Optical conductivity of the two-dimensional Hubbard model

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The optical conductivity $\sigma_1(\omega)$ of the two-dimensional Hubbard model on finite clusters of 4×4 and $\sqrt{10}\times\sqrt{10}$ sites is reported. Experimental features found in the high-T_c cuprate superconductors can be qualitatively reproduced by this model including the presence of mid-infrared spectral weight, a Drude peak whose intensity grows with doping and a total spectral weight that varies slowly as the system is doped away from half filling. We find that to reproduce qualitatively the main experimental features of $\sigma_1(\omega)$, we need to work with a coupling constant of the order of the bandwidth, i.e., $U/t\sim8$–10. Results for the negative-U Hubbard model are included for comparison.

Infrared measurements are an important probe of the dynamics of strongly correlated electronic systems. In particular, the real part of the optical conductivity, $\sigma_1(\omega)$, has provided useful insight into the electronic structure of the cuprate superconductors.[1–3] In the insulating phase, $\sigma_1(\omega)$ shows negligible absorption below a charge-transfer (CT) gap of 1.5–2 eV. As the CuO_2 plane is lightly doped with holes or electrons, there is a rapid growth of spectral weight at low frequencies giving rise to a Drude-like peak and a broad mid-infrared (ir) feature, while the spectral weight in the CT band decreases.[2,3] The integrated conductivity remains approximately constant and thus a redistribution of spectral weight takes place upon doping. A measure of the transfer of spectral weight from the CT band to lower frequencies, used in several experimental papers,[2,3] is a normalized effective carrier density $N_{\rm eff}$ proportional to the integral of $\sigma_1(\omega)$ up to the gap. This quantity was found to rise more rapidly than would be expected from the doped carrier concentration alone. This "anomalous" qualitative behavior was found in both p-type[3] ($La_{2-x}Sr_xCuO_4$) and n-type[2] ($Pr_{2-x}Ce_xCuO_4$) superconductors. These results have raised questions as to whether they can be understood within the framework of the theoretical models presently used to describe the Cu-O superconductors. Here we examine this question for the simplest model which has been proposed to describe these materials, the one-band Hubbard model. In this model we assume that the lower (upper) Hubbard band corresponds to the O $2p$ (Cu $3d$) band of the cuprates and thus the CT gap can be described by an "effective" Hubbard coupling U/t. Using Lanczos techniques, we calculate $\sigma_1(\omega)$ and the Drude weight for finite Hubbard clusters. We find that the behavior of the doped Hubbard model is similar to the experimental results clearly exhibiting a transfer of spectral weight from above the gap to the Drude peak and the mid-ir region. We conclude with results for the negative-U Hubbard model.

The two-dimensional (2D) one-band Hubbard model

$$H=-t\sum_{\langle ij\rangle s}(c^\dagger_{is}c_{js}+c^\dagger_{js}c_{is})+U\sum_i n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

is the simplest model which is believed to contain the essential physical features of the CuO_2 plane. The notation is standard. At half filling, $\langle n\rangle=1$, it is well known that the ground state has long-range antiferromagnetic order. When the system is doped away from half filling, $x=1-\langle n\rangle$, Monte Carlo simulations show the presence of finite-range incommensurate antiferromagnetic correlations.[4] In addition, calculations of the momentum occupation[4] $\langle n_{\mathbf{k}}\rangle$ in the doped region are consistent with a large Fermi surface enclosing $1-x$ electrons. Thus a natural question is whether such a model can exhibit the observed doping dependence of $\sigma_1(\omega)$.

For the Hubbard model, $\sigma_1(\omega)$ can be decomposed into a zero-frequency Drude weight δ function and a regular part,

$$\sigma_1(\omega)=D\delta(\omega)+\frac{\pi e^2}{N}\sum_{n\,(\neq0)}\frac{|\langle n|j_x|0\rangle|^2}{E_n-E_0}\delta(\omega-(E_n-E_0))\ . \tag{2}$$

Here j_x is the paramagnetic current operator

$$j_x=it\sum_{i,s}(c^\dagger_{i+\mathbf{x},s}c_{is}-c^\dagger_{is}c_{i+\mathbf{x},s})\ ,$$

e is the electric charge, and N is the number of sites of the lattice. $\{|n\rangle\}$ denote states of energy $\{E_n\}$ which are excited when j_x acts on the ground state $|0\rangle$ (whose energy is E_0). Using the f-sum rule for the Hubbard model,[5]

$$2\int_0^\infty\sigma_1(\omega)d\omega=(\pi e^2/2N)\langle0|(-T)|0\rangle\ ,$$

where the kinetic operator T is the first term in Eq. (1), one obtains[6]

$$\frac{D}{2\pi e^2}=\frac{1}{4N}\langle0|(-T)|0\rangle-\frac{1}{N}\sum_{n\,(\neq0)}\frac{|\langle n|j_x|0\rangle|^2}{E_n-E_0}\ . \tag{3}$$

Using Lanczos techniques on $\sqrt{10}\times\sqrt{10}$ and 4×4 periodic clusters, we have independently calculated the regular part of $\sigma_1(\omega)$ [whose integral corresponds to the second term on the right-hand side of Eq. (3)] and the kinetic energy, obtaining D from Eq. (3).[7]

Results showing $\sigma_1(\omega)$ versus ω for $U/t=10$ on a 4×4 cluster at various band fillings are shown in Fig. 1. The results for the $\sqrt{10}\times\sqrt{10}$ cluster are qualitatively similar. At half filling, the insulating Hubbard gap is clearly visible. Upon doping, spectral weight is rapidly transferred from the region above the Hubbard gap to the Drude peak at $\omega=0$ and to the midgap region. The presence of this midgap band is very clear in our results and thus its existence can be accounted for within the context of a simple one-band Hubbard model in 2D as previously remarked.[8] Note that similar calculations in 1D have not observed such a large spectral weight in the midgap region[9] and thus its presence is a two- (or higher) dimensional effect. At $x=0.125$ the insulating gap is almost filled since the mid-ir region has a total width comparable with the gap itself.[10] This is reminiscent of previous calculations[11] of the single-particle spectral weight, $N(\omega)$, that showed that hole doping removed single-particle spectral weight from both the upper and lower Hubbard bands and created additional states in the gap extending upwards from the lower Hubbard band. We believe that the additional states found in $N(\omega)$ and those found in the midgap region of $\sigma_1(\omega)$ have a *similar* origin, probably due to the distortions created by holes in an antiferromagnetic background, "string states," which only exist in two or higher dimensions.[12] It is also interesting to notice that for small values of the coupling $U/t\sim4$, the upper Hubbard band and the mid-ir band can hardly be distinguished upon doping. Thus, in order to reproduce experiments [where the upper and midgap bands appear as separate features of $\sigma_1(\omega)$], it is necessary to work in the region $U/t>4$.

Another constraint on U/t is set by the observation that the total spectral weight is approximately independent of doping.[2] The kinetic energy of the Hubbard model which determines this spectral weight through the f-sum rule is shown in Fig. 2(a) for various values of U/t. For large values of U/t, there is a significant change in the total spectral weight with doping which is not compatible with experiments. Thus, to satisfy both the structure in $\sigma_1(\omega)$ and the behavior of the spectral weight, one is led to an intermediate coupling U of order the bandwidth.[13]

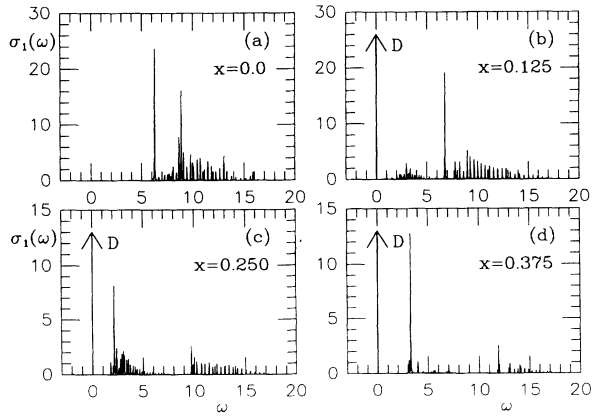

FIG. 1. Real part of the optical conductivity $\sigma_1(\omega)$ for a 4×4 cluster with $U/t=10$ and band fillings ($x=1-\langle n\rangle$) (a) $x=0$ (half-filled band), (b) $x=0.125$, (c) $x=0.250$, and (d) $x=0.375$. A small shift from the real axis ($\epsilon=0.01$) was used to plot the δ functions. The peak at $\omega=0$ represents the Drude peak D. Its intensity in the figure is *not* proportional to its real magnitude, but it is included only for illustration.

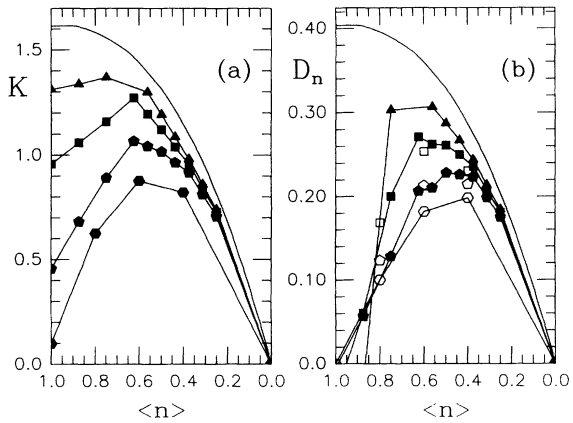

FIG. 2. (a) Kinetic energy per site of the Hubbard model $K=\langle0|(-T)|0\rangle/N$ on a 4×4 cluster as a function of doping for $U/t=4$ (▲), $U/t=8$ (■), and $U/t=20$ (⬟). We also show results for a $\sqrt{10}\times\sqrt{10}$ sites cluster at $U/t=100$ (⬟). The solid line without points corresponds to results for $U/t=0$ in the bulk limit. (b) $D_n=D/(2\pi e^2)$ vs x for various couplings U/t. ▲, ■, and ⬟ denote $U/t=4$, 8, and 20, respectively, on a $4\times4n$ lattice. □, □, and ⬡ indicate results for a $\sqrt{10}\times\sqrt{10}$ site cluster at $U/t=8$, 20, and 100, respectively. The solid line without points denotes the results for $U/t=0$ in the bulk limit.

One measure of the shift of spectral weight from high to low energies is the Drude weight D. Figure 2(b) shows $D_n=D/2\pi e^2$ versus $\langle n\rangle$ for various values of U/t. In an insulating phase D will vanish as $\exp(-N_x/\xi)$ as the linear size N_x of the system increases, as recently seen for 1D Hubbard rings.[9] This is in agreement with our results at half filling where $|D|$ is a small number.[14] Figure 2(b) shows that as the system is doped toward $\langle n\rangle=0.5$, the Drude weight grows rapidly. Increasing the doping further, D_n simply follows the kinetic energy. For very large couplings (but not as large as to induce a transition to a ferromagnetic phase), D_n approximately converges to the result shown in Fig. 2(b) for $U/t=100$. Note that the curve D_n versus doping is smooth and the results for $\sqrt{10}\times\sqrt{10}$ and 4×4 sites are close to each other, and thus we believe its qualitative shape will survive in the bulk limit.

In Fig. 3 we show the sum of the Drude spectral weight D and the midgap spectral weight under $\sigma_1(\omega)$. Normalizing this weight by dividing it by $\pi e^2 t$ gives an effective carrier density in which the unrenormalized mass is $m=(2t)^{-1}$, i.e.,

$$N_{\rm eff}=\frac{1}{\pi e^2 t}\int_0^{\omega_c}\sigma(\omega)d\omega\ . \tag{4}$$

Here ω_c is a frequency just below the upper Hubbard band. The dependence of $N_{\rm eff}$ versus x is shown in Fig. 3 for several values of U/t. An important feature, clearly seen in Fig. 3, is that the system is doped away from half

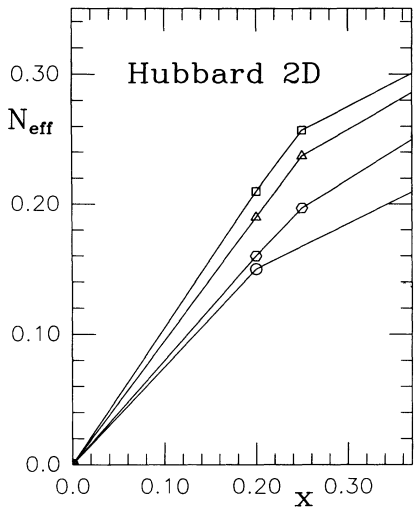

FIG. 3. N_{eff} (i.e., the sum rule of the Drude weight and the midband weight) vs doping for various values of U/t. □ corresponds to $U/t=8$, △ to $U/t=10$, ○ to $U/t=20$, and ○ to $U/t=200$. Doping of $x=0.25$ ($x=0.20$) corresponds to a 4×4 ($\sqrt{10}\times\sqrt{10}$) sites clusters.

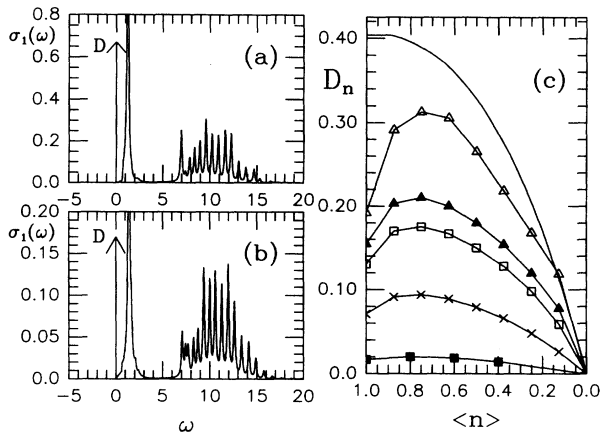

FIG. 4. $\sigma_1(\omega)$ for a 4×4 cluster with $U/t=-10$ and (a) $x=0$, (b) $x=0.125$. We use a small shift from the real axis $\epsilon=0.10$ to plot the δ functions. The peak D at $\omega=0$ has the same meaning as in Fig. 1. (c) The Drude weight $D_n=D/(2\pi e^2)$ for the negative-U Hubbard model vs $\langle n\rangle$. △, ▲, □, ×, and ■ denote results for $U/t=-4$, -8, -10, -20 (4×4 cluster), and -100 ($\sqrt{10}\times\sqrt{10}$ cluster), respectively. The solid line without points corresponds to the result for $U/t=0$ in the bulk limit.

filling, it is the number of *holes* x that determines the spectral weight, and not the total number of electrons as would be the case for the noninteracting system. The dependence of N_{eff} versus x is qualitatively similar to that observed experimentally,[2,3] although the experimental results rise somewhat more rapidly with x. Since the data presented here are the results of a first-principles calculation with only *one* free parameter U/t, we consider Fig. 3 as an encouraging step forward in comparing experiment with Hubbard-model predictions.

It is interesting to contrast the behavior of $\sigma_1(\omega)$ for the positive-U Hubbard model with that for negative U. Figures 4(a) and 4(b) show $\sigma_1(\omega)$ versus ω for $U/t=-10$ at $x=0.0$ and $x=0.125$, and Fig. 4(c) shows the Drude weight $D/2\pi e^2$ versus x for various values of U/t, both obtained on a 4×4 cluster. We know that the ground state of this model at finite doping is superconducting[15] and that the electrons are paired in an s-wave state. $\sigma_1(\omega)$ has spectral weight at energies associated with the breaking of pairs. In addition, as seen in Figs. 4(a) and 4(b), there is low-lying spectral weight in the gap which arises from collective excitations which can exist in the gap because of the absence of a long-range Coulomb interaction in this model. The Drude weight of Fig. 4(c) for the $U<0$ model, does *not* vanish at half filling where the ground state has long-range order in both the charge density and the pair field channels.[15] Note that as $U/t\to\infty$, D vanishes, which is associated with the localization of the pairs in this limit.

Summarizing, we have calculated the optical conductivity of the 2D Hubbard model on finite clusters. For $U>0$, we found that in the undoped case there is a gap in the spectrum. Upon doping, spectral weight is shifted to a Drude peak and the mid-ir region. The intensity of the Drude peak grows quickly with doping. These features are in reasonable qualitative agreement with experiments for a coupling constant U/t of the order of the bandwidth. This behavior can be contrasted with the negative-U Hubbard model which has a finite Drude weight even at half filling, low-lying spectral weight inside the gap, and whose distribution of spectral weight does not vary rapidly as the system is initially doped away from half filling.

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[10]On the 4×4 cluster we observed important finite-size effects (FSE's) working with 14 electrons. In this case the current operator connects the ground state with another state of energy order U/t (that becomes degenerate with the ground state at $U/t=0$) with a matrix element of order 1. Then, its contribution to $\sigma_1(\omega)$ diverges as $U/t\rightarrow0$ and the Drude peak $\rightarrow-\infty$. This is similar to the results observed in Ref. 9 at half filling and it is a FSE that will disappear in the bulk limit. We have simply subtracted this anomalous peak at low energies (located at $\omega=0.453$ at $U/t=10$ and 14 electrons) from our Fig. 1(b) and in the calculation of D_n. We found that this procedure produced results which smoothly connect with those of other dopings. Another approach would have been to use twisted boundary conditions: D. Poilblanc (unpublished).

[11]E. Dagotto, A. Moreo, F. Ortolani, J. Riera, and D. Scalapino (unpublished).

[12]E. Dagotto *et al.*, Phys. Rev. B **41**, 9049 (1990), and references therein.

[13]Note that *independent* calculations have arrived to similar values for U/t. See M. Hybertsen *et al.*, Phys. Rev. B **41**, 11 068 (1990); S. Bacci *et al.* (unpublished).

[14]However, notice that D becomes negative at half filling. This is indeed a finite-size effect. As previously reported [Ref. 9; A. Moreo (unpublished); C. Stafford, A. Millis, and B. Shastry, Phys. Rev. B **43**, 13 660 (1991)], for a half-filled finite system, D can be negative, indicating a paramagnetic response. For the 1D ring, this response was found to decrease as $\exp(-N_x/\xi)$, and we expect that this same behavior will be seen for two-dimensional clusters.

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