Spectral weight function in the Hubbard model for a cubic cluster

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We report the results of a calculation of the spectral weight function of a single hole (or electron) placed in an otherwise half-filled band described by the one-orbital Hubbard model. The calculation is made by exact diagonalization. An eight-site cubic cluster is considered. The density of states is studied as the interaction strength is varied between weak and strong couplings. We observe the spreading of the spectral weight associated with some single-particle eigenstates over a large range of energies, and the appearance of satellite structure at higher excitation energies. Only modest band narrowing is found.

I. INTRODUCTION

This paper reports results of our calculation of the spectral weight function of a single hole or electron placed in an otherwise half-filled band described by a one-orbital Hubbard model Hamiltonian on a cubic lattice. The calculation is made by exact diagonalization for an eight-site system. Our objective is to study the development of the spectral weight function as the electron interaction parameter U varies between weak- and strong-interaction limits.

The discovery of high-temperature superconductivity in copper oxide systems has focused attention on the propagation of holes in an antiferromagnet. La_2CuO_4 is an insulating antiferromagnet, but becomes superconducting when electrons are removed through the replacement of a small percentage of trivalent La by divalent Ba or Sr. The Hubbard Hamiltonian, either in the simplest one orbital form, or with the inclusion of additional terms which recognize the differences between copper and oxygen sites, is often employed to describe this system. Apart from superconductors there are many other transition metal antiferromagnets (NiO, CoO, MnO, etc.) for which a description in terms of some form of Hubbard model may be appropriate.

The antiferromagnetic insulators just mentioned are systems for which the results of conventional local-spin-density band theory are often incorrect. For example, La_2CuO_4 is predicted to be a paramagnetic metal.[1] It is useful to adopt a somewhat different point of view in which electronic structure is investigated with the use of a model Hamiltonian and methods which permit a more complete description of the effects of electron interactions than is provided by band theory.

The more comprehensive procedure for studying the motion of a hole or electron requires calculation of the single-particle Green's function. Since the real and imaginary parts of this function are related by a Hilbert transform, it is sufficient to work with the imaginary part, to which the spectral weight function is proportional. The real part can then be obtained by integration if desired. The spectral weight function is also of interest in itself because a density of states can be obtained from it which includes the effects of interactions.

The fundamental difficulty is that, in common with almost all interesting problems in many-body theory, exact results can be obtained only in limiting circumstances. Our procedure here will be to employ exact diagonalization, which limits us to a system with only a small number of electrons. In other respects, the results are free of approximation beyond the choice of a model Hamiltonian. One must always be concerned, however, as to how the results obtained from calculations on small clusters may be applied to the bulk systems of greater interest.

In this paper we study the one-orbital Hubbard Hamiltonian,[2]

$$H = t \sum_{i,j,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \ . \tag{1}$$

The operators $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) create (destroy) electrons of spin σ on site i; $n_{i\uparrow(\downarrow)}$ is the number operator for electrons of spin up (down) on site i, t is the transfer integral, and U is the electron interaction parameter. The summation in the first term of (1) runs over all nearest neighbors, i and j. It will be convenient in the following to specify all energy quantities as ratios with respect to t; i.e., we may set $t=1$ in (1). We note that for the cubic geometry considered here, the energy spectrum is independent of the sign of t.

The use of small clusters to study the spectral weight function goes back to the work of Harris and Lange.[3] Our calculation involves an eight-site system (a simple cube, with sites at each corner). Although there are no monatomic simple cubic crystals in nature, the simple cubic lattice is frequently studied theoretically because it is the simplest three-dimensional geometry. In the present case, it is convenient to make use of results obtained in previous exact diagonalization calculations for this system in which ground-state energies, thermodynamic properties, and spin correlation functions (but not the spectral weight function) were studied for a wide range of interaction strengths and band fillings.[4,5]

In the strong-interaction limit ($U \gg t$), the t-J model is frequently considered instead of the full Hubbard model,

$$H_{t\text{-}j} = t \sum_{i,j,\sigma} (1-n_{i-\sigma}) c_{i\sigma}^{\dagger} c_{j\sigma} (1-n_{j-\sigma}) + J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j \ . \tag{2}$$

The summations include nearest-neighbor sites. This Hamiltonian approximates a canonically transformed Hubbard Hamiltonian[6] if the exchange parameter $J=2t^2/U$ (some three-site hopping terms are neglected). The additional simplicity of the t-J model results from the exclusion of doubly occupied sites. This greatly reduces the size of the Hilbert space which has to be considered in the diagonalization, and so makes calculations possible for larger clusters than is feasible with the Hubbard model. A high price is paid for the additional simplicity. The t-J model does not connect in any simple way with the noninteracting limit of the Hubbard model: $J=0$ describes the ultra-strong-interaction limit ($U\rightarrow\infty$) of the Hubbard model, while in the large-J limit, heavy holes in a background of spins coupled by a Heisenberg interaction are described. It is, however, very informative, and a major aid in interpretation to connect the large-U results continuously to those for small U. We believe this advantage greatly outweighs the restriction to smaller systems.

Beginning with the classic work of Brinkman and Rice,[7] there have been many calculations of spectral weight functions, on the basis of the t-J model. Most have considered a square lattice. We will not attempt to cite all of these papers here (a substantial list is contained in Ref. 8). One important paper also presents results for the Hubbard model on eight- and ten-site square lattices obtained by exact diagonalization.[8] We are not aware of previous calculations for a cubic lattice by this method although results obtained by other methods have been reported.[9] There is a significant difficulty in interpreting results for an eight-site square lattice (for which we have made some preliminary calculations): the spectrum of single-particle states contains only three levels; two of which are nondegenerate and one which is sixfold degenerate. The high degeneracy is accidental: the maximum degeneracy of single-particle states resulting from the symmetry of a two-dimensional square lattice is two. This leads to an unrealistically large peak in the density of states in the interacting system near the Fermi energy. In contrast, for a cubic cluster, the maximum degeneracy of the single-particle levels (Fig. 1) is three, as is allowed by symmetry, which permits a very natural correspondence with a bulk system.

Freericks and Falicov[10] have pointed out that results obtained for an eight-site cubic cluster may be directly interpreted in terms of a cluster with periodic boundary conditions more appropriate for the discussion of bulk properties by simply multiplying the transfer parameter t by 2. Then the width of the spectrum shown (without this 2) in Fig. 1 becomes $12t$, which agrees with the width obtained from Eq. (1) for single-particle states in an infinite system. We will not insert this factor of 2 explicitly into our results: the reader may wish to remember that when we discuss results obtained for $U=16$, say, that the corresponding value for an infinite system, expressed in units of the appropriate t for the large system, is 32.

Our consideration of cubic rather than square geometry means that we will not try to draw conclusions directly pertaining to high-T_c superconductivity. There

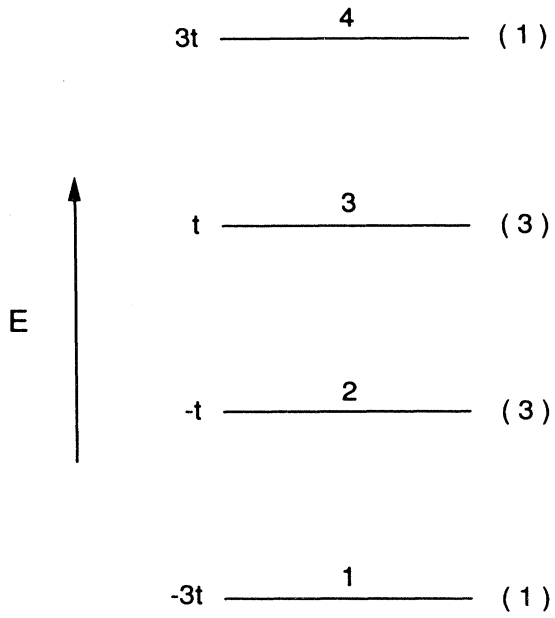

FIG. 1. Illustration of the single-particle levels in the cube. The energies are indicated on the left and the spatial degeneracies in parentheses on the right. Levels are numbered in order of increasing energy.

are, however, generic physical questions which we would like to address. These concern the utility of single-particle eigenstates for the description of the propagation of electrons or holes as the strength of short-range interactions increases. This problem is just as significant in regard to the cubic transition-metal oxides as it is to high temperature superconductivity. Our conclusions, for which evidence is presented below, is that essential aspects of the band structure are surprisingly robust. The opening of a Hubbard gap probably occurs without major disruption of single-particle states away from the Fermi energy. In addition, we find rather modest band narrowing, even for unphysically large U. The two essential changes produced by interactions are the spreading of some single-particle eigenstates over a large region of energies (broadening, in bulk terminology), and the formation of a satellite band at higher excitation energies which includes eigenstates in which propagation is not possible in the noninteracting limit. We remain somewhat uncertain concerning: the utility of a quasiparticle description in the ultra-strong-interaction limit. We find that two of the eigenstates considered give rise to a single strong quasiparticle peak when U is large, while others are spread over a wide range of energies. We are not sure if there is a generalization of this result which applies to an infinite system.

The remainder of this paper is organized as follows. Our calculational procedures are discussed in Sec. II. The results are presented in detail in Sec. III. Our conclusions are summarized in Sec. IV, which also contains

some speculations concerning implications of this work for bulk systems.

II. METHOD

Let us suppose our system contains (exactly) n particles. We denote the eigenstates of the Hamiltonian for n particles by $|\alpha,n\rangle$, in which α implicitly specifies all indices, including conserved quantum numbers, involved in the designation of a state. We will put $\alpha=g$ to denote the ground state (for a specified n). The states are orthonormal

$$\langle \alpha,n|\beta,n\rangle=\delta_{\alpha\beta} . \tag{3}$$

We consider the retarded single-particle Green's function.[11] Let $c_\gamma^\dagger(c_\gamma)$ be the creation (annihilation) operators referring to the single-particle eigenstates $|\gamma,1\rangle$. It is assumed that $|\gamma,1\rangle$ is an eigenstate of a suitable one-particle Hamiltonian. In the present case of the Hubbard model, these states result from a diagonalization of the Hamiltonian in the absence of interactions ($U=0$). We use the notation γ, rather than the more conventional **k** because, for a finite cluster, it is convenient and natural to use real eigenvectors for the single-particle states (and other states as well). The correspondence between γ and **k** in the present case is described below at the beginning of Sec. III. The function describing the propagation of a particle or hole in state γ is

$$G_\gamma^{(\mathrm{ret})}(t-t')=-i\Theta(t-t')\langle [c_\gamma(t)c_\gamma^\dagger(t') + c_\gamma^\dagger(t')c_\gamma(t)]\rangle , \tag{4}$$

in which Θ is a unit step function and $\langle \cdots \rangle$ indicates a ground-state average at zero temperature or an average over a thermal ensemble at finite temperature. The spectral weight function $A_\gamma(\omega)$ is defined in terms of the imaginary part of the Fourier transform of (4):

$$A_\gamma(\omega)=-2\,\mathrm{Im}G_\gamma(\omega) , \tag{5a}$$

where

$$G_\gamma(\omega)=\int_{-\infty}^{\infty} e^{i\omega(t-t')}G_\gamma^{(\mathrm{ret})}(t-t')d(t-t') . \tag{5b}$$

A straightforward calculation leads to

$$G_\gamma(\omega)=\frac{1}{Z}\sum_a e^{-\beta E_a}\left[\sum_b \frac{|\langle a,n|c_\gamma|b,n+1\rangle|^2}{\omega+E_a-E_b+\mu+i\eta} - \sum_d \frac{|\langle a,n|c_\gamma^\dagger|d,n-1\rangle|^2}{\omega-E_a+E_d+\mu-i\eta}\right] . \tag{6}$$

This expression gives the Green's function at finite temperatures in the canonical ensemble; i.e., with the restriction that the states involved have fixed numbers of particles. The quantities involved in Eq. (6) are defined as follows.

The states of the n-particle system are denoted by an index a, those of $n-1$ particles are denoted by d, and those of $n+1$ are denoted by b. The quantity μ is the chemical potential, which in a general case has to be determined separately as a function of temperature. (However, for the situations considered in detail in this paper, μ is independent of temperature and can be determined in advance.) In addition $\beta=(k_BT)^{-1}$, and Z is the partition function

$$Z=\sum_a e^{-\beta E_a} . \tag{7}$$

Finally, η is a small positive quantity. For a bulk system, one would pass to the limit in which η vanishes. The spectral weight is then a sum of δ functions, but one obtains a finite result by summing over a continuous distribution of states of the $(n\pm1)$-particle systems. For a finite system, it is convenient to keep η finite but reasonably small in order to show structure clearly. Alternately η could be made comparable to the spacing between single-particle levels, in order to simulate (roughly) what is to be expected in bulk systems.

In a bulk system, there is no essential difference between the states of the $(n-1)$-, n-, and $(n+1)$-particle systems and n may be dropped as a label. One obtains, after a relabeling of indices,

$$A_\gamma(\omega)=\frac{2\pi}{Z}\sum_{a,b}|\langle a|c_\gamma|b\rangle|^2(e^{-\beta E_a}+e^{-\beta E_b}) \times\delta(\omega+E_a-E_b+\mu) . \tag{8}$$

This is a standard result. However the argument leading from (6) to (8) is not applicable to a finite system in that the states of the n- and $(n\pm1)$-particle systems have different quantum numbers, and moreover, these systems have different numbers of states. Hence we use Eq. (6).

Further, we have the "sum rule," valid at all temperatures:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} A_\gamma(\omega)d\omega=1 . \tag{9a}$$

Equation (9a) is a useful check on numerical computations, however we note that its applicability requires inclusion of contributions from both $(n+1)$- and $(n-1)$-particle systems. In the present problem it is often convenient to consider only the $(n-1)$- [or $(n+1)$]-particle system by themselves. In the case of a single, half-filled band in which the number of single-particle eigenstates equals the number of sites N (times a factor of 2 for spin), we integrate over only one of the terms in (4), and then sum over states of a single spin only to obtain

$$\frac{1}{2\pi}\sum_\gamma\int A_\gamma^{(h)}(\omega)d\omega=\frac{1}{4}N . \tag{9b}$$

The superscript h (holes) implies that only the second term of Eq. (6) has been considered. For use in the remainder of this paper we will refer to the quantity

$$n(\omega)=\frac{1}{2\pi}\sum_\gamma A_\gamma(\omega) , \tag{10}$$

as the density of states.

Equation (6) simplifies substantially if $T=0$. We sup-

pose that the ground state of the n-particle system, now denoted $|g,n\rangle$, is not degenerate. Then we have

$$G_\gamma(\omega)=\sum_b \frac{|\langle g,n|c_\gamma|b,n+1\rangle|^2}{\omega+E_g-E_b+\mu+i\eta} - \sum_d \frac{|\langle g,n|c_\gamma^\dagger|d,n-1\rangle|^2}{\omega-E_g+E_d+\mu-i\eta} . \quad (11)$$

Our calculations are based on Eq. (11), and refer to an eight-particle system on a simple cube. The Hubbard Hamiltonian on a cube possesses particle-hole symmetry, so that it is necessary to compute only one of the terms in eq. (11); the other may be determined immediately from it. The chemical potential, μ, is well known to have the value $U/2$. The system of levels for eight electrons contains 1 state with $S=4$, 63 with $S=3$, 720 with $S=2$, 2352 of $S=1$, and 1764 of $S=0$ (singlets). The ground state is a singlet for all U. In the case there are seven or nine electrons, there are 8 states with $S=\frac{7}{2}$, 216 with $S=\frac{5}{2}$, 1334 with $S=\frac{3}{2}$, and 2352 with $S=\frac{1}{2}$. The $(2S+1)$ degeneracy is not included in these numbers. When the interaction U is large, the states are grouped in manifolds separated by (roughly) U; there are three manifolds for 7 or 9 electrons and four for 8 electrons.

Our calculations are made for positive U only. A somewhat surprising consequence of the symmetry properties of the Hubbard Hamiltonian on a bipartite structure[12] is that the spectral weight function is actually the same for positive and negative values of U.

III. RESULTS AND DISCUSSION

We will report the variation of the spectral weight function for a cube as a function of U. In order to understand its behavior, it is essential to refer to the energy levels of a single particle in a cubic cluster: the energies are -3, -1, 1, and 3 in units of t. The levels with energies of ±1 are triply degenerate, those with energies of ±3 are not degenerate (neglecting spin). These facts are illustrated in Fig. 1. We number the levels in order of increasing energy from the bottom. According to our convention in which the quantity t in the Hamiltonian is positive, in a periodic model, level (1) corresponds to the point R in the Brillouin zone, $\mathbf{k}=(\pi/a,\pi/a,\pi/a)$; (2) to the point $M,\mathbf{k}=(\pi/a,\pi/a,0)$; (3) to $X,\mathbf{k}=(\pi/a,0,0)$; and (4) to the origin, Γ. (Note that in a periodic model, the cluster "t" is to be replaced by "$2t$," as mentioned above.)

In the limit in which $U=0$, the half-filled "band" situation places two particles into level (1) and six in level (2). The spectral weight function has δ function peaks at energies of $-3t$ and $-t$ for holes, and t and $3t$ for electrons.

Figure 2 shows the density of states for $U=1$. Both holes and electrons are included. The following features should be noted.

1. The diagram is symmetric between electron and hole portions, as expected. For electrons, the energy, E, of a peak in the spectral weight function is the energy above the Fermi energy at which an extra electron can propagate. For holes, $-E$, is the energy which has to be added to remove an electron or propagate a hole. We will refer to $|E|$ as the excitation energy.

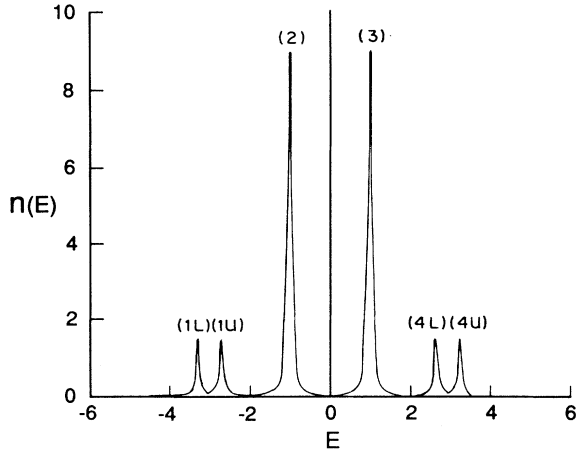

FIG. 2. Density of states for $U=1$. Both holes and electron contributions are shown. The numbers in parentheses indicates the single-particle level associated with the peak. The curves are computed using a width parameter $\eta=0.05$. All energies are ratios with respect to t.

2. The large peaks associated with the triply degenerate states are located almost exactly at the energies where they would be found in a noninteracting system. In particular, the separation between the peaks on the electron and hole sides have not increased, so there is no indication at this point of the formation of a Hubbard gap.

3. The peaks associated with the upper and lower single-particle states have split, but the center of gravity of each split pair is located at the position of the relevant state in the noninteracting system.

4. The area under the peaks shown, satisfies the sum rule, Eq. (9a). Thus, apart from the splitting mentioned above, many-body effects are not significant. The changes produced in the system by the addition or removal of a single particle are well described in terms of occupation of single-particle states. Apart from the splitting, Fig. 2 reproduces Fig. 1.

5. The splitting is a many-body effect, which arises as follows. If one attempts to describe states of the many-body system in terms of occupation of single-particle states; a state in which one hole is present in level (1) is degenerate, in the limit $U=0$, with one in which two holes are present in state (2) and there is an excited electron in state (3). The deep hole can deexcite, creating an electron hole pair. The state with an excited electron-hole pair does not contribute to the spectral weight function when $U=0$. However, for $U\neq0$, the degenerate states are mixed by the interaction. Two states which share single deep hole and shallow hole-electron hole pair characteristics result. Because a degeneracy has been split, the mixing of the states occurs with approximately equal amplitudes, and the coefficients are independent of U for small U, while the amount of the splitting is proportional to U.

It is easy to see that the positions of the quasiparticle peaks are independent of U for small U. More precisely put, if the energy of a quasiparticle peak is expanded in powers of U, the term of first order in U vanishes. To verify this, note that in a system in which all sites are equivalent, we may suppose that in the limit of very small U, and there is one electron per site, all sites are occupied with equal probability, irrespective of spin except for the restrictions imposed by the Pauli principle. Hence the average value of $\langle n_{i\uparrow}n_{i\downarrow}\rangle$ is $\frac{1}{4}$. When one electron is added or removed, the average is $\frac{1}{2}$ ($\frac{1}{2}\pm 1/N$). Hence the energies of the ground states are, for the N-particle system

$$E_g(N)=E_0(N)+NU/4 , \tag{12a}$$

and for the $(N\pm 1)$-particle systems

$$E_g(N\pm 1)=E_0(N\pm 1)+\left[\frac{N}{4}\pm\frac{1}{2}\right]U , \tag{12b}$$

plus corrections of order U^2 and higher. Here, E_0 is the energy of the completely noninteracting system. From Eq. (11) we see that peaks on the hole side occur when

$$E=E_g(N)-E_d(N-1)-\mu , \tag{13}$$

where d is some eigenstate of the $(N-1)$-particle system. Since the chemical potential, $\mu=U/2$ for a half-filled system with electron-hole symmetry, we see that

$$E=E_0(N)-E_d^{(0)}(N-1)+0(U^2) , \tag{14}$$

where $E_d^{(0)}$ is the energy of the noninteracting particle state d with $N-1$ electrons. The energy of $E_d^{(0)}$ is just the sum of the energies of the occupied single-particle states. The desired result follows, and a similar formula applies on the electron side. This argument can break down if the ground state of either the N or $N\pm 1$ particle system is degenerate at $U=0$ but not degenerate for $U\neq 0$. Then, the degeneracy can be split in first order in U, and there can be terms in the ground-state energy of first order in U beyond those given in Eq. (12).

Figure 3 shows the density of states for $U=4$. Comparison of Figs. 2 and 3 shows that while the major peaks remain, the magnitude of the peaks (2) and (3) referring to the highest hole and lowest electron level have been reduced, as also is the case for $(1U)$ and $(4L)$. In contrast, the amplitudes of $(1L)$ and $(4U)$ have increased. Additional structures appear: the most prominent features are associated with configurations forbidden in the noninteracting system (holes in level 3 or electrons propagating in level 2). The separation between the peaks labeled (2) and (3) has increased from $2t$ to $2.5t$. This suggests the beginnings of the formation of a gap associated with antiferromagnetism (as in the work of Kampf and Schieffer[13]). Because the single-particle levels in this small system are separated by a rather large amount $(2t)$, we need a substantial broadening if we are to obtain a density of states which resembles more closely what is obtained in a bulk system. Figure 4 shows the density of states for $U=4$ computed with a width parameter $\eta=0.5$ which resembles qualitatively those obtained in Ref. 13, illustrating the formation of a pseudogap in a SDW system.

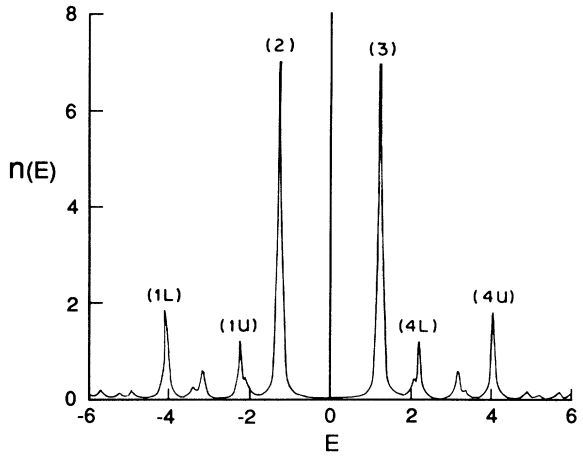

FIG. 3. Density of states for $U=4$, computed with a width parameter $\eta=0.05$.

When the interaction strength is increased, electron-correlation effects become more obvious and lead to new phenomena. Figure 5 shows the density of states for $U=8$. The electron and hole portions (upper and lower Hubbard bands) are clearly separate, with the separation between the peaks labeled (2) and (3) at the top of the lower band and the bottom of the top band having increased to $5.1t$. At this point we have a distinct Hubbard gap. We also see in Fig. 5 the emergence of additional structure. The lower and upper Hubbard bands are broadening, each developing structure at higher excitation energies. This structure is induced by interactions. For example, in the hole band, we see the emergence of peaks associated with single-particle levels 3 and 4 which are not occupied in the noninteracting limit. Correspondingly, there are high energy peaks on the electron side associated with levels 1 and 2 which are fully occupied in the noninteracting limit.

This structure can arise in the following way. We will consider the extra peaks on the hole side. Electron in-

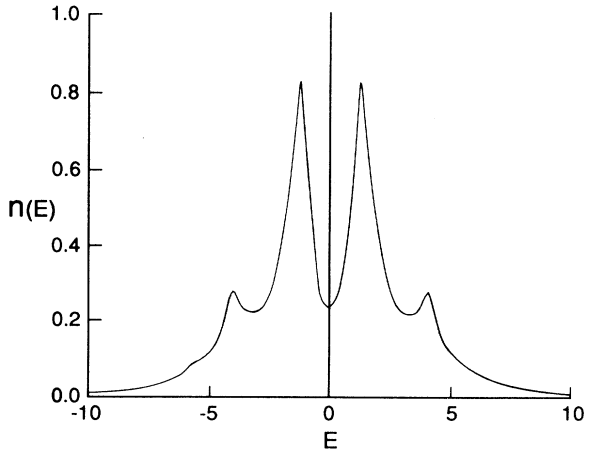

FIG. 4. Density of states for $U=4$, computed with a width parameter $\eta=0.05$.

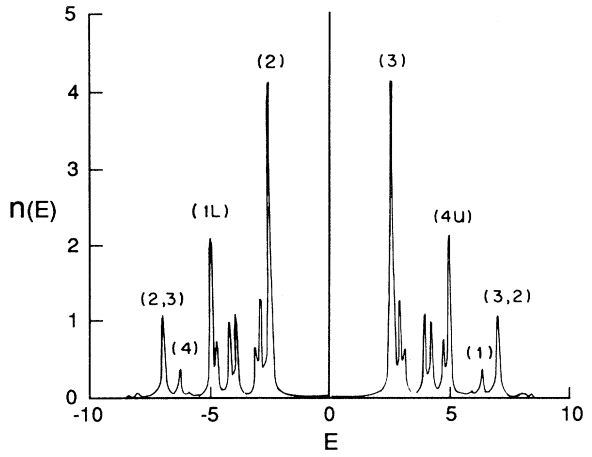

FIG. 5. Density of states for $U=8$, computed with $\eta=0.05$.

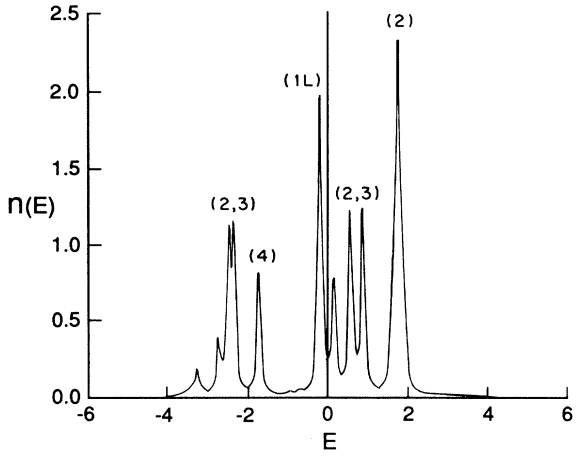

FIG. 6. Density of states for $U=16$, computed with $\eta=0.05$. Only the energy region corresponding to hole states is shown, and the chemical potential has been set to zero.

teractions induce components in the ground-state wave function of the N-electron system in which two (or more) electrons are excited into unoccupied states. The c_γ operator for one of the excited states destroys one of the excited particle states, producing a state of the $(N-1)$-particle system which contains a hole plus an electron hole pair. The peak in the spectral weight function will occur at excitation energies which are larger by the amount required to create the electron-hole pair.

The integrated density of state associated with these eigenstates is, for this U, only about $\frac{1}{3}$ of that associated with the states 1 and 2 for holes and 3 and 4 for electrons. However as U continues to increase, the integrated density of states associated with these forbidden or satellite levels (forbidden in the sense that propagation in them is not possible at $U=0$) increases to become equal to that associated with the allowed levels in the large-U limit.

As the interaction strength is increased still further, the size of the Hubbard gap increases, and we show only the hole portion of the density of states. The electron portion remains identical in appearance. In addition, we drop the chemical potential [put $\mu=0$ in Eq. (10)], so that poles in the denominator occur exactly at the energy difference between the ground state of the N-electron system and the various states of the $(N-1)$-electron system. Figure 6 shows the hole density of states for $U=16$, on this modified excitation energy scale. The peaks at positive energies on this scale result from levels near the bottom of the lowest manifold of states of the $(N-1)$-particle system. When the interaction parameter U is sufficiently large, all the states of the N-particle system are higher in energy than some of the states of the $(N-1)$-particle system (the N-particle system could lower its energy by emission of an electron). The density of states now shows two distinct regions. The upper portion ($E>-0.5$) has large peaks associated with levels 1 and 2. The upper peak, associated with the highest normally occupied level (2) is still quite strong, although the area under this peak is only about $\frac{1}{4}$ as large as in the case of $U=1$. In addition, there is a well-defined peak associated with level (1). The spectral weight functions for these levels are shown separately in Figs. 7 and 8, respectively. It will be observed that there are additional peaks associated with level (2). Although the original quasiparticle peak still persists, much weight has been taken out of it and distributed over additional peaks which occur for a wide range of energies. This would correspond to substantial broadening in the case of a bulk system. In contrast there is a strong peak associated with level 1: the side peaks are much weaker. This is a very well-defined quasiparticle peak with about three times the

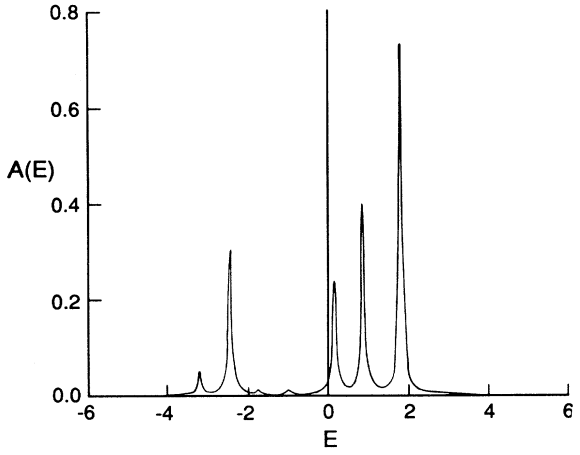

FIG. 7. Spectral weight function for level 2 at $U=16$, computed with $\eta=0.05$. Since this level is threefold degenerate, the vertical scale must be multiplied by 3 to obtain the contribution to the density of states. The factor of $(2\pi)^{-1}$ in Eq. (9a) has been absorbed into A.

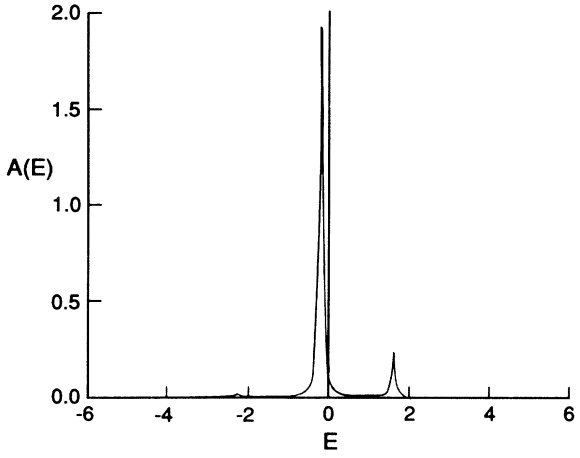

FIG. 8. Spectral weight function for level 1 at $U=16$, computed with $\eta=0.05$.

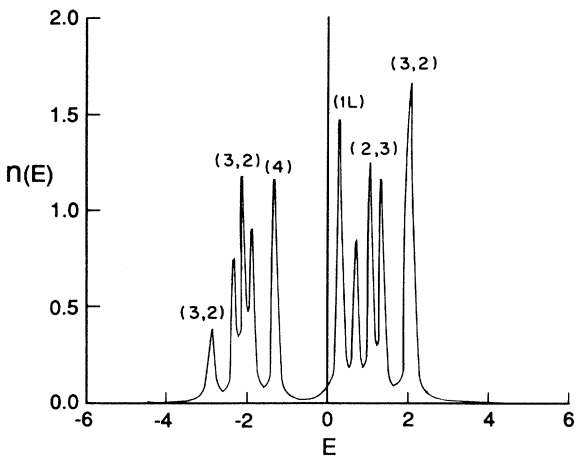

FIG. 9. Density of states for $U=32$, computed with $\eta=0.05$. Hole portion only.

weight of that associated with a single one of the degenerate members of level 2.

There is a significant portion of the hole density of states in Fig. 6 at negative energies (higher and positive excitation energies, however) in which there are large contributions from the "forbidden" levels 3 and 4. (However, peaks associated with levels 2 and 3 appear in both upper and lower energy regions.) A gap has developed between upper and lower (satellite) regions. We will see that as U continues to increase the upper and satellite portions of the density of states become symmetric, and are symmetrically placed above and below $E=0$.

We believe that many physical transition metal antiferromagnets, probably including those such as (pure) La_2CuO_4 which are closely related to high temperature superconductors, are likely to have properties similar to those shown in our Hubbard model calculations in the intermediate range of U/t values. We have sampled this range for $U/t=8$ and $U/t=16$. In this range, essential features of the level structure calculated for small U persist, but there will be significant broadening. The density of states is actually broader than found for small U, in that satellite contributions from forbidden levels appear at higher excitation energies.

Next, we consider the strong-interaction limit. Figures 9, 10, and 11 show the hole portion of the density of states for $U/t=32$, 100, and 1000, respectively. As U continues to increase, the satellite region strengthens and the band shifts slightly higher in energy, so that it is very nearly symmetric, as mentioned above, at $U=1000$. The energy scale is nearly rigid in this range of U. The ground-state energy of the N-electron system differs from 0 by an amount proportional to $(-)t^2/U$, and hence approaches zero slowly as U increases, while the ground manifold of the $(N-1)$-electron system stretches from (roughly) $-3t$ to $3t$.

The two symmetric portions of the density of states are separated by a gap around zero excitation energy. This is apparently a pseudogap. There are a few small peaks, not discernible on the graphs, present for levels 2 and 3—so that it is a region of much reduced density of states, rather than being actually zero. Examination of the energy spectrum shows that there are some states of the seven-electron systems with energies appropriate to produce a peak in the gap: evidently, the matrix element connecting these states to the ground state of the eight-electron system is small.

There is an additional complication: the ground state of the $N-1$ manifold is fully spin aligned for $U>39.5$ (in accord with Nagaoka's theorem[14]). At $U=1000$ in the specific case of the cube with 7 electrons, not only is the ground state "ferromagnetic," but the lowest 13 eigenvalues belong to states which have $S>\frac{1}{2}$, so that the first

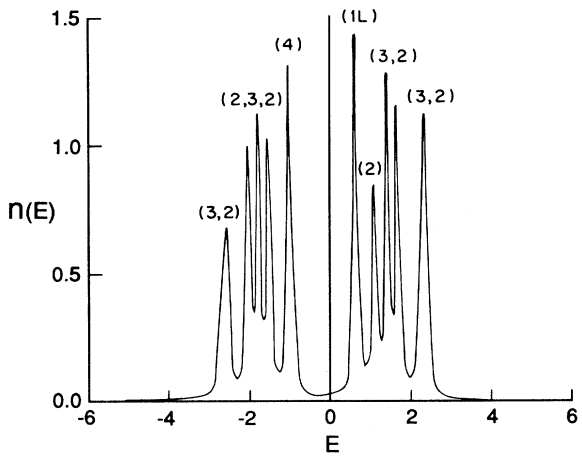

FIG. 10. Density of states for $U=100$, computed with $\eta=0.05$. Hole portion only.

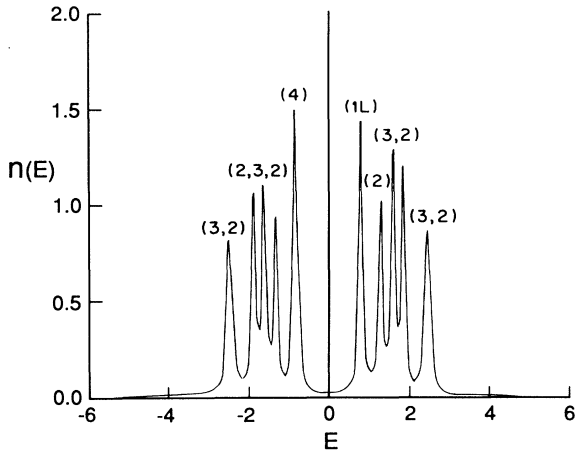

FIG. 11. Density of states for $U=1000$, computed with $\eta=0.05$. Hole portion only.

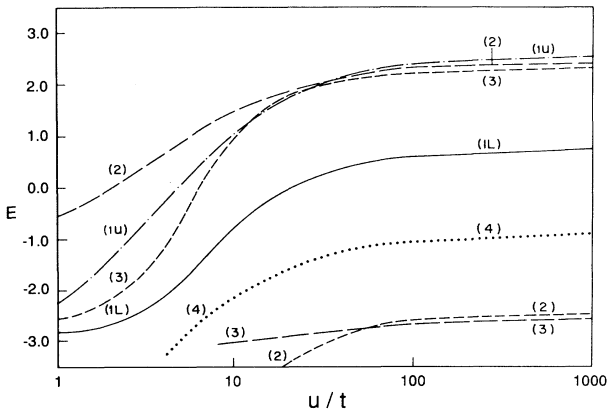

FIG. 12. Energies of principal peaks in the hole density of states as functions of U.

state of $S=\frac{1}{2}$ is above the ground state by $0.36t$, and the highest state of $S=\frac{1}{2}$ is below the top of the lowest manifold by $0.39t$. The energy range covered by states which can be reached from the ground state of the eight-electron system by deleting a single electron is therefore $5.25t$, smaller than the total width of the lowest manifold ($6t$) by 12.5%.

Thus, there is a modest amount of "band narrowing" in this case, which is the result of the presence of states which are not accessible from the singlet ground state of the eight-particle system by removal of a single electron at the top and bottom of the lowest manifold of the seven-electron system. The total width of this lowest manifold remains exactly the width of the single-particle band in the noninteracting system.

The preceding paragraphs should not be interpreted as implying that there is no band narrowing until U increases to the value at which the ground state of the seven-electron system is ferromagnetic. In the case $U=32$, the ground state of the seven-electron system has antiferromagnetic correlations, and both the seven-and eight-electron systems have nearly the maximum average local moments. The total band width here, measured from the lowest energy to the highest energy peak in the density of states is $5.4t$, a reduction of 10% compared to the noninteracting system. For this U, the peak at the top of the hole distribution is still associated with the single-particle level 2; and is at exactly the energy difference between the ground states of the seven-and eight-electron systems. The area under this peak is $\frac{1}{6}$ of the value in the noninteracting system. This is a significant remnant of the quasiparticle picture of the noninteracting system but now the subsidiary peaks in the hole region have almost three times the integrated area. We interpret this, in the context of a bulk system, as indicating large broadening. The area under this peak continues to decrease as U increases.

Essential features of the preceding discussion are summarized in Figs. 12 and 13. Figure 12 shows the position of the principal peaks in the hole portion of the density of states on energy scale used above for large U (i.e., with $\mu=0$). The peaks which occur in the small-U limit are plotted for all values of U; positions of some others which are not readily apparent in our data for small U are plotted only for larger values. First one notices that the energies increase monotonically with U as expected. There are some changes in the order. For example the topmost peak in the noninteracting system is associated with level 2, while for $U=1000$ the upper peak is the remnant of that labeled $1U$ in Fig. 2. This could be interpreted as a reordering of hole levels (change in shape of the hole band), but the small amplitude of these peaks for large U makes us question the utility of this description.

Figure 12 may also be interpreted as indicating that in the large-U limit, there is a small region at the top of the hole portion of the spectrum (actually, the bottom of the hole "band") where the density of states is high. This narrow region, corresponding to the upper peak in Fig.

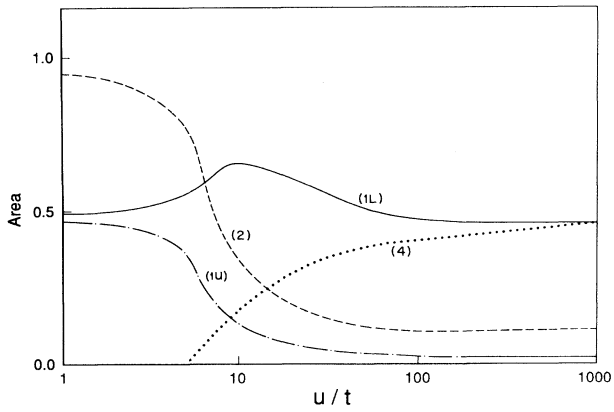

FIG. 13. Areas (dimensionless) under some of the principal peaks in the hole portion of the band (integrated density of states) as functions of U.

11, and whose width in the case $U/t=1000$ is about 10% of the occupied noninteracting band, contains the remnants of the low-excitation-energy peaks from small U. Possibly, discussions of effective mass enhancements pertain to this region.

Figure 12 should be considered in conjunction with Fig. 13, in which the areas under some of the major peaks relating to hole levels are shown. These areas have been normalized in accord with Eq. (9a) so that in the noninteracting system, the integrated density of states for that level is 1. (Each level contains one electron of each spin. The spatial degeneracy of 3 associated with level 2 is not included.) In the small-U limit we have contributions only from levels 2 and 1, the latter being split as described earlier. At large U one might expect in the case of a well-defined quasiparticle that the integrated density would be about $\frac{1}{2}$. (Roughly, all noninteracting levels could be occupied with equal probability, $\frac{1}{2}$ electron or hole of a given spin in each level.) This is the case for two of the levels associated with the top and bottom levels in Fig. 1, but for the other peaks, including all those not plotted in Fig. 13, the integrated area under these peaks is much smaller. It will be observed from Fig. 12 that these well-defined peaks are not related to states at the bottom of the seven-electron manifold. We have a surprisingly complex situation in which, although some rather sharply defined quasiparticles continue to exist at large U, others are distributed over a wide range of energies. The well-defined levels are those nearest to zero excitation energy, rather than being at the bottom or the top of the available range. However, the interpretation which seems most plausible to us is that the persistance of a single peak containing essentially all of the area for two of the single-particle states is a result of the small size and high symmetry of the system for which our calculations have been performed. If this view is correct, one should expect that quasiparticle structure would disappear in the large-U limit for a bulk system.

Finally, we should like to compare our results with those of Dagotto *et al.*,[8] who studied the Hubbard model on 8- and 10-site clusters with periodic boundary conditions representing a square lattice. They considered values of the interaction strength up to $U=40$. The differences in the geometry of the systems under consideration implies that the energies and degeneracies of the simple particle states are different as mentioned previously. However the same general picture of the development of the density of states as U varies emerges from their work as from ours. For small U the peaks are sharp, and are located close to the energies of the single-particle eigenstates. As U increases, a gap forms; the spectral weight for at least some of the eigenstates develops additional peaks, indicating broadening in the bulk limit, and a satellite "band" appears for larger excitation energies. There is also some indication in their work of a gap between the main and the satellite portions of the density of states. We believe the features of the results on which our calculations agree are characteristic of the Hubbard model in general, independent of the specific geometry (except for the consequences of hole-electron symmetry, which is found only in bipartite structures).

IV. CONCLUSIONS

We have calculated the spectral weight functions and the density of states for the one-orbital Hubbard Hamiltonian defined on a simple cube. Values of the interaction parameter ranging from $U/t=1$ to $U/t=1000$ were considered. The results present a picture of the spectral weight function going from weak-interaction limit to ultrastrong interactions.

This is the picture. When the interaction is weak, the peaks in the spectral weight function remain close to the energies of the eigenstates of the noninteracting system. Quasiparticles associated with states close to the Fermi energy are sharp, but if the excitation energy is large enough so that an excited electron or hole is in a state whose energy is enough to permit a hole-electron pair to be created, a splitting of the quasiparticle peak occurs, which, in an infinite system, would correspond to spreading the quasiparticle peak over a range of energies.

As the interaction becomes stronger, additional peaks develop in the spectral weight for states near the Fermi energy (in the noninteracting system). The "original" peak can be identified for all U, but other peaks become of equal or greater importance. The spectral weight associated with eigenstates at the top of the band (in the case of an extra electron) or at the bottom of the band (for a hole) remain concentrated in a small energy range. Satellite peaks emerge at higher excitation energies. These are associated in part, but not exclusively, with propagation in levels not accessible in the noninteracting system; for example, holes in the highest level of the system, which is not occupied when $U=0$. There is an excitation-energy pseudogap between main and satellite regions.

As U continues to increase into the strong-interaction limit, the intensity of the satellite peaks grows, ultimately to become equal to that associated with the main band. In this limit, the hole and electron bands are (separately) symmetric, each consisting of two parts separated by a pseudogap region of low density of states.

Overall, there is some band narrowing in going from weak to strong interactions, but this is not large, amounting to a reduction of the overall width by only a factor of $\frac{1}{8}$. (The band at $U=1000$ has $\frac{7}{8}$ of the width of the free electron manifold.) For extremely large U, the band narrowing can be attributed to the operation of Nagaoka's theorem: the low-lying states of the seven-electron system have $S>\frac{1}{2}$. However, band narrowing becomes evident for U's too small for Nagaoka's theorem to apply.

The results suggest to us that in physical, as opposed to model, systems, for realistic values of the strengths of electron interactions in transition-metal oxides and high-temperature superconductors, the basic picture derived from band-structure calculations is robust and will be qualitatively satisfactory and useful for the interpretation of many experiments, such as those involving photoemission. The most important exception is that there will be a Hubbard gap if the interaction is strong enough (we cannot estimate this from a small cluster calculation) but the band structure will not be greatly disrupted except near the Fermi energy. We think this is consistent with

experiments on transition-metal oxides.[15] Second, satellite structure in the density of states should be found at higher excitation energy if the interactions are strong enough, even in those cases where a one-orbital model may be adequate.

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