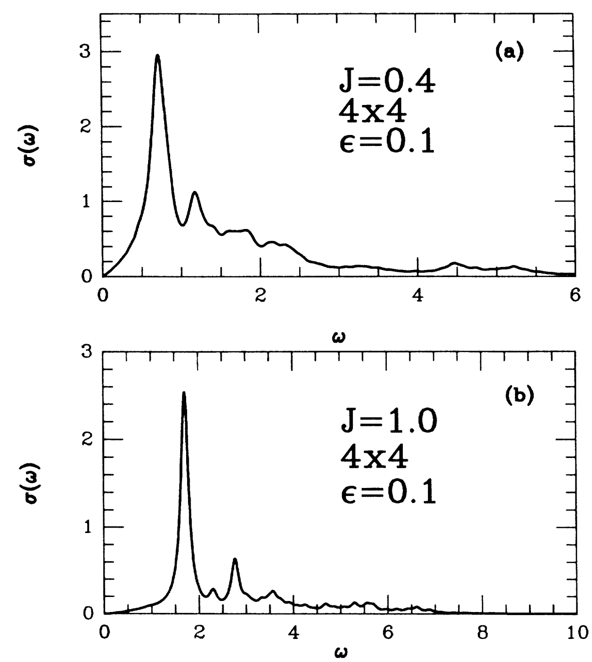

FIG. 4. (a) $\sigma(\omega)$ vs ω for the t-J model on a 4×4 lattice at $J=0.4$ using $\epsilon=0.1$, $t=1$, and PBC. (b) Same as (a) but at $J=1.0$.

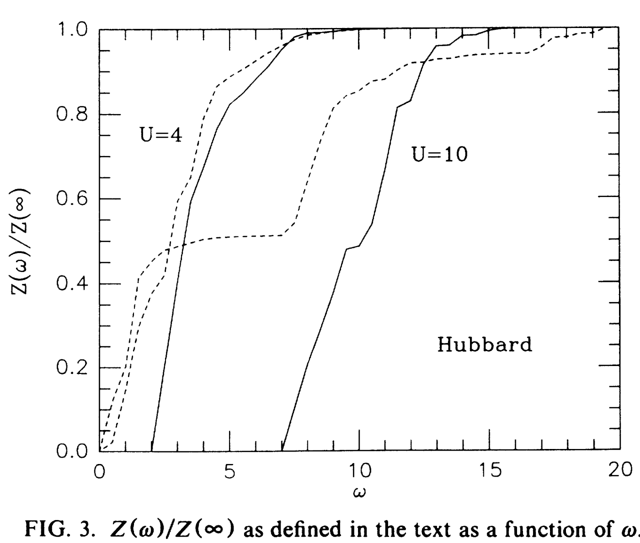

FIG. 3. $Z(\omega)/Z(\infty)$ as defined in the text as a function of ω. The solid lines correspond to half filling while the dashed lines denote results with one hole. $U=4$ and 10 ($t=1$) are shown.

Summarizing, we have studied the optical absorption $\sigma(\omega)$ for both the Hubbard and t-J models. In the one-hole subspace we found a large peak at low energies which we associate with a Drude peak. Additional spectral weight at low energies due to hole excitations may explain the midinfrared experimental features of the new materials. We believe that our conclusions are very general and they will appear in the analysis of other models involving both Cu and O atoms. The present results, combined with the observed shift in the antiferromagnetic peak of the t-J model with doping leading to an incommensurate phase,[12] indicate that some "abnormal" experimental results found in the new materials may have an explanation purely within the context of the Hubbard or t-J models.

We thank D. Scalapino for his collaboration in the early stages of this work and also A. Millis, B. Shastry, E Gagliano, and R. Collins for useful suggestions. This project was supported in part by the NSF Grants No. PHY87-01775 and No. PHY82-17853, and by the Department of Energy Grant No. FG03-88-ER45197, and supplemented by funds from NASA. The computer simulations were done on the CRAY-2 at NCSA, Urbana, Illinois.

[1]G. A. Thomas *et al.*, Phys. Rev. Lett. **61**, 1313 (1988); T. Timusk *et al.*, Phys. Rev. B **38**, 6683 (1988).

[2]S. L. Cooper *et al.*, Phys. Rev. B **40**, 11 358 (1989).

[3]Note, however, that the experimental results are controversial. For example, it may occur that the midinfrared band is mainly due to chains [Z. Schlesinger *et al.* Phys. Rev. B **41**, 11 237 (1990)].

[4]E. Dagotto, A. Moreo, R. Joynt, S. Bacci, and E. Gagliano, Phys. Rev. B **41**, 9049 (1990), and references therein. For a recent review, see E. Dagotto, Int. J. Mod. Phys. B (to be published).

[5]P. F. Maldague, Phys. Rev. B **16**, 2437 (1977). There are many subtle points concerning the study of $\sigma(\omega)$; if we try to derive the sum rule of the Hubbard model with PBC following Maldague, it can be shown that his operator x (a coordinate operator), becomes ill-defined at the boundary since it jumps from L to $-L$ if $2L$ is the length of the lattice. That produces an additional contribution to the sum rule that can be thought of as a surface term. We found numerically that for a finite lattice this term is important at small U (although it disappears if a nonzero momentum is used in the current). However, for FBC there is no problem since there is no hopping term at the boundary. In this case the sum rule is satisfied. There is another interpretation to the result for PBC [D. Poilblanc (private communication); B. Shastry and B. Sutherland (unpublished)] where the difference between the kinetic energy and the integral of $\sigma(\omega)$ as defined in Eq. (3) is associated with the weight of the Drude peak at $\omega=0$. Such a possibility may alter the interpretation of our results for the *t*-*J* model below. The second subtle point concerns the one-hole subspace where the momentum of the ground state [see E. Dagotto *et al.*, Phys. Rev. B **40**, 6721 (1989)] when PBC are used introduces a trivial divergence in $\sigma(\omega)$ at $\omega=0$. To remedy this problem one can simply make an average over all the degenerate states of the hole (zero momentum state). For FBC there are no problems as in the case of the sum rule.

[6]This approximation will work in the normal state where holes behave like free particles (with renormalized masses) but not in the superconducting phase.

[7]S. White *et al.*, Phys. Rev. B **40**, 506 (1989).

[8]D. Baeriswyl, J. Carmelo, and A. Luther, Phys. Rev. B **33**, 7247 (1986).

[9]The results shown in Figs. 2(a) and 2(b) were obtained with FBC in order to satisfy the sum rule [Eq. (4)] but we also obtained results with PBC. For zero hole they are in good agreement with the FBC results if U is large (the sum rule being satisfied within a few percent). For small U the differences are much larger. A similar situation occurs for one hole where clear indications of structure at low energy similar to that of Fig. 2(a) can be observed with PBC. This result together with the small change in the kinetic energy by changing boundary conditions [Fig. 1(a)] leads us to believe that finite-size effects are not very important in the present qualitative analysis at least in strong coupling. Then, $\sigma(\omega)$ seems to be mainly a measure of short-range correlations.

[10]T. M. Rice and F. C. Zhang, Phys Rev. B **39**, 815 (1989); C. Kane *et al.*, *ibid.* **39**, 6880 (1989).

[11]During completion of this work we received a copy of unpublished work from I. Sega and P. Prelovsek, Phys. Rev. B **42**, 892 (1990) where numerical results for the conductivity of the Kondo and *t*-*J* models are discussed with conclusions in agreement with ours.

[12]A. Moreo, E. Dagotto, T. Jolicoeur, and J. Riera, Phys. Rev. B (to be published).