Hubbard model for a cubic cluster

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The ground-state and thermodynamic properties of a simple Hubbard Hamiltonian are studied for an eight-site cubic cluster as functions of the number of electrons and the strength of the electron interaction. The ground-state energy and spin are determined, and the excitation spectrum is computed. Thermodynamic properties including the specific heat, the magnetic susceptibility, and spin correlation functions are calculated. Computations are performed both by explicit diagonalization of the Hamiltonian and by Monte Carlo simulation.

I. INTRODUCTION

This paper reports calculations of the ground-state and thermodynamic properties of the Hubbard model defined on a simple cubic cluster. The Hamiltonian contains only hopping between nearest-neighbor sites on which a single orbital is defined and an interaction U between two electrons on the same site.

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

Here, t is the transfer integral, σ denotes spin, i and j are nearest neighbors, and U is the repulsion parameter (only the case of a repulsive interaction, $U > 0$ is considered here). Our calculations determine the ground state and several thermodynamic functions: the spin susceptibility, the specific heat, and spin-correlation functions; as functions of the parameters of the Hamiltonian, the number of electrons, n, in the system, and temperature.

Even though the model has been the subject of intense study for more than 20 years, there are few exact results for three-dimensional systems. A question which has been quite controversial is whether the system can have a ferromagnetic ground state under any circumstances.[1]

Our point of view is that in view of the difficulty of obtaining definitive results for infinite systems, it is useful and informative to study the Hubbard Hamiltonian on a finite cluster. Then, exact diagonalization is possible and thermodynamic functions can also be computed exactly. In previous work, we have reported results for clusters of four, five, and six sites with various geometries.[2,3] Reference 3 also contains discussion of previous calculations of this type. In the present work, the system under consideration is a cube (eight sites). The importance of this geometry in solid-state physics need no explanation.

A major difficulty in cluster calculations with this Hamiltonian is that the size of the matrices to be diagonalized increases very rapidly with the size of the cluster and the number of particles in the system. We think that this is the reason why there is only one calculation in the literature (of which we are aware) for a cube. Kawabata determined the ground state for a cube containing from two through eight electrons.[4] He found that in certain cases ($n = 4$ and $n = 7$), the ground state has the maximum possible spin for sufficiently large U; while for $n = 5$, the intermediate spin state ("unsaturated ferromagnetism") is the lowest for all $U > 0$. For other occupancies ($n = 2,3,6$), the ground state is either a singlet (even n) or a doublet (odd n).

Another approach to the problem of studying the properties of the Hubbard Hamiltonian has attracted much attention recently. This is the Monte Carlo simulation approach.[5,6] It is based on a discrete formulation of the functional integral approach, and involves a summation over Ising-like random spin variables. We have found it interesting to compare the results of calculations involving explicit diagonalization with those employing Monte Carlo simulation.

In some respects the methods are complementary. The explicit diagonalization approach is restricted to fairly small systems because the size of the Hamiltonian increases extremely rapidly as the number of particles and sites increases. The procedure of Refs. 5 and 6 can be applied to larger systems, but becomes difficult for low temperatures or for large values of U. For systems of the same size, one expects agreement between the diagonalization and Monte Carlo methods. However, in the present work thermodynamic functions are computed, in the diagonalization approach, using a canonical ensemble while the Monte Carlo simulation employs a grand-canonical ensemble. Some differences may arise from this, for the canonical ensembles requires a fixed number of particles in the cluster, while in the grand canonical ensemble, only the average number is fixed, and fluctuations in the number occur. Comparison of the results of the two methods indicates the effect of charge fluctuations.

In the next section, our calculational procedures are outlined. The results are described in Sec. III. A brief summary (Sec. IV) concludes the paper.

II. METHOD

The Hamiltonian (1) is studied on a basis of states $|\hat{n}_{i\sigma}\rangle$ which are diagonal in all the occupation numbers. On this basis, the interaction U occurs only on the diagonal and t on the off-diagonal terms. Then the energy of any state may be expressed alternatively as

$$E = U\varepsilon(t/u) \ , \tag{2a}$$

or

$$E = t\varepsilon'(U/t) , \tag{2b}$$

where (2a) is convenient if $U > t$, and (2b) is convenient if $t > U$. In the case of a simple cube,

$$E(t) = E(-t) .$$

Let n be the number of electrons in the system, N the number of sites (eight in this case) and $n' = 2N - n$. Electron-hole symmetry yields

$$E_{n'} = E_n + (N - n)U . \tag{3}$$

Therefore it is sufficient to calculate the properties of the system for $t > 0$ and $n \leq N$. We will first discuss calculations based on explicit diagonalization of the Hamiltonian and second, the Monte Carlo calculations.

Our computer program diagonalizes the Hamiltonian within subspaces of fixed S_z (or $n_\uparrow - n_\downarrow$). For a system with eight sites, these matrices can become very large. For example, for $n = 8$ and $S_z = 0$, the dimension of the Hamiltonian is 4900×4900. Therefore, it was necessary to form symmetrized combinations of basis states which enable us to restrict the numerical diagonalization to much smaller submatrices. This factorization will be discussed in detail elsewhere.

All the eigenvalues and eigenvectors were obtained. Thermodynamic properties were then calculated in a canonical ensemble. The functions studied included the spin susceptibility,

$$\chi = \frac{2}{n}\frac{1}{ZT}\sum_j e^{-\beta E_j} m_j^2 . \tag{4a}$$

The index j denotes an eigenstate and m_j is given by

$$m_j = \tfrac{1}{2}(n_\uparrow - n_\downarrow)_j , \tag{4b}$$

so that m_j represents S_z in units of $\hbar$ for the jth eigenstate. The quantity Z is the partition function,

$$Z = \sum_j e^{-\beta E_j} , \tag{5}$$

and $\beta = 1/kT$, k being Boltzmann's constant and T, the temperature.

The specific heat is given by

$$C = \frac{1}{kT^2 Z}\left[\sum_j E_j^2 e^{-\beta E_j} - \frac{1}{Z}\left[\sum_j E_j e^{-\beta E_j}\right]^2\right] . \tag{6}$$

Spin-correlation functions are defined here as follows:

$$L_{\mu\nu}(j) = \tfrac{1}{4}\langle j \mid (n_{\mu\uparrow} - n_{\mu\downarrow})(n_{\nu\uparrow} - n_{\nu\downarrow}) \mid j\rangle , \tag{7}$$

in which μ and ν denote sites. Then we form the thermal average

$$\langle L_{\mu\nu}(T)\rangle = \frac{1}{Z}\sum_j e^{-\beta E_j} L_{\mu\nu}(j) . \tag{8}$$

In the cube, there are only four different correlation functions, depending on whether μ and ν are the same, or first, second, or third neighbors. We denote these functions as L_0, L_1, L_2, and L_3, respectively. L_0 is the "local moment."

In addition to these calculations involving explicit diagonalization of the Hamiltonian, we have performed Monte Carlo simulations using the method of Hirsch.[5] Our calculations were made for a $2 \times 2 \times 2$ system, i.e., the same cube as considered in the diagonalization method. The specific procedures are essentially the same as those of Ref. 5, and will not be described in detail here. Because the size of the system considered in the two sets of calculations is the same, substantial agreement is expected. Differences in results illustrated of the effect of fluctuations in the number of particles on the thermodynamic properties. Recently, Hirsch has reported Monte Carlo simulations for much larger systems (up to $6 \times 6 \times 6$), but only for the half-filled band case.[6]

III. RESULTS

A. Ground-state spin

Our results for the spin of the ground state are summarized in Table I. They are in agreement with those of Kawabata.[4] A magnetic state, in the sense that $S > \frac{1}{2}$, is found for occupancies $n = 4$ ("quarter-filled band") and $n = 7$ if U/t is sufficiently large, and for $n = 5$ for all positive values of U. The results for the cube are different from those for some other systems we have studied in that in the present case, the spin changes abruptly from minimum to maximum value when there is a jump, rather than passing through intermediate spin values (unsaturated ferromagnetism), as was found to be the case for the octahedron, for example. In addition, we consider the value of U/t for which the transition occurs to be quite large. The "band width," $W = 6t$, so that in the case $n = 4$, we must have $U/W > 37$ to get a magnetic state.

Many aspects of these results (but not all) can be qualitatively explained in terms of occupancy of single particle levels. The energies and degeneracies of the single particle levels for the cube are listed in Table II. First, it is interesting to compare these energies with those for an (infinite) simple cubic lattice with nearest-neighbor interactions of strength $t/2$. This gives

$$E \sim t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] . \tag{9}$$

It will be observed, first, that the energies in Table II correspond to those obtained from Eq. (9) at the symmetry points of the Brillouin zone (R, M, X, and Γ); second, that these degeneracies are the same as the number of inequivalent points; and third that the energies are also the energies at which Van Hove singularities occur in the den-

TABLE I. Ground-state spin for occupancies $2 \leq n \leq 8$ as functions of $z = t/U$.

$n = 2$	$S = 0$, all z
$n = 3$	$S = \frac{1}{2}$, all z
$n = 4$	$S = 2$, $z < 0.004\,48$
	$S = 0$, $z > 0.004\,48$
$n = 5$	$S = \frac{3}{2}$, all z
$n = 6$	$S = 0$, all z
$n = 7$	$S = \frac{7}{2}$, $z < 0.0253$
	$S = \frac{1}{2}$, $z > 0.0253$
$n = 8$	$S = 0$, all z

TABLE II. Energies of the different single-particle states (divided by t) for a cube. The number in parenthesis is the degeneracy.

$-3(1)$	$-1(3)$	$1(3)$	$3(1)$

sity of states.[7] The single particle energies in the cubic cluster can therefore be regarded as roughly representative of a simple s band in a perfect crystal.

If the system contains two electrons, it is clear that less energy is required to form a singlet state, since $2|t|$ is required to promote an electron into the second state of Table II. Hence for small values of U/t, a singlet ground state would be expected to occur. However, one might suppose that if $U \gg |t|$, it would be energetically favorable to form a triplet state, since in this simplest form of the Hubbard model, the interaction does not affect the energy of a fully spin aligned state but it may increase the energy of a singlet state. In fact in the case of $n=2$ this does not happen. A correlated singlet state is formed whose energy is independent of U in the large-U limit, implying that it is possible for the particles to avoid each other's site completely. The energy of this singlet state is $-2\sqrt{7}t$ in the large-U limit, which is always lower than that of the triplet state ($-4t$).

Similar behavior occurs for $n=3$. It is obvious from Table II that the doublet must have lower energy than the quartet for small U. Again at large U, the lowest doublet has an energy independent of U which is lower than that of the quartet. In fact for all values of $n \leq 8$, it is possible to form one or more correlated singlets (even n) or doublets (odd n) whose energy is independent of U for large U. It is not obvious, however, whether the energy of this state will be lower than that of a state of higher spin.

When there are four particles ("quarter-filled band") we do find that for very large U, the "ferromagnetic" state (maximum alignment) is lowest. Since the first excited single particle state is triply degenerate, one might expect that a particularly stable situation would arise when these states are filled. This is an example of Hund's rule applied to the cluster, treated as a single atom.[8] It is then not surprising that for $n=5$, a particularly stable situation would occur when there are two particles in the lowest single particle state, and the remaining three occupy the first excited state with parallel spin. The point which is not obvious is that this quartet state is the ground state for all $U>0$; however what happens is that the lowest doublet state of the five-particle system requires the same occupancy of single-particle states; but the lower spin configuration experiences a greater repulsive interaction even when U is small.

Increasing n to 6 produces a case in which a substantial promotion energy is required to produce a magnetic state. In this case the singlet remains the ground state for all U. At $n=7$, we again have a Hund's rule situation in which both degenerate single particle states can be full for $S=\frac{7}{2}$; this state is the ground state for large U, in spite of the substantial difference in single-particle energy required by this occupancy. The occurrence of the high spin ground state in this case is consistent with Nagaoka's result that for a simple cubic lattice (and some others) ferromagnetism is possible for a system with one particle less than that required for a half-filled band when U is sufficiently large.[9] Finally, when $n=8$, the half-filled band seems always to favor a low-spin ground state.

One feature of the $n=6$ system deserves note. There is a change in the degeneracy and therefore of the spatial symmetry of the ground state at $z=0.0162$. For smaller z (large U/t), the ground state is a singlet; for higher z, the state is a doublet. The effect of this transition on spin-correlation functions will be discussed below.

The simple-cubic lattice with nearest-neighbor interactions only is not a particularly favorable system for the occurrence of band ferromagnetism. The density of states has a high, flat portion in the middle of the band,[7] in contrast to the face-centered-cubic structure, for example, where there is a sharp spike at either the top or the bottom, depending on the sign of t. Likewise the conditions for the occurrence of a maximum spin state in the cluster are more stringent (in terms of values of U/t required) than for the tetrahedral and octahedral clusters we have studied previously.[3] The difference between the cluster types in this respect appears to be due to the different pattern of degeneracies of the single particle levels.

B. Ground-state correlation functions

Ground-state spin-correlation functions generally decrease as U/t varies between localized and itinerant limits. This unsurprising statement requires some elaboration and qualification, the most important being that in cases where there is a change in the spin of the ground state, or a change in the spatial symmetry; there is a dramatic change in these functions except that the change in the local moment is small. These remarks are illustrated in Figs. 1 and 2.

Spin-correlation functions for $n=7$ are shown in Fig. 1. For small values of z ($z<0.0253$), the system is in the

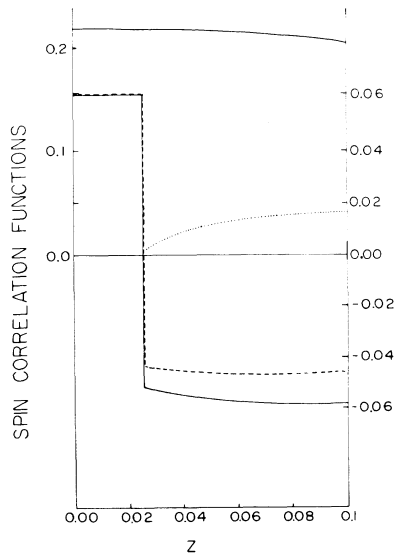

FIG. 1. Ground-state spin-correlation functions as function of $z=t/U$ for $n=7$. Local moment (L_0 solid line), left-hand scale; other functions (L_1, solid line; L_2, dots; L_3, dashes), right-hand scale.

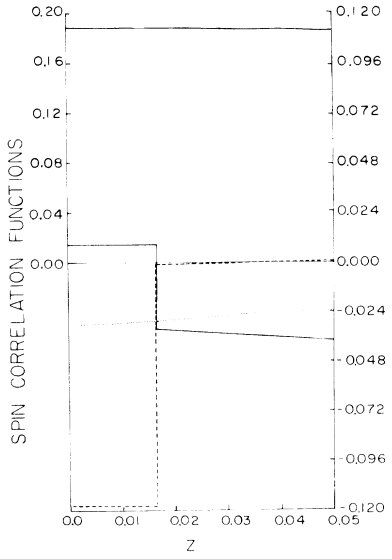

FIG. 2. Ground-state spin-correlation functions as functions of z for $n=6$. Curves are drawn as in Fig. 1.

"ferromagnetic" state. In this case, the spin correlation functions are independent of U. The local moment is $\frac{7}{32}$ (each site has a probability $\frac{7}{8}$ of being occupied). The first-, second-, and third-neighbor correlation functions are positive and equal to each other. This situation describes uniform magnetization. When z increases beyond 0.0253, the ground state has $S=\frac{1}{2}$. There is only a small change in the local moment, but a dramatic change in the other functions: L_1 and L_3 become negative, while L_2 is weakly positive. This arrangement is characteristic of antiferromagnetic order. The subsequent dependence of these functions on U is not monotonic, but for values of z beyond the limited range shown, the functions decrease to zero.

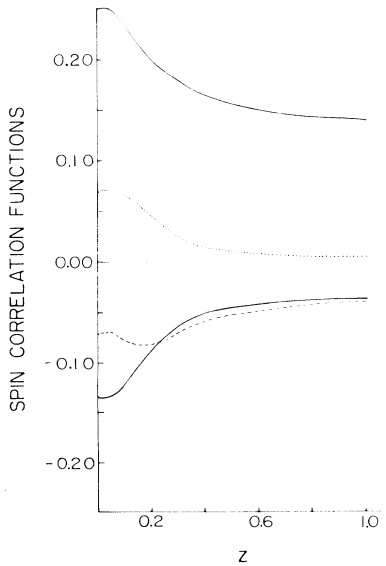

FIG. 3. Ground-state spin-correlation functions for the half-filled band as functions of z. Curves are drawn as in Fig. 1.

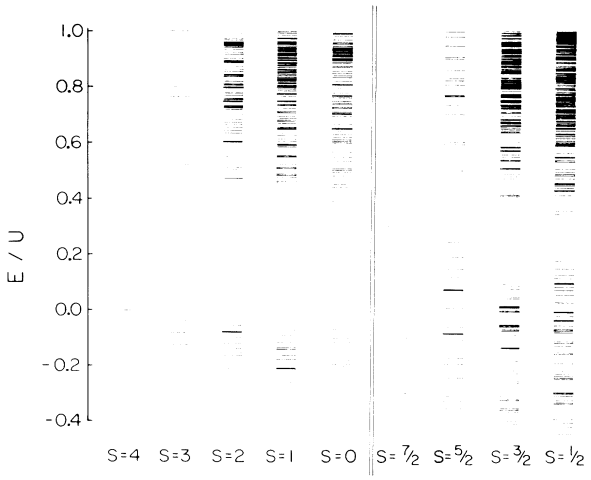

FIG. 4. Energy spectra for $z=0.1$ for $n=8$ (left) and $n=7$ (right). States are classified by spin. Spatial degeneracies are not shown.

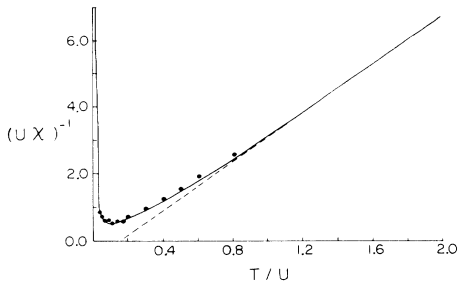

FIG. 5. Reciprocal magnetic susceptibility as a function of temperature in units of U for the half-filled band in the case $z=0.2$. Solid curve, results for explicit diagonalization; dots, results of Monte Carlo calculations.

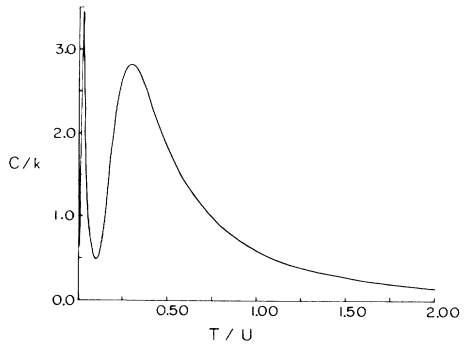

FIG. 6. Specific heat for the half-filled band case with $z=0.1$ as a function of the ratio of temperature to interaction strength.

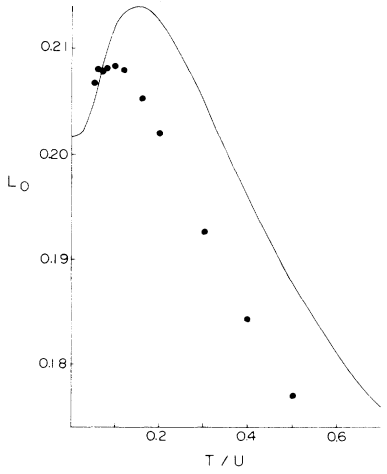

FIG. 7. Local moment L_0 as function of temperature for the half-filled band and $z=0.2$. Dots are the result of Monte Carlo calculations. The scale has been chosen to emphasize differences.

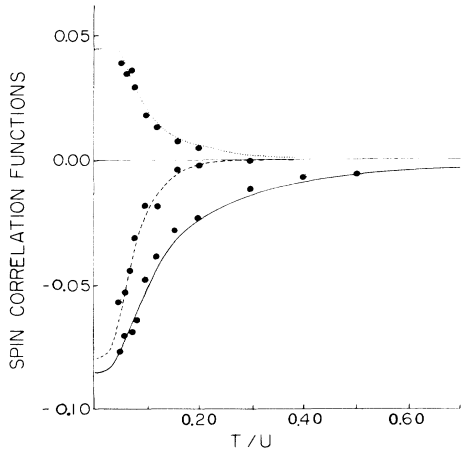

FIG. 8. First-, second-, and third-neighbor correlation functions (L_1, L_2, and L_3) as functions of temperature for the half-filled band and $z=0.2$. Dots are the result of Monte Carlo calculations.

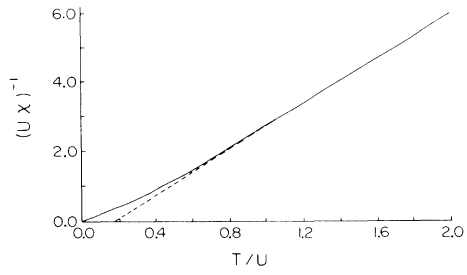

FIG. 9. Temperature dependence of the magnetic susceptibility for $n=7$ and $z=0.0222$.

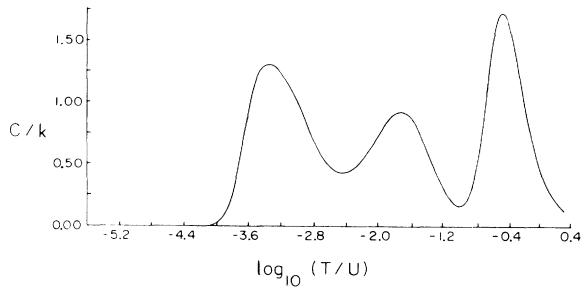

FIG. 10. Temperature dependence of the specific heat for $n=7$ and $z=0.0222$. Note the logarithmic scale of temperature.

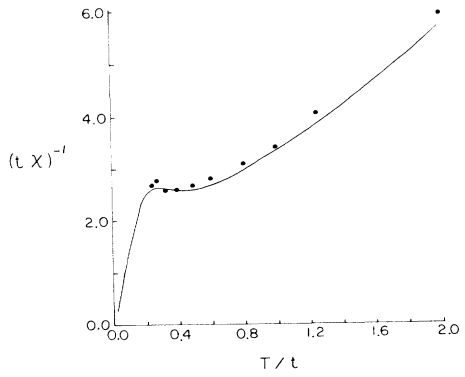

FIG. 11. Temperature dependence of the magnetic susceptibility for $n=7$ and $U/t=4$. Dots are the result of Monte Carlo calculations.

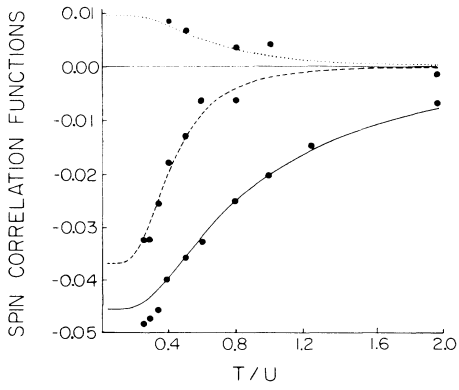

FIG. 12. First-neighbor (L_1, solid lines), second-neighbor (L_2, dotted line), and third-neighbor (L_3, dashed line) spin-correlation functions for $n=7$ and $U/t=4$. Large dots are the results of Monte Carlo calculations.

In the case $n=6$, the ground state is a singlet for all z. However there is a change from a nonspatially degenerate ground state (smaller z) to a doubly degenerate state (larger z) at $z=0.0162$. When this occurs, the pattern of spin correlation changes (Fig. 2). Again, the local moment is only weakly affected (as is L_1); but L_2 changes from positive to negative with an increase in magnitude, and L_3 increases form a larger negative value to a value close to zero, becoming positive as z increases further.

The half-filled band case ($n=8$) is less dramatic. The zero-temperature local moment and spin-correlations functions are shown in Fig. 3. It will be observed that the third-neighbor correlation function L_3 is not monotonic as a function of z, but increases in magnitude with z for small z. The sign pattern of the correlations: first and third neighbors, negative; second neighbors, positive, is consistent with antiferromagnetism. Note also that as U increases from zero, correlations remain weak until, roughly, U is in the range of $3t-5t$. The correlations are fully developed when U is about $20t$, and there is little further change for values of U greater than this.

C. Excitation spectrum

A diagram showing the energy spectrum for $E \leq U$ is shown for the cases $n=7$ and 8 for $z=0.1$ in Fig. 4. Consider the case $n=8$ first. There is a relatively sparse group of low-lying levels ($E<0$) which are separate from a much more dense group of higher levels by a gap of about $0.4U$. These low-lying levels correspond to the possible ways in which l "up" spins and $8-l$ "down" spins ($l \leq 8$) can be distributed on eight sites without having two on any site. It it within this manifold that an effective Heisenberg Hamiltonian would be valid. The higher energy group has one site doubly occupied, and is correspondingly more numerous. The separation between the groups is the Hubbard gap, which becomes equal to U only in the limit $z=0$. If the corresponding diagram is drawn for $z=0.2$, no gap is visible.

In the case $n=7$ the lower group of states is both more numerous and spread more widely in energy. This occurs because for $n=7$, there is always one vacant site (in the basis set). For a given vacancy, there exists a set of spin rearrangement states in which seven spins are assigned without any two being on the same site. However, when the Hamiltonian is diagonalized the vacancy is spread over different sites, e.g., the hole is mobile; and the energy of a state depends not only on the spin pattern, but also on the k vector of the "mobile hole." For the value of z chosen for the figure, the gap has almost disappeared, but for larger U/t; the separation of the states into those without and with a double occupancy becomes quite clear.

D. Thermodynamic properties

We consider here the temperature dependencies of the magnetic susceptibility, the spin correlation functions, and the specific heat. We shall proceed by discussing the half-filled band ($n=8$) first, and smaller values of n subsequently. The results that will be specifically discussed here are a relatively small sample of those obtained. We have chosen parameter values for the illustrations which, we believe, illustrate the most important physics.

The susceptibility is shown in Fig. 5 for $t/U=0.2$ and $n=8$. The curve resembles what would be expected for an antiferromagnet except that as $T \to 0$, χ^{-1} approaches infinity instead of going to a finite limit. This behavior is characteristic of a finite system with a singlet ground state for which the susceptibility has to vanish at $T=0$. The dots are results from the Monte Carlo calculation. The agreement is reasonably good everywhere, excellent at low temperatures, but with small differences at higher temperatures. We think that the differences are due to the fact that the Monte Carlo calculation employs a grand canonical ensemble which makes some allowance for charge fluctuations, which are more important at higher temperatures. The dashed line indicates the extrapolation of a linear least-squares fit to the high temperature portion of the curve. It is evident that the susceptibility obeys a Curie-Weiss law of the form

$$\chi^{-1}=C^{-1}(T-\Theta) .$$

where Θ is a paramagnetic Curie temperature. Note that Θ is positive (as would be expected if the ground state were ferromagnetic) even though the ground state is a singlet with fairly strong antiferromagnetic correlations at low temperatures (as will be discussed below). The value of Θ obtained by a least-squares fit to the high-temperature points is approximately $0.16U$.

The specific heat for the case of $n=8$, $z=0.1$ is shown in Fig. 6. Here we see the characteristic two-peak structure found in numerical calculations for smaller systems, going back to the calculations of Shiba and Pincus.[10] The low-temperature peak is associated with the lowest set of spin rearrangement levels in Fig. 3, and it is in this temperature region that strong spin correlations develop between different sites.

The local moment and neighboring atom spin correlation functions are shown for $n=8$ and $z=0.2$ in Figs. 7 and 8. Again we compare results of quantum Monte Carlo calculations with those obtained from explicit diagonalization. It is seen that there is generally good agreement between the two sets of calculations for the first-, second,- and third-neighbor spin-correlation functions but that the Monte Carlo calculations give a smaller local moment except at the lowest temperature studied. This we attribute to the effect of charge fluctuations which become small at low temperatures. The value of U/t for the case shown (5), is not particularly large, and was chosen in order to illustrate the effect of fluctuations on the moment.

Next we consider the case of $n=7$. In this case, the ground state has the maximum spin for $z<0.0253$. One expects and finds quite different temperature dependences of the magnetic susceptibility at low temperatures depending on the nature of the ground state. Figure 9 shows the susceptibility for the case $z=0.0222$ ($U/t=45$). This case was not accessible to our Monte Carlo calculations. At high temperature (T of the order of U or greater) a Curie Weiss law is accurately obeyed, which extrapolates to a paramagnetic Curie temperature determined by a least-squares fit to be $T_c \approx 0.19U$). For lower temperature, there the departures from this behavior, and as $T \to 0$, the susceptibility obeys a Curie law rather than a

Curie-Weiss law. This is a result of the finite size of the system.

The specific heat for the same values of the parameters is shown in Fig. 10. In this case, there are three peaks in the low-temperature specific heat. The lowest peak is due to a set of four closely spaced levels, some of which are triply degenerate, beginning at an energy of about $0.001U$ above the ground state. These levels are essentially just spin rearrangements. In the present case, the ground state can be regarded has having a single hole in a (spin-aligned) band. The energy required to promote this hole to its first excited translational state is $0.044U$ in the example shown, and it is probable that states involving translational motion of the hole are involved in the second peak.

In contrast, Fig. 11 shows the susceptibility as a function of temperature for the case of $U/t=4$, for which the ground state has $S=\frac{1}{2}$. In this case we also have Monte Carlo results down to fairly low temperatures. Again, there is rather good agreement between the Monte Carlo and explicit diagonalization calculations although there are relatively small differences at high temperatures that can be attributed to implicit inclusion of charge fluctuations in the Monte Carlo results. At low temperature we see that χ^{-1} starts to increase, then turns over and follows a Curie law to $T=0$. This behavior was also found for the octahedral cluster discussed in Ref. 3. An increase in χ^{-1} at low temperature is characteristic of antiferromagnets; a bulk metallic antiferromagnet would have χ^{-1} finite at $T=0$. We argue that the increase in χ^{-1} can be regarded as the cluster equivalent of the onset of antiferromagnetism but the fact that the cluster is finite with an odd number off electrons forces a Curie law at the lowest temperatures. First-, second,- and third-neighbor spin-correlation functions are shown for these parameters in Fig. 12. Here there is also good agreement between Monte Carlo and explicit diagonalization calculations although there is noticeable statistical noise in the Monte Carlo results. The sign pattern of the correlation functions is the same as for the half-filled band and is that expected for antiferromagnetism. Generally, all of the correlation functions are smaller in magnitude than in the half-filled band case. The first-neighbor function decays rather slowly with increasing temperative, while the second-, and third-neighbor functions change rapidly in the range of temperature of the order $0.2t$ to $0.4t$, which corresponds (according to Fig. 11) to the temperature range in which χ^{-1} is increasing. These results support our discussion of this cluster in terms of antiferromagnetism.

We shall discuss our results for smaller occupancies ($n=6$, 5, and 4) more briefly. The magnetic susceptibility is shown for $n=6$ in Fig. 12. Again, there is rather good agreement between explicit diagonalization and Monte Carlo calculations with small differences at high temperatures. In the case of $n=6$ (Fig. 13), the ground state is a singlet for all U, and the case illustrated shows behavior characteristic of antiferromagnetism. At temperatures just above the minimum, there is a region in which Curie-Weiss behavior with negative intercept (paramagnetic Néel temperature) is found, but at much higher temperatures, we find a positive intercept as discussed previously for $n=8$.

Spin-correlation functions are shown for $n=5$ and $U/T=4$ in Fig. 14. The ground state for $n=5$ has $S=\frac{3}{2}$ (unsaturated ferromagnetism) for all U. In the case illustrated the spin-correlation functions are quite small in magnitude (we regard this as indicative of a highly itinerant situation). There are significant discrepancies between Monte Carlo and explicit diagonalization results indicating important charge fluctuations. It is particularly interesting in this case that the first neighbor spin correlation function is always negative. This result is actually independent of U. The second-neighbor function changes sign near $T=0.2t$. We see from this that it may be difficult to draw qualitative inferences concerning magnetic alignment in the ground state from measurements of spin-correlation functions at high temperature.

This observation is reinforced by the behavior of the spin-correlation functions for $n=4$ and U/t, sufficiently large for the system to be ferromagnetic. All correlation functions are positive although small at low temperatures, but both the first- and second-neighbor functions change sign at higher temperatures.

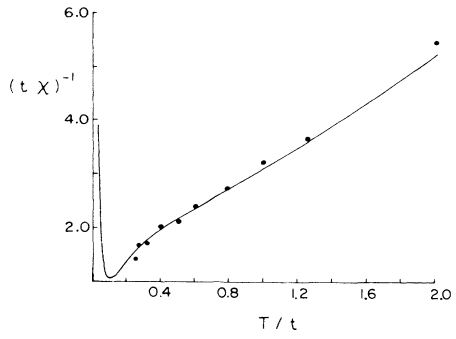

FIG. 13. Temperature dependence of the magnetic susceptibility for $n=6$ and $U/t=4$. Dots are the results of Monte Carlo calculations.

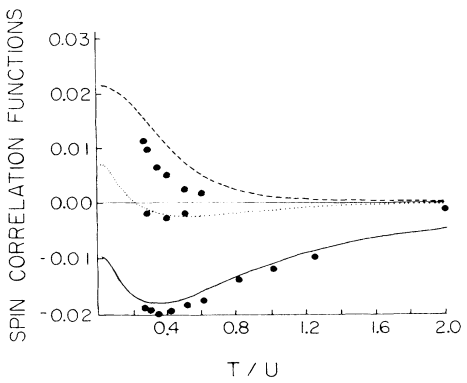

FIG. 14. Temperature dependence of spin-correlation functions for $n=5$ and $U/t=4$. Curves are drawn as in Fig. 12.

IV. SUMMARY

When the simplest form of Hubbard model with a single nondegenerate orbital and nearest-neighbor interactions only is considered on a simple-cubic cluster of eight sites, the calculated ground-state and thermodynamic functions describe several types of magnetic behavior, depending on the number of particles in the system and the ratio U/t. For $n=7$ or $n=4$ we find a maximum spin ground state when U/t is sufficiently large, but for $n=5$, an unsaturated ferromagnetic ground state is obtained for all positive values of U. Antiferromagnetic spin correlations are found in other cases. Then the temperature dependent magnetic susceptibility resembles that for a bulk antiferromagnet except at very low temperatures, where finite-size effects dominate. A Curie-Weiss law with a negative paramagnetic Curie (Néel) temperature holds in a restricted temperature range. When the ground state has other than the minimum spin, a Curie-Weiss law with a positive Curie temperature applies. In all cases we have examined, the susceptibility at temperatures large compared to the band width obeys a Curie-Weiss law with positive T_c.

The specific heat typically has a two-peak structure, but in one case, we have found three. The local moment decays quite gradually with temperature at low temperature while the first-, second-, and third-neighbor spin-correlation functions decrease much more rapidly. There is no obvious way in which the nature of the ground state can be readily inferred from the spin-correlation functions at high temperature. Comparison of calculations performed by explicit diagonalization and utilizing the canonical ensemble with Monte Carlo simulations employing the grand-canonical ensemble indicate that the most important effect of charge fluctuations is to reduce the local moment at high temperatures; otherwise there is rather good agreement between results of the two approaches.

Finally, we note that overall qualitative similarities between the results of the present calculation for a cube and previous calculations by ourselves and others for smaller systems. The similarity resides in the fact that the same type of magnetic properties occur: for example, Curie-Weiss behavior of the susceptibility and the occurrence of two peaks in the specific heat. The existence of these characteristics is substantially independent of the geometry and the number of particles, but the specifics, such as the kind of order which occurs for a given interaction strength, the numerical value of the paramagnetic Curie temperature, etc. do depend strongly on the details of the system.

ACKNOWLEDGMENT

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