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Cluster approach to the extended Hubbard model

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The eigenvalue problem of the two-site and three-site extended Hubbard Hamiltonian, which contains the intra-atomic repulsion U, the nearest-neighbor repulsion V, the isotropic exchange J, the anisotropic exchange J', the hopping term t, the semihopping term S, and the double hopping term D, has been solved exactly and the grand partition function is obtained. The magnetic and thermodynamic quantities such as the magnetic susceptibility and the specific heat are calculated for arbitrary electron density. Several features believed to have wider validity have been deduced from this cluster model.

I. INTRODUCTION

A cluster-type approach to the narrow-band Hubbard model[1,2] has been suggested by several authors.[3-7] In thse cluster approaches, the eigenvalue problem of a finite number of sites is treated exactly. The grand partition function can then be obtained and the magnetic and thermodynamic properties calculated accordingly. In most cases, only the effects of the hopping term t and the intrasite correlation term U in the half-filled model have been considered. Chen and Cheng[8] have extended the calculation to arbitrary electron densities and included the effect of the direct intersite Coulomb repulsion term. Shiba[5] has shown that, for the simple Hubbard model with only U and t, as the size of the cluster increases the specific-heat curve remains qualitatively the same agreeing with the result of self-consistent approximation.[9] Chui and Bray[10] have developed a computer renormalization-group calculation on the one-dimensional finite chain, and the $2k_F$ and $4k_F$ correlation functions for the cluster model were calculated.

In this investigation we include in the cluster model all the interaction terms[11] which were neglected by Hubbard in his original work.[1] Among these interaction terms all assigned reasonable numerical magnitude[12]; the most significant one is the intersite isotropic exchange term J, especially concerning the magnetic properties of the system. That this is so will be borne out in the calculation of the magnetic and thermodynamic quantities in the cluster model.

In Secs. II and III we solve the two-site extended Hubbard model analytically and the three-site model numerically for arbitrary electron densities. The magnetic and thermodynamic quantities are computed and discussed in Sec. IV. A brief conclusion including the general features of the results of the cluster model that we believe to be valid for the actual many-body system is given in Sec. V.

II. TWO-SITE MODEL

The one-band Hubbard Hamiltonian in Wannier representation is usually written in the form

$$\hat{H}=t\sum_{ij}C^{\dagger}_{i\sigma}C_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $\langle ij\rangle$ indicates sum over nearest neighbor only, $C^{\dagger}_{i\sigma}$ creates an electron in the Wannier state centered about the lattice site i with spin σ, and $n_{i\sigma}=C^{\dagger}_{i\sigma}C_{i\sigma}$. U is the intra-atomic Coulomb interaction (correlation) and t is the transfer integral (hopping energy). For the two-site model we consider two particular neighboring sites and allow the number of electrons to vary in this two-site cluster by introducing a chemical potential μ into the Hamiltonian. Therefore, the information of interaction between the cluster and the rest of the system is also included in the chemical potential.

The extended Hubbard Hamiltonian of the two-site system in the two-site system in the presence of a uniform magnetic field B is

$$\begin{aligned}\hat{H}_{ts}=t&\sum_{\sigma}(C^{\dagger}_{1\sigma}C_{2\sigma}+C^{\dagger}_{2\sigma}C_{1\sigma})+U\sum_{i=1,2}n_{i\uparrow}n_{i\downarrow}+Vn_1n_2+J(n_{1\uparrow}-n_{1\downarrow})(n_{2\uparrow}-n_{2\downarrow})\\&+J'(C^{\dagger}_{1\uparrow}C_{1\downarrow}C^{\dagger}_{2\downarrow}C_{2\uparrow}+C^{\dagger}_{2\uparrow}C_{2\downarrow}C^{\dagger}_{1\downarrow}C_{1\uparrow})+D(C^{\dagger}_{1\uparrow}C_{2\uparrow}C^{\dagger}_{1\downarrow}C_{2\downarrow}+C^{\dagger}_{2\uparrow}C_{1}\;C^{\dagger}_{2\downarrow}C_{1\downarrow})\\&+S\sum_{\sigma}[C^{\dagger}_{1\sigma}C_{2\sigma}(n_{1,-\sigma}+n_{2,-\sigma})+C^{\dagger}_{2\sigma}C_{1\sigma}(n_{1,-\sigma}+n_{2,-\sigma})]-\gamma B\sum_{i=1,2}(n_{i\uparrow}-n_{\downarrow})-\mu\sum_{1=1,2}\sum_{\sigma}n_{i\sigma}\,,\end{aligned} \tag{2}$$

where V is the direct Coulomb interaction (intersite repulsion), J is the isotropic exchange interaction, J' is the anisotropic exchange interaction, D is the double hopping term, S is the semihopping term, and γ is the magnetic moment of the electron.

The eigenvalue problem of Eq. (2) can be solved exactly. There are 16 nondegenerate eigenvalues and eigenstates, all listed in the Appendix. From the known eigenvalues the grand partition function Q can be written down immediately. The chemical potential μ can then be determined via Q in the usual manner. If $2f=n$ denotes the average number of particles per site, the chemical potential μ can be calculated from the equation

$$\begin{aligned} &e^{4\beta\mu}(1-4f)\,e^{-\beta(2U+4V)} \\ &\quad + e^{3\beta\mu}(3-4f)\,e^{-\beta(U+2V)}\cosh\beta(t+2S) \\ &\quad + Ae^{2\beta\mu}(1-2f) + e^{\beta\mu}(1-4f)\cosh\beta t - f = 0\,, \end{aligned} \tag{3}$$

where

$$A = \tfrac{1}{2}[2e^{-\beta(J+V)} + e^{-\beta(U-D)} + e^{-\beta(V-J-J')} + (e^{-\beta E_+} + e^{-\beta E_-})] \tag{4}$$

in terms of f, T, and the interaction parameters.

The magnetic susceptibility χ and the specific heat C_v also follow immediately from knowledge of Q and μ. These quantities for different values of f will be computed and discussed in Sec. IV. In the limit of the narrow band, the parameter U is much larger than the other coupling parameter t, J, J', V, S, D. The spectrum of the two-site cluster can then be roughly divided into three groups of levels, the spacing between successive groups are of order U while the spacing between levels within the same group are of order t^2/U. In particular, at $f=\frac{1}{2}$ and with only U, t present we find that among the six eigenvalues, the ground state $|\psi_{10}\rangle$ has minimal $|S_z|$ and an eigenvalue E_{10} approximately t^2/U below zero [Appendix, Eq. (3)]. The first excited level is degenerate; there are three states $|\psi_6\rangle$, $|\psi_8\rangle$, and $|\psi_{11}\rangle$, some of which, e.g., $|\psi_6\rangle$ and $|\psi_{11}\rangle$ have maximal $|S_z|$ and they all are located at energies ~0. These two levels will interchange with each other if we introduce a negative J of appropriate magnitude. The highest excited states are $|\psi_7\rangle$ and $|\psi_9\rangle$; their energies are approximately of the order of U above zero. The nature of such a spectrum will manifest itself in the thermal and magnetic properties of the system.

III. THREE-SITE MODEL

In order to judge the result of the two-site model, we now enlarge the cluster and consider the three-site model. Magnetic and thermodynamic quantities will be calculated again and compared with those of the two-site model.

The Hamiltonian of the three-site model in a linear chain structure including only the nearest-neighboring interaction is similar in nature to Eq. (2), except for the inclusion of the third site.

There are $4^3=64$ eigenvalues and eigenvectors corresponding to the fact that there are four states per site. Since the Hamiltonian is isotropic in spin space, the total spin S and its z component S_z are good quantum numbers. The 64×64 Hamiltonian matrix can thus be reduced into block form: 28 eigenvalues can be obtained analytically. The rest can also be reduced into four 9×9 matrices, two of which are identical and these three 9×9 matrices have been diagonalized numerically.

In order to investigate the effect of the different boundary conditions on the clusters, we have also considered the three-site model in ring geometry. The Hamiltonian matrix exhibits more symmetry than that for the linear chain, and the eigenvalues and eigenstates are also different.

All these eigenvalues and eigenstates for both types of boundary condition have been obtained explicitly[12] but will not be listed in its totality here. They will be used to calculate the thermal and magnetic quantities in Sec. IV.

By analyzing the eigenvalues and eigenvectors of the three-site models, we find similar features as those in the two-site model. Numerically it is found that the ground state is usually the state with minimal $|S_z|$. The state with maximum $|S_z|$ can become the ground state if we introduce a sufficiently negative isotropic exchange interaction J. We also find both analytically and numerically, for $V=0$, the one-particle states and the five-particle states have the same excitation spectra, except for a constant of shift of $2U$; so do the two- and four-particle states, except for a shift of U. However, for $V\neq 0$, this feature is lost for the linear model simply due to the fact that a particle at the central site interacts via V differently than a particle at an end site with its neighbors. In the case of ring geometry, because of the cyclic symmetry, the above-mentioned feature is recovered even for $V\neq 0$. The shift of the spectrum of the five-particle states relative to that of the one-particle state is now $2U+8V$; the shift of the four-particle spectrum relative to the two-particle spectrum is $U+4V$. These are the amount of energy increase when we put two or four particles in the states with two or one particle already present, respectively.

There is another significant feature about the excitation spectrum at $f=\frac{1}{2}$. From the numerical calculation, we find that the twenty eigenstates for the half-filled case are divided into two groups. There is an energy spacing of the order of several t^2/U

between the ground state and the lowest excited levels. Among the latter levels some of them have maximal $|S_z|$ and some have minimal $|S_z|$. Their positions will interchange if we introduce a sufficiently negative J into the Hamiltonian. The energy gap between the first excited states and the highest state is of the order of U. This particular feature will manifest itself in the calculation of magnetic and thermodynamic quantities in the next section. The calculation of the grand partition function, the chemical potential, the magnetic susceptibility, and the specific heat of the three-site model are similar to that for the two-site model, except that we have to sum over $4^3 = 64$ eigenvalues in the three-site model. The numerical calculation and discussions will be given in the next section.

IV. NUMERICAL RESULTS AND DISCUSSIONS

To start calculating magnetic and thermodynamic quantities we have to evaluate first the chemical potential of the system at different occupation numbers. At $f=\frac{1}{2}$ the situation is particularly simple. It is found that the chemical potential is $U/2+V$ for the two-site model, and $U/2+2V$ for the three-site model in the ring geometry provided the semihopping term S is neglected. This is a consequence of the particle-hole symmetry that also leads to similar excitation spectra for the states with occupation number f and for those with occupation number $1-f$. Following from this fact, we find that all magnetic and thermodynamic quantities are symmetric with respect to $f=\frac{1}{2}$, the half-filled case, unless S is introduced.

The behavior of magnetic and thermodynamic quantities in the cluster model can all be understood from the excitation spectra. As we mentioned in the previous section, the state with minimal $|S_z|$ are the ground states unless we introduce a sufficiently negative isotropic J. In Figs. 1 and 2 we have shown the magnetic susceptibility curves of the two-site model and of the three-site model for $f=\frac{1}{2}$, with only U, t present. We see that in the two-site case, there is a low-temperature peak for the magnetic susceptibility. This is due to the transition from the ground state of antiparallel spins with $S_z=0$ to the parallel-spin states with $S_z \neq 0$ of the nearly first excited level. In contrast, in the three-site model the susceptibility decreases monotonically as T increases because there is no qualitative change from the ground level of minimal $|S_z| \neq 0$ to the first excited levels since all of them have $|S_z| \neq 0$. As we introduce a negative J the original ground state is replaced by the state with maximal $|S_z|$. In general a negative J enhances the magnetic susceptibility for both the two- and three-site model. In the two-site model a negative J also has the effect of removing the low-temperature peak of the magnetic susceptibility when plotted against temperature, resulting in a monotonically decreasing behavior corresponding to the nature of the ground state. For the non-half-filled case such as $f=\frac{1}{3}$ (or $f=\frac{2}{3}$) we show that there is also a low-temperature peak in the susceptibility curve (Fig. 3). Again this is primarily due to a transition from the antiparallel-spin

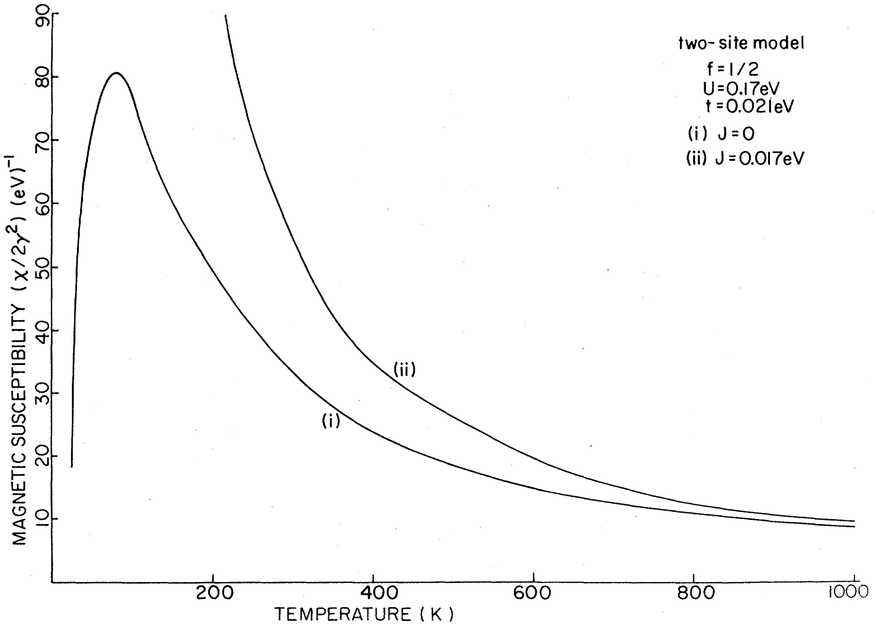

FIG. 1. Magnetic susceptibility curves of the two-site model for the half-filled case.

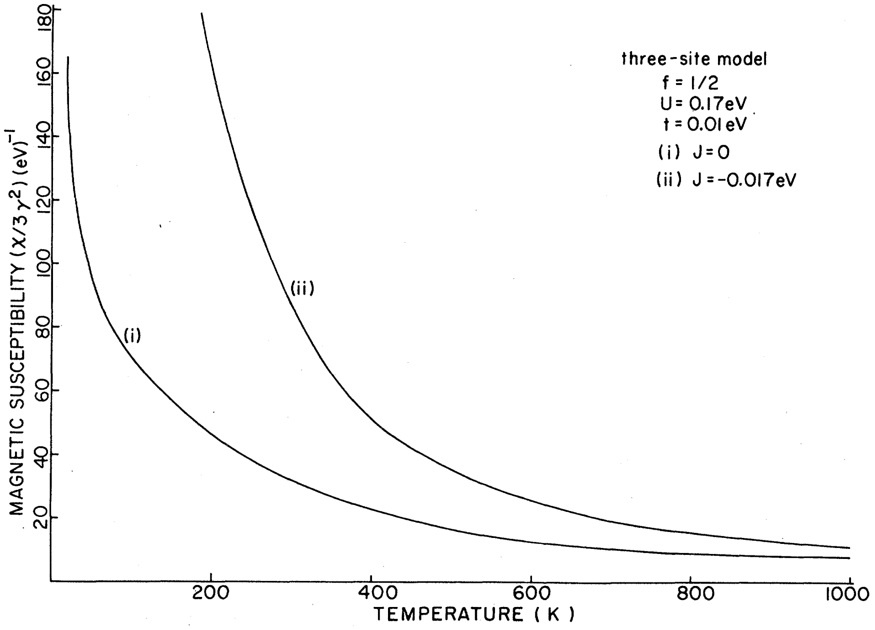

FIG. 2. Magnetic susceptibility curves of the three-site model for the half-filled case.

ground state with $S_z = 0$ to the parallel-spin excited states of two (or four) particles in the three-site model and will be changed by the introduction of negative J. These qualitatively different types of behavior of the susceptibility are merely caused by the even and odd nature of the number of particles in the states due to the finiteness of the cluster. Therefore, we believe that such fine structure will be diminished if we increase the size of the cluster. We also find some interesting properties for nonintegral occupation. In Fig. 4 for $f = 0.455$, we find in the two-site model a "shoulder" in the magnetic susceptibility curve. This is due to the averaging of the contribution from one-particle states with nonzero S_z and two-particle states with vanishing S_z (see Fig. 2), recalling the monotonic

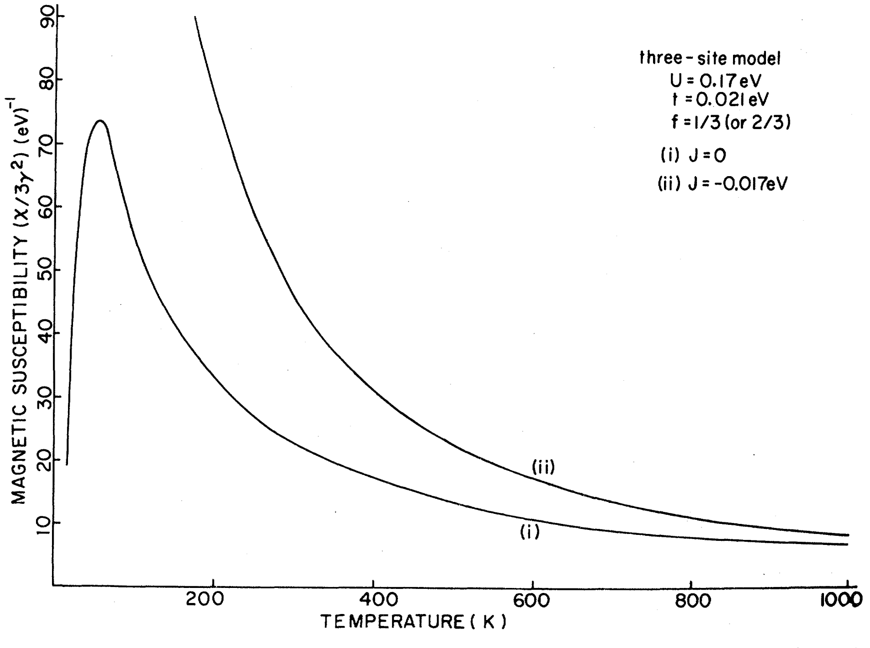

FIG. 3. Magnetic susceptibility curves of the three-site model for the case $f = \frac{1}{3}$ (or $\frac{2}{3}$).

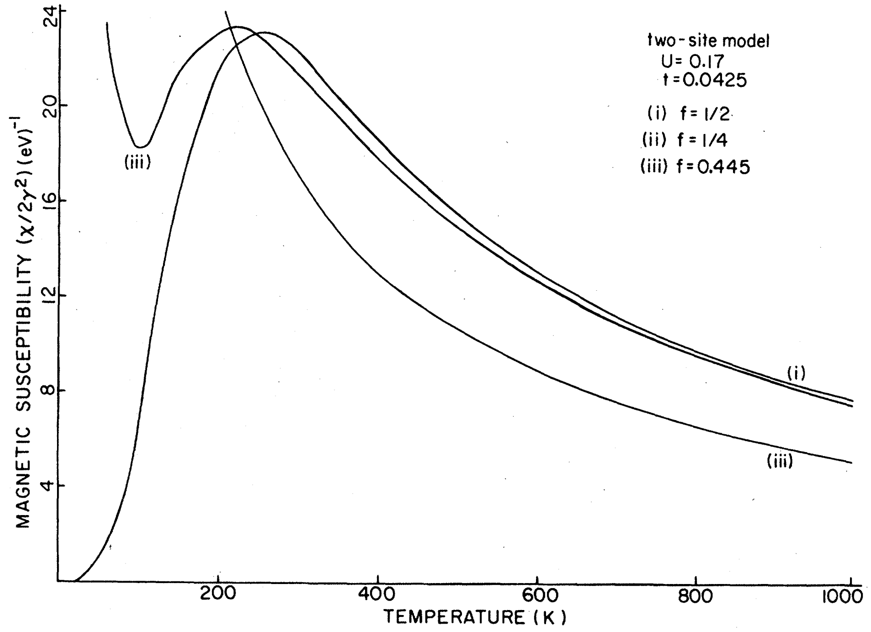

FIG. 4. Magnetic susceptibility curves of the two-site model for the case of integral and nonintegral occupation numbers.

and the peaked natures of the susceptibility associated individually with these two types of states. We find that this kind of phenomena will occur for f close to $\frac{1}{3}$ in the three-site model. The effects of the other parameters are quantitatively small if we keep their values in the same order as t and will not be discussed further.

The specific-heat curve can be interpreted in the same manner. In Fig. 5 we find that in both the two-site and the three-site models for $f=\frac{1}{2}$, the specific-heat curves are very similar to each other qualitatively. They both have a low-temperature and a high-temperature peak. The width and the height of the peaks depend on the ratio of U to t. These two peaks can be adequately explained by the two distinct energy spacings in the excitation

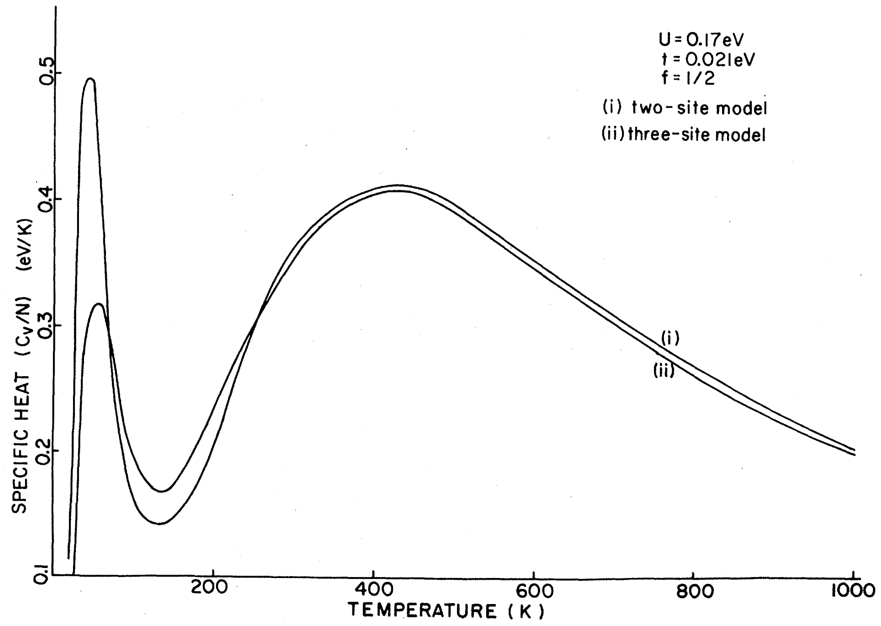

FIG. 5. Specific-heat curves of both the two-site and three-site models for half-filled case with only U,t present.

spectra for the half-filled case. Therefore, this feature remains valid even when the cluster gets larger. This is different from the explanation of Shiba and Pincus.[11] They interpreted the low-temperature peak as arising from the antiferromagnetic short-range order and the high-temperature peak from the metal-insulator transition. As we include more interaction parameters, we find that the only parameter that changes the result qualitatively is the isotropic exchange J. If J is negative, the specific-heat curve has qualitative changes due to the rearrangement of the eigenvalues mentioned above (Fig. 6). But if J is positive, the energy spectrum is just shifted upward with no qualitative modification, leading only to quantitative changes in the thermodynamic quantities. The effects of other parameters are not very significant as long as they remain the same order of magnitude as t.

We have studied the non-half-filled case in the three-site model, say $f=\frac{1}{3}$ (or $f=\frac{2}{3}$) (Fig. 7). We find that there are also two peaks on the specific-heat curves. This phenomena can also be explained by inspecting the eigenvalue spectrum. In the case when only U and t are present, the arrangement of the eigenvalues is more or less the same as that of the half-filled case. A group of states center around zero with energy with approximately t^2/U, the other group of states are located above zero with energy gap of the order of U. The ground state is again the antiparallel-spin states; the parallel-spin states are located exactly at zero. Therefore, the excitation spectrum and the specific heat can change significantly only when we introduce a negative J.

The nonintegral occupation number cases are also studied. In Fig. 8 we plot the specific-heat curves of the two-site and the three-site model for $f=0.345$. We find that the curves are not quite alike. Thus is because in the two-site model the contribution would primarily be from the one-particle states while in the three-site model it would primarily be from the two-particle states. Since the nature of the spectra for them are qualitatively different, therefore, we expect the specific-heat curves to be rather different. This shows that for f not close to $\frac{1}{2}$ the cluster may not give a reliable description of the thermal properties of the actual many-body system.

V. CONCLUSION

We have solved the two-site and the three-site extended Hubbard narrow-band model with all the nearest-neighbor interactions exactly. From analyzing the eigenvalues and eigenvectors, several interesting general features are worth noting. First, the ground state is usually the minimal $|S_z|$ configuration unless a ferromagnetic isotropic exchange interaction J is introduced. This minimal $|S_z|$ configuration usually includes an admixture of states in which some sites are doubly occupied with antiparallel spins in order to take advantage of the off-diagonal t transitions among the appropriately phased singly occupied and doubly occupied states. As the cluster becomes larger, the

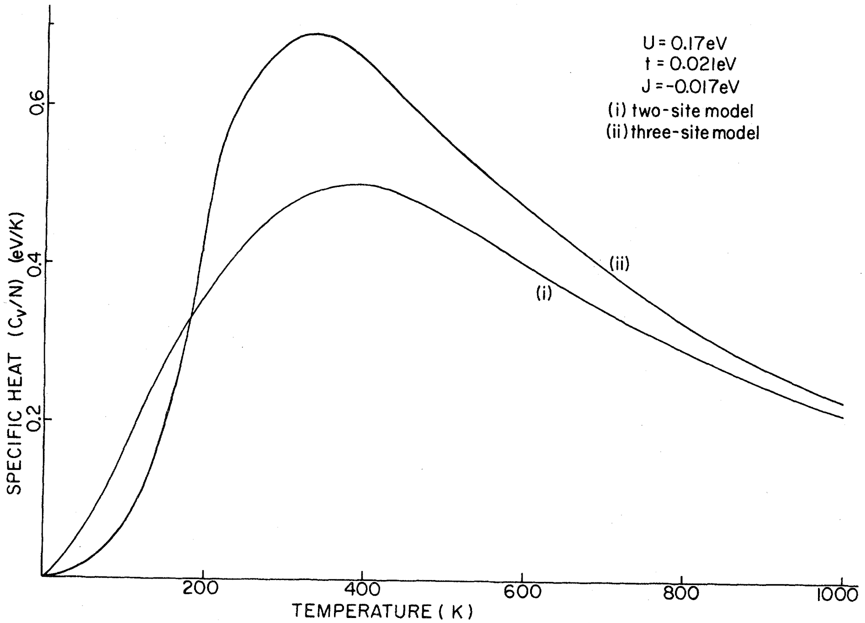

FIG. 6. Specific-heat curves of both the two-site and three-site models for the half-filled case with U, t, and J present.

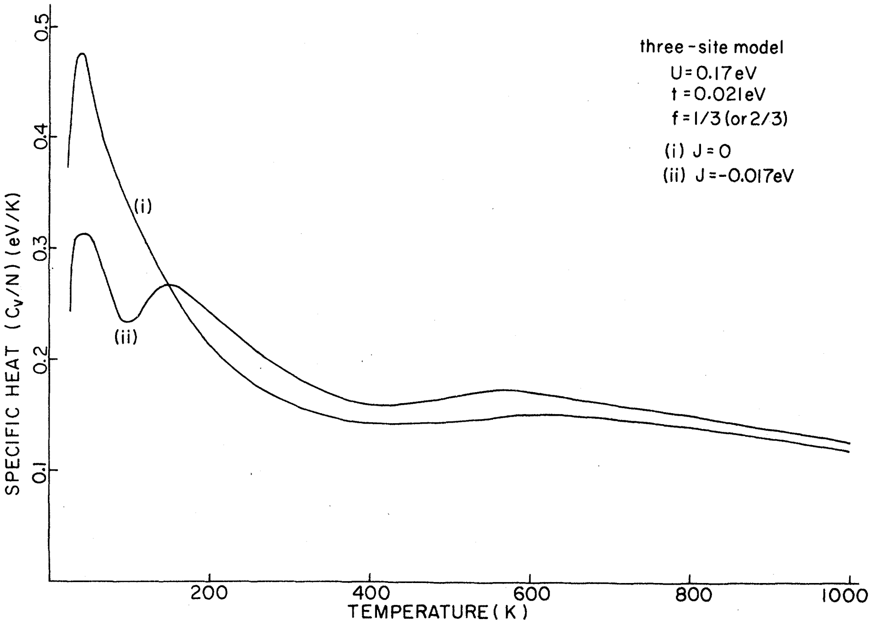

FIG. 7. Specific-heat curves of the three-site model for the case $f=\frac{1}{3}$.

off-diagonal effect may be even more dominant in the determination of the ground state as long as U remains finite simply because the number of such transitions increases faster than the number of diagonal U terms. Second, the excitation spectra of the states corresponding to occupation number f are always similar to those with occupation number $1-f$, that is, the excitation spectrum is symmetric with respect to $f=\frac{1}{2}$, provided that the semihopping term S is not included. This leads to the consequence that the chemical potential of a general cluster model with ring geometry is a constant $U/2+2V$. Also, the magnetic and the thermodynamic quantities are symmetric with respect to $f=\frac{1}{2}$. Third, the excitation spectra of the cluster models at $f=\frac{1}{2}$ are qualitatively similar. For

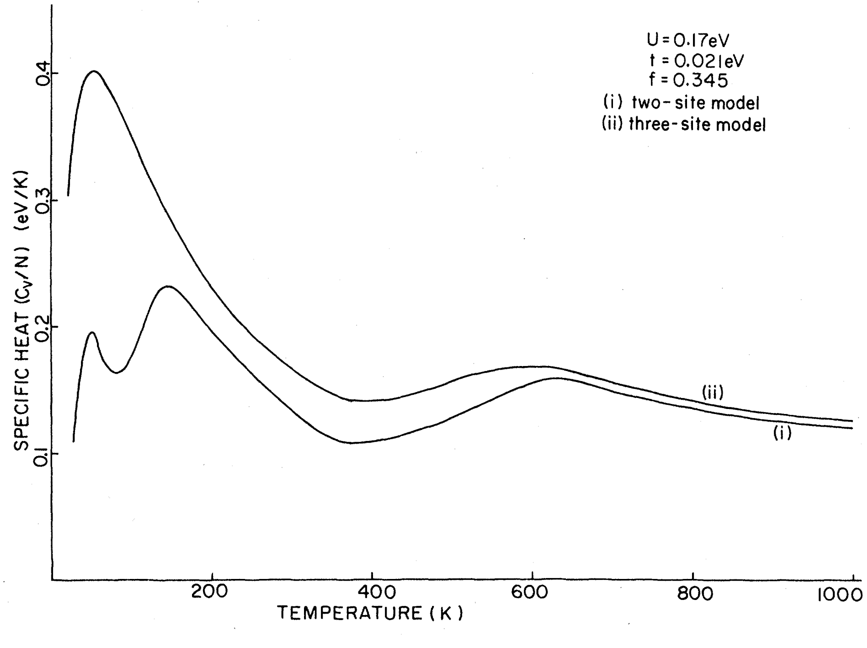

FIG. 8. Specific-heat curves of the two-site and three-site models for $f=0.345$ with only U,t present.

the two- and three-site models, they arrange themselves into two groups. One group is closely spaced within a width of order of several t^2/U, the other group is separated by a gap of order U. This leads to the specific-heat curves with the low-temperature and high-temperature peaks on the curves corresponding to those two energy spacings. The magnetic susceptibility in the case of reasonable value of $J<0$ is essentially of the Curie form, monotonically decreasing as temperature increases. This is to be contrasted with the result of Ref. 8 with the presence of only U, V, and T, which shows that the Curie form is obtained only by assuming an unphysically large V. The presence of a positive J does not alter the qualitative features of the specific heat, but a negative J does because the levels of the excitation spectrum are then rearranged. But these cluster models will not be valid for occupation numbers far away from $f=\frac{1}{2}$ because of the qualitative difference in the result shown by the different small clusters. Other features of the magnetic susceptibility which varies according to even or odd sites in the cluster are also pointed out.

In subsequent calculations, the mean-field approximation will be applied to the cluster model. By using the Hartree-Fock approximation, a self-consistency condition is obtained by assuming the thermal average of the spin-deviation operator of the cluster to be equal to that of the surrounding sites. Equations governing the relationship between the interaction parameters and the transition temperature will be found. We find that both the ferromagnetic and the antiferromagnetic transition temperature increases as $|J|$ and U increase, but they decrease as t increases. These mean-field cluster results will be presented as a sequel to the present work.

APPENDIX

The eigenvalues and eigenstates of the two-site model are listed as follows. (The representation that $|11\rangle\,|10\rangle$ means that in the left site both spin states are occupied by one electron and on the right site, the spin-up state is occupied while the spin-down state is empty.)

(i) Zero-particle state:

$$E_1=0\,,\quad |\Psi_1\rangle=|00\rangle|00\rangle\,. \tag{1}$$

(ii) One-particle states:

$$\begin{aligned}
E_2&=t-\gamma B-\mu\,, & |\Psi_2\rangle&=\frac{1}{\sqrt{2}}(|10\rangle\,|00\rangle+|00\rangle\,|10\rangle)\,,\\
E_3&=-t-\gamma B-\mu\,, & |\Psi_3\rangle&=\frac{1}{\sqrt{2}}(|10\rangle\,|00\rangle-|00\rangle\,|10\rangle)\,,\\
E_4&=t+\gamma B-\mu\,, & |\Psi_4\rangle&=\frac{1}{\sqrt{2}}(|10\rangle\,|00\rangle+|00\rangle\,|01\rangle)\,,\\
E_5&=-t+\gamma B-\mu\,, & |\Psi_5\rangle&=\frac{1}{\sqrt{2}}(|01\rangle\,|00\rangle-|00\rangle\,|01\rangle)\,.
\end{aligned} \tag{2}$$

(iii) Two-particle states:

$$\begin{aligned}
E_6&=J+V-2\gamma B-2\mu\,, & |\Psi_6\rangle&=|10\rangle\,|10\rangle\,,\\
E_7&=U-D-2\mu\,, & |\Psi_7\rangle&=\frac{1}{\sqrt{2}}(|11\rangle\,|00\rangle-|00\rangle\,|11\rangle)\,,\\
E_8&=V-J-J'-2\mu\,, & |\Psi_8\rangle&=\frac{1}{\sqrt{2}}(|10\rangle-|01\rangle-|01\rangle\,|10\rangle)\,,\\
E_9&=E_+-2\mu\,, & |\Psi_9\rangle&=\frac{1}{\sqrt{N_+}}[2(t+S)|11\rangle\,|00\rangle-(U+D-E_+)|10\rangle|01\rangle-(U+D-E_+)|01\rangle\,|10\rangle+2(t+S)|00\rangle\,|11\rangle]\,,\\
E_{10}&=E_--2\mu\,, & |\Psi_{10}\rangle&=\frac{1}{\sqrt{N_-}}[2(t+S)|11\rangle\,|00\rangle-(U+D-E_-)|10\rangle\,|01\rangle-(U+D-E_-)|01\rangle\,|10\rangle+2(t+S)|00\rangle\,|11\rangle]\,,\\
E_{11}&=J+V+2\gamma B-2\mu\,, & |\Psi_{11}\rangle&=|10\rangle\,|01\rangle\,.
\end{aligned} \tag{3}$$

(iv) Three-particle states:

$$\begin{aligned}
&E_{12}=(t+2S)+U+2V-\gamma B-3\mu\ , \quad |\Psi_{12}\rangle=\frac{1}{\sqrt{2}}(|11\rangle\,|10\rangle-|10\rangle\,|11\rangle)\ ,\\
&E_{13}=-(t+2S)+U+2V+\gamma B-3\mu\ , \quad |\Psi_{13}\rangle=\frac{1}{\sqrt{2}}(|11\rangle\,|10\rangle-|10\rangle\,|11\rangle)\ ,\\
&E_{14}=(t+2S)+U+2V+\gamma B-3\mu\ , \quad |\Psi_{14}\rangle=\frac{1}{\sqrt{2}}(|11\rangle\,|01\rangle+|10\rangle\,|11\rangle)\ ,\\
&E_{15}=-(t+2S)+U+2V+\gamma B-3\mu\ , \quad |\Psi_{15}\rangle=\frac{1}{\sqrt{2}}(|11\rangle\,|01\rangle-|01\rangle\,|11\rangle)\ ,
\end{aligned} \tag{4}$$

(v) Four-particle state:

$$E_{16}=2U+4V-4\mu\ , \quad |\Psi_{16}\rangle=|11\rangle\,|11\rangle\ , \tag{5}$$

where

$$\begin{aligned}
&E_{+}=\tfrac{1}{2}\{(U+D+V-J+J')+[(U+D-V+J-J')^2+16(t+S)^2]^{1/2}\}\ ,\\
&E_{-}=\tfrac{1}{2}\{(U+D+V-J+J')-[(U+D-V+J-J')^2+16(t+S)^2]^{1/2}\}\ ,\\
&N_{+}=2[8(t+S)^2+(U+D-V+J-J')(U+D-E_{+})]\ ,\\
&N_{-}=2[8(t+S)^2+(U+D-V+J-J')(U+D-E_{-})]\ .
\end{aligned} \tag{6}$$

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