High-Temperature Thermodynamics of the Strongly Correlated Hubbard Model at Arbitrary Electron Density

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We consider the Hubbard model for electron correlations in solids in the narrow-band regime where the intra-atomic Coulomb repulsion is large compared to the bandwidth. A high-temperature pertubation expansion in the bandwidth is performed to lowest order for the grand partition function. This procedure is carried out both for one-dimensional systems, of interest for the tetracyanoquinodimethan (TCNQ) charge-transfer salts, and for a three-dimensional cubic lattice. Both the specific heat and magnetic susceptibility are computed as functions of temperature and electron density.

INTRODUCTION

The Hubbard model[1] for metallic magnetism and, in general, for electron correlation in solids, has been adopted by various authors[2] as a satisfactory model to describe the behavior of the charge-transfer salts in which experiments[3] indicate that correlation effects may be dominant. In fact, these materials [e.g. tetracyanoquinodimethan (TCNQ) salts] often crystallize in the form of linear chains of closed-shell cations separated by stacks of molecular anions with unparied electrons. The electrons can transfer along the chains via π overlaps, thus providing a possible physical realization of the model described by the one-dimensional Hubbard Hamiltonian, which can be written in its simplest form as

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{i,\sigma} (c^\dagger_{i\sigma} c_{i+1,\sigma} + \text{c.c.}) . \qquad (1)$$

Here U is the Coulomb repulsion that operates when two electrons occupy the same orbital, t is the electron transfer integral connecting states localized on nearest-neighbor molecules, $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ are, respectively, creation and annihilation operators for an electron of spin σ on the ith site, and $n_{i\sigma}$ is the number of electrons with spin σ on the ith site.

However, this model, although simple in form, is not easy to handle mathematically even for a linear chain and often one cannot obtain any exact results but is obliged to resort to approximations. There do exist a few exact solutions for infinite-chain problems. Lieb and Wu[4] obtained the ground-state energy in an analytic form for the half-filled case (one electron per site) and proved that the ground state is both antiferromagnetic and insulating. Takahashi[5] and Ovchinnikov[6] calculated (also for a half-filled band) the magnetic susceptibility at zero temperature and some elementary excitations, respectively. Their work has been subsequently extended to an arbitrarily filled system by Shiba,[7] who gave the ground-state energy and the zero-temperature magnetic susceptibility, and by Coll,[8] who calculated some low-lying excitations.

Unfortunately, no exact solution exists for the finite-temperature properties of the Hubbard model, either arbitrarily filled or simply half-filled (except for some special values of the parameters t and U).[9–12] On the other hand, these thermodynamic properties have recently been the object of an increasing interest because it is precisely the thermal behavior that appears to be most remarkable in the charge-transfer salts. As an example, N-methylphenazinium (NMP) (TCNQ) exhibits a "metal-insulator transition" which has been observed by Epstein *et al.*[13] and discussed within the context of the Hubbard model.

Therefore it is quite natural that in an attempt to interpret the available experimental results and to make some significant predictions, various approximate approaches have been proposed. First of all, it should be mentioned that Hubbard presented a treatment of the correlation effect in his paper on the Mott transition.[1] Basically, he applied a modification of the coherent-potential approximation[14–18] (CPA) to this case. Although it is well known[15] that in one-dimensional systems the CPA is not a good approximation for the density of states, Hubbard's work provides a useful framework if only the gross features of the electronic structure are important. This is certainly true at high temperatures where Hubbard's approximate theory can be used for a semiquantitative comparison with more accurate descriptions. Subsequently, Shiba and Pincus[19] studied the half-filled Hubbard model for linear chains and rings containing two

to six atoms, by performing exact machine computations. For these finite systems and for several values of the ratio U/t they calculated exactly the specific heat, magnetic susceptibility, entropy, internal energy, and some correlation functions. The results obtained in this way indicated that when $U/t \geq 1$ it is possible to distinguish two temperatures ranges: a low-temperature region, in which the short-range antiferromagnetic ordering is dominant, and a high-temperature region, in which the gradual formation of local moments occurs around $U/4k_B$ (k_B is the Boltzmann constant). When U/t becomes smaller than 1, the two regions tend to overlap and the thermal properties of the model differ only slightly from those of the noninteracting system. Following this work, Hone and Pincus[20] concentrated on the strongly correlated limit ($U/t \gg 1$) and studied the high-temperature behavior, both static and dynamic, of the half-filled Hubbard model by carrying out a high-temperature perturbation expansion in t/U and in t/k_BT (T is the temperature). The results are in good agreement with the exact calculations for finite linear chains[19] and although restricted to high temperatures, they extend far enough to include the metal-insulator transition.

In the present paper we generalize this analysis to a system with an arbitrary concentration of electrons. This generalization is motivated by our concern with doped charge-transfer salts (CTS) as well as with CTS which crystallize in chains occupied with an average of less than one electron per site (e.g., one-quarter-filled band) such as (quinolinium)$(TCNQ)_2$.[3] With the same method we also investigate the magnetic susceptibility of a simple cubic lattice. This latter study relates to the question of the conditions for ferromagnetism in a simple tight-binding metal.

In Sec. II we review the high-temperature-expansion method and describe its application to our problem. In Sec. III we present and discuss the numerical results for the temperature dependence of the specific heat and the magnetic susceptibility. In Sec. IV we calculate the magnetic susceptibility for a three-dimensional simple cubic lattice and a brief discussion in Sec. V concludes this work.

II. HIGH-TEMPERATURE EXPANSION

We assume that in the Hamiltonian (1), $t/U \ll 1$ and we consider the temperature region in which $t/k_BT \ll 1$. With these restrictions our Hamiltonian can be thought of as consisting of two terms:

$$H = H_0 + H' , \tag{2}$$

where H_0 is the exactly soluble part,

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow} , \tag{3}$$

and H' is to be treated as a perturbation,

$$H' = t \sum_{i,\sigma} (c^\dagger_{i\sigma} c_{i+1,\sigma} + \text{c. c.}) . \tag{4}$$

It is shown in standard works on statistical mechanics[21] that the grand partition function of a system of interacting particles described by a Hamiltonian $H = H_0 + H'$ is given (under rather general conditions) by the infinite-order expansion

$$Z = e^{-\beta\Omega_0}\left(1 + \sum_{n=1}^{\infty} (-1)^n \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \times \int_0^{\tau_{n-1}} d\tau_n \, \langle H'(\tau_1) H'(\tau) \cdots H'(\tau_n) \rangle_0\right) , \tag{5}$$

where $\beta = 1/k_BT$, Ω_0 is the thermodynamic potential for the unperturbed system, and $\langle\ \rangle_0$ represents an average over the grand canonical ensemble of the unperturbed system, but using the correct chemical potential. $H'(\tau)$ is the perturbative part of the Hamiltonian which in the interaction picture becomes

$$H'(\tau) = e^{\tau H_0} H' e^{-\tau H_0} . \tag{6}$$

We shall now apply (5) to the Hubbard model. Having made the strong-correlation and high-temperature assumptions, we are allowed to truncate the expansion for Z to the lowest-order term in τ. Further, by inspection of Eq. (4), we notice that the lowest-order nonvanishing term in t involves the transfer of an electron from one site to a nearest neighbor and then its return, i.e., it is of order t^2. Thus the grand partition function of our system is reduced to

$$Z \simeq e^{-\beta\Omega_0} (1 + \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \, \langle H'(\tau_1) H'(\tau_2) \rangle_0) . \tag{7}$$

It is now easy to evaluate Z by considering all possible electron occupancies of a pair of adjacent sites and we obtain

$$\beta\Omega = -\ln Z = -\frac{N_A}{\beta}\left[\ln z_0 + \frac{2(\beta t)^2}{z_0^2}\left(e^{\beta\mu} + e^{-\beta U + 3\beta\mu}\right)\cosh\beta h + \frac{4}{z_0^2}\left(\frac{\beta t^2}{U}\right) e^{2\beta\mu}\left(1 - e^{-\beta U}\right)\right] , \tag{8}$$

where Ω is the thermodynamic potential, N_A is the number of sites in the chain, μ is the chemical potential, z_0 is the site partition function

$$z_0 = 1 + 2e^{\beta\mu}\cosh\beta h + e^{2\beta\mu - \beta U} , \tag{9}$$

and $h = \mu_B B$ is the product of the Bohr magneton and an external constant magnetic field B.

The next step is to evaluate μ. For the half-filled band we have simply $\mu = \frac{1}{2}U$, by particle-hole symmetry. But for an arbitrarily filled band, μ must be calculated as a function of the electron density and temperature from the thermodynamic relation

$$N = -\left.\frac{\partial\Omega}{\partial\mu}\right|_{\beta,V,h}, \tag{10}$$

where N is the number of electrons in the chain. From (8) and (10) we obtain the equation

$$\rho = \frac{2(x+x^2e^{-\beta U})}{z_0} + \frac{2x}{z_0^2}\left[(\beta t)^2(1+3x^2e^{-\beta U}) + 4(1-e^{-\beta U})(\beta t^2/U)x\right] - \frac{8(x+x^2e^{-\beta U})}{z_0^3}\left[(\beta t)^2(x+x^3e^{-\beta U}) - 2(1-e^{-\beta U})(\beta t^2/U)x^2\right], \tag{11}$$

where $x = e^{\beta\mu}$ and ρ is the electron density ($\rho = N/N_A$). We have solved Eq. (11) numerically for $\rho = 0.1$, 0.25, 0.5, 0.75, 0.9; and for $t/U = 0$, $\frac{1}{12}$, and $\frac{1}{8}$. In this way we have obtained the temperature dependence of the chemical potential μ (and thus of the thermodynamic potential Ω) as a function of the electron density and the correlation strength. From these results it is straightforward to compute the specific heat

$$c_V = k_B\beta^2 \frac{\partial^2}{\partial\beta^2} \ln Z \tag{12}$$

and the static magnetic susceptibility

$$\chi = \lim_{h\to 0} -N_A\mu_B^2 \frac{\partial^2\Omega}{\partial h^2} . \tag{13}$$

For particular values of the electron density ρ, i.e., for an almost empty band and for a quasi-half-filled band, we have also derived approximate algebraic expressions which complement our description of the specific heat and the magnetic susceptibility.

In Sec. III we present and discuss our results for the temperature dependence of these thermodynamic properties.

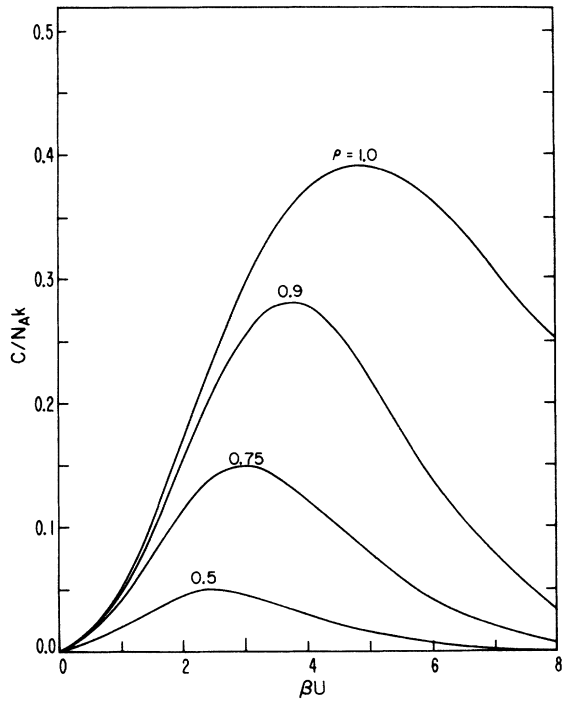


FIG. 1. Temperature dependence of specific heat in the atomic limit ($t = 0$) for electron densities ranging from 0.5 to 1.

III. SPECIFIC HEAT AND MAGNETIC SUSCEPTIBILITY

Figures 1 – 5 show the temperature dependence of the specific heat for different electron densities, from a quasiempty band to a half-filled band, and for different ratios t/U (0, $\frac{1}{12}$, $\frac{1}{8}$). We remind the reader that, at least for large U/t, a peak is expected in the specific heat at a temperature corresponding to the onset of appreciable thermal excitation of doubly occupied sites. For the limiting case $t = 0$ this is simply the Schottky anomaly associated with the simple electronic spectrum of two sharp levels separated by an energy U. This general feature persists as the sharp levels broaden into bands for large U/t. In order to separate the effects of changes in electron density and of Coulomb correlation, we first consider the modification of this peak by changes in ρ for the atomic limit ($t = 0$). In Figs. 1 and 4 we observe not only the obvious decrease in height to be expected with decreasing density, but also a shift of position toward higher temperatures. This behavior persists at very small densities (see Fig. 4) and, for a nearly empty band ($\rho = 0.1$), the peak occurs roughly at $T = U/2k_B$, while for the half-filled band it occurs at a temperature slightly lower than $U/4k_B$. Thus a decrease in electron density results in an increase of the thermal energy required to impose a significant number of doubly occupied sites. The effects of Coulomb correlation are illustrated in Figs. 2, 3, and 5. If the band is more than one-quarter filled ($\rho = 1$, 0.9, 0.75) the peak position changes, but only slightly, with respect to the corresponding curves for the atomic limit. An increase in the electron correlation, however, corresponds to a lower peak in the half-filled and nearly-half-filled cases, while for all other cases the peak height increases with U/t.

More drastic is the effect of correlation at low densities. Even for the quarter-filled band we notice a progressive disappearance of the peak

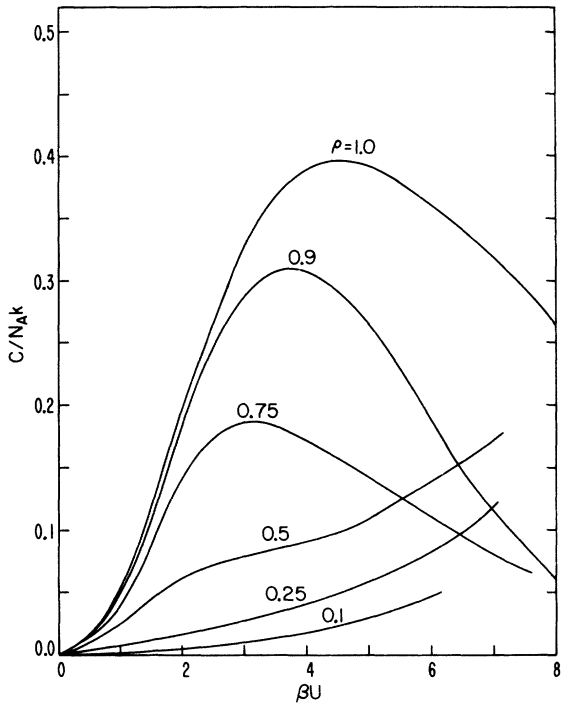


FIG. 2. Temperature dependence of the specific heat for $t/U=\frac{1}{12}$ and for electron densities $\rho=1$, 0.9, 0.75, 0.5, 0.25, 0.1.

while t/U increases, and the tendency to form a new maximum at lower temperature is evident. For lower electron densities (see Fig. 5) these effects are more pronounced. With $\rho=0.1$ and even for t/U as small as $\frac{1}{12}$ the specific-heat peak evident for $t=0$ has been washed out, and c_V is monotonically increasing. In Fig. 5(b) we see how far this process has advanced already by the time $t/U=\frac{1}{100}$. The rise of c_V beyond $\beta U\approx 6$ indicates the development of a second, low-temperature specific-heat maximum, whose origin is probably the antiferromagnetic short-range ordering. As t/U increases, this contribution overwhelms the high-temperature peak, leading to the monotonic behavior seen in Fig. 5(a). For these low densities ($\rho\leq 0.1$) we have been able to use the analytic approximation.

$$c_V/N_A k_B=\rho(2(\beta t)^2+\tfrac{1}{4}\rho\{(U\beta)^2\,[1-2(\beta t)^2]e^{-\beta U}$$
$$-12(\beta t)^2\,[2-e^{-\beta U}-(\beta U)e^{-\beta U})\}),$$

whose validity is restricted by the condition $\rho\ll 1$. Finally we may remark that low electron densities seem to correspond to an over-all behavior "shifted" towards higher temperatures.

Let us now turn to the magnetic susceptibility whose temperature behavior is illustrated in Figs. 6–8. From these graphs it is apparent that in our temperature domain the corrections to a simple

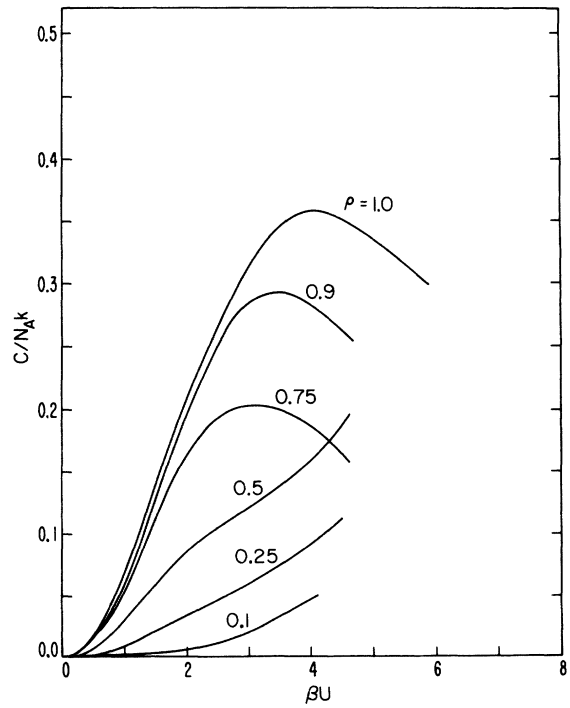


FIG. 3. Temperature dependence of the specific heat for $t/U=\frac{1}{8}$ and for electron densities $\rho=1.$ 0.9, 0.75, 0.5, 0.25, 0.1.

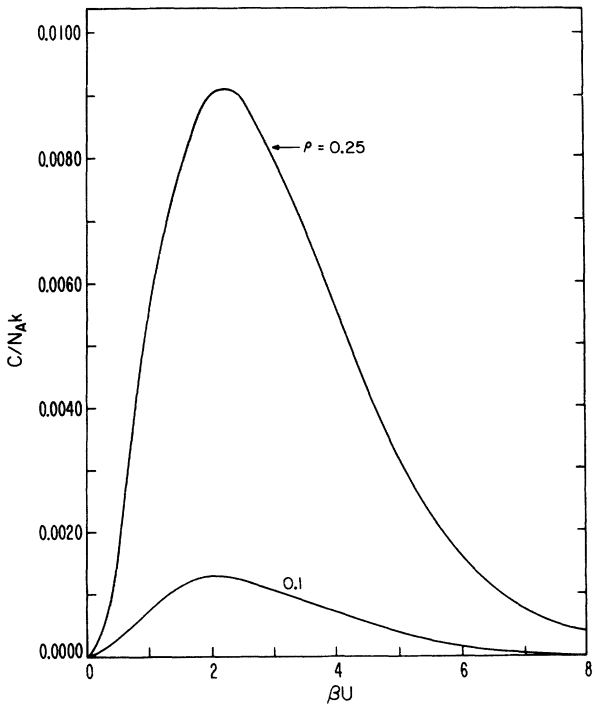
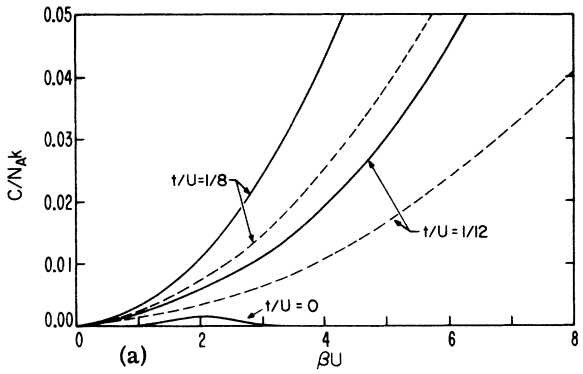


FIG. 4. Temperature dependence of the specific heat for $t=0$ at low electron densities.

Curie law are small at any density for both $t=0$ and $t \neq 0$. For a half-filled band this is not surprising. In fact if the temperature is well above the chemical potential $\frac{1}{2}U$ the electrons are nondegenerate and the Curie law is to be expected.[20] Moreover, the conduction electrons remain nondegenerate at lower temperature since the band gap U/t is large. In fact, as it is shown in Ref. 10 when U/t is increased, the appearance of the Pauli paramagnetism contribution is shifted towards lower temperatures; so we cannot expect to see the saturation characteristic of a Pauli behavior in the magnetic susceptibility at least for a half-filled band. We may add that the magnetic susceptibility



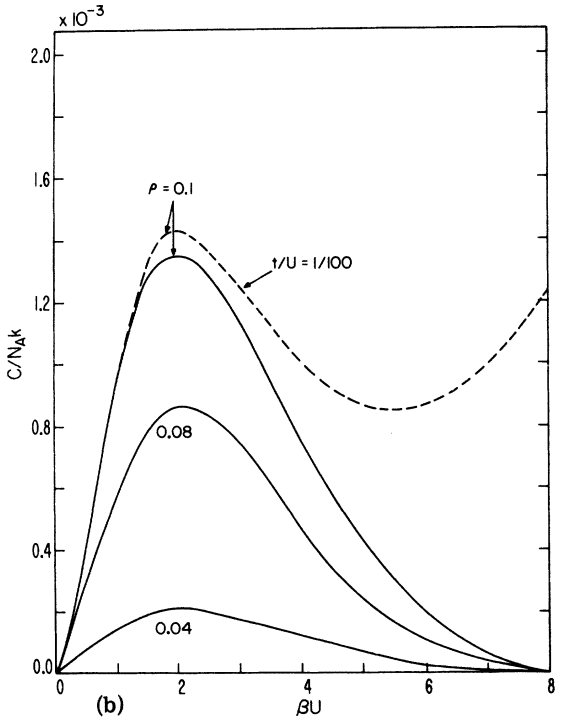


FIG. 5. (a) Temperature dependence of specific heat for $\rho=0.1$ (solid curves) and for $\rho=0.05$ (dashed curves). (b) Specific heat at very low electron densities for $t=0$ (solid curves) and for $t/U=\frac{1}{100}$ (dashed curve).

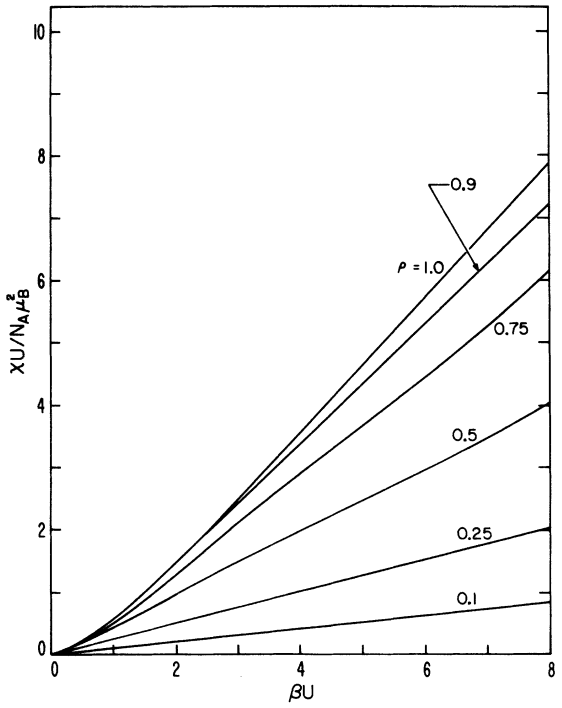


FIG. 6. Magnetic susceptibility in the atomic limit ($t=0$).

for electron densities very close to $\rho=1$ can be obtained algebraically by solving Eq. (11) in the

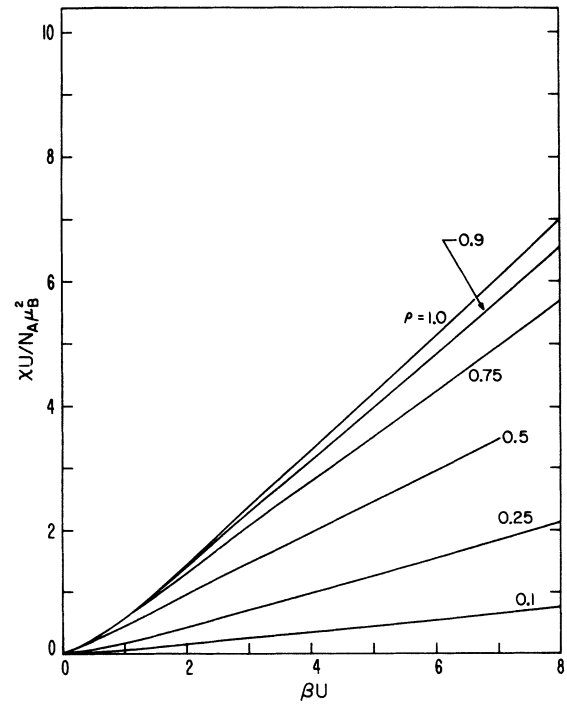


FIG. 7. Magnetic susceptibility for $t/U=\frac{1}{12}$.

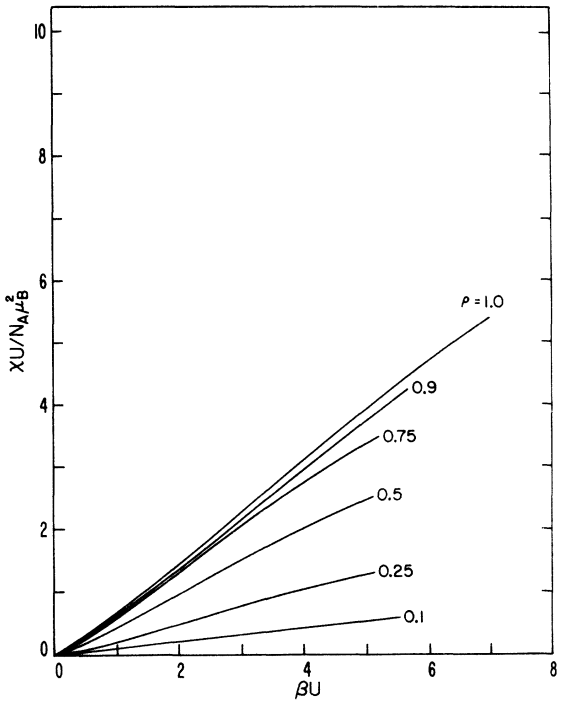


FIG. 8. Magnetic susceptibility for $t/U = \frac{1}{8}$.

approximation $1-\rho \ll 1$ and is given by

$$X = N_A \mu_B^2 \beta \left[1 - (1-\rho)(1 - 4\beta t^2/U) - 2\beta t^2/U\right] .$$

Although the validity of this expression is further restricted by the condition $(1-\rho)^{-2} \ll e^{\beta U}$ it is apparent from it that we have a Curie-Weiss -type susceptibility. The Weiss temperature has a value $\theta \approx 2t^2\rho/U$, which is in accord with a description of the system in terms of Heisenberg Hamiltonian with antiferromagnetic exchange constant $\approx 2t^2\rho/U$.

Next we turn our attention to lower electron densities. First of all, it is useful to make reference to one of the few available exact results concerning the susceptibility of the Hubbard model at arbitrary density, i.e., Ref. 7. In Fig. 4 of Ref. 7 we notice that the zero-temperature magnetic susceptibility per spin for a given ratio t/U increases sharply as the electron density is lowered. Thus, if we assume that the over-all behavior of χ does not change qualitatively with ρ, we may expect the peak position to decrease with ρ.[22]

So, even for low densities, we cannot expect to see any appearance of the maximum in χ. This maximum corresponds to the low-temperature peak in the specific heat; in the region where the second peak of the specific heat was found, there is only a gradual change of the Curie constant. For very low electron densities $\rho < 0.1$ we again find an algebraic solution,

$$\chi = \mu_B^2 N_A \rho\beta \left\{1 - \tfrac{1}{2}\rho\left[e^{-\beta U} + 4(\beta t^2/U)(1 - e^{-\beta U}) - 2(\beta t)^2 e^{-\beta U}\right]\right\},$$

which may be related to the behavior of a Heisenberg antiferromagnet with exchange of the order of $2t^2\rho/U$. In fact, for rather low temperatures, i.e., $e^{\beta U} \gg 1$, this equation takes the form

$$\chi \propto \beta(1 - \theta/T),$$

with

$$\theta \approx (2t^2/U)\rho .$$

We may finally remark that the decrease of the susceptibility with the electron correlation is in agreement with the calculations[22] for finite chains and rings.

IV. SIMPLE CUBIC LATTICE

So far we have considered only second-order terms in t. To this order we take into account only hopping to nearest neighbors and back so the crystal structure enters only trivially through the number of nearest neighbors. If we want to extend our considerations to a simple cubic lattice to observe the effects of higher-order dimensional topologies we must include terms of order t^4 in the evaluation of the expansion (5). We have no terms of odd order in t because there are no closed paths on the lattice with an odd number of near-neighbor steps. The evaluation of Ω is rather lengthy but straightforward. As before we compute the traces in a representation where $n_{i\sigma}$ is diagonal and obtain

$$-\beta\Omega/N_A = \ln z_0 + (6/z_0^2)\left[(\beta t)^2 + (\beta t)^4\right](x + x^3 e^{-\beta U})\cosh\beta h + (12/z_0^2)(\beta t^2/U)x^2(1 - e^{-\beta U}) + (2/z_0^4)(\beta t)^4$$
$$\times (x\cosh\beta h + 4x^2\cosh 2\beta h + x^3\cosh 3\beta h + x^5 e^{-\beta U}\cosh 3\beta h + 4x^6 e^{-2\beta U}\cosh 2\beta h + x^7 e^{-3\beta U}\cosh\beta h). \quad (14)$$

Next we evaluate the chemical potential $\mu(\rho, t/U, \beta)$ from Eq. (10), a computation which in general must again be done numerically. The magnetic susceptibility for arbitrary electron density ρ can then be found from Ω by Eq. (13). The results for $t/U = \frac{1}{12}$ and $t/U = \frac{1}{8}$ are shown in Figs. 9 and 10, respectively. On the other hand, for low densitites we can solve Eq. (10) algebra-

ically, as in the one-dimensional problem, and we obtain

$$\chi = \mu_B N_A \rho\beta \{1 - \tfrac{1}{2}\rho [e^{-\beta U} + 12(\beta t^2/U)(1 - e^{-\beta U}) - 6(\beta t)^2 e^{-\beta U} - 8(\beta t)^4]\} . \quad (15)$$

There are qualitative changes in the magnetic properties of the system as the electron density is varied. In fact, we can see some evidence for a transition from antiferromagnetic to ferromagnetic behavior with decreasing ρ, at sufficiently low temperatures. This is to be expected from the work of Nagaoka,[23] who studied the ground state of the nearly-half-filled band ($|1-\rho| \ll 1$) Hubbard model for small t/U. In particular, he found for the simple cubic lattice that the ground state is ferromagnetic only under the (approximate) condition

$$2t/U < 0.49(1-\rho) - 0.40(1-\rho)^{5/3} \quad (1-\rho \ll 1). \quad (16)$$

This upper bound on t/U clearly increases initially with $(1-\rho)$. Nagaoka also gave arguments to suggest that at lower densities, where these first terms in an expansion in $(1-\rho)$ are no longer adequate, the upper bound on t/U would decrease again to zero at some $\rho > 0$, in agreement with Kanamori's low-density predictions.[24]

Our high-temperature expansion is, of course, not useful very near a ferromagnetic phase transition, where $\chi \to \infty$. However, we do see a change in the sign of the curvature of $\chi(\beta)$ at low temperatures with decreasing ρ. The upward curvature for $\rho \leq 0.5$ suggests the development of ferromagnetic short-range correlations, whereas the negative curvature for $\rho \geq 0.75$ reflects antiferromagnetic behavior. If we take for example the curves for $t/U = \frac{1}{8}$, where the transition between ferromagnetic and antiferromagnetic behavior is more apparent, we may estimate roughly that it occurs at $\rho \simeq 0.6$. For $t/U = \frac{1}{12}$ the critical value of ρ appears to be somewhat higher. If we continue to apply Eq. (16) for this relatively large value of t/U we find $\rho < 0.75$ for a ferromagnetic ground state, in excellent agreement with our interpretation of Fig. 9. Extension of Nagaoka's results to $t/U = \frac{1}{8}$ is less reliable, of course, but he does imply a decrease in the value of ρ required for ferromagnetism.

Furthermore, an approximate analytic solution of Eq. (10) for μ is possible for $e^{-\beta U/2} \ll (1-\rho) \ll 1$. After substitution of this value of μ into Eq. (14) for Ω and subsequent differentiation we find

$$\chi = N_A \mu_B^2 \beta \{1 - (1 \quad \rho)[1 - 12\,(\beta t^2/U) - \tfrac{3}{2}(\beta t)^4] - 6(\beta t^2/U)\}$$

for

$$e^{-\beta U/2} \ll 1 - \rho \ll 1 . \quad (17)$$

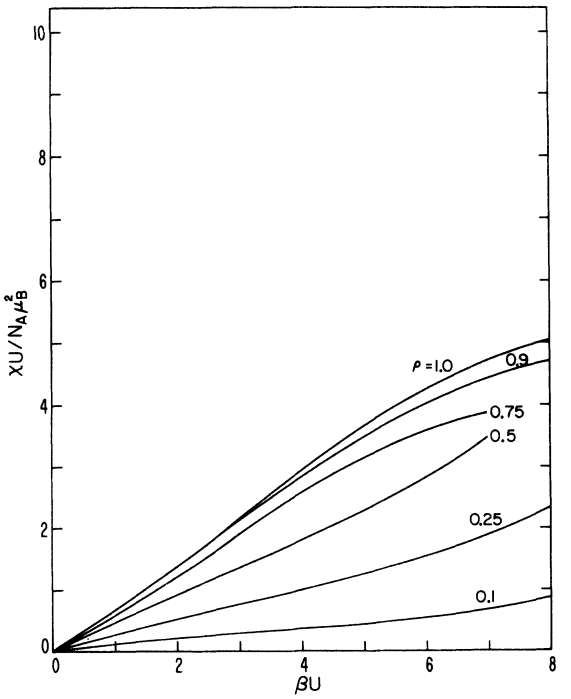


FIG. 9. Temperature dependence of the magnetic susceptibility for a simple cubic lattice ($t/U = \frac{1}{12}$).

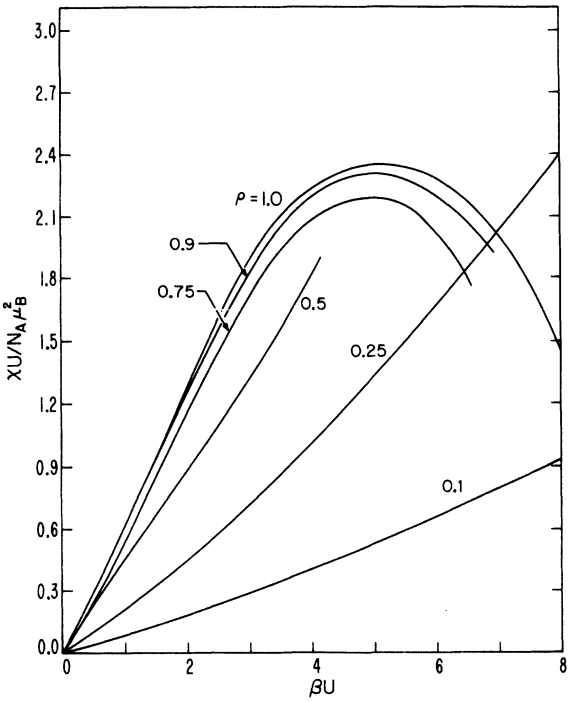


FIG. 10. Temperature dependence of magnetic susceptibility for a simple cubic lattice ($t/U = \frac{1}{8}$).

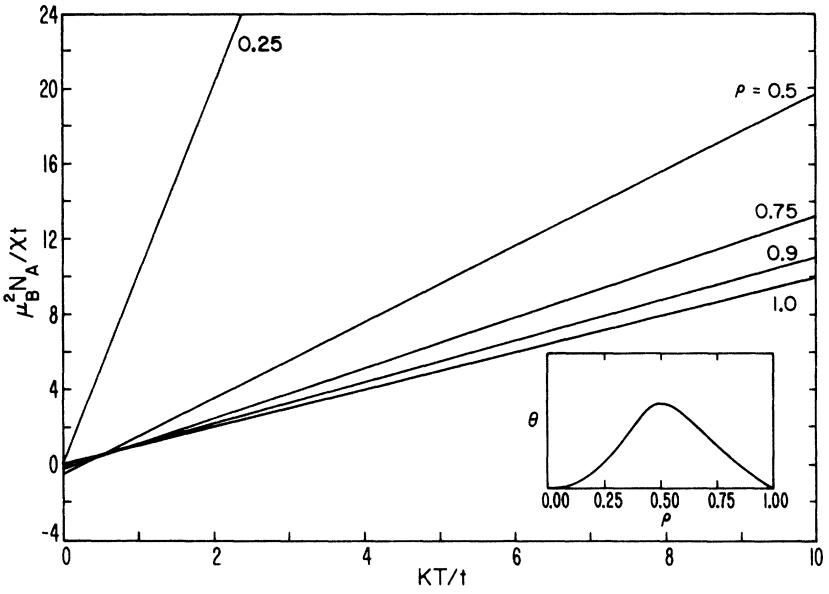


FIG. 11. Temperature dependence of the inverse magnetic susceptibility for a simple cubic lattice for $U=\infty$. The inserted graph of the Curie temperature θ vs electron density ρ has been obtained by extrapolating to zero temperature and should be regarded only as qualitative.

Unless $U/t \gg 1$ the restrictions on $1-\rho$ plus our basic assumption $\beta t \ll 1$ severely limit the temperature domain in which Eq. (17) can be applied. However, the result does provide a simple approximate criterion for the onset of ferromagnetic behavior—that the expression within curly brackets becomes greater than unity. For $1-\rho \ll 1$ the condition is

$$(2t/U)(\beta t)^{-3} \approx \tfrac{1}{2}(1-\rho) . \tag{18}$$

We are interested in the behavior at as large a value of β as possible. For $\beta t = 1$, which is the lowest temperature for which one might claim any validity for the theory, the condition (18) becomes

$$2t/U \approx \tfrac{1}{2}(1-\rho) , \tag{19}$$

which is essentially identical to the criterion (16) obtained by Nagaoka for a ferromagnetic ground state. This extraordinary agreement must be viewed as fortuitous, but our qualitative interpretation is apparently correct.

Let us now consider the almost empty band. According to Kanamori's theory, [24] the ground state of a simple cubic lattice is not ferromagnetic for densities below a certain small value. Thus we may suspect that even for finite temperatures the onset of ferromagnetic behavior takes place for some value of ρ different from zero. However, Eq. (15) seems to contradict this statement as the magnetic susceptibility is still of ferromagnetic type at very low densities. However, this applies to the high-temperature region and therefore the question remains open as to whether or not the system has a ferromagnetic ground state for densities below $\rho = 0.1$.

Finally we turn our attention to Fig. 11, where the inverse magnetic susceptibility is plotted versus the temperature in the extreme-correlation ($U=\infty$) case. Here we expect, and actually find, a ferromagnetic behavior over the entire range of electron densities. By extrapolating to zero temperature we may infer also that the Curie temperature has a maximum roughly at $\rho = \frac{1}{2}$ and decreases somewhat symmetrically as ρ approaches its extreme values. However, the inserted graph of the Curie temperature versus electron density should be regarded only as qualitative.

V. CONCLUSION

In the previous sections we have performed a high-temperature expansion of the chemical potential and the thermodynamic potential in order to make some definite statements about the basic thermal properties of the Hubbard model. Both the effects of the carrier concentration and of the electron correlation have been taken into account and the following picture has emerged. For one-dimensional uniform systems the magnetic susceptibility is not qualitatively affected, in the high-temperature region, either by a change in electron density or in t/U. The susceptibility is progressively reduced with ρ and slightly reduced with the electron correlation. This last statement is in agreement with finite-chain calculations. [19] More interesting is the behavior of the specific heat. In fact for low electron densities the high-temperature peak is shifted towards $T = U/2k_B$ and tends to decrease in height. The low-temperature maximum begins its formation at higher temperatures and for a quasiempty band completely determines the shape of $C/N_A k_B$. While a low electron

correlation tends to reduce the high-temperature peak if the band is half-filled or quasi-half-filled, it has the opposite effect for intermediate densities. Quite different is the picture obtained for the magnetism in a simple cubic lattice. The ferromagnetic-antiferromagnetic transition, induced by electron density change at zero temperature and studied by Nagaoka, has been found to take place at finite temperature also. Another transition at very low carrier concentration, although improbable, is not excluded and the problem remains open.

Finally we mention that the high-temperature thermodynamic properties of the Hubbard model are being studied independently by Bulaevskii and Khomskii.[25]

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