Thermodynamic Properties of the One-Dimensional Half-Filled-Band Hubbard Model*

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In order to investigate the thermal properties (specific heat, magnetic susceptibility, entropy, internal energy, and some correlation functions) of the one-dimensional half-filled-band Hubbard model, we have studied linear chains and rings containing two to six atoms, by performing machine calculations. Supplementing the low-temperature behavior obtained from the exact solution for the infinite chain by Lieb and Wu, our results should be suggestive of the properties of the infinite system throughout the entire temperature domain. It is shown that when the ratio of the correlation energy U to the total width Δ of the band of single-particle excitations is larger than 1, the specific heat has two peaks. The high-temperature peak arises from the gradual metal-insulator transition (or the gradual formation of local moments), while the low-temperature peak is associated with the antiferromagnetic short-range ordering. When U/Δ becomes small, the two peaks merge into one. This picture is consistent with all other thermal properties, including correlation functions. The high-temperature properties are compared with the results predicted by Hubbard's approximate theory based on the truncation of the equations of motion of the Green's functions.

I. INTRODUCTION

There has been considerable work on the Hubbard Hamiltonian, which is a simple model for studying the origin of metallic magnetism and also the metal-insulator transition (Mott transition). The Hubbard Hamiltonian in its simplest form consists of two terms[1]:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1\,, \qquad \mathcal{H}_0=-\sum_{i,j,\sigma} t_{ij} C_{i\sigma}^{\dagger} C_{j\sigma}\,,$$
$$\mathcal{H}_1=U\sum_i n_{i\uparrow} n_{i\downarrow}\,, \qquad n_{i\sigma}\equiv C_{i\sigma}^{\dagger} C_{i\sigma}\,. \tag{1.1}$$

The first term, annihilating an electron with spin σ at the jth site and then creating it at the ith site, describes the hopping motion of electrons. It is usually assumed that the band is single and that the transfer is allowed only between nearest-neighbor sites. The correlation between electrons is represented by the second term, which shows that, if two electrons with opposite spin are on the same site, the energy increases by the amount U. Although this model looks very simple, the solution is not trivial. On the contrary, there are few firm results.

The investigation of this system began when the effect of correlation on the conditions for ferromagnetism was examined by Hubbard,[1] Gutzwiller,[2] and Kanamori[3] from different viewpoints. Hubbard is the first to have noticed the possibility of a metal-insulator transition in the system described by Eq. (1.1). He employed a Green's-function truncation scheme to show that, when the electron-to-atom ratio is one (i.e., half-filled system) and $U > U_{cr}$, the system is an insulator at 0 °K. He also showed that, if $U > U_{cr}$, the system is metallic. U_{cr} is determined by the transfer integral and is, in general, the order of magnitude of the unperturbed bandwidth.

It is well known, in this connection, that in the half-filled system with fairly large value of U each atom is occupied by one electron, and the degeneracy of the 2^N states (N is the total number of atoms) is lifted by the transfer of electrons, which results in an antiferromagnetic ground state. Also, if we confine ourselves within a small region, where the electron-to-atom ratio is very close to unity and also U is quite large, Nagaoka[4] has proved some exact results for the ground state.

Hubbard's work has stimulated active discussions on this model, and many papers have appeared since then. Parallel to theoretical studies much experimental investigation on the metal-nonmetal transition has been reported,[5-8] and this has recently been one of the most actively pursued fields. But we must emphasize again that, in spite of these works, we unfortunately still have few well-founded theoretical results for this model. In this situation, any exact results on the Hubbard model are very helpful, even if the system is rather special.

Therefore it is quite interesting that Lieb and Wu[9] succeeded in obtaining the exact ground state of the one-dimensional Hubbard model with arbitrary values of U. This theory proves that in the half-filled case the ground state is always insulating, if U is finite. Following this work, the lowest excited states (spin-wave spectrum)[10] and magnetic susceptibility at absolute-zero temperature[11] were determined. But unfortunately there are no exact finite-temperature results, although they are highly desirable. This is one of the motivations for this paper.

One-dimensional (or more generally low-dimen-

sional) many-body systems are fascinating, not only because of their mathematical tractability, but also because the underlying physics is different from that in higher-dimensional systems. Here the short-range ordering plays a more important role than in higher-dimensional systems. Many investigations of one-dimensional *localized*-spin systems have been carried out, both experimentally and theoretically, from this viewpoint. The study of the one-dimensional antiferromagnetic Heisenberg model with spin $\frac{1}{2}$ is especially worthy of attention, since it is intimately connected with the one-dimensional half-filled-band Hubbard model which we discuss. It is well known that for this system, the beautiful exact solution of the ground state,[12,13] the spin-wave spectrum,[14] and the susceptibility at zero temperature[15] have been obtained. As for the thermodynamic properties, Bonner and Fisher[16] gave an extensive analysis, which has been very useful for understanding the experimental results on one-dimensional antiferromagnets such as $Cu(NH_3)_4SO_4 \cdot H_2O$,[17] $KCuF_3$,[18] and $Cu(C_6H_5COO)_2 \cdot 3H_2O$.[19] Comparing the situation in the one-dimensional Hubbard model (a model of an *itinerant*-electron system) with that in the *localized*-spin system which we briefly surveyed above, one easily notices that the study of finite-temperature properties of the one-dimensional half-filled-band Hubbard model is desirable, but lacking. This paper is devoted to this study.

The experimental search for one-dimensional itinerant-electron systems which realize to some extent the Hubbard model is interesting, but at present there is only an attempt by Epstein *et al.*,[20] who try to interpret their experimental results of specific heat, etc., on the organic charge-transfer salt *N*-methylphenazinium tetracyanoquinodimethane (TCNQ) in terms of the one-dimensional Hubbard model. Much work is still necessary to clarify this situation, but this again motivates us to study the thermal properties of the Hubbard model. In a real system, needless to say, thermal excitations of molecular motions complicate the situation at finite temperatures. On the theoretical side, we feel it necessary to clarify, first of all, the thermodynamic properties of the one-dimensional Hubbard model, in which the lattice is assumed for simplicity to be rigid.

In this paper we study such properties as magnetic susceptibility, specific heat, entropy, internal energy, and correlation functions in the one-dimensional half-filled-band Hubbard model as a function of temperature. Our approach to this problem is the same as that of Bonner and Fisher. In other words, we perform exact machine calculations for finite systems, and extrapolate to the properties of the infinite system by increasing the number of atoms of the system. It should be noted, in this connection, that Mattheiss[21] performed a calculation for a benzene ring consisting of six hydrogen atoms. This was done to investigate the effect of configuration interaction and to justify the use of the Heisenberg exchange operator, but no study was made of thermodynamic properties. An important lesson learned from Bonner and Fisher is that in one-dimensional systems, strongly interacting through a short-range force such as a Heisenberg model with nearest-neighbor interactions, the thermodynamic behavior is mainly determined by the short-range ordering, and therefore the properties of the infinite system can be determined from those of finite systems. In fact, they calculated finite-temperature properties of the one-dimensional Heisenberg chain with two to eleven spins and skillfully extrapolated them to the infinite chain. Since the one-dimensional half-filled-band Hubbard model with extremely large values of U is equivalent to the one-dimensional antiferromagnetic Heisenberg model as far as low-temperature properties are concerned, it is quite natural to follow this method. But, as is easily noticed, the Hilbert space we have to handle is larger than the localized-spin system. Thus we only actually treated a finite system consisting of two to six atoms. Supplementing the properties at zero temperature, which is difficult to find from our calculations, by the exact solution, we can nevertheless construct the behavior of various quantities of the infinite chain throughout the entire temperature domain. We can determine the dependence of the thermodynamic behavior of the one-dimensional half-filled-band Hubbard model on the relative magnitude of U to the total bandwidth Δ. The problem of convergence is delicate and it depends on the quantity calculated as well as on the magnitude of the parameters.

An outline of this paper is as follows: Numerical calculations of specific heat, magnetic susceptibility, entropy, and internal energy of finite systems are given in Sec. II, and here a picture of thermal properties of the infinite one-dimensional half-filled-band Hubbard model is obtained. That picture is examined by the calculation of some relevant correlation functions, and the results are presented in Sec. III. Section IV is devoted to a comparison of our results with the predictions, based on Hubbard's approximate theory.[1] The latter is expected to give good results when U/Δ is large and the temperature is high enough to ignore the coupling of single-particle excitations with collective spin-wave excitations. In Sec. V other subjects, which may have an intimate connection with our study, are briefly discussed.

II. SPECIFIC HEAT, SUSCEPTIBILITY, ENTROPY, AND INTERNAL ENERGY OF ONE-DIMENSIONAL FINITE SYSTEMS

We assume that in the one-dimensional Hubbard

model which we discuss, the hopping of an electron occurs only between nearest-neighbor atoms. In other words, the transfer integral in Eq. (1.1) has the form

$$t_{ij} = t\ (>0) \quad \text{for} \quad |i-j| = 1$$
$$= 0 \qquad \text{otherwise} . \tag{2.1}$$

Thus the unperturbed (i.e., $U=0$) one-particle energy spectrum is given by

$$E_k = -2t\cos ka , \tag{2.2}$$

with the wave number k and the lattice constant a. The density of states of the infinite system diverges at the band edges in the way characteristic of one dimensionality as

$$\rho(\epsilon) = \frac{N}{\pi} \frac{1}{[(\frac{1}{2}\Delta)^2 - \epsilon^2]^{1/2}} \quad \text{for} \quad |\epsilon| \leq \tfrac{1}{2}\Delta$$
$$= 0 \qquad \text{otherwise} , \tag{2.3}$$

where N is the number of atoms and Δ is the total width of the band, i.e., $\Delta = 4t$.

The principle of the calculation of thermodynamic properties of a finite system is very simple. If we obtain all energy eigenvalues and eigenfunctions of the system, elementary statistical mechanics for the canonical ensemble can be used to calculate all the required quantities. Eigenvalues and eigenfunctions are obtained directly from diagonalizing the eigenvalue matrix. The maximum number of atoms of the system that we can handle is determined in principle by the upper limit of the size of the matrix that can be diagonalized by machine. The total number of eigenvalues of the half-filled system is given by $(2N)!/(N!)^2$, which is equal to 924 for $N=6$. In the localized-spin system with spin $\frac{1}{2}$ the total number of eigenvalues is 2^N. Thus, as far as the total number of eigenvalues is concerned, the half-filled-band Hubbard model consisting of six atoms is almost equivalent to a localized-spin system with ten spins. In our system each atom can be doubly occupied or vacant. Therefore, the Hilbert space is larger than in the Bonner and Fisher case with the same number of atoms.

The size of the eigenvalue matrix can of course be reduced by maximum use of the symmetry, which depends on the boundary condition imposed. We actually considered the two kinds of boundary conditions: (a) chain—a finite system with open ends, (b) ring—a finite system with cyclic boundary conditions.

All eigenvalues were calculated for chains consisting of two to five atoms, while for rings calculations were made for $N=3$–6.[22] As our Hamiltonian [Eq. (1.1)] is isotropic in spin space, the total spin S and its z component S_z are good quantum numbers. The geometry of the system further

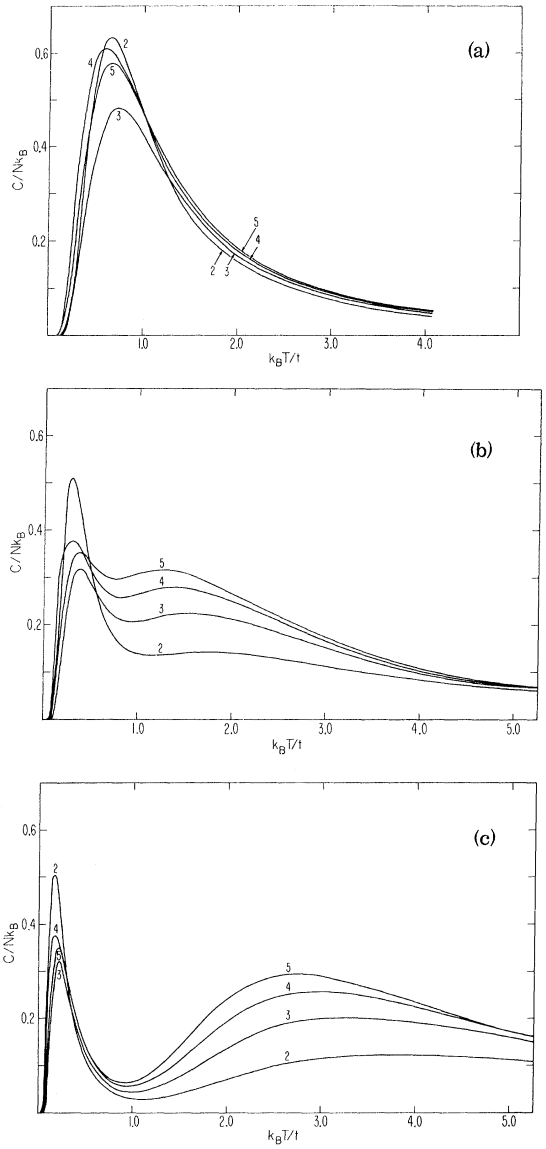


FIG. 1. Specific heat C/Nk_B of chains containing two to five atoms vs temperature for three typical values of U/t: (a) $U/t=0.5$, (b) $U/t=4.0$, and (c) $U/t=8.0$.

reduces the size of the matrix. For instance, in the case of the $N=6$ ring, the symmetry is C_{6v}. Therefore, we can use the irreducible representations of this group to reduce the size of the eigenvalue matrix. In this way we actually calculated all eigenvalues and, if necessary, eigenfunctions, for the finite systems mentioned above, and then, using these results, computed the thermodynamic quantities. The programs were checked with the $U=0$ results.

The numerical results for the temperature dependence of specific heat, magnetic susceptibility, entropy, and internal energy can now be presented

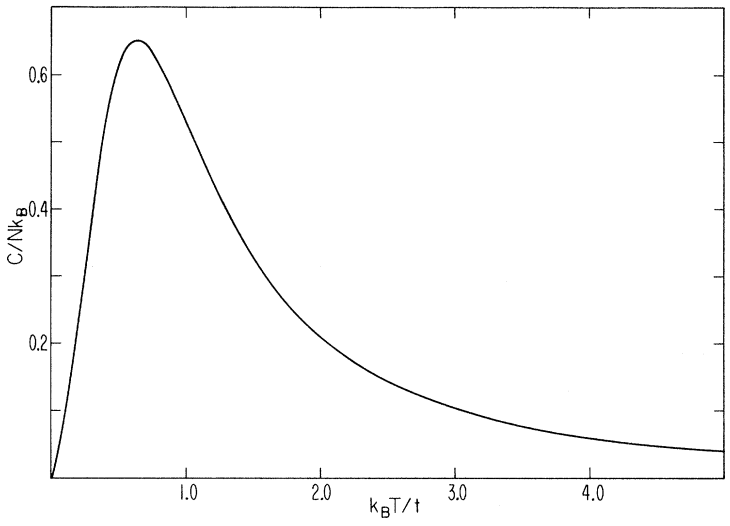


FIG. 2. Temperature dependence of the specific heat C/Nk_B of the infinite chain for $U/t=0$.

and discussed.

A. Specific Heat

Figures 1(a)–1(c) show the temperature dependence of the specific heat of chains at typical values of U/t. Comparing these figures with each other, one can easily notice how the features of the specific heat vs temperature change with the relative magnitude of U to t. The specific heat has a peak at slightly lower temperature than t/k_B when U is small compared with Δ, while when the magnitude of U is increased beyond Δ, the peak splits into two. This characteristic change of the specific heat clearly suggests the rearrangement of energy levels. We believe the low-temperature peak arises from the antiferromagnetic short-range ordering and the high-temperature peak comes from the gradual metal-insulator transition (or gradual formation of local moments). This conclusion is supported by the calculations of other thermal properties and correlation functions (Sec. III), as well as by an approximate calculation for the high-temperature region (Sec. IV).

It is not easy to unambiguously extrapolate these results for finite systems to the infinite system. But some facts known for the infinite chain are helpful in guessing the specific heat of the infinite chain from Figs. 1(a)–1(c). In the case $U=0$ (i.e., one-dimensional noninteracting electrons), the specific heat of the infinite chain can be calculated easily. The result (Fig. 2) shows the initial linear increase of the specific heat, a peak at $k_BT/t\simeq 0.65$, and the gradual decrease at high temperatures. In our calculations for finite systems the specific heat falls exponentially at low temperature, of course, because of the discreteness of energy levels. Since the spin-wave frequency is linearly proportional to the wave number in the small-wave-number region, irrespective of the magnitude of U,[10] and since Bonner and Fisher also predict the linear increase of the specific heat, we believe that in our system the specific heat at low temperature is linear and the coefficient increases with U/Δ. Comparing Figs. 1(a)–1(c) with Fig. 2 we reach the following conclusions on the effect of correlation: In the region $U/\Delta \lesssim 1$ the correlation makes the peak slightly lower and enhances the specific heat at high temperature ($k_BT/t>1$). In the region $U/\Delta \gtrsim 1$ (or $U/t \gtrsim 4$) the specific heat consists of two peaks. The low-temperature peak in the case of $U/t=8$, the origin of which we believe is the antiferromagnetic short-range ordering, is consistent with Bonner and Fisher's result. In fact, according to these authors, the specific heat C/Nk_B of the infinite antiferromagnetic Heisenberg chain has a peak at $k_BT/|J|\simeq 1$, the height of which is ~ 0.35. Applying a simple perturbation theory to the half-filled-band Hubbard model with extremely large U, we find that the effective antiferromagnetic exchange $|J|$ is given by $2t^2/U=0.25t$ for $U/t=8$. (We use Bonner and Fisher's definition of the exchange integral.) Therefore the low-temperature peak in Fig. 1(c) is consistent with that of Bonner and Fisher.

For the high-temperature peak in Figs. 1(b) and 1(c), the convergence is so slow that it is not easy to predict the behavior of the infinite chain precisely. We believe this peak arises from single-particle excitations which create holes and doubly occupied states in our system. Such excitations clearly change the magnitude of the local moment at each site. Furthermore, once a hole or double-occupied state is formed, it moves rather freely with a kinetic energy of the order of t. For these reasons we ascribe the second peak in the specific heat to the gradual formation of local moments (or gradual metal-insulator transition). In fact, we

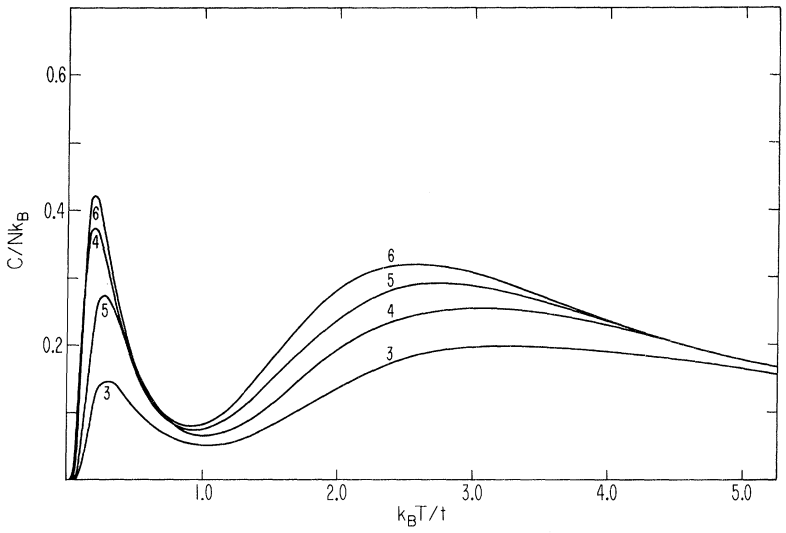


FIG. 3. Variation of specific heat C/Nk_B with temperature for rings with three to six atoms. The ratio U/t is taken as 8.0.

will study the nature of this peak by calculating the temperature dependence of the magnitude of local moment at each site (Sec. III), as well as by Hubbard's approximate truncation of the equations of motion of Green's functions as applied to the present case (Sec. IV). According to the latter the high-temperature broad peak is located at a temperature slightly lower than $U/4k_B$.

Figure 3 shows the specific heat of rings for $U/t = 8$. As is easily noticed, its essential features are the same as in the case of chains. But if we compare our low-temperature peaks in Fig. 3 with Bonner and Fisher's results, we find that our peak for $N = 6$ is higher than that for $N = 4$, in contrast to theirs. In order to clarify this, we examined the case of an extremely large U, $U/t = 20$, and found that for this case the peak for $N = 6$ is lower than that for $N = 4$, and that the heights of these peaks are the same as Bonner and Fisher's. In this sense the case of $U/t = 8$ (i.e., $U/\Delta = 2$) is not a large-U limit.

B. Magnetic Susceptibility

The picture we presented in connection with two peaks found in the specific heat is confirmed further by calculating the magnetic susceptibility. The magnetic susceptibility of chains with two to five atoms and rings with five and six atoms is shown in Figs. 4(a)–4(c), where the even-odd effect is clear in the very low-temperature region. The susceptibility of the infinite chain at zero temperature[11] derived from the exact solution by Lieb and Wu is shown in the same figures. By using this exact result we can describe the temperature dependence of the susceptibility of the infinite chain throughout the entire temperature domain. Again, the result for noninteracting electrons ($U/t = 0$) given in Fig. 5 is helpful in understanding the effect of correlation. The susceptibility of noninteracting electrons has a bump at $k_B T/t \simeq 0.65$ because of the van Hove singularity at the band edges [see Eq. (2.3)]. When U/t is increased, the susceptibility is enhanced and at the same time the position of maximum shifts toward lower temperature. In the case of very large U/t the position of maximum is found around $k_B T \simeq |J|$ ($\simeq 2t^2/U$), consistent with Bonner and Fisher's calculation. The low-temperature peak in the specific heat observed in $U/\Delta \geq 1$ corresponds to the maximum of the susceptibility. In the region $k_B T \sim U/4$, where we found the second peak in the specific heat, there is no trace of anomaly except for a gradual change of the Curie constant.

C. Entropy

Figures 6(a)–6(c) show the temperature dependence of entropy for the same values of U/t as before. We believe that, in the infinite chain, the entropy increases linearly at low temperature, judging from the behavior of entropy of noninteracting electrons and pure Heisenberg antiferromagnets.[16] Notice that in the case of $U/t = 8$ ($U/\Delta = 2$), roughly speaking, the entropy can be separated into two parts, i.e., the region below $k_B T/t \sim 1$ and the region above that. The former, having essentially the same temperature dependence as in the Heisenberg antiferromagnet, arises from collective spin-wave excitations, while the rapid increase in the latter is due to single-particle excitations which create holes and doubly occupied states. Apparently, Fig. 6(b) with $U/t = 4$ ($U/\Delta = 1$) corresponds to just the critical case, in which the entropies due to collective spin-wave excitations and single-particle excitations are strongly mixed with one another.

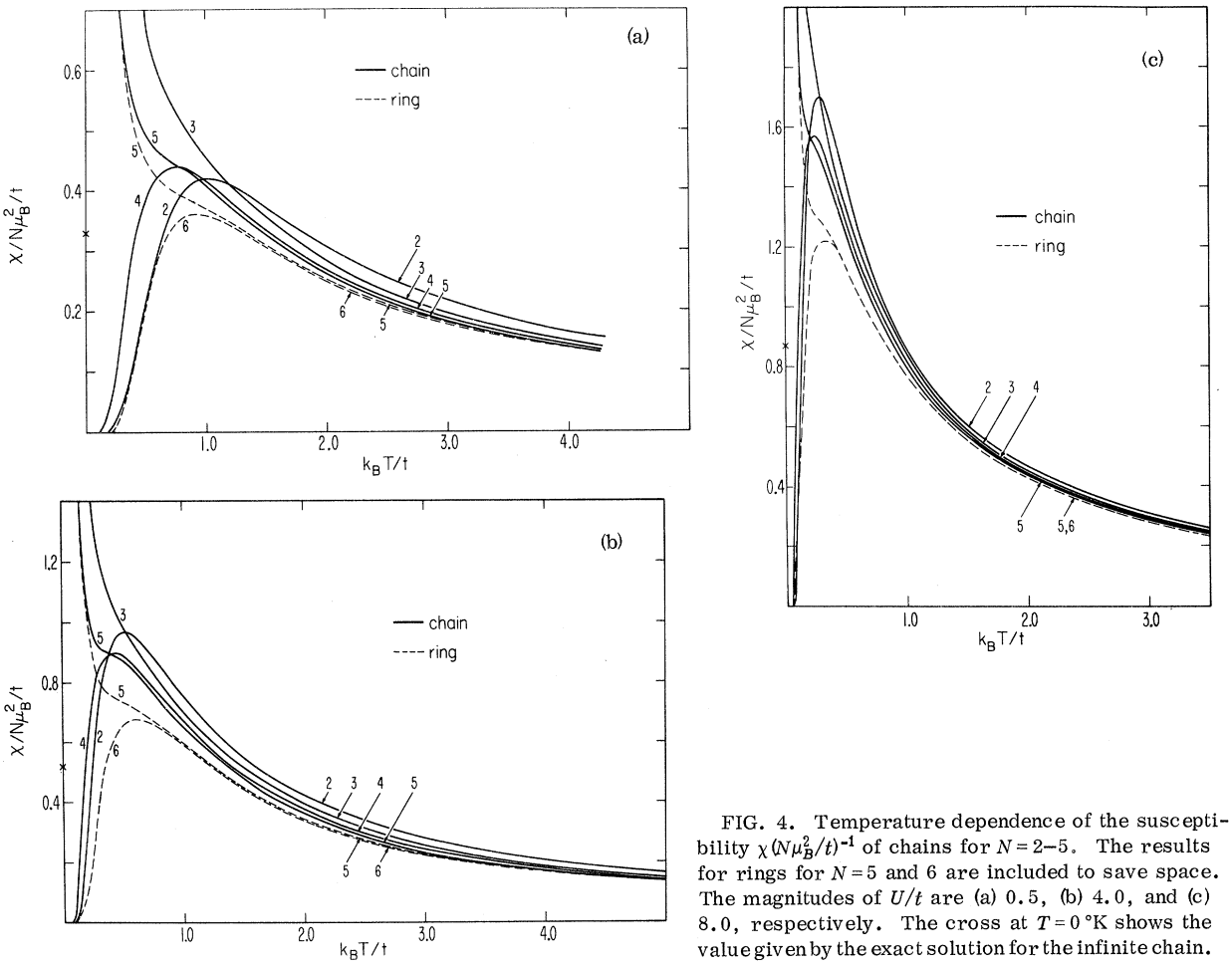


FIG. 4. Temperature dependence of the susceptibility $\chi(N\mu_B^2/t)^{-1}$ of chains for $N=2$–5. The results for rings for $N=5$ and 6 are included to save space. The magnitudes of U/t are (a) 0.5, (b) 4.0, and (c) 8.0, respectively. The cross at $T=0$ °K shows the value given by the exact solution for the infinite chain.

D. Internal Energy

An example of the temperature dependence of the internal energy of rings with three to six atoms is shown in Fig. 7. Here the exact solution of the ground-state energy for the infinite chain is included. The sharp increase of the internal energy, which starts from $k_BT/t\sim 1$, is related to the high-temperature peak in the specific heat [Fig. 1(c)] and the second step of the increase of entropy [Fig. 6(c)], and it arises again from single-particle excitations, which cost additional energy of the order of U.

Summing up the numerical calculations for the thermodynamic properties of finite systems, we find that when $U/\Delta \gtrsim 1$ the temperature dependence of specific heat, entropy, and internal energy can be separated into two nearly independent regions. The low-temperature part comes from the antiferromagnetic short-range ordering,[23] and the high-temperature part reflects excitations which form holes and double-occupied states, or, conversely, it reflects the local moment formation or the gradual metal-nonmetal transition. When U/Δ is decreased beyond the critical region located around $U/\Delta\sim 1$, the essential feature of thermal properties can be described by a slight modification of the behavior of a noninteracting electron system, i.e., enhancement of the magnetic susceptibility, etc.

III. TEMPERATURE DEPENDENCE OF CORRELATION FUNCTIONS

In the previous section a feeling for the thermal properties of the one-dimensional half-filled-band Hubbard model was drawn from the calculation of various thermodynamic quantities of finite systems. Although the results are consistent with our picture, the interpretation may seem indirect. In order to obtain detailed information we determine the temperature dependence of some correlation functions relevant to the study of the nature of the system.

The correlation function considered is

$$L_\delta(T)=(1/N)\sum_j \langle \vec{S}_j\cdot\vec{S}_{j+\delta}\rangle , \tag{3.1}$$

where $\vec{S}_j$ is the spin operator at the jth site:

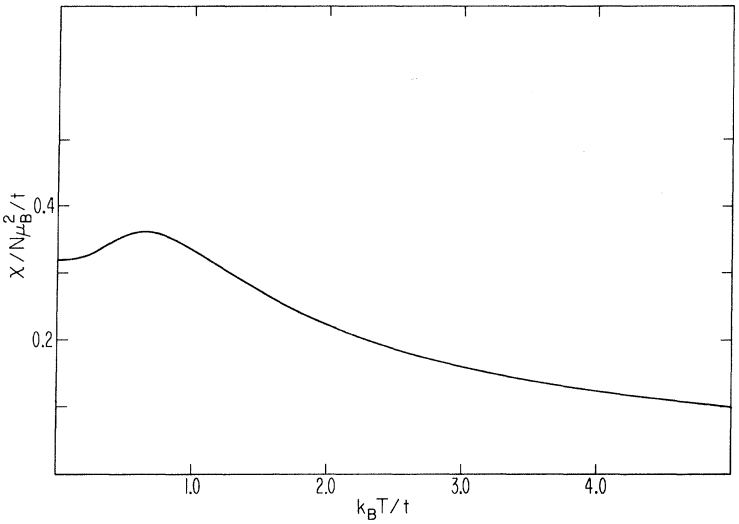


FIG. 5. Temperature dependence of the susceptibility of the infinite chain for $U/t = 0$.

$$\vec{S}_j \equiv \sum_{\sigma\sigma'} \langle \sigma | \vec{S} | \sigma' \rangle C_{j\sigma}^{\dagger} C_{j\sigma'} , \tag{3.2}$$

and the symbol $\langle\,\rangle$ denotes the average over the canonical ensemble. The meaning of the quantity $L_\delta(T)$ is clear. First of all, $L_0(T)$ shows the magnitude of spin at each site (or the degree of localization of electrons). For a completely localized electron system, in which each site is occupied by a single electron, L_0 is equal to $\frac{3}{4}$, while for a noninteracting electron system we have $L_0 = \frac{3}{8}$. Therefore the temperature dependence of L_0 gives information on the degree of localization of electrons. On the other hand, $L_\delta(T)$ $(\delta \neq 0)$ is the spin correlation on different sites as a function of temperature.

We now present numerical results for L_0, L_1, and L_2 for a six-atom ring, which is the largest system considered in the present work and has a good symmetry for calculating L_δ.

1. *Magnitude of Local Moments*

The temperature dependence of L_0 for some typical values of U/t is shown in Fig. 8. From this figure we are able to draw the following conclusions:

(i) As the temperature is increased, L_0 gradually decreases at high temperature, i.e., electrons gradually delocalize. This "transition" is gradual, and, roughly speaking, the characteristic temperature of the "transition" coincides with the position of the high-temperature peak of the specific heat. Thus we conclude that the high-temperature peak in the specific heat is associated with the gradual localization of electrons (or gradual metal-insulator transition).

(ii) The behavior at low temperature, for instance, the region $k_BT/t < 1$ in the case of $U/t = 8$, deserves special attention. This result tells us that the degree of localization is the largest, not in the ground state, but at some intermediate temperature! We believe that this occurs for the following reason: The ground state is antiferromagnetic. The antiferromagnetic coupling arises from virtual hopping of electrons, which is clear from the formula for the effective exchange energy, $|J| = 2t^2/U$, in the extremely strong U case. This virtual transfer makes the degree of localization smaller. On the other hand, in the ferromagnetic state, no virtual hoppings can occur. Therefore this state has a completely localized wave function and $L_0 = \frac{3}{4}$. So the degree of localization of the ground state is smaller than in one of the excited states. Incidentally, $L_0(T = 0\,^\circ\mathrm{K})$ can be calculated by using the exact solution. The cross in Fig. 8 is the point obtained in this way for the case of $U/t = 8$, which is very close to our result of $N = 6$ ring.

(iii) In the infinite chain L_0 must go to $\frac{3}{8}$ at infinite temperature. In our ring with six atoms, however, this is not the case. This difference is due to a size effect. In fact, it is easy to show that, at extremely high temperature $k_BT \gg U$, we have

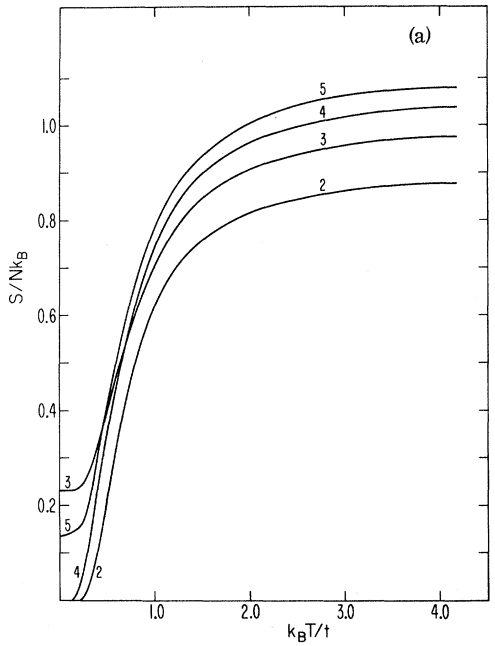
$$L_0 \to \tfrac{3}{8}\, 2N/(2N-1) , \tag{3.3}$$

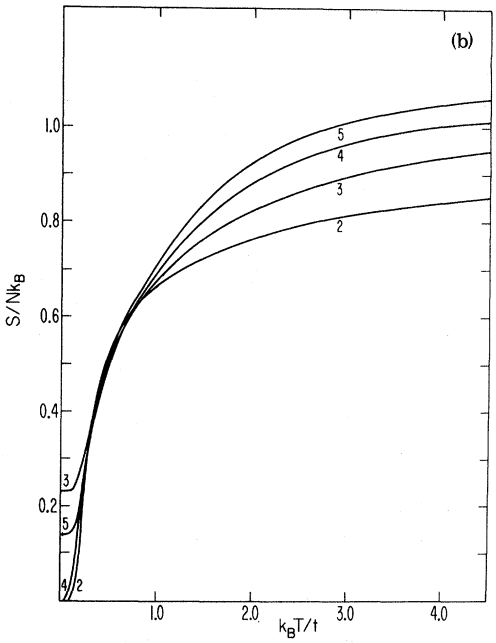
with the fixed total number N of atoms. The right-hand side is a slowly converging function of N, and in the present case with $N = 6$ this formula gives $\frac{3}{8} \cdot \frac{12}{11}$, which is shown as the arrow in Fig. 8.

(iv) As mentioned above, $L_0(T = 0\,^\circ\mathrm{K})$ for the infinite chain can be obtained from the exact solution for the ground-state energy.[9] The average of $N^{-1}\sum_j n_{j\uparrow} n_{j\downarrow}$ in the ground state is related to the ground-state energy $E(U)$ in a simple way:

$$\frac{1}{N}\sum_j \langle n_{j\uparrow} n_{j\downarrow} \rangle = \frac{1}{N}\frac{\partial E(U)}{\partial U} . \tag{3.4}$$

Therefore $L_0(T = 0\,^\circ\mathrm{K})$ is given by





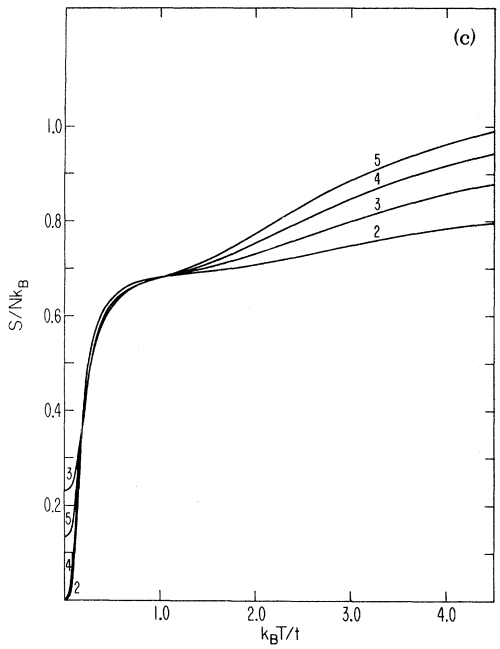


FIG. 6. Entropy vs temperature for chains containing two to five atoms. The relative magnitude of correlation to the transfer integral U/t is (a) 0.5, (b) 4.0, and (c) 8.0, respectively.

$$L_0(T=0\,^\circ\mathrm{K})=\frac{3}{4}-\frac{3}{2}\,\frac{1}{N}\,\frac{\partial E(U)}{\partial U}\ . \qquad (3.5)$$

By using this formula we calculated $L_0(T=0\,^\circ\mathrm{K})$ for the infinite chain as a function of U/t. The result is shown in Fig. 9. This gives the degree of localization of electrons in the ground state.

2. *Spin Correlation on Different Sites L_1 and L_2*

Knowledge about the spin ordering can be obtained from $L_6(T)$ ($\delta \neq 0$). Figure 10 shows the temperature dependence of the nearest-neighbor spin correlation L_1 and the next-nearest-neighbor spin correlation L_2 for $N=6$ ring. This figure clearly demonstrates how far the antiferromagnetic ordering persists when the temperature is raised.

(a) The characteristic temperature of the decrease of spin correlation, which one might call "Néel temperature," can be estimated from this figure. Using, for simplicity, the expression for the effective exchange interaction $|J|$ in the strong U case

$$|J| \simeq 2t^2/U$$

gives $|J|/t \simeq 0.25$ for $U/t=8$ and $|J|/t \simeq 0.5$ for $U/t=4$, which is consistent with the characteristic temperature estimated from the figure.

(b) Notice that L_1 has an appreciable magnitude even at high temperatures. In contrast with this, L_2 is almost zero in the region where the specific heat has the second peak.

(c) In the infinite antiferromagnetic Heisenberg chain we can calculate $L_1(T=0\,^\circ\mathrm{K})$ by using the exact solution,[12,13] which gives

$$L_1(T=0\,^\circ\mathrm{K})=\tfrac{1}{4}-\ln 2\ . \qquad (3.6)$$

In Fig. 10 this value is shown for comparison. Unfortunately, an exact solution for $L_1(T=0\,^\circ\mathrm{K})$ of the infinite one-dimensional Hubbard model does not exist.

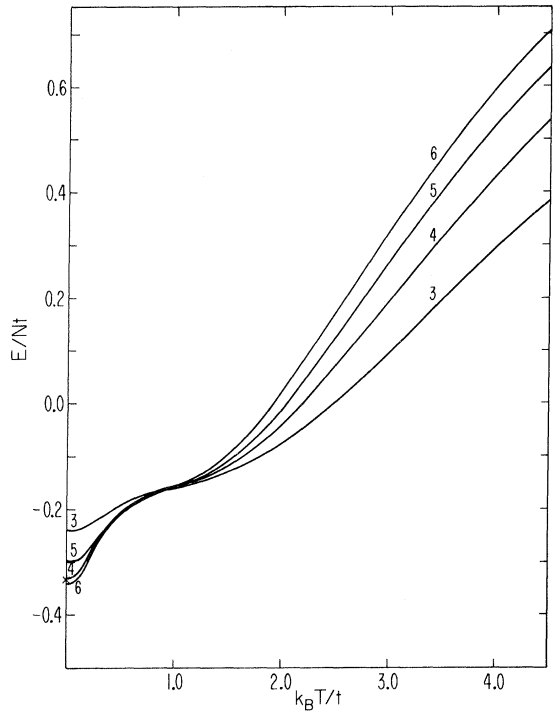


FIG. 7. Internal energy of rings with three to six atoms as a function of temperature. U/t is chosen as 8.0.

IV. COMPARISON OF HIGH-TEMPERATURE BEHAVIORS WITH RESULTS PREDICTED BY HUBBARD'S APPROXIMATE THEORY

In Sec. II we showed that, when $U/\Delta \geq 1$, two types of excitations—collective spin-wave excitations and single-particle excitations—contribute to the thermodynamic quantities almost independently. In the low-temperature region, where spin-wave excitations are dominant, Bonner and Fisher's calculations were useful in understanding our results. On the other hand, at high temperatures, the convergence of our results for finite systems is too slow to accurately extrapolate to the infinite system. In such a situation even an approximate theory may be helpful, if it is relevant to this temperature region. In this section we show the results which Hubbard's approximate theory[1] (his "improved" approximation) predicts, and compare them with exact calculations for finite systems. It turns out that his theory semiquantitatively reproduces our results for the thermal properties in the high-temperature region, if U is large compared with t.

Hubbard proposed an approximate treatment of the correlation effect in his paper on the Mott transition.[1] The basic assumption behind his truncation scheme of the Green's functions is that, when U/t is large, the motion of an electron, say, with up-spin strongly perturbed by the presence of electrons with down-spin, is so randomly modulated that we may apply a theory of disordered alloys, now famous under the name of the coherent potential approximation (CPA),[24–28] to this case by slightly modifying it. Some of the important features of his theory are as follows:

(i) It gives the exact result for $t=0$ (sometimes called the atomic limit) and only approximately gives the linear term in t.

(ii) Coupling with collective spin-wave excitations, which are important at low temperature, is neglected.

(iii) When U/t is small, it gives a metallic ground state. On the other hand, the exact solution

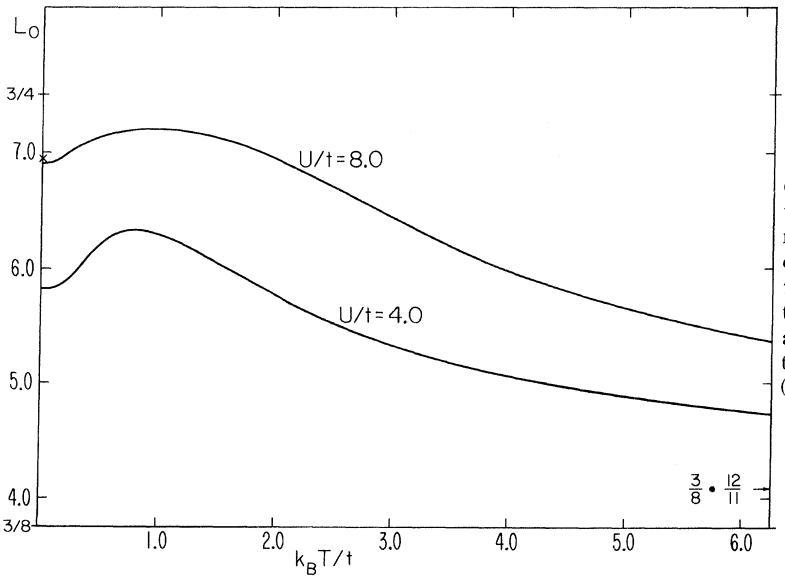


FIG. 8. Temperature dependence of the correlation function L_0, which characterizes the magnitude of local moments. The total number of atoms is six, and typical values of parameter U/t are chosen. The cross at $T=0$ °K shows the value which the exact solution for the infinite chain predicts. The arrow shows the limiting value of L_0 at high temperature given by the formula (3.3), i.e., $(\frac{3}{8}\cdot\frac{12}{11})=0.409$.

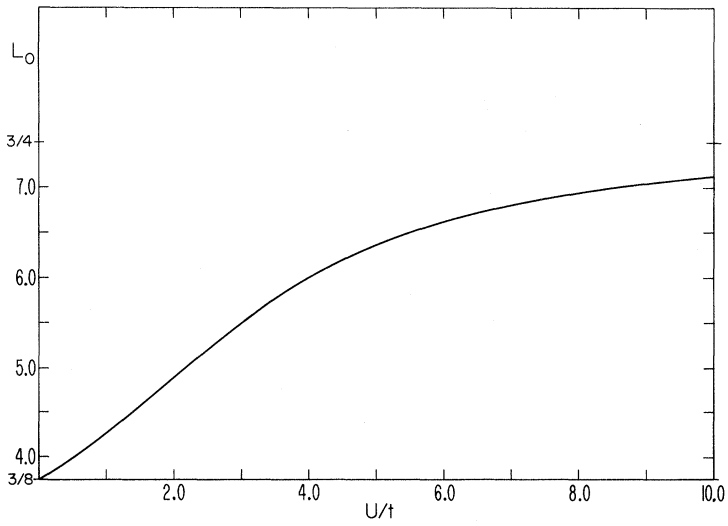


FIG. 9. Correlation function L_0 at $T=0$ °K vs U/t for the infinite chain.

for the one-dimensional system has an insulating ground state.

It is well known[25] that in one-dimensional disordered systems the CPA is not a good approximation for the density of states. So one may argue that, in this sense, Hubbard's theory applied to one-dimensional systems is not reliable. But in our discussions on thermodynamic properties at high temperatures only the gross features of the electronic structure are important. Thus even his approximate theory should be adequate.

In this section we assume that the system is paramagnetic, since we are interested in the high-temperature region. There are some attempts[29,30] to extend Hubbard's theory (his first work on the correlation effect) to the antiferromagnetic phase. But at low temperatures, the detailed structure of the electronic state neglected in his theory may play an important role.

According to Hubbard, the one-particle Green's function with wave vector $\vec{k}$, energy ω, and spin σ for the Hamiltonian [Eq. (1.1)], plus a Zeeman term due to the uniform magnetic field, can be written as

$$G_{\vec{k}\sigma}(\omega)=\frac{1}{F_\sigma(\omega+\sigma\mu_B H)-\epsilon_{\vec{k}}} \qquad (\sigma=+ \text{ or } -)\,, \quad (4.1)$$

where the inverse of the locator $F_\sigma(\omega)$ is related to the "atomic self-energy" $\Omega_\sigma(\omega)$ by

$$\frac{1}{F_\sigma(\omega)}=\frac{\omega-U(1-\langle n_{-\sigma}\rangle)-\Omega_\sigma(\omega)}{[\omega-\langle n_{-\sigma}\rangle\Omega_\sigma(\omega)][\omega-U-(1-\langle n_{-\sigma}\rangle)\Omega_\sigma(\omega)]-\Omega_\sigma^2(\omega)\langle n_{-\sigma}\rangle(1-\langle n_{-\sigma}\rangle)}\,. \quad (4.2)$$

The "atomic self-energy" $\Omega_\sigma(\omega)$, which describes the scattering processes, consists of three distinct contributions:

$$\Omega_\sigma(\omega)=\Omega'_\sigma(\omega)+\Omega'_{-\sigma}(\omega)-\Omega'_\sigma(U-\omega)\,, \quad (4.3)$$

where the first term of the right-hand side is called the scattering correction and the second and third terms are the resonance broadening corrections. Now the self-energy $\Omega'_\sigma(\omega)$ is connected with $F_\sigma(\omega)$ by the self-consistency equation

$$\Omega'_\sigma(\omega)=F_\sigma(\omega)-[(1/N)\textstyle\sum_{\vec{k}} G_{\vec{k}\sigma}(\omega)]^{-1}\,. \quad (4.4)$$

This is a brief summary of mathematics of Hubbard's theory. These four equations [Eqs. (4.1)–(4.4)] form a set of equations in Hubbard's theory.

Since in our case the unperturbed density of states $\rho(\omega)$ given in (2.3) is simple and symmetric with respect to its center, and our system is assumed half filled, these coupled equations can be simplified to a large extent. In fact, by using (2.3) we find that

$$\frac{1}{N}\sum_{\vec{k}} G_{\vec{k}\sigma}(\omega)=\frac{i}{[(\tfrac{1}{2}\Delta)^2-F_\sigma(\omega)^2]^{1/2}}\,. \quad (4.5)$$

Thus, choosing the origin of the energy at $U/2$, we obtain the following cubic equation for the locator $F(\omega)$ in the case of zero magnetic field:

$$6\omega F^3+(9[\omega^2-(\tfrac{1}{2}\Delta)^2]-\{16\omega^2+6[\omega^2-(\tfrac{1}{2}U)^2]\})F^2$$
$$+\{8\omega[\omega^2-(\tfrac{1}{2}U)^2]+18\omega(\tfrac{1}{2}\Delta)^2\}F$$
$$+\{-[\omega^2-(\tfrac{1}{2}U)^2]^2-9\omega^2(\tfrac{1}{2}\Delta)^2\}=0\,. \quad (4.6)$$

It is easy to find the density of states $D(\omega)$,

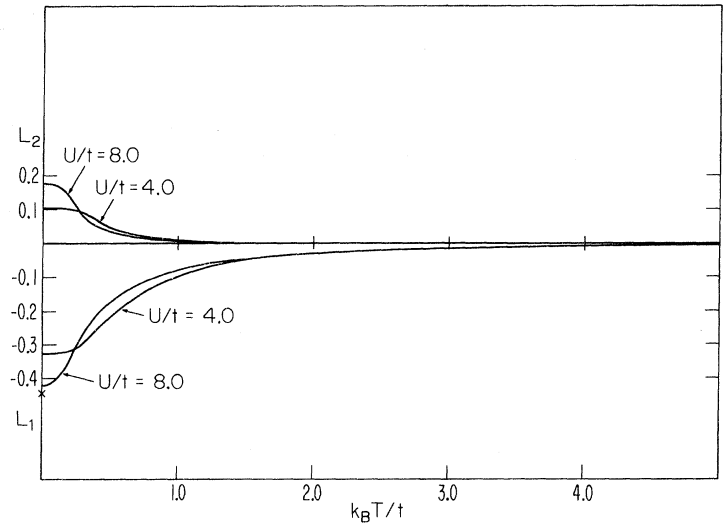


FIG. 10. Temperature dependence of the correlation function $L_\delta(\delta=1, 2)$, which gives us the information on the spin correlation on different sites. The total number N of atoms is six. The cross shows the value of L_1 for the infinite antiferromagnetic Heisenberg chain obtained from the exact solution (Refs. 12 and 13) (see the text). The upper part of this figure shows L_2 and the lower part indicates the temperature dependence of L_1.

$$D(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\frac{1}{N}\sum_k G_k(\omega)\,, \tag{4.7}$$

by solving Eq. (4.6). Figure 11 shows the profile of $D(\omega)$ for two typical values of U/t. The critical value, at which the energy gap first appears at $\omega = 0$, is given by

$$U_{cr}/\Delta = \tfrac{1}{2}\sqrt{6}\ . \tag{4.8}$$

Incidentally, this value is larger than the value $\frac{1}{2}\sqrt{3}$ obtained by Hubbard,[1] assuming that $\rho(\omega)$ is elliptic, because in our case the unperturbed density of states is very large at the band edges.

Once the locator $F(\omega)^{-1}$ is found from Eq. (4.6), it is straightforward to calculate specific heat, magnetic susceptibility, etc. Here we sketch the derivation of the formulas needed to calculate these quantities and show our numerical results.

A. Specific Heat

The average of the energy,

$$\langle \mathcal{H} \rangle = -\sum_{ij\sigma} t_{ij}\,\langle C^\dagger_{i\sigma} C_{j\sigma}\rangle + U\sum_j \langle n_{j\uparrow} n_{j\downarrow}\rangle\,, \tag{4.9}$$

can be expressed in terms of a one-particle Green's function in the form[31]

$$\begin{aligned}\langle \mathcal{H} \rangle &= \sum_k \int_{-\infty}^{\infty} d\omega f(\omega)(\omega+\epsilon_k)\left(-\frac{1}{\pi}\right)\mathrm{Im}\,G_k(\omega) + \tfrac{1}{2}UN \\ &= \int_{-\infty}^{\infty} d\omega f(\omega)\left(-\frac{1}{\pi}\right)\mathrm{Im}\left((\omega+F)\sum_k \frac{1}{F-\epsilon_k}\right) + \tfrac{1}{2}UN\,,\end{aligned} \tag{4.10}$$

where the Fermi distribution function is $f(\omega)$. Since the chemical potential always stays at zero irrespective of temperature, we have for the specific heat

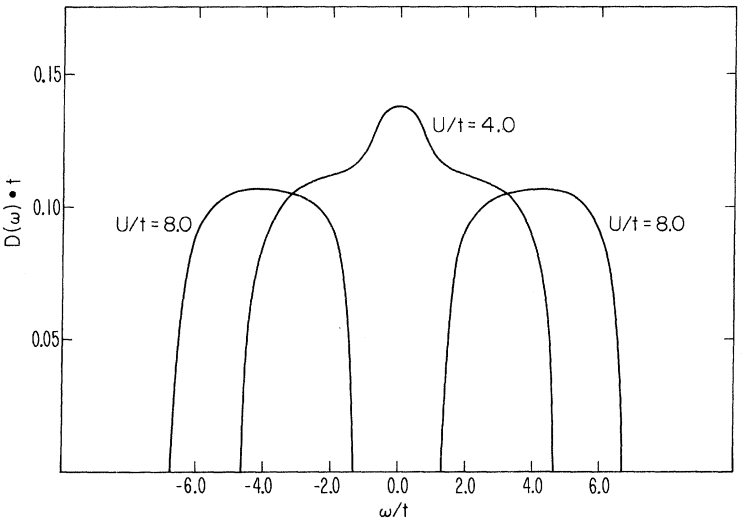


FIG. 11. Density of states $D(\omega)$ of one-particle excitations which Hubbard's approximate theory predicts for the one-dimensional half-filled-band Hubbard model. The system is assumed to be paramagnetic. Two typical values of U/t are chosen.

$$\frac{C}{Nk_B}=\int_{-\infty}^{\infty}\frac{d\omega}{k_BT}\,\frac{\omega}{k_BT}\left(2\cosh\frac{\omega}{2k_BT}\right)^{-2}\left(-\frac{1}{\pi}\right)\times\mathrm{Im}\left((\omega+F)\frac{1}{N}\sum_k\frac{1}{F-\epsilon_k}\right)\,. \quad (4.11)$$

B. Static Uniform Magnetic Susceptibility

In order to determine the expression for the susceptibility, we must retain all linear terms in the magnetic field. In Hubbard's formulation the scattering processes included in $\Omega_\sigma(\omega)$ are changed by the magnetic field through the average number of electrons $\langle n_\sigma\rangle$. Thus there are extra contributions besides the shift of the energy bands due to the magnetic field. Carefully retaining linear terms in Eqs. (4.1)–(4.4), we finally find that

$$\frac{\chi}{2\mu_B^2N}=\int d\omega\left(-\frac{\partial f}{\partial\omega}\right)\left(-\frac{1}{\pi}\right)\mathrm{Im}\,Z\Big/\left[1+U\int d\omega f(\omega)\left(-\frac{1}{\pi}\right)\mathrm{Im}\left(\frac{(\frac{1}{2}U)^2-(\omega-F)^2}{(\frac{1}{2}U)^2-(1-ZF)(\omega-F)^2}Z^3F\right)\right]\,, \quad (4.12)$$

where $Z=(1/N)\sum_k G_k(\omega)$. In the above expression the numerator comes from the shift of energy band, while the second term in the denominator arises from the change of the scattering processes.

C. Magnitude of Local Moments

It is not difficult to obtain the formula for the magnitude of local moments L_0 introduced in Sec. III:

$$L_0(T)=(3/N)\textstyle\sum_j\langle(S_j^z)^2\rangle = (3/2N)\sum_j\langle n_{j\uparrow}(1-n_{j\downarrow})\rangle\,, \quad (4.13)$$

where the average $\langle n_{j\uparrow}(1-n_{j\downarrow})\rangle$ can be calculated from the retarded Green's function $\langle\langle(1-n_{j\downarrow})C_{j\uparrow};\ C_{j\uparrow}^\dagger\rangle\rangle$ by using the spectral theorem

$$\langle n_{j\uparrow}(1-n_{j\downarrow})\rangle=\int_{-\infty}^{\infty}d\omega f(\omega)\,(-1/\pi)\times\mathrm{Im}\,\langle\langle\,(1-n_{j\downarrow})\,C_{j\uparrow};\,C_{j\uparrow}^\dagger\rangle\rangle\,. \quad (4.14)$$

Here the retarded Green's function $\langle\langle A;\ B\rangle\rangle$ is defined by

$$\langle\langle A;\ B\rangle\rangle=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\,(-i)\,\langle[A(t),\ B(0)]_+\rangle\,, \quad (4.15)$$

where $[\ ,\ ]_+$ denotes the anticommutator, and $A(t)$ is the Heisenberg representation of the operator A. Since in Hubbard's theory the Green's function $\langle\langle(1-n_{j\downarrow})C_{j\uparrow};\ C_{j\uparrow}^\dagger\rangle\rangle$ is related to the one-particle Green's function $\langle\langle C_{j\uparrow};\ C_{j\uparrow}^\dagger\rangle\rangle$ by a simple expression, we easily find that

$$L_0(T)=\frac{3}{4}\int_{-\infty}^{\infty}d\omega f(\omega)\left(-\frac{1}{\pi}\right)\mathrm{Im}\frac{\frac{1}{2}U-\omega+F}{\frac{1}{2}U}\sum_k G_k(\omega)\,. \quad (4.16)$$

Figures 12–14 show the temperature dependence of the specific heat, susceptibility, and the magnitude of local moments, respectively, at a typical value of U/t. In this theory the contribution to the specific heat is associated with single-particle excitations across the so-called Hubbard gap. The susceptibility decreases at low temperature because of this gap. However, spin-wave contributions which are neglected in this Hubbard theory are actually important for the low-temperature behavior of the specific heat as well as the susceptibility. For the same reason, the decrease of the magnitude of local moments clearly observed in Fig. 8 is lacking in Fig. 14. Comparing these figures

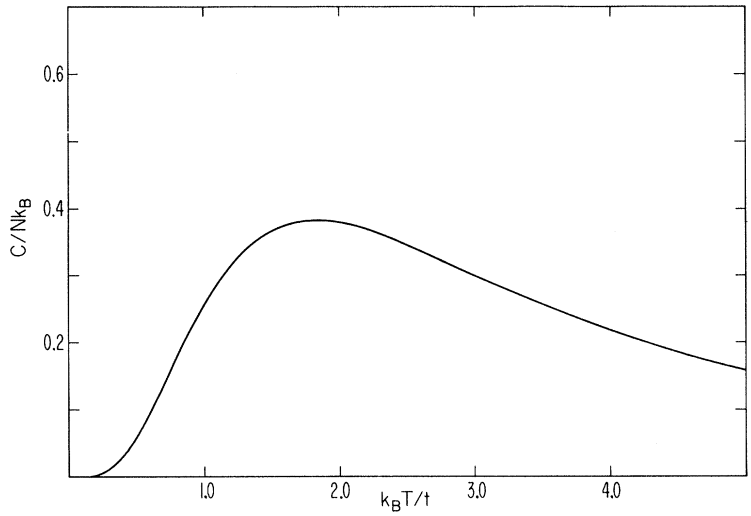


FIG. 12. Temperature dependence of specific heat according to Hubbard's approximation. The system is assumed to be paramagnetic. The parameter U/t is taken as 8.

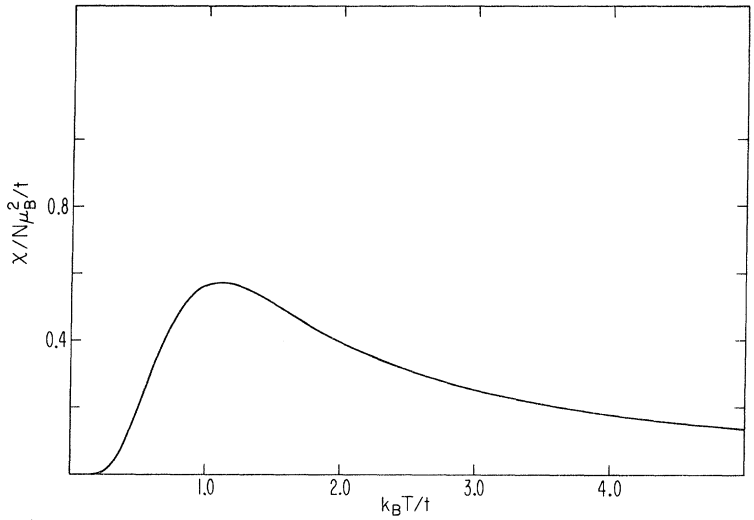


FIG. 13. Variation of the susceptibility $\chi/(N\mu_B^2/t)$ with temperature, which Hubbard's approximation gives under the assumption that the system is paramagnetic throughout the entire temperature domain.

with the results for finite systems shown in Secs. II and III, we find that, in the high-temperature region, say, $k_B T > 1.5t$, Hubbard's theory gives fairly good results, when $U/t = 8$, judging from our exact calculations. We believe the reason for this is that at high temperatures most states contribute with almost equal weight, and therefore the motion of an electron may be regarded in some sense as random. In the calculation of the specific heat [see, for instance, Fig. 1(c)] the convergence is so slow that it is difficult to extrapolate to the infinite chain. But with the aid of Hubbard's theory we guess that the second peak of the specific heat is located at slightly lower temperature than $U/4k_B$.

V. DISCUSSION

In order to obtain a feeling for the finite-temperature properties of the one-dimensional half-filled-band Hubbard model, we have calculated various thermodynamic quantities and correlation functions. The picture we have obtained is the following: When $U/\Delta \gtrsim 1$, we can discriminate two temperature regions. In the high-temperature region around $U/4k_B$ the gradual formation of local moments occurs, while in the low-temperature region the short-range antiferromagnetic ordering is dominant for the thermal behavior. When U/Δ becomes small, passing through the intermediate region located around 1, the two regions overlap with each other and the thermal properties of our system are essentially the same as those of the noninteracting system, except for some slight modifications such as the enhancement of the susceptibility, etc.

When U is small compared with Δ, we can apply

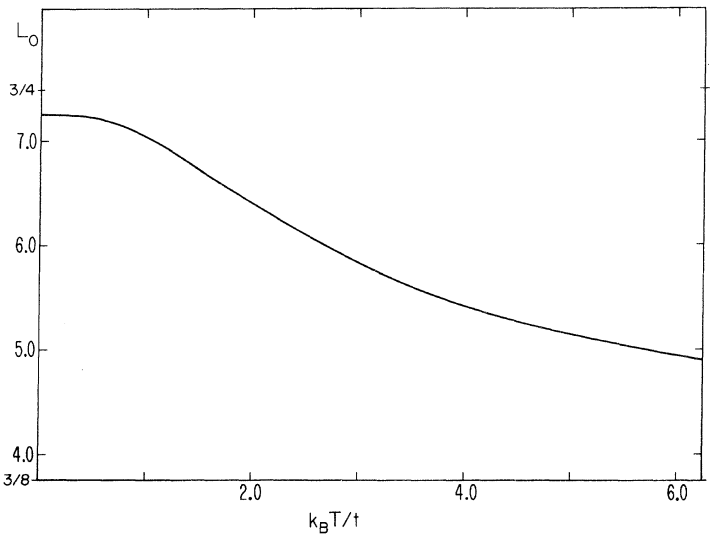


FIG. 14. Magnitude of local moments L_0 vs temperature according to Hubbard's approximation for paramagnetic state.

the molecular-field approximation (or, more generally, the random-phase approximation) to our system. Although the molecular-field approximation predicts long-range antiferromagnetic ordering at low temperatures, the order parameter is so small in this region of U that the singularity at the Néel point is not appreciable. In fact, we find that for $U/\Delta \lesssim \frac{1}{2}$ the random-phase approximation gives semiquantitatively reasonable results.[32]

The behavior of the thermodynamic properties, including some correlation functions, for $U/\Delta \gtrsim 1$ is interesting in connection with a controversial problem of localized-spin-like behaviors in itinerant-electron ferromagnets. Some authors[33,34] have tried to approach this question by using the functional integral method, but unfortunately this has not vastly improved the situation. For the itinerant-electron antiferromagnet there is an attempt[35] based on the molecular-field approximation, but it is also far from convincing. Although our model is very simple, we hope our results have clarified some aspects of the complicated intermediate situation between localized and itinerant magnetism.

As our studies are restricted to the one-dimensional system, we cannot say anything convincing beyond this, but we conjecture from our results that in three-dimensional system, when U/Δ is large, the formation of local moments in the high-temperature region will still stay gradual and broad, while the antiferromagnetic correlation at low temperature will turn into a long-range ordering.

Note added in proof. In this work we applied the canonical ensemble method, which is appropriate to "real" molecules. The results of the application of the grand canonical ensemble, which is more useful for extrapolation to the infinite system, will be published in the near future.

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†On leave from Department of Physics, Faculty of Science, Osaka University, Osaka, Japan.

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[22]We limited ourselves to less than six atoms. Judging from the paper by Bonner and Fisher and our results, it is necessary to extend the calculation to ten or twelve atoms in order to get extrapolations quantitatively as reliable as those of Bonner and Fisher. But a ring of $N=10$ was too large for us to handle. For semiquantitative conclusions a ring with less than six atoms is sufficient.

[23]We have not given any rigorous proofs that the ordering is short ranged in the infinite system. But since our system is one dimensional and isotropic and has short-range interactions, it is natural to believe that there is no long-range order in the infinite one-dimensional Hubbard model.

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Nonlinear Effects in the Critical Dynamics of Easy-Axis Ferro- and Antiferromagnets *

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Approximate kinetic equations have been derived for the critical dynamical variables of easy-axis ferro- and antiferromagnets. Particular attention is paid to nonlinear couplings and their influence on the dynamics of the long-wavelength fluctuations of the order parameter. The nonlinear nature of the problem is reflected in the inverse reduced-susceptibility matrix. When only the linear susceptibilities are retained the equations reduce to those of Schwabl and Michel. Including both linear and nonlinear susceptibilities leads to a number of new effects. Among these are the renormalization of the decay rates, a change below T_c in the relative weights of the two central peaks in the linear dynamical susceptibility of the antiferromagnetic order parameter, and the introduction of a high-frequency background in the order-parameter power spectrum. Provided the thermodynamic scaling laws are obeyed, these effects are essentially independent of temperature. An experimental test of the theory involving measurements of the width of the imaginary part of the dynamic susceptibility of the ferromagnetic order parameter at corresponding temperatures above and below T_c is proposed.

I. INTRODUCTION

According to the current interpretation,[1] insofar as the critical dynamics is concerned, magnetic systems undergoing second-order phase transitions fall into two categories. In the first category are the so-called conventional systems, which are characterized by the property that, as the critical point is approached from the high-temperature side, the fluctuations in the order parameter decay at a rate which, in the first approximation, is inversely proportional to the corresponding susceptibility. The unconventional or strong-coupled systems are those where the decay rate has a weaker temperature dependence. Easy-axis ferro- and antiferromagnets are in the first category, while isotropic and planar ferro- and antiferromagnets are in the second. (In applying these criteria it must be kept in mind that when the anisotropy is weak, e.g., MnF_2, fully conventional behavior may be realized only at temperatures very close to T_c; at higher temperatures the dynamics may resemble that of isotropic systems.[2])

The purpose of this paper is to examine in detail the critical dynamics of conventional systems, with particular emphasis on the nonlinear effects. The approach will be sufficiently general to encompass both ferro- and antiferromagnets at temperatures above and below the critical temperature. The starting point in the analysis is a set of kinetic equations for the critical dynamical variables which was obtained recently by Kawasaki.[3] As discussed by him the critical dynamical variables are those variables whose long-wavelength fluctuations decay very slowly near the critical point. Included in this set are the hydrodynamic variables as well as the order parameter, if the latter is not conserved. In addition, in a nonlinear theory one must also include products of these variables. For easy-axis ferromagnets the critical variables are combinations of the energy density and the magnetic-moment density along the preferred axis. If the Hamiltonian has the property of being invariant with respect to spin rotations about the preferred axis, then the order parameter is also a hydrodynamic variable. In the case of easy-axis antiferromagnets the critical dynamical variables are normally the energy density, the magnetization density (provided the system has the rotational symmetry mentioned above), and the staggered-moment density along the preferred axis. Since the uniform field susceptibility of an antiferromagnet remains finite at the critical point, the fluctuations in the magnetization do not behave anomalously. Furthermore, in the absence of an external field, which we will henceforth assume, there is no linear thermodynamic coupling between the magnetization and either the staggered magnetization or the energy. Although nonlinear