(1954).
[8]K. Yosida, Phys. Rev. 106, 893 (1957).
[9]M. S. Fullenbaum and D. S. Falk, Phys. Rev. 157, 452 (1967).
[10]H. Keiter, Z. Physik 223, 289 (1969).
[11]J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149, 491 (1966).
[12]J. A. Gardner and C. P. Flynn, Phil. Mag. 15, 1233 (1967).

PHYSICAL REVIEW B VOLUME 6, NUMBER 3 1 AUGUST 1972

Magnetic Susceptibility at Zero Temperature for the One-Dimensional Hubbard Model*

H. Shiba†
Department of Physics, University of California, Los Angeles, California 90024
(Received 22 February)

The magnetic susceptibility at absolute-zero temperature for the one-dimensional Hubbard model is studied exactly as a function of the concentration of electrons by using Lieb and Wu's theory for this system. Our analysis essentially follows Griffiths's method for the magnetic susceptibility of the one-dimensional Heisenberg antiferromagnet, and is a generalization of Takahashi's calculation to the systems with an arbitrary concentration of electrons. The ground-state energy and the magnitude of local moments at each site are also studied. Combined with the results on the susceptibility, they should suggest how the effect of the Coulomb interaction on the properties of the system at low temperatures changes with the concentration of electrons.

I. INTRODUCTION

One-dimensional systems are fascinating for various reasons. They are usually easier to handle mathematically than higher-dimensional systems. One can often give exact statements without resorting to approximations.[1] Moreover, in some cases and for some properties, they are remarkably different from higher-dimensional systems. The one-dimensional Hubbard model, a model of interacting itinerant electrons, is not an exception.

The one-dimensional Hubbard Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 ;$$
$$\mathcal{H}_0 = -\sum_{ij\sigma} t_{ij}\, c_{i\sigma}^{\dagger} c_{j\sigma} , \qquad (1.1)$$
$$\mathcal{H}_1 = U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} ,$$

where t_{ij} is assumed to be t for $|i-j|=1$ (nearest-neighbor hopping) and zero otherwise. For this model Lieb and Wu[2] first gave an exact analysis on the ground state by essentially the same approach as that for the one-dimensional Heisenberg spin system[3,4] and for the one-dimensional fermion gas with δ-function interactions.[5]

In our Hamiltonian (1.1) there are three fundamental parameters for the thermodynamic properties of the system, that is, the strength of the Coulomb interaction relative to the transfer integral U/t, the concentration of electrons N/N_a (N and N_a are the total number of electrons and lattice points, respectively), and the temperature of the system k_BT. Let us review previous work on this system and then make the purpose of the paper clear, using these parameters.

A. Case (i): Half-Filled Band ($N/N_a = 1$)

1. Absolute-Zero Temperature ($k_BT = 0$)

The ground-state energy was obtained in an analytic form by Lieb and Wu.[2] According to them, the ground state is antiferromagnetic and insulating. Following this work, the spin-wave spectrum and the magnetic susceptibility at zero temperature were calculated by Ovchinnikov[6] and Takahashi,[7] respectively. By these calculations the properties of the one-dimensional half-filled Hubbard model were clarified almost completely as far as the absolute-zero temperature is concerned.

2. Finite Temperature ($k_BT \neq 0$)

Unfortunately, no exact solution is available for finite-temperature properties of the infinite system. But the thermodynamic properties of finite chains were calculated exactly by Shiba and Pincus.[8] Based on this calculation, we can guess a gradual "transition" from the paramagnetic and metallic state at high temperatures to the antiferromagnetic and insulating state at low temperatures.

B. Case (ii): System with $N/N_a \neq 1$

According to the Lieb-Mattis theorem[9] the ground state of our system is a singlet irrespective of the concentration of electrons. Even if $N/N_a \neq 1$, Lieb and Wu's theory should be useful and, in fact, it predicts a metallic ground state. But the dependence of the ground-state energy and other quan-

tities at $T=0$ on the concentration N/N_a has not yet been examined.

This paper is devoted exactly to the case (ii). Since the Hubbard model is often discussed in connection with the origin of the itinerant-electron magnetism, the magnetic properties of this Hamiltonian are especially interesting. Therefore, a special emphasis in this paper is placed on the study of the magnetic susceptibility. In other words, the dependence of the magnetic susceptibility of the system on U/t and N/N_a is our main concern. Many elaborate but approximate theories[10–12] have been proposed on the role of the correlation effect in metallic magnetism, based on the three-dimensional version of the Hubbard Hamiltonian. We believe that *exact* calculations of the properties of the one-dimensional Hubbard model must be interesting. For the half-filled case, Takahashi calculated the magnetic susceptibility at zero temperature, as mentioned before. The present paper is an extension of his work to arbitrary concentrations of electrons.

In Sec. II we give a short summary of Lieb and Wu's work and then calculate the ground-state energy as well as the magnitude of magnetic moments at each site as a function of N/N_a and U/t. This section may be regarded as the introductory part of Sec. II. In Sec. III we study the magnetic susceptibility of our system without any restrictions to the concentration of electrons, using Lieb and Wu's formulation and following Griffiths's analysis[13] on the magnetic susceptibility at zero temperature of the one-dimensional Heisenberg antiferromagnet. A brief discussion is given in Sec. IV.

II. GROUND-STATE ENERGY AS A FUNCTION OF THE CONCENTRATION OF ELECTRONS

Lieb and Wu[2] gave an excellent analysis of the ground state of the system (1.1) and a good starting point to the exact discussion on the behaviors at zero temperature. According to their conclusion, the lowest state of the one-dimensional Hubbard model with a fixed magnetization is described by the coupled equations for two "distribution functions," $\rho(k)$ and $\sigma(\Lambda)$,

$$2\pi\rho(k)=1+\cos k\int_{-B}^{B}\frac{8u\,\sigma(\Lambda)\,d\Lambda}{u^2+16(\sin k-\Lambda)^2}\ , \tag{2.1}$$

$$\int_{-Q}^{Q}\frac{8u\,\rho(k)\,dk}{u^2+16(\Lambda-\sin k)^2}=2\pi\sigma(\Lambda)+\int_{-B}^{B}\frac{4u\,\sigma(\Lambda')\,d\Lambda'}{u^2+4(\Lambda-\Lambda')^2}\ , \tag{2.2}$$

where $u=U/t$, and the parameters B and Q are determined by the conditions

$$\int_{-Q}^{Q}dk\,\rho(k)=N/N_a\ , \tag{2.3}$$

$$\int_{-B}^{B}d\Lambda\,\sigma(\Lambda)=M/N_a\ , \tag{2.4}$$

with the total number of down-spin electrons M. Once these coupled equations are solved, the lowest energy is obtained by the formula

$$E=-2tN_a\int_{-Q}^{Q}dk\cos k\,\rho(k)\ . \tag{2.5}$$

Using this formulation we will calculate the magnetic susceptibility at zero temperature in Sec. III. In this section we discuss the ground-state energy and the magnitude of local moments at each site (defined later) at arbitrary values of N/N_a.

First of all, from the Lieb-Mattis theorem we know that the ground state of our system (1.1) is a singlet, that is, $M/N=\frac{1}{2}$, which corresponds to $B=\infty$.[2] Now we can reduce the coupled integral equations (2.1) and (2.2) into a single one. Introducing the Fourier transform of $\sigma(\Lambda)$ and substituting it into Eqs. (2.1) and (2.2), we get

$$2\pi\rho(k)=1+\cos k\int_{-Q}^{Q}dk'\,\rho(k')\int_{-\infty}^{\infty}d\omega\,\frac{e^{i\omega(\sin k-\sin k')}}{e^{|\omega|u/2}+1}\ . \tag{2.6}$$

It is convenient for later purposes to define the function

$$\begin{aligned}R(x)&\equiv\frac{1}{4\pi}\int_{-\infty}^{\infty}dy\ \frac{1}{e^{|y|}+1}\ e^{ixy/2}\\&=\frac{1}{4\pi}\int_{-\infty}^{\infty}dt\ \frac{\operatorname{sech}\frac{1}{2}\pi t}{1+(x+t)^2}\\&=\frac{1}{\pi}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{2n}{x^2+(2n)^2}\end{aligned} \tag{2.7}$$

as in the study of the one-dimensional antiferromagnetic Heisenberg model.[13] Thus, Eq. (2.6) can be written in the form

$$2\pi\rho(k)=1+\cos k\int_{-Q}^{Q}dk'\,\rho(k')\times\frac{8\pi}{u}R\left(\frac{4(\sin k-\sin k')}{u}\right)\ . \tag{2.8}$$

Although this equation is difficult to solve in a compact form except for the half-filled case ($Q=\pi$), it is easy to obtain the solution by the iteration method or numerically, or to examine some limiting cases. In fact, approximating Eq. (2.8) by a set of 41 coupled linear algebraic equations, we calculated N/N_a in Eq. (2.3) and the ground-state energy per site E/N_a. The results are shown in Figs. 1 and 2. From Fig. 1 the relation between the concentration of electrons N/N_a and Q in the ground state is found. As easily noted, $U/t=0$ is a singular point. From Fig. 2, which shows the ground-state energy as a function of N/N_a, we can point out some features of the effect

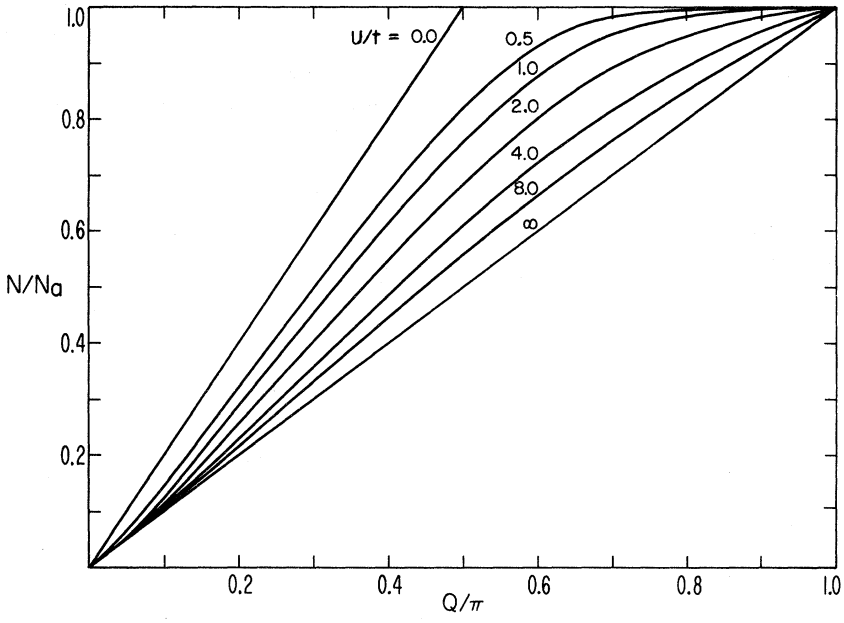

FIG. 1. Relation between N/N_a and Q at some typical values of U/t.

of correlation.

(i) At a low density of electrons ($N/N_a \lesssim 0.4$) the effect of correlation on the ground-state energy is not so large, because electrons occupy the states at the bottom of the band, where there is a high density of states, and therefore they can avoid each other without much cost of their kinetic energies. The effect of correlation is the most evident in the half-filled case.

(ii) When U/t increases, the system can gain energy only by migration processes of electrons through vacant sites, and thus the position of the minimum of the ground state as a function of N/N_a shifts from $N/N_a = 1.0$ to 0.5. Although our system is a simple one-dimensional one, with a single orbital, this result should be, in principle, suggestive of the effect of correlation on the cohesive energy of transition metals.[14]

(iii) The energy of the lowest state with the maximum total spin coincides with the $U/t = \infty$ curve in

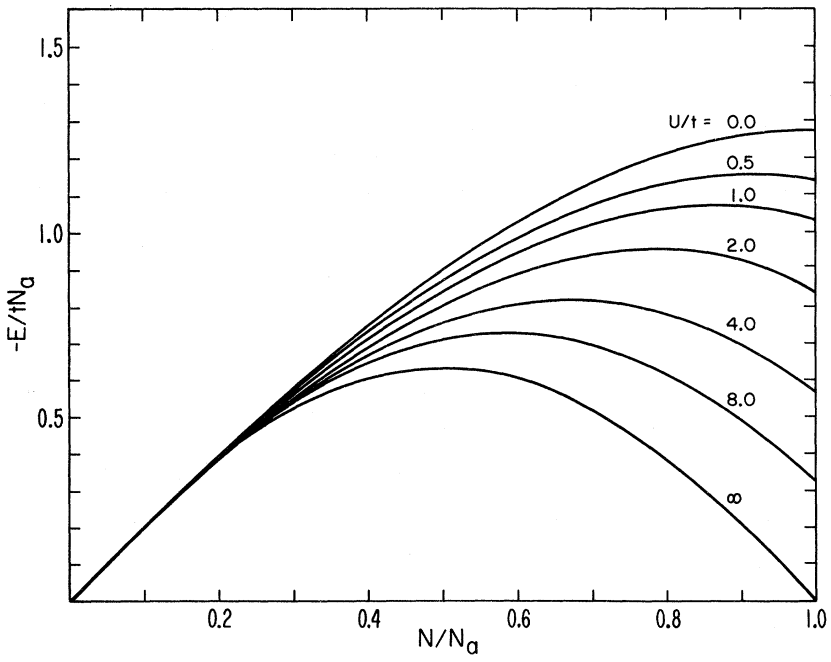

FIG. 2. Concentration dependence of the ground-state energy at typical values of U/t. At $U/t = 0$, the ground-state energy is given by $-(4/\pi)\sin\{\frac{1}{2}\pi N/N_a\}$ while $E/tN_a = -(2/\pi)\sin\{\pi N/N_a\}$ at $U/t = \infty$.

Fig. 2. Physically, this is natural.

Let us study the strong U limit ($u \gg 1$), starting from Eq. (2.8) and expanding in power of $1/u$. We can easily obtain

$$2\pi\rho(k) = 1 + \cos k \frac{4}{u} \ln 2 \frac{Q}{\pi} + O\left(\frac{1}{u^2}\right) \quad . \tag{2.9}$$

Substituting this equation into (2.3) and (2.5) and determining Q up to the order of $1/u$, we have

$$\frac{E}{tN_a} \cong -\left[\frac{2}{\pi}\sin\left(\pi\frac{N}{N_a}\right) + \frac{4\ln 2}{u}\left(\frac{N}{N_a}\right)^2 \times\left(1 - \frac{\sin(2\pi N/N_a)}{2\pi N/N_a}\right)\right] \quad . \tag{2.10}$$

In the half-filled case ($N/N_a = 1$), Eq. (2.10) reproduces the ground-state energy of the one-dimensional Heisenberg antiferromagnet with the exchange coupling $J = 2t^2/U$.[3,4]

Another quantity, which is useful to understand the ground state and is easy to derive from Eqs. (2.5) and (2.6), is the magnitude of local moments at each site introduced in Ref. 8:

$$L_0 = (1/N_a)\sum_j \langle(\tilde{S}_j)^2\rangle \, , \tag{2.11}$$

where $\tilde{S}_j$ is the spin operator at the jth site: $\tilde{S}_j = \sum_{\sigma\sigma'}\langle\sigma|\tilde{S}|\sigma'\rangle c^\dagger_{j\sigma} c_{j\sigma'}$ and the average $\langle\cdots\rangle$ is taken in the ground state. This quantity is related to the ground-state energy by

$$L_0 = \frac{3}{4}\frac{N}{N_a} - \frac{3}{2}\frac{1}{N_a}\frac{\partial E(U)}{\partial U} \, , \tag{2.12}$$

as easily proved. Note that in Eq. (2.12) Q also depends on U. In fact, from the condition of the fixed number of electrons we obtain

$$\frac{\partial Q}{\partial U} = -\frac{1}{2\rho(Q)}\int_{-Q}^{Q} dk \frac{\partial\rho(k)}{\partial U} \quad . \tag{2.13}$$

By using this expression, the derivative $\partial E(U)/\partial U$ is written in the form

$$\frac{1}{N_a}\frac{\partial E(U)}{\partial U} = 2\int_{-Q}^{Q} dk\,(\cos Q - \cos k)\frac{\partial\rho(k)}{\partial u} \, , \tag{2.14}$$

where $\partial\rho(k)/\partial u$ is obtained as the solution of the integral equation

$$2\pi\frac{\partial\rho(k)}{\partial u} = \cos k\int_{-Q}^{Q} dk'\,\rho(k')\left(\frac{4}{u}\right)^2 \Phi\left(\frac{4(\sin k - \sin k')}{u}\right) + \cos k\int_{-Q}^{Q} dk' \frac{\partial\rho(k')}{\partial u} \times\left[\frac{8\pi}{u}R\left(\frac{4(\sin k - \sin k')}{u}\right) - \frac{4\pi}{u}R\left(\frac{4(\sin k - \sin Q)}{u}\right) - \frac{4\pi}{u}R\left(\frac{4(\sin k + \sin Q)}{u}\right)\right] , \tag{2.15}$$

with

$$\Phi(x) \equiv \sum_{n=1}^{\infty}(-1)^{n+1} n \frac{x^2 - (2n)^2}{[x^2 + (2n)^2]^2} \quad . \tag{2.16}$$

Thus, it is easy to get the quantity L_0.

Figure 3 shows the dependence of the magnitude of local moments at each site on the concentration of electrons at various values of U/t. In the noninteracting system ($U/t = 0$), L_0 is given by

$$L_0 = \tfrac{3}{4}(N/N_a)(1 - \tfrac{1}{2}N/N_a) \, , \tag{2.17}$$

while in the strong U limit we obtain

$$L_0 \simeq \frac{3}{4}\frac{N}{N_a} - \frac{6\ln 2}{u^2}\left(\frac{N}{N_a}\right)^2\left(1 - \frac{\sin(2\pi N/N_a)}{2\pi N/N_a}\right) \quad . \tag{2.18}$$

Again the effect of correlation on L_0 is small in the low density of electrons, and it becomes evident when N/N_a approaches unity.

III. MAGNETIC SUSCEPTIBILITY AT ZERO TEMPERATURE

The magnetic susceptibility gives important information on this system. For the half-filled case, Takahashi[7] calculated the susceptibility and showed how it changes from the Pauli paramagnetic behavior to that of localized spins as U/t increases. It is interesting to study the magnetic susceptibility for $N/N_a < 1$. The Griffiths method,[13] which Takahashi followed in his analysis, is still found useful even when $N/N_a < 1$.

In the study of the susceptibility we can assume that the magnetization induced by an external field is small, and therefore B remains quite large in Eqs. (2.1)–(2.4). The increase of energy due to the magnetization of the system, which is directly connected with the magnetic susceptibility, is determined by the asymptotic behavior of $\sigma(\Lambda)$ in the region $\Lambda \gg 1$.

Let us rewrite Eqs. (2.1)–(2.4) into a convenient form for this purpose. Integrating both sides of Eq. (2.2) over Λ from $-\infty$ to $+\infty$, and using the relations (2.3) and (2.4), we get

$$S \equiv \tfrac{1}{2}N/N_a - M/N_a = \int_B^{\infty} d\Lambda\,\sigma(\Lambda) \quad . \tag{3.1}$$

The integral equation for $\sigma(\Lambda)$ is obtained by substituting Eq. (2.1) into (2.2) in the form

$$2\pi\,\sigma(\Lambda) = (1/2\pi)\,g_Q^{(0)}(\Lambda) - \int_{-B}^{B} d\Lambda'\,S_Q(\Lambda,\Lambda')\,\sigma(\Lambda') \, , \tag{3.2}$$

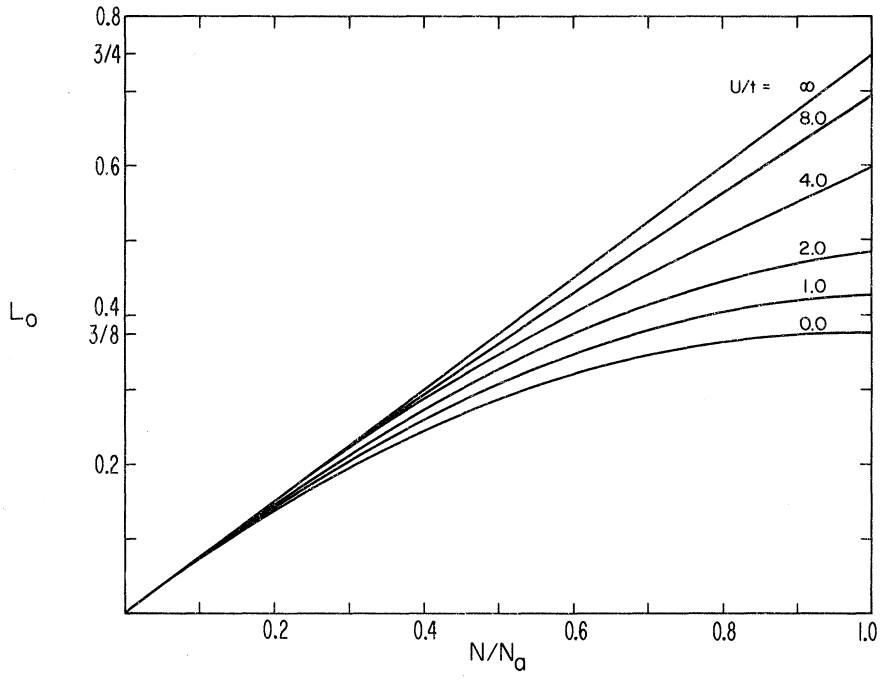

FIG. 3. Magnitude of local moments at each site L_0 versus the concentration of electrons N/N_a. When $U/t=\infty$, L_0 is equal to $\frac{3}{4}N/N_a$. On the other hand, L_0 is given by $\frac{3}{4}(N/N_a)(1-\frac{1}{2}N/N_a)$, when $U/t=0$.

where

$$g_Q^{(n)}(\Lambda) \equiv \int_{-Q}^{Q} dk \cos^n k \frac{8u}{u^2+16(\sin k-\Lambda)^2} \quad (3.3)$$

and the kernel is defined by

$$S_Q(\Lambda,\Lambda') = \frac{4u}{u^2+4(\Lambda-\Lambda')^2} - \int_{-Q}^{Q} \frac{dk}{2\pi} \cos k \frac{8u}{u^2+16(\Lambda-\sin k)^2} \times \frac{8u}{u^2+16(\Lambda'-\sin k)^2} . \quad (3.4)$$

It is useful to introduce a new function $\sigma^{(n)}(\Lambda)$ as the solution of the integral equation

$$\sigma^{(n)}(\Lambda) = (1/2\pi) g_Q^{(n)}(\Lambda) - \int_{-\infty}^{\infty} d\Lambda' S_Q(\Lambda,\Lambda')\sigma^{(n)}(\Lambda') . \quad (3.5)$$

Then $\sigma^{(n)}(\Lambda)$ can be expressed in terms of the resolvent kernel $s_Q(\Lambda,\Lambda')$ defined by

$$s_Q(\Lambda,\Lambda') = S_Q(\Lambda,\Lambda') - \int_{-\infty}^{\infty} d\Lambda'' S_Q(\Lambda,\Lambda'')s_Q(\Lambda'',\Lambda') = S_Q(\Lambda,\Lambda') - \int_{-\infty}^{\infty} d\Lambda'' s_Q(\Lambda,\Lambda'')S_Q(\Lambda'',\Lambda') . \quad (3.6)$$

In fact, it is easy to show

$$\sigma^{(n)}(\Lambda) = \frac{1}{2\pi} g_Q^{(n)}(\Lambda) - \int_{-\infty}^{\infty} \frac{d\Lambda'}{2\pi} s_Q(\Lambda,\Lambda') \frac{1}{2\pi} g_Q^{(n)}(\Lambda') . \quad (3.7)$$

By using these newly introduced functions and integrating the product of $s_Q(\Lambda_1,\Lambda)$ and Eq. (3.2) over Λ from $-\infty$ to $+\infty$, we obtain

$$\sigma(\Lambda) = \sigma^{(0)}(\Lambda) + \int_{|\Lambda'|>B} \frac{d\Lambda'}{2\pi} s_Q(\Lambda,\Lambda')\sigma(\Lambda') . \quad (3.8)$$

Similarly, the integration of the product of $\sigma(\Lambda)$ and Eq. (3.5) over Λ from $-B$ to B yields

$$\frac{E}{tN_a} = \frac{E_0(Q)}{tN_a} + 2\int_{|\Lambda|>B} \frac{d\Lambda}{2\pi} \sigma(\Lambda)(2\pi)^2\sigma^{(2)}(\Lambda) , \quad (3.9a)$$

$$\frac{N}{N_a} = \frac{N_0(Q)}{N_a} - \int_{|\Lambda|>B} \frac{d\Lambda}{2\pi} \sigma(\Lambda)(2\pi)^2\sigma^{(1)}(\Lambda) , \quad (3.9b)$$

where $E_0(Q)$ and $N_0(Q)$ are the ground-state energy and the total number of electrons at a fixed value of Q, respectively, i.e.,

$$\frac{E_0(Q)}{tN_a} = -\frac{2}{\pi}\sin Q - 2\int_{-\infty}^{\infty} \frac{d\Lambda}{2\pi} \sigma^{(0)}(\Lambda) g_Q^{(2)}(\Lambda) , \quad (3.10a)$$

$$\frac{N_0(Q)}{N_a} = \frac{Q}{\pi} + \int_{-\infty}^{\infty} \frac{d\Lambda}{2\pi} \sigma^{(0)}(\Lambda) g_Q^{(1)}(\Lambda) . \quad (3.10b)$$

The quantities $E_0(Q)$ and $N_0(Q)$ were actually calculated in Sec. II. In order to evaluate the second term in Eqs. (3.9a) and (3.9b) we have to know $\sigma^{(n)}(\Lambda)$ and $\sigma(\Lambda)$ for $\Lambda \gg 1$. Starting from Eqs. (3.6) and (3.7), solving the latter by iteration and rearranging terms, we find that

$$\sigma^{(n)}(\Lambda) = \frac{1}{u}\int_{-Q}^{Q}\frac{dk}{2\pi}\cos^n k\,\mathrm{sech}\frac{2\pi(\Lambda-\sin k)}{u} + \int_{-\sin Q}^{\sin Q}\frac{dt}{2\pi}\int_{-\sin Q}^{\sin Q}\frac{dt'}{2\pi}\,\frac{2\pi}{u}\,\mathrm{sech}\frac{2\pi(\Lambda-t)}{u} \times L_Q(t,t')\int_{-Q}^{Q}\frac{dk}{2\pi}\cos^n k\,\frac{4}{u}R\left(\frac{4(\sin k - t')}{u}\right), \tag{3.11}$$

where $L_Q(t, t')$ is the solution of the equation

$$L_Q(t,t') = \delta(t-t') + \int_{-\sin Q}^{\sin Q} dt''\,\frac{4}{u}R\left(\frac{4(t-t'')}{u}\right)L_Q(t'',t') \ . \tag{3.12}$$

Now it is clear that for $\Lambda \gg 1$, $\sigma^{(n)}(\Lambda)$ decays exponentially. In fact, the asymptotic form of $\sigma^{(n)}(\Lambda)$ in $|\Lambda| \gg 1$ is given by

$$\sigma^{(n)}(\Lambda) \simeq (2/u)\,e^{-2\pi|\Lambda|/u} I_Q^{(n)}(u) \ , \tag{3.13}$$

where

$$I_Q^{(n)}(u) = \int_{-Q}^{Q}\frac{dk}{2\pi}\cos^n k\,e^{2\pi(\sin k)/u} + \int_{-\sin Q}^{\sin Q} dt\,e^{2\pi t/u}\int_{-\sin Q}^{\sin Q} dt' L_Q(t,t') \times\int_{-Q}^{Q}\frac{dk}{2\pi}\cos^n k\,\frac{4}{u}R\left(\frac{4(\sin k - t')}{u}\right) \ . \tag{3.14}$$

The next task is to simplify Eq. (3.8) for $|\Lambda| > B \gg 1$.

Defining the function $P(\Lambda)$ by

$$\sigma(\Lambda+B) \equiv \frac{2}{u} I_Q^{(0)}(u) P(\Lambda)\,e^{-2\pi B/u} \tag{3.15}$$

and using the asymptotic expression for $\sigma^{(0)}(\Lambda)$ [Eq. (3.13)], we have

$$P(\Lambda) = e^{-2\pi\Lambda/u} + \int_{-\infty}^{\infty}\frac{d\Lambda'}{2\pi}\,P(\Lambda') \times[s_Q(B+\Lambda, B+\Lambda') + s_Q(B+\Lambda, -B-\Lambda')] \tag{3.16}$$

for $\Lambda > 0$. But this equation is further simplified in the case where $B \gg 1$, Λ and $\Lambda' > 0$, since we can apply the following approximations:

$$s_Q(B+\Lambda, B+\Lambda') + s_Q(B+\Lambda, -B-\Lambda') \simeq s_Q(B+\Lambda, B+\Lambda') \simeq (8\pi/u)R[4(\Lambda-\Lambda')/u] \ . \tag{3.17}$$

Here we ignored exponentially small terms. Substituting this into Eq. (3.16), we obtain

$$P(\Lambda) = e^{-2\pi\Lambda/u} + \int_0^{\infty} d\Lambda'\,\frac{4}{u}R\left(\frac{4(\Lambda-\Lambda')}{u}\right)P(\Lambda') \tag{3.18}$$

or

$$P\left(\frac{u}{4}x\right) = e^{-\pi x/2} + \int_0^{\infty} dx' R(x-x')\,P\left(\frac{u}{4}x'\right) . \tag{3.18'}$$

Now Eqs. (3.9a), (3.9b), and (3.1) can be written in the form

$$\frac{E}{N_a t} = \frac{E_0(Q)}{N_a t} + \frac{8b_0}{u}\,e^{-4\pi B/u}\,I_Q^{(2)}(u)\,I_Q^{(0)}(u) \ , \tag{3.19a}$$

$$\frac{N}{N_a} = \frac{N_0(Q)}{N_a t} - \frac{4b_0}{u}\,e^{-4\pi B/u}\,I_Q^{(1)}(u)\,I_Q^{(0)}(u) \ , \tag{3.19b}$$

$$S = a_0 e^{-2\pi B/u} I_Q^{(0)}(u) \ , \tag{3.19c}$$

where a_0 and b_0 are given by

$$a_0 = \tfrac{1}{2}\int_0^{\infty} dx\,p(\tfrac{1}{4}ux) \tag{3.20a}$$

and

$$b_0 = \pi\int_0^{\infty} dx\,e^{-\pi x/2}\,p(\tfrac{1}{4}ux) \ , \tag{3.20b}$$

respectively. The important point here is that Eq. (3.18') is exactly the same as that in Griffiths's work,[13] his equation (43), and that a_0 and b_0 are the same quantities with the same notation. So there is actually no need to solve (3.18) or (3.18'). Substituting Eq. (3.19c) into (3.19a) and (3.19b), we find that

$$\frac{E}{tN_a} = \frac{E_0(Q)}{tN_a} + S^2\,\frac{(2\pi)^2}{u}\,\frac{I_Q^{(2)}(u)}{I_Q^{(0)}(u)} \ , \tag{3.21a}$$

$$\frac{N}{N_a} = \frac{N_0(Q)}{N_a} - S^2\,\frac{(2\pi)^2}{2u}\,\frac{I_Q^{(1)}(u)}{I_Q^{(0)}(u)} \ . \tag{3.21b}$$

Here the use was made of the relation $b_0/a_0^2 = \frac{1}{2}\pi^2$ conjectured by Griffiths[13] and proved rigorously by Yang and Yang.[15] In Eqs. (3.21a) and (3.21b) there is a deviation of Q due to the magnetization S from the value in the singlet ground state. The change of Q is determined by the condition that the total number of electrons should be constant. Substituting the deviation of Q obtained in this way into Eq. (3.21a), we find that

$$\frac{E}{tN_a} = \frac{E_0(Q)}{tN_a} + (2\pi S)^2\left[\frac{1}{u}\,\frac{I_Q^{(2)}(u)}{I_Q^{(0)}(u)} + \frac{1}{2u}\,\frac{I_Q^{(1)}(u)}{I_Q^{(0)}(u)}\left(\frac{\partial E_0(Q)}{\partial Q}\Big/\frac{\partial N_0(Q)}{\partial Q}\right)\right] . \tag{3.22}$$

Here Q is related to N/N_a through the relation we found in Sec. II, i. e.,

$$N/N_a = N_0(Q)/N_a \ .$$

The second term in Eq. (3.22) represents the increase of the energy due to the magnetization. Adding the Zeeman term and minimizing the total energy with respect to S, we find our final expression for the susceptibility

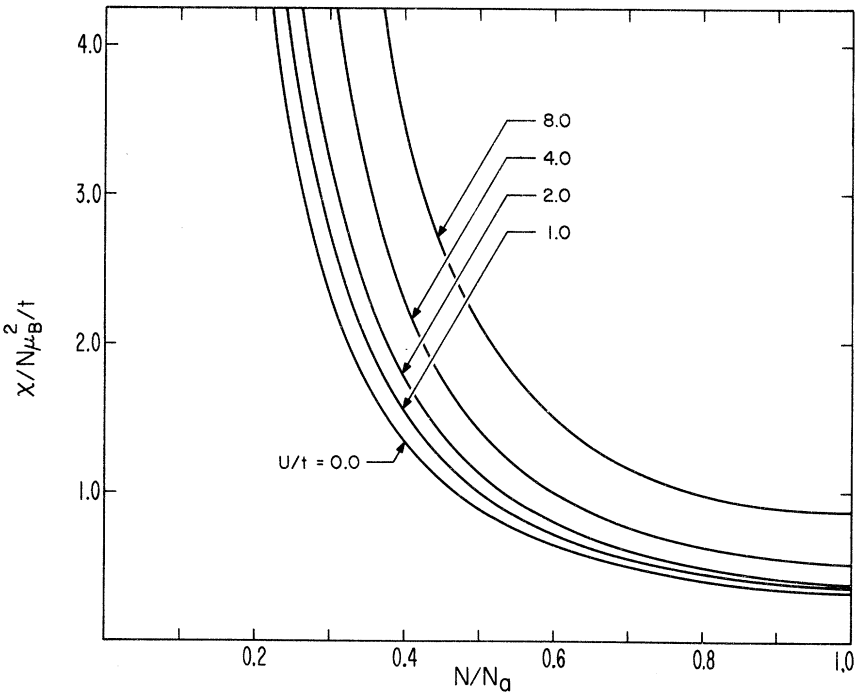

FIG. 4. Magnetic susceptibility per electron $\chi/(N\mu_B^2/t)$ vs N/N_a. All curves diverge as a function of N/N_a only at $N/N_a=0$.

$$\frac{\chi}{N_a\mu_B^2/t}=\left[2\pi^2\left(\frac{1}{u}\,\frac{I_Q^{(2)}(u)}{I_Q^{(0)}(u)}+\frac{1}{2u}\,\frac{I_Q^{(1)}(u)}{I_Q^{(0)}(u)}\,\frac{\partial E_0(Q)}{\partial Q}\Big/\frac{\partial N_0(Q)}{\partial Q}\right)\right]^{-1}. \quad (3.23)$$

By using the formula (3.23) we can calculate the magnetic susceptibility at arbitrary values of U/t and N/N_a. Details of the numerical calculation are described in the Appendix. Figure 4 shows our results for the susceptibility per electron versus N/N_a at typical values of U/t, while Fig. 5 shows the dependence of the susceptibility on U/t with fixed values of N/N_a. From these figures it is evident that with the decrease of the concentration of electrons and/or with the increase of U/t the system is more easily magnetized. This tendency is consistent with the results for the energy (Fig. 2) and can be explained by the fact that when N/N_a decreases and/or U/t increases, one can get a small amount of magnetization without much cost of energy. In Fig. 4, all the curves of the susceptibility diverge at $N/N_a=0$ simply because of the divergence of the density of states at band edges.

Let us study some limiting cases.

a. Half-filled case ($Q=\pi$). It is easy to find

$$I_Q^{(0)}=I_0(2\pi/u)\,,\qquad I_Q^{(1)}=0\,,$$

and

$$I_Q^{(2)}=(u/2\pi)\,I_1(2\pi/u)\,,$$

where $I_\nu(x)$ is the Bessel function of imaginary argument of the order ν. Therefore, (3.23) gives

$$\frac{\chi}{N_a\mu_B^2/t}=\frac{1}{\pi}\,\frac{I_0(2\pi/u)}{I_1(2\pi/u)}\,, \quad (3.24)$$

which is Takahashi's result[7] for the half-filled case.

b. Strong U limit ($U/t\gg 1$). In this limit the approximation

$$I_Q^{(n)}\simeq\int_{-Q}^{Q}\frac{dk}{2\pi}\cos^n k$$

is appropriate. Furthermore, we have

$$\frac{1}{N_a}\,\frac{\partial E_0}{\partial Q}\simeq-\frac{2}{\pi}\cos Q$$

and

$$\frac{1}{N_a}\,\frac{\partial N_0}{\partial Q}\simeq\frac{1}{\pi}\,.$$

Therefore, the susceptibility in the strong U limit is proportional to u in the way

$$\frac{\chi}{N_a\mu_B^2/t}\simeq\frac{u}{\pi^2}\left(1-\frac{\sin 2Q}{2Q}\right)^{-1}\simeq\frac{u}{\pi^2}\left(1-\frac{\sin(2\pi N/N_a)}{2\pi N/N_a}\right)^{-1}. \quad (3.25)$$

Note exactly the same factor $1-[\sin(2\pi N/N_a)]/(2\pi N/N_a)$ appeared in Eq. (2.10). When $N/N_a=1$, the right-hand side of Eq. (3.25) represents the Griffiths formula for the susceptibility of the one-dimensional antiferromagnet with the nearest-neighbor coupling $J\simeq 2t^2/U$, while in the low-density limit Eq. (3.25) gives

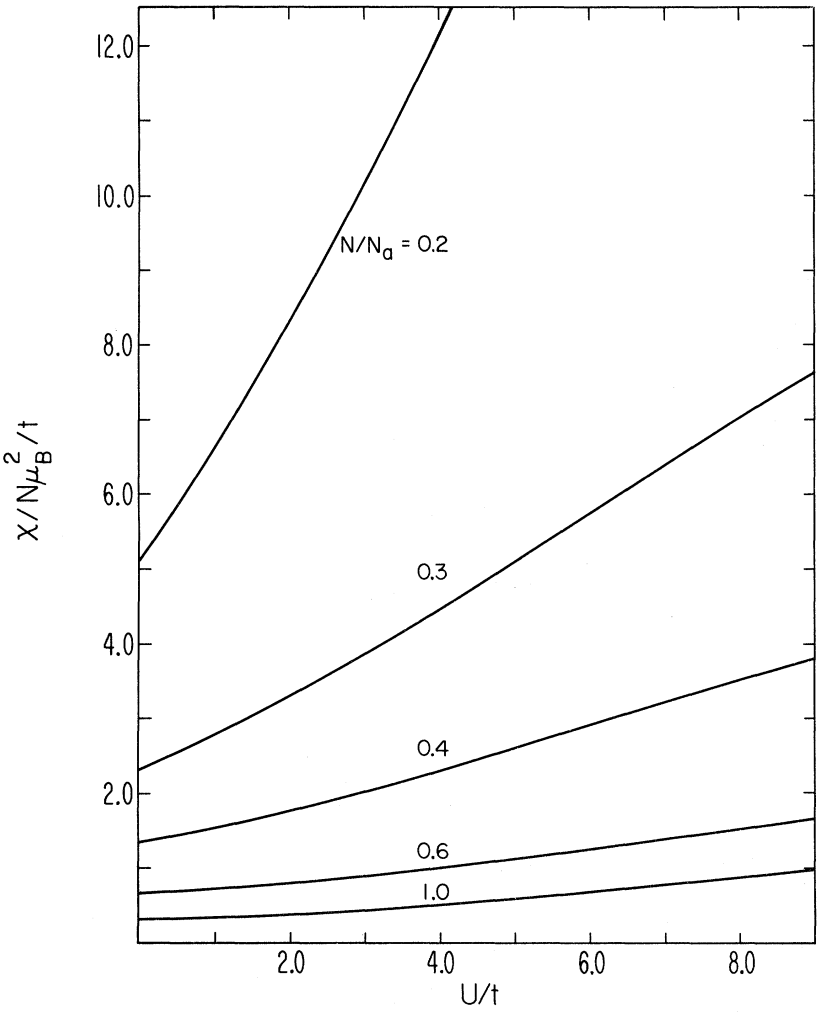

FIG. 5. Susceptibility per electron $\chi/(N\mu_B^2/t)$ vs U/t at some fixed values of N/N_a.

$$\frac{\chi}{N_a \mu_B^2/t} \simeq \frac{3}{2\pi^4} \frac{u}{(N/N_a)^2} \,. \tag{3.26}$$

c. Weak U limit ($U/t \ll 1$). As evident in Fig. 1, the relation between Q and N/N_a is singular in this limit. Carefully examining each factor, we obtain, from Eq. (3.23),

$$\frac{\chi}{N_a \mu_B^2/t} \simeq \frac{1}{\pi} \frac{1}{\sin Q}$$

$$\simeq \frac{1}{\pi} \left[\sin\left(\frac{\pi}{2} \frac{N}{N_a}\right)\right]^{-1}, \tag{3.27}$$

which is nothing but the Pauli paramagnetism of the one-dimensional noninteracting electron system.

IV. DISCUSSION

In this paper we have studied the properties of the one-dimensional Hubbard model at absolute-zero temperature as a function of the concentration of electrons N/N_a and the strength of correlation relative to the hopping integral U/t, calculating the magnetic susceptibility as well as the ground-state energy and the magnitude of local moments at each site. Our calculations are based on Lieb and Wu's theory, and therefore they are exact.

Since our model is a one-dimensional system, some of our conclusions should be inherent in one dimensionality, while others are applicable irrespective of dimensionality. The three-dimensional version of our Hubbard model is believed to have a ferromagnetic or antiferromagnetic ground state with a long-range ordering under certain conditions of the concentration of electrons and the strength of correlation. In fact, Penn[16] showed such possibilities, employing the random phase approximation. On the other hand, in our one-dimensional system, the ground state is always a singlet and is "smooth" as a function of N/N_a (mathematically speaking, $N/N_a = 1$ is a singular point). This is due to the fact that our model is a one-dimensional one

with a single orbital. But as far as general aspects of the effect of correlation are concerned, our results should be suggestive beyond one dimensionality.

Our study in this paper has been restricted to absolute-zero temperature. Combining the results with the conclusions on the finite-temperature properties of the half-filled case, [8] we can give some conjectures on finite-temperature properties of the one-dimensional Hubbard model with $N/N_a < 1$.

(i) The high-temperature peak of the specific heat per atom, [8] which was found in the half-filled case for $U/t \gtrsim 4$, must be observed, as far as N/N_a is not too small. But the height of the peak will decrease with the decrease of N/N_a, because the probability of finding doubly occupied states becomes small. As for the low-temperature peak the coefficient of the linear increase with temperature must become large with the decrease of N/N_a, and the height of the peak will decrease.

(ii) When N/N_a decreases, the susceptibility per electron increases at low temperatures, and it must decrease rapidly with temperature.

ACKNOWLEDGMENTS

The author is indebted to Professor P. A. Pincus for valuable discussions and his critical reading of the manuscript. It is a pleasure to thank Professor T. Holstein and Professor R. Orbach for their hospitality.

APPENDIX

Here an outline of our numerical calculation of the susceptibility is described.

The quantities $I_Q^{(n)}(u)$, $\partial E_0(Q)/\partial Q$, and $\partial N_0(Q)/\partial Q$ appearing in Eq. (3.23) can be expressed in terms of the solutions of integral equations. In fact, we can write Eq. (3.14) in the form

$$I_Q^{(n)}(u) = \int_{-Q}^{Q} \frac{dk}{2\pi} \cos^n k \, \psi(k) , \tag{A1}$$

where $\psi(k)$ is the solution of the equation

$$\psi(k) = e^{2\pi(\sin k)/u} + \int_{-Q}^{Q} dk' \cos k' \times \frac{4}{u} R\left(\frac{4(\sin k - \sin k')}{u}\right) \psi(k') , \tag{A2}$$

as one can easily check by the iteration method. As for $\partial E_0(Q)/\partial Q$ and $\partial N_0(Q)/\partial Q$, the same technique as in the calculation of L_0 is useful. From Eqs. (2.3) and (2.5) we obtain

$$\frac{\partial E_0(Q)}{\partial Q} = -4\cos Q \, \rho(Q) - 2\int_{-Q}^{Q} dk \cos k \, \frac{\partial \rho(k)}{\partial Q} \tag{A3}$$

and

$$\frac{\partial N_0(Q)}{\partial Q} = 2\rho(Q) + \int_{-Q}^{Q} dk \, \frac{\partial \rho(k)}{\partial Q} . \tag{A4}$$

Here use was made of the relation $\rho(k) = \rho(-k)$. Performing the differentiation of both sides of Eq. (2.9) by Q, we find the equation

$$2\pi \frac{\partial \rho(k)}{\partial Q} = \cos k \, \rho(Q) \left[\frac{8\pi}{u} R\left(\frac{4(\sin k - \sin Q)}{u}\right) + \frac{8\pi}{u} R\left(\frac{4(\sin k + \sin Q)}{u}\right)\right] + \cos k \int_{-Q}^{Q} dk' \frac{\partial \rho(k')}{\partial Q} \frac{8\pi}{u} R\left(\frac{4(\sin k - \sin k')}{u}\right) . \tag{A5}$$

In our numerical calculations the integral equations (A2) and (A5) were replaced again by 41 coupled linear algebraic equations and then $I_Q^{(n)}$, $\partial E_0(Q)/\partial Q$, and $\partial N_0(Q)/\partial Q$ were evaluated.

---

*Work supported in part by the National Science Foundation, GP-21290, and the Office of Naval Research, under Contract No. N00014-69-A-0200-4032.

†Present address: Department of Physics, Faculty of Science, Osaka University, Toyonaka, Japan.

[1]See, for instance, L. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966).

[2]L. H. Lieb and F. Y. Wu, Phys. Rev. Letters 20, 1445 (1968).

[3]H. Bethe, Z. Physik 71, 205 (1931).

[4]L. Hulthen, Ark. Mat. Astron. Fys. 26A, No. 11 (1938).

[5]C. N. Yang, Phys. Rev. Letters 19, 1312 (1967).

[6]A. A. Ovchinnikov, Zh. Eksperim. i Teor. Fiz. 57, 2144 (1970) [Sov. Phys. JETP 30, 1160 (1970)].

[7]M. Takahashi, Progr. Theoret. Phys. (Kyoto) 42, 1098 (1969); 43, 1619 (1970).

[8]H. Shiba and P. A. Pincus, Phys. Rev. B5, 1966 (1972); H. Shiba, Progr. Theoret. Phys. (Kyoto) (to be published).

[9]L. H. Lieb and D. C. Mattis, Phys. Rev. 125, 164 (1962).

[10]J. Hubbard, Proc. Roy. Soc. (London) A276, 238 (1963); A281, 401 (1964).

[11]M. C. Gutzwiller, Phys. Rev. Letters 10, 159 (1963).

[12]J. Kanamori, Progr. Theoret. Phys. (Kyoto) 30, 275 (1963).

[13]R. B. Griffiths, Phys. Rev. 133, A768 (1964).

[14]J. Friedel, in *Theory of Magnetism in Transition Metals*, edited by W. Marshall (Academic, New York, 1967), p. 283.

[15]C. N. Yang and C. P. Yang, Phys. Rev. 151, 258 (1966).

[16]D. R. Penn, Phys. Rev. 142, 350 (1966).