Dynamic conductivity of strongly correlated electrons: The Hubbard model on a cubic lattice

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The frequency-dependent (optical) conductivity of the Hubbard model on a three-dimensional cubic lattice is studied through calculations on a small cluster. The interaction strength is varied between the weak- and strong-coupling limits. Results are reported for the half-filled band, and for small hole dopings away from half filling. The formation of a Hubbard gap is observed. Results are related to aspects of the current discussion of the metal-insulator transition in bulk systems.

I. INTRODUCTION

This paper is concerned with the frequency-dependent (optical) conductivity of strongly correlated electrons described by the simple, one-orbital Hubbard model in three dimensions. We investigate these quantities using exact numerical calculations for a small cluster.

The optical conductivity of the Hubbard model has been the subject of much recent study in view of possible applications to cuprate superconductors. Most of the work has concerned one- and two-dimensional models.[1-17] Much less attention has been given to three-dimensional systems. Many calculations have used some type of an exact diagonalization procedure (such as the Lanczos algorithm). Because those calculations are limited to a small number of sites, it is apparent that the linear extent of the systems that can be investigated is much greater in one- or two-dimensional cases. The calculations reported here involve a cube with eight sites. Because the wavelengths of infrared and optical phonon are very large compared to the lattice constants of crystals, the wave vector $\mathbf{q}$ of a photon emitted or absorbed can generally be neglected, and one considers the conductivity only in the case $q=0$. We will refer to this as the optical conductivity.

In general, one would like to study the conductivity σ as a function of the band filling and the interaction strength U. There are three ranges of energy: (1) low (ω close to zero), in which one investigates the so-called "Drude weight," (2) intermediate energies $\omega \sim t$ [t is the hopping integral; see Eq.(5) (below)], and (3) high energies, $\omega \sim U$, in which case one has transitions across the Hubbard gap.

If dissipative processes are ignored,

$$\sigma(\omega)=D\delta(\omega)+\sigma_{\rm reg}(\omega) , \tag{1}$$

in which D (a real constant) is the Drude weight and $\sigma_{\rm reg}$ is regular as $\omega \to 0$. The first term corresponds to the possibility of free acceleration in a static field. In a classic paper, Kohn[18] showed that, for a large system, D would vanish for an insulator while it would be finite for a metal, with the value

$$D=\pi e^2 n/m^* , \tag{2}$$

where n is the number of carriers per unit volume, and m^* is the optical effective mass.

In the Hubbard model for a large system with a half-filled band, D is expected to be zero for sufficiently large U, and in the case of a one-dimensional system, it should be zero for all $U>0$. For other band fillings, D should not be zero. In the case of a finite system, there are significant complications, which are discussed in several of the references,[6,11,13-15] which occur when periodic boundary conditions are imposed. For a half-full band, one finds for a ring with $4n$ sites $D<0$, and for a ring with $4n+2$ sites, $D>0$.[15] However, $|D|$ decays rapidly (essentially exponentially) with the size of the ring.[14] In the case of one-dimensional systems with open boundary conditions, $D=0$.

For other band fillings for which D would not be zero for a large system, the nonzero value of D obtained for a finite system with periodic boundary conditions is meaningful. In the case of open boundary conditions, for which D is, strictly speaking, zero, it is shown in Ref. 13 that there is a peak in the optical conductivity at low frequency ("Drude precursor") such that a D can be extracted by integrating over this peak, and this value of D is in agreement with that obtained when periodic boundary conditions are employed.

In all cases, the real part of the conductivity in the Hubbard model is constrained by the sum rule[1] (in units in which $\hbar=1$),

$$\int_0^\infty {\rm Re}\sigma_{\alpha\alpha}(\omega)d\omega=\frac{\pi e^2\Delta^2}{2V}\langle 0|(-T_\alpha)|0\rangle , \tag{3a}$$

in which Δ is the nearest-neighbor distance, which will be taken to be unity in the numerical calculations which follow, V is the volume assigned to the system, and T_α is the contribution to the noninteracting part of the Hamiltonian which we call the kinetic energy from motion in the direction specified by the index α. In a cubic system, σ is independent of α. Further, as a convention, we will take $V=N\Delta^3$ where N is the number of sites. Equation (3a) simplifies

$$\int_0^\infty {\rm Re}\sigma(\omega)d\omega=\frac{\pi e^2}{6N\Delta}\langle 0|(-T)|0\rangle , \tag{3b}$$

where T is the full kinetic energy.

Equation (3b) should be contrasted with the usual form of the f sum rule[19]

$$\int_0^\infty \mathrm{Re}\sigma(\omega)d\omega=\frac{\pi}{2}\frac{ne^2}{m} \tag{4}$$

(m being the free-electron mass). When Eqs. (1) and (2) are compared with Eq. (4), it is necessary to adopt the convention that the integral over positive frequencies includes $\frac{1}{2}$ of the δ function at $\omega=0$; i.e., there is a contribution to (4) of $D/2$. It will also be observed that the right-hand side of (4) is independent of the electron interaction, while the right-hand side of (3b) depends on the interaction, and in fact can vanish (e.g., for a half-filled band as $U\rightarrow\infty$). The discrepancy is a consequence of the one-band characteristics of the simple Hubbard model: The optical conductivity of actual solids at energies of more than a few volts is dominated by transitions to higher bands, which are not included in the present model. Even in many of the physical systems to which the Hubbard model is intended to apply (antiferromagnetic transition-metal compounds), the model cannot describe the charge-transfer transitions (oxygen p states to metal d) which often define the onset of strong absorption.[20] In this paper, we will discuss optical transitions across the Hubbard gap, but it is not clear if there are experimental observations of this.

The Hubbard model as defined on an eight-site (3d) cubic cluster has been studied previously. Kawabata determined the spin of the ground state as a function of U/t for filling from two to eight electrons.[21] Spin-correlation functions and thermodynamic properties were obtained in Ref. 22. The spectral weight function for the same system is described in Refs. 23 and 24. We will not cite here the far more voluminous literature on the Hubbard model on two-dimensional (2D) square lattices of various sizes but a review of some related aspects of the 2D problem is contained in Ref. 24.

The remainder of this paper is organized as follows. Section II contains a discussion of the theory underlying the calculation of the optical conductivity, and a brief description of the computational methods employed. Our results are described in Sec. III. The paper concludes with a brief summary in Sec. IV.

II. THEORY AND CALCULATIONAL METHODS

The simple Hubbard model is defined by the Hamiltonian

$$H=t\sum_{\langle i,j\rangle,\sigma}c_{i\sigma}^\dagger c_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}\ . \tag{5}$$

The notation is standard. We consider one orbital localized on each site. Hopping, characterized by a transfer integral t, is permitted between nearest-neighbor sites. Interactions occur only between two electrons of opposite spin on the same site, and are measured by a parameter U.

In order that this paper should be comprehensible and reasonably self-contained, we review briefly some of the formal aspects of the calculation of the dynamic conductivity. Much of the discussion is based on Ref. 13.

The current operator is obtained by the procedure of Kohn.[18] We consider the interaction with a weak electric field described by a position-independent vector potential $\mathcal{A}$. Then a gauge transformation is introduced which eliminates the vector potential from the Hamiltonian but modifies the phase of the orbitals. The result is that the hopping matrix elements in Eq. (5) are multiplied by a phase factor, so that (5) becomes

$$H=t\sum_{\langle ij\rangle,\sigma}e^{-ie\mathcal{A}\cdot(\mathbf{R}_i-\mathbf{R}_j)}c_{i\sigma}^\dagger c_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}\ . \tag{6}$$

We now suppose that $\mathcal{A}$ is small, and expand the first term through second order in $\mathcal{A}$. The current J_α is defined by

$$J_\alpha=-\frac{\partial H}{\partial\mathcal{A}_\alpha}=N(j_\alpha^{(P)}+j_\alpha^{(D)})\ . \tag{7}$$

(α is a rectangular component and N is the number of sites). The current consists of two parts: one which is independent of $\mathcal{A}$, $j^{(P)}$ (sometimes called the paramagnetic current), and one of first order in $\mathcal{A}$, $j^{(D)}$ (the diamagnetic current). We are including only nearest-neighbor hopping in (5), so $\mathbf{R}_i-\mathbf{R}_j$ is a nearest-neighbor lattice vector, Δ_{ij}. In the cubic system of interest here, our convention is that $|\Delta|=1$, and Δ_{ij} lies along a cube axis. For convenience, we take $\mathcal{A}$ to define the x direction. Then,

$$j_x^{(P)}=\frac{iet}{N}\sum_{\langle ij\rangle,\sigma}\Delta_{ij,x}c_{i\sigma}^\dagger c_{j\sigma}\ , \tag{8a}$$

$$j_x^{(D)}=\frac{te^2}{N}\mathcal{A}\sum_{\langle ij\rangle,\sigma}\Delta_{ij,x}^2c_{i\sigma}^\dagger c_{j\sigma}=\frac{e^2\mathcal{A}}{N}T_x\ , \tag{8b}$$

where T_x is the contribution from the first term of (5) due to motion in the x direction.

The "observed" currents are found with the use of the density matrix ρ,

$$\langle j_x\rangle=\mathrm{Tr}[\rho(j_x^{(P)}+j_x^{(D)})]\ . \tag{9}$$

The trace in (9) is evaluated to first order in $\mathcal{A}$, using a standard procedure[19] in which one retains only terms of first order in $\mathcal{A}$. One obtains the complex conductivity tensor $\sigma_{\alpha\beta}$,

$$\sigma_{\beta\alpha}=\frac{e^2}{iN(\omega+i\eta)}\langle T_\alpha\rangle_0\delta_{\alpha\beta}+\frac{i}{\omega+i\eta}\Pi_{\alpha\beta}\ , \tag{10}$$

where η is an infinitesimal positive quantity, $\langle\ \rangle_0$ indicates an average with the density matrix in the absence of the field (ground-state average at $T=0$), and $\Pi_{\alpha\beta}$, the current-current correlation function, is given by

$$\Pi_{\alpha\beta}=\frac{1}{N}\sum_m\langle 0|j_\beta^{(P)}|m\rangle\langle m|j_\alpha^{(P)}|0\rangle\times\left[\frac{1}{\omega+E_0-E_m+i\eta}-\frac{1}{\omega-E_0+E_m+i\eta}\right]\ . \tag{11}$$

In a cubic system, only the diagonal terms ($\alpha=\beta$) in the optical conductivity are different from zero.

We may now let η tend to zero, and separate σ into its

real and imaginary parts.

$$\sigma_{\alpha\alpha}(\omega)=\sigma_R(\omega)+i\sigma_I(\omega) . \tag{12}$$

The real part σ_R is singular at $\omega=0$. This leads to an expression for the Drude weight D [Eq. (1)],

$$D=\frac{\pi}{N}\left[e^2\langle -T_\alpha\rangle+2\sum_m \frac{|\langle 0|j_\alpha|m\rangle|^2}{E_0-E_m}\right] . \tag{13a}$$

The index α can be dropped for a cubic system, giving

$$D=\frac{\pi}{3N}\left[e^2\langle -T\rangle+2\sum_m \frac{|\langle 0|\mathbf{j}|m\rangle|^2}{E_0-E_m}\right] . \tag{13b}$$

For a two-dimensional square lattice, the factor 3 in the denominator becomes 2. For $\omega>0$, we have

$$\sigma_R=\frac{\pi}{3\omega}\frac{1}{N}\sum_m |\langle 0|\mathbf{j}|m\rangle|^2\delta(\omega+E_0-E_m) \quad (\omega>0) , \tag{14}$$

$$\sigma_I=\frac{1}{3N\omega}\left\{e^2\langle -T\rangle+\sum_m |\langle 0|\mathbf{j}|m\rangle|^2\left[\frac{1}{\omega+E_0-E_m}-\frac{1}{\omega-E_0+E_m}\right]\right\} , \tag{15}$$

in which the sum over m is to be interpreted as a principle-value integral in the case of a large system. In a finite system, singularities are avoided by approximating the principal value using

$$\mathrm{Re}\frac{1}{\omega\pm E_0\mp E_m+i\eta}=\frac{\omega\pm E_0\mp E_m}{(\omega\pm E_0\mp E_m)^2+\eta^2} ,$$

in which a small but finite value of η is retained. The real dielectric function is obtained from σ_I by (cgs units)

$$\epsilon(\omega)=1-4\pi\sigma_I/\omega . \tag{16}$$

The real and the imaginary parts of the conductivity are connected by the Kramers-Kronig relations. One of these asserts that

$$\sigma_I(\omega)=-\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty}\frac{\sigma_R(\nu)}{\nu-\omega}d\nu \tag{17}$$

[and $\sigma_R(-\nu)=\sigma_R(\nu)$]. We find from (17) that in the limit $\omega\to\infty$

$$\lim_{\omega\to\infty}[\omega\sigma_I(\omega)]=\frac{2}{\pi}\int_0^\infty\sigma_R(\nu)d\nu . \tag{18}$$

It then follows from (15) that

$$\int_0^\infty\sigma_R(\nu)d\nu=\frac{\pi}{6N}e^2\langle -T\rangle , \tag{3b'}$$

which is the f sum rule discussed in the Introduction.

We can now combine Eqs. (3b'), (13b), and (14) to deduce that if there is no state degenerate with the ground state

$$\sum_m \frac{|\langle 0|\mathbf{j}|m\rangle|^2}{E_m-E_0}|=\frac{e^2}{2}\langle -T\rangle . \tag{19}$$

This result can also be obtained through use of commutation rules to evaluate the sum. However, then Eq. (13b) implies that $D=0$, as discussed previously.

Numerical calculations for the eight-site cubic cluster were performed using exact diagonalization. The Hamiltonian, defined on this structure, possesses electron-hole symmetry. It is necessary for this small cluster to employ open boundary conditions. Therefore, the numerical value of D resulting from evaluation of Eq. (13b) must be zero. This is a useful check on the numerical calculations.

In principle, the conductivity for a finite system is a sum of δ functions. In order to keep the results finite, the parameter η in Eq. (11) was set equal to 0.05.

III. RESULTS

We will consider first the calculated conductivity in the half-filled band case, then, for systems with one or two holes. In order to understand the results, it is essential to understand the level spectrum of the noninteracting system. This is illustrated in Fig. 1. As a convention, and for convenience, we will assume that the parameter t in Eq. (5) is equal to $+1$. This is equivalent to scaling U, and all energies by t, i.e., $U\to U/t$. The single-particle spectrum contains four levels: the lowest, spatially nondegenerate, energy -3; two triply degenerate levels of energy -1 and $+1$; and a nondegenerate level of energy $+3$. The symmetries of the levels from lowest to highest are Γ_2', Γ_{25}', Γ_{15}, and Γ_1. If the sign of t is negative the order of the symmetries is reversed but nothing else changes. The current operator belongs to Γ_{15}. In the half-filled band case with $U=0$, the lowest two single-particle levels are filled. This situation is reminiscent of a

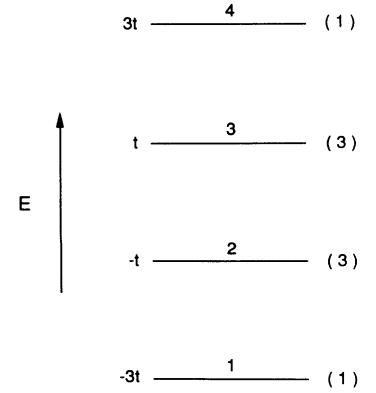

FIG. 1. Energy-level diagram for the single-particle states.

semiconductor rather than a metal. In the one- and two-hole cases, the second level is not completely filled: these cases correspond to metals.

The discussion of Sec. II indicated the importance of the quantity $\langle -T \rangle$, the ground-state expectation value of the noninteracting part of the Hamiltonian. Our results for this quantity are given in Table I. Equation (3b) asserts, on the basis of this data, that the optical absorption vanishes as $U \rightarrow \infty$ in the half-filled band limit, but not for the other occupancies.

The numerical values contained in Table I have a simple explanation for $U=0$. In this case one is simply adding particles one at a time to the levels as illustrated in Fig. 1. The first two particles go into the level with $E=-3t$; the remainder go into the level with $E=-t$. When U is nonzero but small, $\langle -T \rangle$ remains close to its value in the noninteracting limit, but as U increases ($U>6$), $\langle -T \rangle$ develops a maximum at $n=5$.

We would like to interpret this data so as to be relevant to current discussion of the behavior of the quantity n/m^* [(electron density)/(effective mass)] near a metal-insulator transition.[25] However, there are two limitations which result from the small size of the system we consider: (1) a sharp transition is not to be expected even at $T=0$ in a finite system, unless there is a change in symmetry of the ground state due to a crossing of levels. This does not occur in the half-filled band case in the present model. (2) A gradual transition is partially obscured as a result of the gaps in the single-particle spectrum illustrated in Fig. 1.

In spite of these problems, the following interpretation is plausible: Since (for $U \leq 4$), $\langle -T \rangle$ increases monotonically with an increasing number of particles for fixed U, and also since the absorption for small U has a straightforward interpretation in terms of single-particle transitions, it is reasonable to define an effective mass as the ratio of $\langle -T \rangle$ for $U=0$ and fixed n to that for nonzero U:

$$m^*(n,U)=\langle -T \rangle_0 / \langle -T \rangle_U \ . \tag{20}$$

This m^* is not the usual effective mass of band theory because the band mass has been scaled out; rather, it is a measure of the effect of interactions on the integrated optical absorption. Figure 2 shows that, for small U, m^* remains close to but larger than unity for all n.

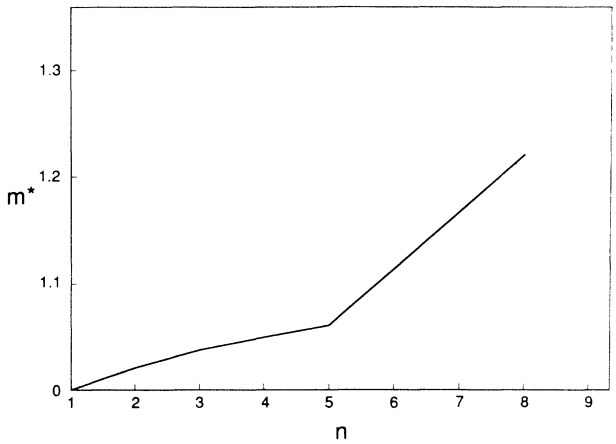

FIG. 2. Variation of the dimensionless effective mass defined by Eq. (20) with occupancy for $U=4t$. The sharp change of slope at $n=5$ is probably a finite-size effect.

However, the situation is different for large U, since $\langle -T \rangle$ has a maximum at $n=5$, and decreases rapidly as the half-filled limit is approached. Calculations of the spectral weight function for this system[23,24] show the existence of a narrow band of quasiparticle states for large U whose width decreases only slowly for large U. In these circumstances, we believe it is reasonable to consider that the decrease of $\langle -T \rangle$ is due to a decreasing effective number of carriers. We believe these data support the idea that a metal-insulator transition occurs only in the half-filled band case, and as $n \rightarrow 0$, rather than as $m^* \rightarrow \infty$.

In the noninteracting limit, $U=0$, the only energy at which optical absorption can occur is $\omega=2$ (in units of t), corresponding in the cases of interest here (eight, seven, and six electrons) to a transition between Γ'_{25} and Γ_{15} levels. As U increases, absorption is spread over a range of energies. However, in the half-filled case, the absorption moves steadily to higher energies. Figure 3 shows the calculated optical conductivity for $U=1,4,8,12$, and 100. The strength of the absorption drops, as required by the data of Table I, and also as is apparent from the factor

TABLE I. The ground-state expectation value of the negative of the first term in Eq. (5). $\langle -T \rangle / N$ is given for all band fillings and selected values of U.

U \ n	1	2	3	4	5	6	7	8
0	0.375	0.75	0.875	1.0	1.125	1.25	1.375	1.5
1	0.375	0.748 16	0.871 43	0.994 42	1.119 93	1.237 31	1.361 44	1.485 09
2	0.375	0.744 15	0.863 28	0.982 36	1.105 53	1.205 99	1.321 41	1.439 14
4	0.375	0.734 53	0.843 08	0.953 36	1.061 76	1.121 33	1.180 41	1.246 88
6	0.375	0.725 62	0.824 36	0.926 38	1.015 43	1.038 07	1.019 89	0.990 38
8	0.375	0.718 15	0.808 98	0.903 86	0.975 98	0.968 57	0.888 72	0.797 83
10	0.375	0.712 03	0.796 65	0.885 51	0.946 51	0.913 34	0.791 10	0.669 33
12	0.375	0.706 99	0.786 74	0.870 56	0.919 73	0.869 83	0.718 60	0.577 44
16	0.375	0.699 29	0.772 02	0.848 04	0.884 11	0.807 53	0.620 91	0.452 55
32	0.375	0.683 79	0.743 98	0.804 20	0.821 10	0.699 46	0.465 88	0.239 04
100	0.375	0.669 52	0.720 04	0.765 93	0.772 36	0.616 53	0.375	0.078 02

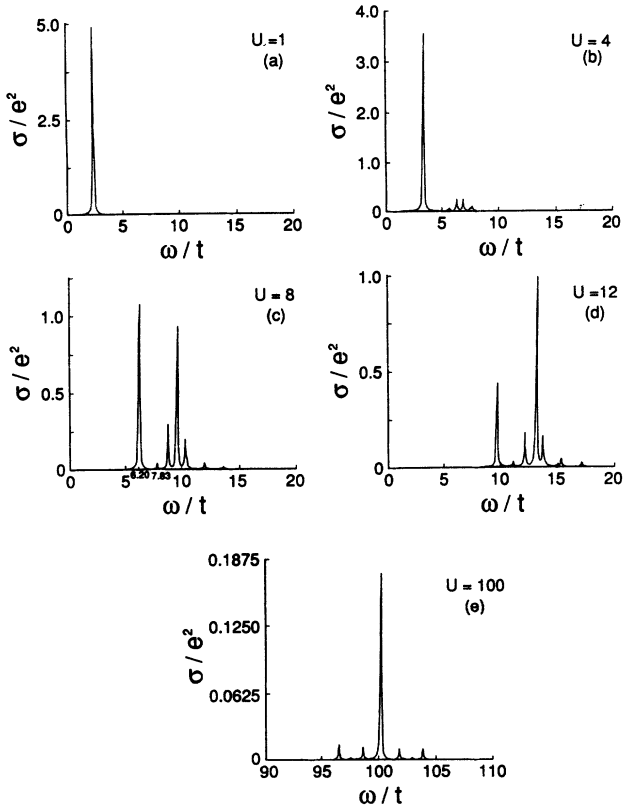

FIG. 3. Optical conductivity for the half-filled band case of different values of U: (a) $U=1$; (b) $U=4$; (c) $U=8$; (d) $U=12$; (e) $U=100$. Curves are computed with a broadening (η) of 0.05. In all cases, the Hubbard parameter U and the frequency ω are given in units of the hopping integral t.

ω^{-1} in Eq. (10). In the half-filled case, for $U>8$ (roughly), antiferromagnetism is established in the sense that the antiferromagnetic structure factor is within 10% of its limit as $U\rightarrow\infty$. The spectrum of the Hamiltonian then has a separate, low-lying manifold of states which are spin rearrangements. These states are not accessible optically. Optical absorption requires transitions to a higher manifold whose states involve a real (as opposed to virtual) double occupancy, and this requires an energy of the order of U. The energy of the lowest peak is plotted as a function of U in Fig. 4. The real dielectric function will show resonance behavior associated with the conductivity peaks.

We now turn to the consideration of systems with one and two holes in a half-filled band. Figure 5 shows the optical conductivity for the one-hole case for $U=1,4,8,12$, and 32.

We observed, previously, $D=0$ as a consequence of the boundary conditions. At $U=0$, all of the absorption is concentrated in a peak at $\omega=2$, a single-particle transition. As U increases this peak broadens and splits. This position of the lowest major peak is shown in Fig. 4. In addition, absorption develops at higher energies, and becomes associated with transitions into the upper Hubbard band.

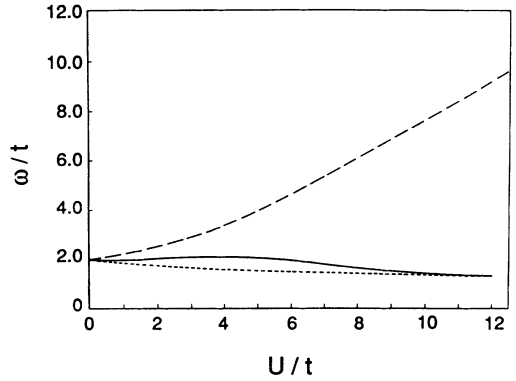

FIG. 4. Energy of the lowest (major) peak in the optical conductivity peak is shown as a function of U. Long-dashed line, half-filled band; solid line, one-hole case; short-dashed line, two holes. All quantities are in units of t.

Up to about $U=6$ (note that the "bandwidth" is also 6), the lowest absorption peak remains at $\omega=2$. Evidently, optical absorption at the energy of the single-particle transition persists until U is about the size of the bandwidth. As U increases further, this peak moves to lower energies. For $U\geq 10$, there is a clear separation of the lower and upper Hubbard bands. There are several absorption peaks in each band. We think it is plausible that this peak structure is a consequence of the finite size of the system we consider, and that, in the limit of a large system the absorption would be distributed more uniformly over both the lower and upper bands. Comparison of Figs. 3(c) and 5(c) or 3(d) and 5(d) shows that for a given value of U, doping leads to a transfer of absorption from higher to lower energy. The data of Table I show that the integrated absorption is not constant with doping, but the change is not large for $U\sim 6$ or 8, i.e., for

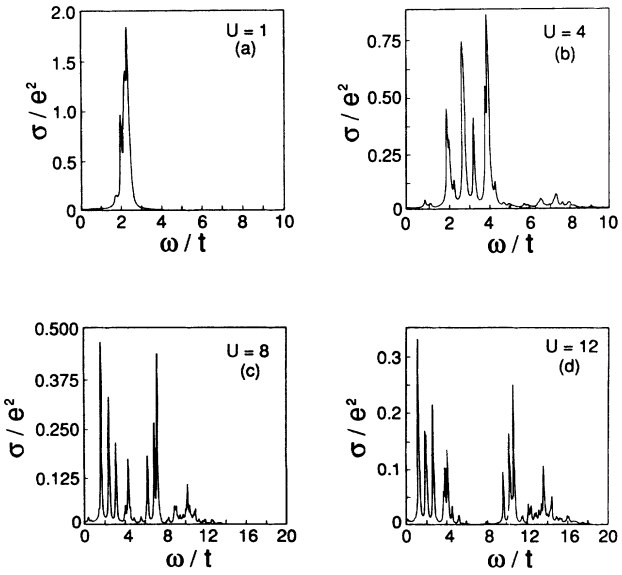

FIG. 5. Optical conductivity for one hole in the half-filled band for selected values of U: (a) $U=1$; (b) $U=4$; (c) $U=8$; (d) $U=12$.

values of U similar to the bandwidth. The one-hole system remains metallic with a narrow quasiparticle band persisting to large U.[22] In this specific case, the ground state becomes the Nagaoka[26] ferromagnetic state for $U > 39.5$.[22] Since this is a noninteracting state, the absorption for $U > 39.5$ reverts to a single peak at $\omega = 2$, but now corresponding to a transition between Γ_{15} and Γ_1 single-particle states.

Following Moreo and Dagotto,[12] we define the scaled integrated absorption up to frequency ω,

$$Z(\omega) = \frac{6N}{\pi e^2 \langle -T \rangle} \int_0^{\omega} \sigma_R(\omega') d\omega' \ . \tag{21}$$

It follows from Eq. (3b') that $Z(\infty) = 1$. We show the function $Z(\omega)$ for selected values of U in the one-hole case in Fig. 5. For a small value of U [Fig. 5(a)], almost all the absorption occurs in a small energy range near $\omega = 2$, consistent with the discussion above. As U increases [Figs. 6(c) and 6(d)], a plateau forms close to $Z = \frac{1}{2}$. This results from the separation of the manifold of states into lower and upper Hubbard bands. As is seen from the figures, there is some indication of a plateau for $U = 8$, and it is clearly established for $U = 12$. The interested reader may wish to consult Fig. 4 of Ref. 22 (also reprinted as Fig. 8.5.4 in Ref. 19) which shows that the spectrum of spin-$\frac{1}{2}$ states for $n = 7$ contains a Hubbard gap for $U = 10$. When the gap forms, the integrated absorption is about equally divided between upper and lower Hubbard bands.

As U continues to increase, the plateau widens and the Hubbard gap approaches U. Then most of the integrated absorption is concentrated in the lower band.

Wagner, Hanke, and Scalapino[13] (WHS) have pointed out that when open boundary conditions are employed, one can still estimate the Drude weight by integrating over the low-energy absorption ("Drude precursor"), which they interpret (see their Fig. 12) as the absorption in the lower Hubbard band. Their result, for a one-dimensional system, appears to agree rather well with the value of D in the metallic case obtained when periodic boundary conditions are employed.

There could be some ambiguity in defining the "Drude precursor" because the absorption for this finite system exhibits a complex multipeak structure. It is possible that some of this intermediate-energy absorption in the lower Hubbard band becomes a midinfrared feature in a large system,[12,16] as seen in cuprate superconductors. However, if we integrate over the lower Hubbard band as in WHS, the Drude precursor has one-half of the total absorption when the Hubbard bands separate, and the full absorption for large U.

We now consider the case of two holes in the half-filled band. The conductivity is shown for four different values of U, in Fig. 7, and the integrated absorption is shown in Fig. 8. As in the one-hole situation, the absorption begins at $U = 0$ with a single peak at $\omega = 2$, and spreads to both higher and lower frequencies as U increases. The major absorption peak of lowest energy, whose position is shown in Fig. 4, moves away from the energy of the single-particle transition more rapidly than in the one-hole case, but for large U, beyond the range shown in Fig. 4, the peak for two holes is slightly above that for one hole.

A Hubbard gap is apparent in the optical conductivity for two holes for somewhat smaller values of U than for one hole. It is already evident for $U = 6$ for two holes, but does not appear until about $U = 8$ or 10 for one hole. This difference is probably a feature of the small system we consider in which the holes are spatially constrained.

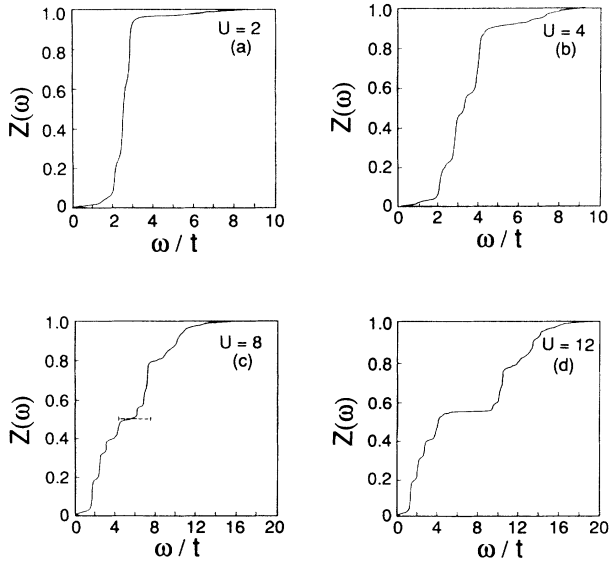

FIG. 6. Dimensionless integrated absorption $Z(\omega)$ [Eq. (21)] as a function of frequency for one hole in the half-filled band for different values of U: (a) $U = 2$; (b) $U = 4$; (c) $U = 8$; (d) $U = 12$. In (c), the dashed line indicates a plateau where the Hubbard gap develops.

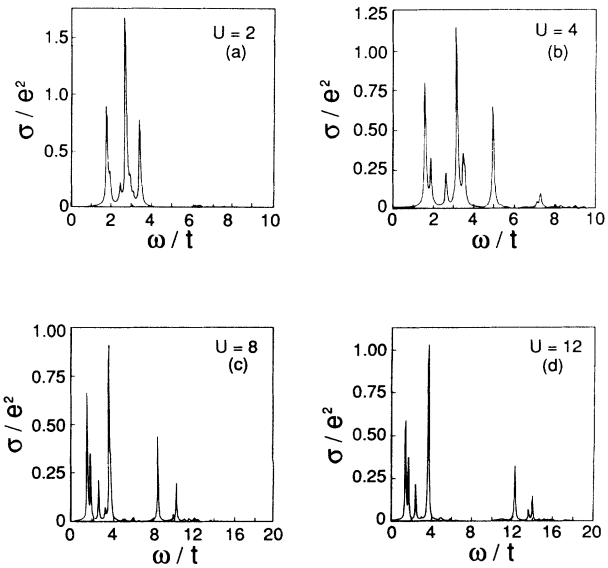

FIG. 7. Optical conductivity for two holes in a half-filled band for selected values of U: (a) $U = 2$; (b) $U = 4$; (c) $U = 8$; (d) $U = 12$.

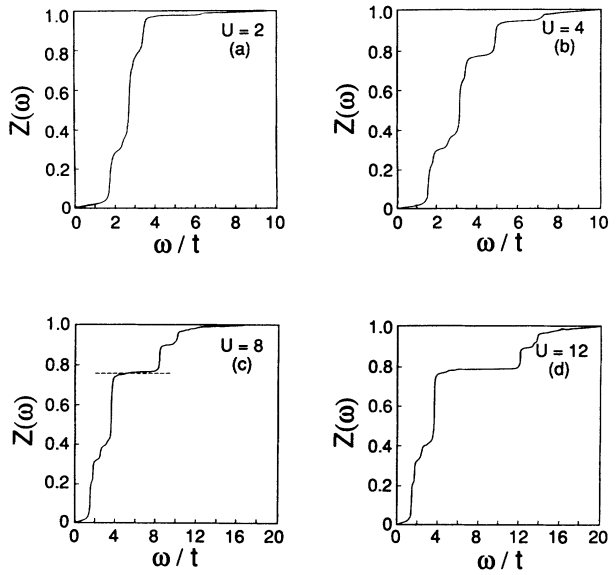

FIG. 8. Integrated absorption $Z(\omega)$ [Eq. (21)] as a function of frequency for two holes in the half-filled band for (a) $U=2$; (b) $U=4$; (c) $U=8$; (d) $U=12$. In (c), the dashed line indicates the plateau corresponding to the Hubbard gap.

It is probably of greater significance that when U is large enough so that the Hubbard bands are clearly identified, the widths of the lower bands are very nearly equal to 6 in both cases which is the single-particle bandwidth [compare Figs. 5(d) and 7(d)]. The manifold of two-particle states is wider than this, about 10. The states in the upper portion of this manifold are not accessible optically from the ground state. The integrated absorption (Fig. 8) also differs in the two-particle case. When the manifolds separate as U increases, the integrated absorption associated with the lower manifold is roughly three times that associated with the upper. This implies, when the data of Table I are considered (and excluding the one-hole case where $U=100$ for which the ground state is the high spin state) that the integrated absorption associated with the lower band is roughly twice as large in the two-hole case than for one hole. If the absorption integrated over the lower band in the cluster is interpreted as generalizing to a quantity proportional to the number of carriers for a large system, we see that this quantity should be considered to be the number of holes rather than the number of electrons. This result is in agreement with that of Ref. 16 for the 2D Hubbard model. This, we believe, supports the view that the metal-insulator transition is characterized by $n \rightarrow 0$ rather than $m^* \rightarrow \infty$.

IV. SUMMARY

We have investigated the frequency-dependent conductivity of the one-orbital Hubbard model in three dimensions by means of exact numerical calculations on an eight-site cubic cluster. We studied a wide range of interaction strengths (U) ranging from weak coupling to strong coupling. The small size of the cluster made it necessary to consider the specific features of this system, such as the actual single-particle level spectrum, carefully in our analysis of the results.

We found that, in the half-filled band case, the optical absorption began (for $U=0$) at the energy of the lowest allowed single-particle transition, and moved to higher energies steadily as U increased. For large U, the absorption occurs near $\omega=U$, resulting from transitions in which a double occupancy occurs.

In the case in which one hole is present in a half-filled band, we see clearly the splitting of the absorption into two portions whose intensity is initially roughly equal, corresponding to transitions into the lower and upper Hubbard bands. The splitting becomes apparent around $U \sim 10$, i.e., somewhat larger than the overall width of the single-particle states. As U continues to increase, the Hubbard gap approaches U, and the absorption associated with the upper Hubbard band becomes small. However, in the specific geometry, considered here, the Nagaoka high spin state occurs for large U, and the absorption from the ground state becomes of the single-particle type.

The results for the absorption when two holes are present are qualitatively similar to those for one hole, but there are obvious quantitative differences, particularly in regard to the magnitude of the absorption. The Hubbard gap was apparent in the absorption for the two-hole case for slightly smaller U than in the one-hole case. Also, absorption due to transitions into the upper Hubbard band was weaker by roughly a factor of 2 compared to the one-hole case. For small U, the integrated absorption is a monotonically increasing function of the number of electrons in the band, so interaction effects can reasonably be described in terms of an effective mass which increases with U. However, for large U, the pattern changes, and the absorption decreases as one approaches the half-filled band. The behavior is consistent with a picture in which the effective number of carriers goes to zero linearly with "doping," i.e., with the number of holes in the half-filled band.

Although details of the calculated optical conductivity, such as the location and area under specific peaks, depend on the specifics of the small cluster considered, there is significant evidence that many general features do not. Comparison of the present results for a small 3D system with those of Ref. 16 for a 4×4 2D system show similar behavior which we believe is generic: For half filling, transitions occur only to states in the upper Hubbard band. When the system has holes, spectral weight is transferred to low energies. A Drude term appears and there is optical absorption within the lower Hubbard band, which may be related to the midinfrared feature observed in high-T_c superconductors. Perhaps most importantly, the approximate linear dependence of the effective number of carriers on hole doping from the half-filled band for sufficiently large U is also observed in the 2D case.

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