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The One-Dimensional Hubbard Model for Large or Infinite U

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The magnetic properties of the one-dimensional Hubbard model with a hard-core interaction on a ring (periodic boundary conditions) are investigated. At finite temperatures it is shown to behave up to exponentially small corrections as a pure paramagnet. An explicit expression for the ground-state degeneracies is derived. The eigenstates of this model are used to perform a perturbational treatment for large but finite interactions. In first order in U^{-1} an effective Hamiltonian for the one-dimensional Hubbard model is derived. It is the Hamiltonian of the one-dimensional Heisenberg model with antiferromagnetic couplings between nearest neighbor spins. An asymptotic expansion for the ground-state energy is given. The results are valid for arbitrary densities of electrons.

KEY WORDS: Paramagnetism; Hubbard model; hard-core interaction; partition function; magnetization; ground states; Heisenberg model.

1. INTRODUCTION

From the theoretical point of view one-dimensional models are often fascinating, since in many cases it is possible to obtain exact results. This is also true for the Hubbard model.[1] It describes itinerant electrons on a lattice with an on-site interaction. Whereas not too much is known about the properties of the Hubbard model in more than one dimension, it is solvable in one dimension using the Bethe Ansatz. This was shown by Lieb and Wu,[2] who derived the so-called nested Bethe Ansatz equations. Unfortunately it is difficult to solve these equations. Lieb and Wu obtained the ground state in the thermodynamic limit for a half-filled band and the

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excitations may be classified in this case as well (see ref. 3 and the references therein). Irrespective of the density of the electrons, the theorem of Lieb and Mattis[4] tells us that the ground state is a singlet. This result was recently extended to finite temperatures by Aizenman and Lieb[5] in the sense that the magnetization is always less than the pure paramagnetic value. Further, Shiba[6] and Carmelo and Baeriswyl[7] used the thermodynamic limit of the nested Bethe Ansatz equations to obtain expansions for several quantities in the limit of strong interaction. These results are valid for all densities and we will come back to them later.

In the special case of a hard-core interaction the theorem of Lieb and Mattis is not valid. Instead, Aizenman and Lieb[5] showed that in the case of a ring (periodic boundary conditions) and for an odd number of particles there is one among the degenerate ground states for which the total spin takes the maximal value. For all finite temperatures the magnetization exceeds the pure paramagnetic value. There is a tendency toward a ferromagnetic behavior. In contrast, one may show that for a chain with open ends all the spin configurations are degenerate and the system is paramagnetic.[5] This means that the tendency toward a ferromagnetic behavior for the system with periodic boundary conditions must be weak, since a change of the boundary conditions should not produce a large effect.

In Section 2 we discuss the symmetries of a model of itinerant one-dimensional electrons on a lattice with a hard-core repulsion (e.g., the one-dimensional Hubbard model) in some detail and we show that the partition function factorizes up to exponentially small corrections into an electronic part and a magnetic part. The latter is that of a pure paramagnet. This result is used to show that the difference of the magnetization from the paramagnetic value is exponentially small, depending on the number of electrons. [$X(N)$ will be called exponentially small if and only if $\delta > 0$ exists such that $X(N)\exp(\delta N)$ tends to 0 in the limit where N tends to infinity.] In Section 3 we construct the eigenstates of the one-dimensional Hubbard model with hard-core interactions and we discuss the electronic properties of the system. We give an explicit expression for the degeneracies of the ground states in the subspaces where the z component of the total spin of the system is fixed. Further, we calculate the thermodynamic potentials in the thermodynamic limit. The free energy density is given by a sum of the free energy density of spinless fermions and that of a paramagnet. The eigenstates are used in Section 4 to derive an effective Hamiltonian for the one-dimensional Hubbard model in the limit of strong interaction. The effective Hamiltonian is the Hamiltonian of the Heisenberg model with antiferromagnetic couplings. This result yields an expansion for the ground-state energy of the one-

dimensional Hubbard model which differs from the one given in refs. 6 and 7. Our result is obtained by an ordinary perturbational treatment. The radius of convergence of the perturbational series tends to 0 in the thermodynamic limit and therefore our expansion of the ground-state energy is only asymptotically true. Unfortunately, nothing is known about the convergence of the series expansion for the ground-state energy given in ref. 7 and the difference remains as an open problem. In the same way as for the Hubbard model, an effective Hamiltonian for the one-dimensional tJ-model[8,9] in the small-J limit may be obtained.

2. HARD-CORE INTERACTIONS, MAGNETIC PROPERTIES

The Hamiltonian of the one-dimensional (extended) Hubbard model is given by

$$H = -\sum_{x,\sigma} t_x(a^+_{x+1\sigma}a_{x\sigma} + a^+_{x\sigma}a_{x+1\sigma}) + U\sum_x n_{x+}n_{x-} + V(\{n_x\}) \quad (2.1)$$

$a^+_{x\sigma}$ ($a_{x\sigma}$) are the creation (annihilation) operators for electrons with spin σ on the site x and $n_{x\sigma} = a^+_{x\sigma}a_{x\sigma}$, $n_x = n_{x+} + n_{x-}$. They obey the usual anticommutation relations for fermions. The model describes electrons on a one-dimensional lattice with an on-site interaction and a hopping between nearest neighbor sites. U is a positive real number, t_x are non-vanishing real numbers. $V(\{n_x\})$ is a finite potential that depends on the occupation numbers only. It may be, for example, a long-range interaction or a single-particle potential of the form $\sum v_x n_x$ with finite real numbers v_x. In the usual Hubbard model one has $V = 0$ and $t_x = t > 0$. In the following L denotes the number of sites, N the number of electrons. We will restrict ourselves to the case $N \leqslant L$. In the case of a chain with open ends, the sum in (2.1) goes from 1 to $L-1$; in the case of periodic boundary conditions the sites are taken to be integers modulo L, so that the sum goes from 1 to L and $x + L = x$. The Hamiltonian conserves the number of electrons with spin + (−), which we denote by N_+ (N_-). In the case of a hard-core interaction ($U = \infty$) the Hamiltonian takes the form

$$H_0 = P_0\left[-\sum_{x,\sigma} t_x(a^+_{x+1\sigma}a_{x\sigma} + a^+_{x\sigma}a_{x+1\sigma}) + V(\{n_x\})\right]P_0 \quad (2.2)$$

where P_0 is the projector onto the states with no doubly occupied sites,

$$P_0 = \prod_x (1 - n_{x+}n_{x-}) \quad (2.3)$$

In this and in the following section we discuss the properties of the Hamiltonian (2.2). We introduce the operators

$$S_{a,n} = (2N)^{-1} \sum_{x=1}^{L} \sum_{j=1}^{N} \exp\left[2\pi i j \left(a - \sum_{y=1}^{x} n_y\right)\Big/ N\right] \tau_{x,n}, \qquad a = 1, \ldots, N \tag{2.4}$$

where

$$\begin{aligned} \tau_{x,0} &= n_x = a_{x+}^+ a_{x+} + a_{x-}^+ a_{x-} \\ \tau_{x,1} &= a_{x+}^+ a_x \quad + a_{x-}^+ a_{x+} \\ \tau_{x,2} &= -i(a_{x+}^+ a_x \quad - a_x^+ \; a_{x+}) \\ \tau_{x,3} &= a_{x+}^+ a_{x+} - a_x^+ \; a_x \end{aligned} \tag{2.5}$$

In the subspace of no doubly occupied sites and for fixed a, the operators $S_{a,0}$, $S_{a,1}$, $S_{a,2}$, and $S_{a,3}$ generate a $u(2)$ algebra, i.e., $P_0[S_{a,0}, S_{a,i}]P_0 = 0$, $i = 1, 2, 3$, and $P_0 S_{a,i} S_{a,j} P_0 = iP_0 S_{a,k} P_0/2$, where (i, j, k) is a cyclic permutation of $(1, 2, 3)$. In the subspace of no doubly occupied sites the ath electron is defined by counting up the electrons from the site $x = 1$. Here $\mathbf{S}_a = (S_{a,1}, S_{a,2}, S_{a,3})$ represents the spin operators of the ath electron. They do not change the occupation numbers n_x and therefore they commute with $V(\{n_x\})$ and with P_0. Further, one obtains the commutation relations

$$\left[S_{a,n}, P_0 \sum_{\sigma} (a_{x+1\sigma}^+ a_{x\sigma} + a_{x\sigma}^+ a_{x+1\sigma}) P_0\right] = 0, \qquad 1 \leqslant x < L \tag{2.6}$$

and

$$\begin{aligned} S_{a,n} P_0 \sum_{\sigma} (a_{1,\sigma}^+ a_{L,\sigma} + a_{L,\sigma}^+ a_{1,\sigma}) P_0 \\ = P_0 \sum_{\sigma} (a_{1,\sigma}^+ a_{L,\sigma}) P_0 S_{a+1,n} + P_0 \sum_{\sigma} (a_{L,\sigma}^+ a_{1,\sigma}) P_0 S_{a-1,n} \end{aligned} \tag{2.7}$$

If we take an open chain with Dirichlet boundary conditions, (2.6) shows that the Hamiltonian (2.2) commutes with the operators $S_{a,n}$. The Hamiltonian is invariant under the transformations generated by the algebra $[u(2)]^N$. As a consequence, all spin configurations are degenerate and the system behaves as a pure paramagnet. In the case of periodic boundary conditions this is not longer true. Because of (2.7), the Hamiltonian (2.2) commutes only with the operators of a subalgebra of $[u(2)]^N$, namely with the operators that do not change under cyclic

permutations of the particles. We will call this subalgebra $([u(2)]^N)_c$. The components S_x, S_y, and S_z of the total spin

$$S_x = \sum_a S_{a,1} = \sum_x \tau_{x,1} \tag{2.8a}$$

$$S_y = \sum_a S_{a,2} = \sum_x \tau_{x,2} \tag{2.8b}$$

$$S_z = \sum_a S_{a,3} = \sum_x \tau_{x,3} \tag{2.8c}$$

of the system are elements of that algebra.

In the following we will discuss a system with periodic boundary conditions. A further symmetry operator of the Hamiltonian (2.2) is the operator that performs the cyclic permutation of the spins. It may be written as

$$C = \sum_{\sigma_1 \cdots \sigma_N} \sum_{x_1 < \cdots < x_N} a^+_{x_1\sigma_N} a^+_{x_2\sigma_1} \cdots a^+_{x_N\sigma_{N-1}} a_{x_N\sigma_N} \cdots a_{x_1\sigma_1} \tag{2.9}$$

Since $C^N = 1$, C has the eigenvalues $C_r = \exp(2\pi i r/N)$, $r = 1,..., N$. It commutes with S_x, S_y, and S_z so that the eigenvalues of S^2, S_z, and C may be used to classify the eigenstates of the Hamiltonian (2.2). C commutes with the elements of the symmetry group generated by the algebra $([u(2)]^N)_c$. Therefore we may characterize a spin configuration of an eigenstate of H_0 by its eigenvalue of C. All spin configurations with the same eigenvalue c_r are degenerate. Let $f(N/d, N_-/d)$ be the number of spin configurations with a given value of $S_z = m = N/2 - N_-$ that are invariant under cyclic permutations $C^{N/d}$ but not under $C^{N/dp}$ with a p such that $dp \mid N$ (dp divides N). One has

$$\sum_{d \mid N, N_-} f(N/d, N_-/d) = \binom{N}{N_-} \tag{2.10}$$

which is the number of spin configurations for fixed m. From (2.10) one obtains

$$f(N, N_-) = \sum_{d \mid N, N_-} \mu(d) \binom{N/d}{N_-/d} \tag{2.11}$$

where $\mu(d)$ is the Möbius function. (2.11) follows using formulation of the Möbius inversion formula for functions of more than one integer (see Appendix A). Some obvious properties of $f(N, N_-)$ are

$$f(N, N_-) = f(N, N - N_-) \tag{2.12a}$$

$$f(N, N) = f(N, 0) = \delta_{N,1} \tag{2.12b}$$

$$N \mid f(N, N_-) \tag{2.12c}$$

To obtain a spin configuration for a given r and $S_z = m$ one has to take a linear combination of N/d configurations that are invariant under $C^{N/d}$, where d is a divisor of r, N, and N . The number of spin configuration for fixed r and $S_z = m$ is therefore given by

$$d_{N,r,m} = \sum_{d \mid r, N, N} (d/N) f(N/d, N\ /d) \tag{2.13}$$

Some properties of $d_{N,r,m}$ are

$$d_{N,r,m} = d_{N,r,-m} \tag{2.14a}$$

$$d_{N,1,m} \leqslant d_{N,r,m} \leqslant d_{N,0,m} \tag{2.14b}$$

(2.14a) follows from (2.12a). The first equality in (2.14b) holds if and only if r, N, and N are relative prime. The second equality in (2.14b) holds if and only if r is a multiple of the greatest common divisor of N and N . Summing over r in (2.13), one obtains

$$\begin{aligned}
\sum_{r=0}^{N\ 1} d_{N,r,m} &= \sum_{r=0}^{N\ 1} \sum_{d \mid N, N} \sum_{e \mid N/d, N\ /d, r} (e/N)\, \mu(d) \binom{N/de}{N\ /de} \\
&= \sum_{r=0}^{N\ 1} \sum_{e \mid N, N} \sum_{d \mid e, r} \binom{N/e}{N\ /e} (d/N)\, \mu(e/d) \\
&= \sum_{e \mid N, N} \binom{N/e}{N\ /e} \sum_{d \mid e} \mu(d) \\
&= \binom{N}{N_-}
\end{aligned} \tag{2.15}$$

as it should be. The last step follows from (A.8).

The partition function is defined as

$$Z(\beta, h) = \mathrm{Tr}[\exp(-\beta H_0 + \beta h S_z)] \tag{2.16}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature and h is a uniform magnetic field in the z direction. Let E_n be the eigenvalues of H_0. The number of eigenstates of H_0 with the eigenvalues E_n in the subspace of states with eigenvalue c_r of C and eigenvalue m of S_z may be written as $\mu_{n,r} d_{N,r,m}$ with an integer $\mu_{n,r} \geqslant 0$. The partition function takes the form

$$Z(\beta, h) = \sum_{n,r,m} \mu_{n,r} d_{N,r,m} \exp(-\beta E_n + \beta h m) \tag{2.17}$$

We introduce

$$Z_0(\beta, h) = \sum_{n,r} \mu_{n,r} \exp(-\beta E_n)\, 2^N [\cosh(\beta h/2)]^N / N \tag{2.18}$$

which will be used as an estimate for $Z(\beta, h)$. To obtain an upper bound for the partition function, we use the second relation (2.14b),

$$\begin{aligned} d_{N,r,m} &\leqslant d_{N,0,m} \\ &= \sum_{e \mid N, N} \sum_{d \mid e} \binom{N/e}{N/e} (d/N)\, \mu(e/d) \\ &= \sum_{e \mid N, N_-} \binom{N/e}{N_-/e} \Phi(e)/N \end{aligned} \tag{2.19}$$

$\Phi(n)$ is the Euler totient function that is defined as the number of positive integers not exceeding and relative prime to n (see, e.g., ref. 10, p. 826). An upper bound for the partition function is now given by

$$\begin{aligned} Z(\beta, h) &\leqslant \sum_{n,r,N_-} \sum_{d \mid N, N_-} \Phi(d) \binom{N/d}{N_-/d} \mu_{n,r} \exp[-\beta E_n + \beta h(N/2 - N_-)]/N \\ &= \sum_{n,r} \sum_{d \mid N} \sum_{N_- = 0}^{N/d} \Phi(d) \binom{N/d}{N_-} \mu_{n,r} \exp[-\beta E_n + \beta h d(N/2d - N_-)]/N \end{aligned} \tag{2.20}$$

This result leads finally to

$$Z(\beta, h) \leqslant Z_0(\beta, h) \left\{ 1 + \sum_{\substack{d > 1 \\ d \mid N}} \Phi(d) [2 \cosh(\beta h d/2)]^{N/d} [2 \cosh(\beta h/2)]^{-N} \right\} \tag{2.21}$$

The equality in (2.20) and (2.21) holds if and only if $N = 1$.

A lower bound for the partition function may be obtained from (2.14b) as well. We have

$$d_{N,r,m} \geqslant d_{N,1,m} = f(N, N_-)/N \tag{2.22}$$

Using (2.17), one may perform the same manipulations as in (2.20) to obtain

$$Z(\beta, h) \geqslant \sum_{n,r} \sum_{d \mid N} \sum_{N_- = 0}^{N/d} \mu(d) \binom{N/d}{N_-} \mu_{n,r} \exp[-\beta E_n + \beta h d(N/2d - N_-)]/N \tag{2.23}$$

which may be written in the form

$$Z(\beta, h) \geqslant Z_0(\beta, h) \left\{ 1 + \sum_{\substack{d \mid N \\ d > 1}} \mu(d) [2 \cosh(\beta h d/2)]^{N/d} [2 \cosh(\beta h/2)]^{-N} \right\} \tag{2.24}$$

The equality in (2.23) and (2.24) holds if and only if $N=1$. These results may be formulated as follows.

Theorem 1. The partition function of the (extended) Hubbard model (2.2) with a hard-core repulsion and $N>1$ obeys the relations

$$Z_0(\beta, h)\, Y_<(\beta h) < Z(\beta, h) < Z_0(\beta, h)\, Y_>(\beta h) \tag{2.25}$$

with

$$Y_>(x) = 1 + \sum_{\substack{d>1 \\ d \mid N}} \Phi(d)[2\cosh(xd/2)]^{N/d}[2\cosh(x/2)]^{-N} \tag{2.26a}$$

and

$$Y_<(x) = 1 + \sum_{\substack{d>N \\ d \mid N}} \mu(d)[2\cosh(xd/2)]^{N/d}[2\cosh(x/2)]^{-N} \tag{2.26b}$$

Remarks. (i) For fixed x, $Y_>(x)-1$ and $1-Y_<(x)$ become exponentially small in the limit of large N. This shows that up to exponentially small corrections the partition function of the one-dimensional Hubbard model with hard-core interactions factorizes and the magnetic part is that of a pure paramagnet. The factorization becomes exact in the thermodynamic limit, where the upper and the lower bounds tend to the same value.

(ii) In the case $V=0$, $t_x = t > 0$ the thermodynamic potentials may be calculated in the thermodynamic limit using the explicit form of the eigenenergies of the Hamiltonian. This is done in the following section.

(iii) The bounds in Theorem 1 cannot be used as good estimates in the limit where βh tends to infinity and N is fixed. In this limit $Y_<(\beta h)=0$ and $Y_>(\beta h)=N$. The reason is that no assumption about the eigenvalues E_n of the Hamiltonian was made.

From now on we let $N>1$. In the same way as (2.26) was obtained, one may derive bounds for the derivatives of $Z(\beta, h)$. One has

$$\beta^{-k} \frac{d^k}{dh^k} Z(\beta, h) = \sum_{n,r,m} \mu_{n,r} d_{N,r,m} m^k \exp(-\beta E_n + \beta h m) \tag{2.27}$$

Since $m^{2l} \geqslant 0$, we may calculate the upper and lower bounds for the right-hand side of (2.27) for $k = 2l$ in the same way as we have calculated the upper and lower bounds for the partition function. One obtains

$$\beta^{-2l} \frac{d^{2l}}{dh^{2l}} Z(\beta, h) < \beta^{-2l} \frac{d^{2l}}{dh^{2l}} (Z_0(\beta, h)\ Y_>(\beta h)) \tag{2.28a}$$

$$\beta^{-2l} \frac{d^{l}}{dh^{2l}} Z(\beta, h) > \beta^{-2l} \frac{d^{2l}}{dh^{2l}} (Z_0(\beta, h)\ Y_<(\beta h)) \tag{2.28b}$$

If k in (2.27) is odd, one may use

$$\beta^{-2l-1} \frac{d^{2l+1}}{dh^{2l+1}} Z(\beta, h)$$

$$= \left(\frac{N}{2}\right) \beta^{-2l} \frac{d^{2l}}{dh^{2l}} Z(\beta, h) - \sum_{n,r,m} \mu_{n,r} d_{N,r,m} m^{2l} \left(\frac{N}{2} - m\right) \exp(-\beta E_n + \beta h m) \tag{2.29}$$

to calculate upper and lower bounds in this case. Since $m^{2l}(N/2 - m) \geqslant 0$, the derivation is the same as before. One obtains finally

$$\beta^{-2l-1} \frac{d^{2l+1}}{dh^{2l+1}} Z(\beta, h)$$

$$< \beta^{-2l-1} \frac{d^{2l+1}}{dh^{2l+1}} (Z_0(\beta, h)\ Y_<(\beta h))$$

$$+ \left(\frac{N}{2}\right) \beta^{-2l} \frac{d^{2l}}{dh^{2l}} Z_0(\beta, h)(Y_>(\beta h) - Y_<(\beta h)) \tag{2.30a}$$

$$\beta^{-2l-1} \frac{d^{2l+1}}{dh^{2l+1}} Z(\beta, h)$$

$$> \beta^{-2l-1} \frac{d^{2l+1}}{dh^{2l+1}} (Z_0(\beta, h)\ Y_>(\beta h))$$

$$+ \left(\frac{N}{2}\right) \beta^{-2l} \frac{d^{2l}}{dh^{2l}} Z_0(\beta, h)(Y_<(\beta h) - Y_>(\beta h)) \tag{2.30b}$$

The magnetization is given by

$$M(\beta, h) = \beta^{-1} \frac{d}{dh} \ln Z(\beta, h) \tag{2.31}$$

and the expectation value of S^2 of the system without a magnetic field may be calculated as

$$\langle S^2 \rangle(\beta, 0) = 3[Z(\beta, 0)]^{-1} \beta^{-2} \frac{d^2}{dh^2} Z(\beta, h)\Big|_{h=0} \tag{2.32}$$

One has the following result.

Corollary 1. The difference of the magnetization from the paramagnetic value for a model described by the Hamiltonian (2.2) is exponentially small. The magnetization obeys the relations

$$M(\beta, h) < M_0(\beta, h) + (N/2)[Y_>(\beta h)/Y_>(\beta h) - 1] + Y'_>(\beta h) \tag{2.33a}$$

$$M(\beta, h) > M_0(\beta, h) + (N/2)[Y_<(\beta h)/Y_<(\beta h) - 1] + Y'_<(\beta h) \tag{2.33b}$$

where

$$M_0(\beta, h) = \beta^{-1}(d/dh) \ln Z_0(\beta, h) = N \tanh(\beta h/2)/2 \tag{2.34}$$

is the paramagnetic value.

This follows from (2.31) and from the bounds on the partition function (2.25) and its first derivative [i.e., (2.30) for $l=0$]. But, as in the case of Theorem 1, this result gives no estimate for the magnetization in the limit where βh tends to infinity and N is fixed. For zero temperature, the magnetization is given by the maximal value S_z in the subspace of the ground states. It is shown below that for the Hubbard model (i.e., $V=0$, $t_x = t > 0$), $h > 0$, and $T=0$ we have $M = N/2$ if N is odd and $M = N/2 - 1$ if N is even, whereas the pure paramagnetic value is given by $M_0 = N/2$ in this case.

As was mentioned in the introduction, the second theorem of Aizenman and Lieb[5] shows that the magnetization of systems described by (2.2) with an odd number of particles exceeds the paramagnetic value. This result follows from a certain "clique structure" of the partition function. That structure may be obtained within our formulation as well. Inserting (2.11), (2.13) into (2.17), one obtains

$$Z(\beta, h) = \sum_{e \mid N} D_e(\beta)[2 \cosh(\beta e/2)]^{N/e} \tag{2.35}$$

where

$$D_e(\beta) = \sum_{n,r} \mu_{n,r} \exp(-\beta E_n) \sum_{d \mid e, r} d\mu(e/d)/N \tag{2.36}$$

Aizenman and Lieb showed that $D_e(\beta) > 0$ if N is odd and $t_x > 0$. In this case $M(\beta, h) > M_0(\beta, h)$ follows easily. On the other hand, if N is even, $D_e(\beta)$ might be negative for some e and it is not possible to obtain a bound for $M(\beta, h)$ using (2.35), (2.36).

In a similar way, using (2.28) in the case where $l = 1$, we obtain the following result.

Corollary 2. The expectation value of S^2 differs from the paramagnetic value by exponentially small corrections. It obeys the relations

$$\langle S^2 \rangle(\beta, 0) < 3N/4 + [Y_<(0)]^{-1} Y''_>(0) \tag{2.37a}$$

$$\langle S^2 \rangle(\beta, 0) > 3N/4 + [Y_>(0)]^{-1} Y''_<(0) \tag{2.37b}$$

The value $3N/4$ is again the paramagnetic value, which may be obtained by replacing Z with Z_0 in (2.32).

3. HARD-CORE INTERACTIONS, ELECTRONIC PROPERTIES

From now on we discuss the properties of the usual Hubbard model, i.e., V is set to 0 in (2.1) and (2.2) and $t_x = t > 0$ independent of x. Results for $t < 0$ may be obtained in a similar manner.

The Hamiltonian of the one-dimensional Hubbard model us usually diagonalized using the Bethe Ansatz. The case of hard-core interactions is much simpler than the case of finite U. The normalized eigenstates of H_0 may be written in the form

$$\begin{aligned} &|r; k_1 \cdots k_N; \sigma_1 \cdots \sigma_N\rangle \\ &\quad = L^{-N/2} \sum_P (-)^P n_{\{\sigma\}}^{1/2} N^{-1} \sum_{j=1}^{N} \exp(2\pi i r j/N) \\ &\qquad \times \sum_{x_1 < x_2 < \cdots < x_N} \exp\left(i \sum_a x_a k_{P_a} \right) a^+_{x_1 \sigma_{j+1}} \cdots a^+_{x_N \sigma_{j+N}} |0\rangle \end{aligned} \tag{3.1}$$

Here the first sum runs over all $N!$ permutations, and $n_{\{\sigma\}}$ is the smallest number of cyclic permutations that leave the spin configuration invariant. It is clear that $n_{\{\sigma\}} | N$. The spin indices are understood modulo N, i.e., $\sigma_j = \sigma_{j+N}$. Because of the periodic boundary conditions, the wavenumbers k_a must satisfy the condition

$$\exp(ik_a L + 2\pi i r/N) = 1 \tag{3.2}$$

The energy of the state (3.1) is given by

$$E(\{k_a\}) = -2t \sum_a \cos k_a \tag{3.3}$$

and the eigenvalue of this state with respect to C is $c_r = \exp(2\pi i r/N)$. One cannot choose r arbitrarily, it has to satisfy the condition $(N/n_{\{\sigma\}}) | r$. In the case $N_- = N$ or $N_- = 0$, for example, $n_{\{\sigma\}} = 1$ and only the value $r = 0$ is possible. In this case the sum over j in (3.1) is a sum over equal contributions and the states (3.1) are Slater determinants of single-particle states with momenta k_a. It should be mentioned that the states (3.1) form a complete orthonormal set of states without doubly occupied sites.

The form (3.1) of the eigenstates is similar to the usual Bethe Ansatz. The electronic part of the wave function is the same; the spin part of (3.1) is constructed using the symmetry described in Section 2. It should be mentioned that these states are eigenstates of S_z but not of S^2. A similar structure for the eigenstates of H_0 was used by Doucot and Wen,[11] using the language of first quantization.

The ground state is obtained by the symmetric distribution of the wave numbers around 0, i.e.,

$$\{k_j\} = \{-\pi(N-1)/L, \ldots, \pi(N-1)/L\} \tag{3.4}$$

The ground state is a state with $r = 0$ for N odd and $r = N/2$ for N even. The ground-state degeneracy is thus completely determined by the symmetry described in Section 2. From (2.11), (2.13), and (2.19), we obtain the following result.

Corollary 3. If $N < L$ the ground-state degeneracy for fixed $S_z = N/2 - N_-$ is given by

$$d_{N_-}^{(0)} = d_{N,0,N/2-N_-} = \sum_{e \mid N, N_-} \binom{N/e}{N_-/e} \Phi(e)/N \tag{3.5a}$$

if N is odd, and

$$d_{N_-}^{(0)} = d_{N,N/2,N/2-N_-} = \sum_{e \mid N, N_-} \sum_{d \mid e, N/2} (d/N)\, \mu(e/d) \binom{N/e}{N_-/e} \tag{3.5b}$$

if N is even.

Remark. In the case where N is odd, the maximal value of S_z is $N/2$, whereas it is $N/2 - 1$ if N is even. This result follows since $d_{N,0,N/2} = 1$ if N is odd and $d_{N,N/2,N/2} = 0$ if N is even, but $d_{N,N/2,N/2} = 1$ if N is even.

Only in the case of a half-filled band, i.e., for $N=L$, does one obtain a different result. In this case the ground-state energy given by (3.3) is zero and does not depend on r. In fact, all the spin configurations are degenerate in this case. Further, (3.4) shows that the ground state has zero momentum.

It should be mentioned that the energy differences of the states with lowest energy for a different r are of the order r^2/N^2L and are therefore much smaller than the energy difference of the two lowest lying eigenvalues for the same r, which is of the order $1/L$.

The expression (3.3) for the energy of the eigenstates may be used to calculate the thermodynamic potentials in the thermodynamic limit. The partition function $Z_0(\beta, h)$, which was introduced in (2.18), may be written as

$$Z_0(\beta, h) = N^{-1}[2\cosh(\beta h/2)]^N \sum_r Z_{N,r/N}(\beta) \tag{3.6}$$

where

$$Z_{N,u}(\beta) = \sum_{0 \leqslant n_1 < \cdots < n_N < L} \exp\left\{2\beta t \sum_a \cos[2\pi(n_a - u)/L]\right\} \tag{3.7}$$

We introduce

$$Y_u(\beta, z) = \sum_N z^N Z_{N,u}(\beta) \tag{3.8}$$

which may be written as

$$Y_u(\beta, z) = \prod_n (1 + z\exp\{2\beta t \cos[2\pi(n-u)/L]\}) \tag{3.9}$$

In the thermodynamic limit we define

$$p(\beta, z) = \beta^{-1} \lim_{L\to\infty} L^{-1} \ln Y_u(\beta, z) \tag{3.10}$$

$Y_u(\beta, z)$ may be interpreted as the grand canonical partition function of a system of noninteracting one-dimensional spinless fermions with single-particle energies $-2t\cos[2\pi(n-u)/L]$, $n=1,\ldots, L$. The function $p(\beta, z)$ is the pressure. It may be written in the form

$$p(\beta, z) = \beta^{-1} \int_0^1 dx \ln(1 + z\exp\{2\beta t \operatorname{cosd}[2\pi(x-u)]\}) \tag{3.11}$$

and does not depend on u. The reason is that, as mentioned above, the energies for different r become degenerate in the thermodynamic limit. The

free energy density is related to the pressure by a Legendre transformation in the chemical potential $\mu = \beta^{-1} \ln(z)$ to its conjugate variable c, the concentration of the electrons. It turns out that the free energy density of the one-dimensional Hubbard model with hard-core interaction is in the thermodynamic limit given by the sum of the free energy densities of a system of noninteracting spinless fermions and a systems of noninteracting spins, such that the densities of the spins and of the spinless fermions are the same.

4. THE CASE OF LARGE U

The case of large but finite U may be treated perturbatively with the hopping term of the Hamiltonian (2.1) as the perturbation. The part of H that is proportional to U has the eigenvalues nU, $n \geqslant 0$, with the eigenprojectors P_n. The P_n project onto the subspaces with n doubly occupied sites. Since the eigenvalues nU are highly degenerate, one has to perform a degenerate perturbation expansion. To first order one has to diagonalize H_0 given in (2.2). Because of the symmetry described in Section 2, the eigenstates (3.1) are highly degenerate. This degeneracy may be lifted at least partially by the second order of the perturbational calculation. To second order one has to calculate the matrix elements of (see, e.g., ref. 12)

$$P_0 H' P_0 = -P_0 H S_0 H P_0 \tag{4.1}$$

where S_0 is the reduced resolvent

$$S_0 = \sum_{n>0} (Un)^{-1} P_n \tag{4.2}$$

Since $P_0 H P_n = 0$ for $n > 1$, H' may easily be calculated and one obtains

$$\begin{aligned} H' &= H_1' + H_2' \\ H_1' &= -2(t^2/U) \sum_x n_x n_{x+1} \\ &\quad + (t^2/U) \sum_{x,\sigma,\sigma'} (a^+_{x+1\sigma} a^+_{x\sigma'} a_{x\sigma} a_{x-1\sigma'} + \text{h.c.}) \\ H_2' &= 2(t^2/U) \sum_{x,\sigma,\sigma'} a^+_{x+1\sigma} a^+_{x\sigma'} a_{x\sigma} a_{x+1\sigma'} \\ &\quad - (t^2/U) \sum_{x,\sigma} (a^+_{x+1\sigma} n_x a_{x-1\sigma} + \text{h.c.}) \end{aligned} \tag{4.3}$$

h.c. denotes the Hermitian conjugate of the preceding term. The decomposition of H' was chosen such that $P_0 H_1' P_0$ is invariant under the

symmetries generated by $([u(2)]^N)_c$. If for some reason the second parts of H_1' and H_2' are neglected, $H_0 + H'$ is the Hamiltonian of the tJ model.[8,9] The matrix elements of H' between two degenerate eigenstates of H_0 may be calculated without difficulties. The details are given in Appendix B. The result is

$$\begin{aligned}
&\langle r; k_1 \cdots k_N; \sigma_1' \cdots \sigma_N' | H' | r; k_1 \cdots k_N; \sigma_1 \cdots \sigma_N \rangle \\
&\quad = -2(t^2/U)(n_{\{\sigma\}} n_{\{\sigma'\}})^{1/2} N^{-2} \sum_{j,j'} \sum_{a} \exp[2\pi i r(j-j')/N] I_a \\
&\qquad \times (\delta_{\sigma_{j'+a}', \sigma_{l+a}} \delta_{\sigma_{j'+a+1}', \sigma_{j+a+1}} - \delta_{\sigma_{j'+a}', \sigma_{j+a+1}} \delta_{\sigma_{j'+a+1}', \sigma_{l+a}}) \\
&\qquad \times \prod_{a' \neq a, a+1} \delta_{\sigma_{j'+a'}', \sigma_{j+a'}}
\end{aligned} \tag{4.4}$$

where the coefficient I_a is given by

$$\begin{aligned}
I_a = L^{-N} \sum_{P} (-)^P \sum_{P'} (-)^{P'} \sum_{x_1 < \cdots < x_N} \exp\left[i \sum_{\beta} x_\beta (k_{P_\beta} - k_{P_\beta'}) \right] \\
\times [1 - \cos(k_{P_a} + k_{P_{a+1}})] \, \delta_{x_a + 1, x_{a+1}}
\end{aligned} \tag{4.5}$$

We may replace the sum over $x_1 < \cdots < x_N$ in (4.5) by a sum over $x_2 < \cdots < x_N < x_1 + L$. Then one may introduce $y_{a-1} = x_a$, $a = 2, \ldots, N$, $y_N = x_1 + L$ as new summation variables. After an obvious change in the summation over P and P' one obtains the same expression as in (4.5), but with a replaced by $a-1$. This shows that I_a does not depend on a, $I_a = I$. Summing (4.5) over a and diving by N, we obtain

$$\begin{aligned}
I &= L^{-N} N^{-1} \sum_{a,a'} \sum_{P} (-)^P \sum_{P'} (-)^{P'} \sum_{x_1 < \cdots < x_N} \exp\left[i \sum_{\beta} x_\beta (k_{P_\beta} - k_{P_\beta'}) \right] \\
&\quad \times [1 - \cos(k_{P_a} + k_{P_{a'}})] \delta_{x_a + 1, x_{a'}} \\
&= L^{-N} N^{-1} \sum_{a,a'} \sum_{P} (-)^P \sum_{x_1, \ldots, x_N} \exp\left[i \sum_{\beta} x_\beta (k_\beta - k_{P_\beta}) \right] \\
&\quad \times [1 - \cos(k_a + k_{a'})] \delta_{x_a + 1, x_{a'}}
\end{aligned} \tag{4.6}$$

The sum over $x_1, \ldots, x_N$ is easily performed and one obtains

$$I = L^{-1} N^{-1} \sum_{a,a'} (\cos k_a - \cos k_{a'})^2 \tag{4.7}$$

The matrix elements (4.4) may finally be written as

$$(4t^2/U) \langle r, \sigma_1' \cdots \sigma_N' | H_{\text{eff}} | r, \sigma_1 \cdots \sigma_N \rangle \tag{4.8}$$

where

$$H_{\text{eff}} = I \sum_a (\mathbf{S}_a \cdot \mathbf{S}_{a+1} - 1/4) \tag{4.9}$$

and

$$|r, \sigma_1 \cdots \sigma_N\rangle = n_{\{\sigma\}}^{1/2} N^{-1} \sum_j \exp(2\pi i r j/N) |\sigma_{j+1} \cdots \sigma_{j+N}\rangle \tag{4.10}$$

Up to a constant $-IN/4$, H_{eff} is the Hamiltonian of the one-dimensional antiferromagnetic Heisenberg model with periodic boundary conditions. The matrix elements of H_{eff} are taken between two eigenstates of the operator that performs a cyclic permutation of the spins. This operator commutes with H_{eff}. In order to obtain the eigenstates of the Hubbard model up to second order in the perturbational treatment, we have to diagonalize the Hamiltonian of the Heisenberg model with N spins. The ground state is an eigenstate of S^2 with the eigenvalue $s(s+1)$, where $s=0$ if N is even or $s=\frac{1}{2}$ if N is odd. This is in agreement with the theorem of Lieb and Mattis.[4]

It should be mentioned that the result (4.8), (4.9) was derived for a finite system and that it may give the wrong ground-state energy in the thermodynamic limit. Since the energy gap between the ground states for different r is $O(N^{-3})$, the convergence radius for the perturbational series is $O(N^{-4})$ and tends to zero in the thermodynamic limit. In the thermodynamic limit the lowest energies in the different subspaces where r is fixed become degenerate and it is not sufficient to calculate the matrix elements of H' between the degenerate eigenstates of H_0 for fixed r. Nevertheless, the thermodynamic limit of I may easily be calculated and one obtains

$$I = c\{1 + \sin(2\pi c)/2\pi c - [\sin(\pi c)/\pi c]^2\} \tag{4.11}$$

where c is the electron density in the thermodynamic limit. Using that the ground-state energy per particle of the Heisenberg model is in the thermodynamic limit given by $I/4 - I \ln 2$, we obtain the ground-state energy per site of the Hubbard model

$$E = -2t \sin(\pi c)/\pi - 4 \ln 2 (t^2/U)\, cI \tag{4.12}$$

This does not coincide with the result of Shiba[6] (see also ref. 7)

$$E = -2t \sin(\pi c)/\pi - 4 \ln 2 (t^2/U)\, c^2[1 - \sin(2\pi c)/2\pi c] \tag{4.13}$$

Equation (4.13) follows if one takes the thermodynamic limit of the nested Bethe Ansatz equations obtained by Lieb and Wu and expands in powers

of $(1/U)$. This means that the thermodynamic limit is taken first, whereas our result is obtained by first expanding and then taking the thermodynamic limit. As was argued above, our result can be only asymptotically true in the thermodynamic limit. Unfortunately, nothing is known about the convergence of the $1/U$ expansion that yields (4.13).[7] We may remark that (4.12) gives a lower value for the ground-state energy than (4.13) if and only if c is smaller than c_0, which is the solution of the equation $\tan(\pi c_0) = 2\pi c_0$. One has $c_0 \approx 0.371$. For small c the second term in (4.12) is of the order c^2, whereas the second term in (4.13) is of the order c^4. For $c = 1$, (4.12) and (4.13) coincide.

A similar calculation may be performed for the one-dimensional tJ-model.[8,9] The kinetic energy of this model, i.e., the part of the Hamiltonian that is proportional to t, is given by (2.2). A perturbational treatment of the term that is proportional to J is therefore completely analogous to the calculations above. The only difference is that $4t^2/U$ is replaced by J and some of the terms in H' are neglected in the tJ-model, namely the second terms in the expressions for H_1' and H_2' in (3.7). The result for the tJ-model is

$$J\langle r, \sigma_1' \cdots \sigma_N' | H_{tJ,\text{eff}} | r, \sigma_1 \cdots \sigma_N \rangle \tag{4.14}$$

where

$$H_{tJ,\text{eff}} = I_{tJ} \sum_a (\mathbf{S}_a \cdot \mathbf{S}_{a+1} - 1/4) \tag{4.15}$$

and

$$I_{tJ} = L^{-1} N^{-1} \sum_{a,a'} [1 - \cos(k_a - k_{a'})] \tag{4.16}$$

In the thermodynamic limit one obtains

$$I_{tJ} = c\{1 - [\sin(\pi c)/\pi c]^2\} \tag{4.17}$$

Putting $c = 1 - \delta$, it may be seen that I_{tJ} differs from I in the order δ. Such a result was expected, since the two parts of H' that are neglected in the tJ-model are of the order δ.[8,9]

APPENDIX A

The Möbius function $\mu(d)$ defined as (see, e.g., ref. 10, p. 826)

$$\begin{aligned} \mu(d) &= 1 && \text{if } d = 1 \\ &= (-1)^k && \text{if } d \text{ is a product of } k \text{ distinct primes} \\ &= 0 && \text{if } d \text{ is divisible by a square} > 1 \end{aligned} \tag{A.1}$$

obeys the following proposition.

Proposition (Möbius Inversion Formula). Let $f(n)$ and $g(n)$ be complex-valued arithmetic functions of a natural number. Then

$$f(n) = \sum_{d|n} g(d) \tag{A.2}$$

if and only if

$$g(n) = \sum_{d|n} \mu(d) f(n/d) \tag{A.3}$$

This is equivalent to the following proposition.

Proposition. Let $f(n_1,..., n_m)$ and $g(n_1,..., n_m)$ be complex-valued arithmetic functions of m natural numbers. Then

$$f(n_1,..., n_m) = \sum_{d|n_1,...,n_m} g(n_1/d,...,n_m/d) \tag{A.4}$$

if and only if

$$g(n_1,..., n_m) = \sum_{d|n_1,...,n_m} \mu(d) f(n_1/d,..., n_m/d) \tag{A.5}$$

Proof. Let n be the largest common divisor of $n_1,..., n_m$ and let $n_i = nm_i$, $i = 1,..., m$. Then (A.4) reads

$$\begin{aligned} f(m_1 n,..., m_m n) &= \sum_{d|n} g(m_1 n/d,..., m_n n/d) \\ &= \sum_{d|n} g(m_1 d,..., m_m d) \end{aligned} \tag{A.6}$$

and (A.5) reads

$$g(m_1 n,..., m_n n) = \sum_{d|n} \mu(d) f(m_1 n/d,..., m_m n/d) \tag{A.7}$$

The equivalence of (A.6) and (A.7) is a simple consequence of the equivalence of (A.2) and (A.3). This proves the equivalence of (A.4) and (A.5). On the other hand, the equivalence of (A.2) and (A.3) follows from the equivalence of (A.4) and (A.5). This shows that the second proposition is equivalent to the Möbius inversion formula.

The Möbius function obeys

$$\sum_{d|n} \mu(d) = \delta_{n,1} \tag{A.8}$$

which follows, for instance, from (A.2), (A.3) with $f(n) = 1$ and $g(n) = \delta_{n,1}$.

APPENDIX B

We calculate the matrix elements of H' in (4.3) between different degenerate eigenstates of H_0. For the first term in H_1' we obtain

$$\langle r, k_1 \cdots k_N, \sigma_1' \cdots \sigma_N' | \sum_x n_x n_{x+1} | r, k_1 \cdots k_N, \sigma_1 \cdots \sigma_N \rangle$$
$$= L^{-n} (n_{\{\sigma\}} n_{\{\sigma'\}})^{1/2} N^{-2} \sum_P (-)^P \sum_{P'} (-)^{P'} \sum_{j,j'} \exp[2\pi i r(j-j')/N]$$
$$\times \sum_{x_1 < \cdots < x_N} \left(\sum_a \delta_{x_a+1, x_{a+1}} \right) \exp\left[i \sum_a x_a (k_{P_a} - k_{P_a'}) \right] \prod_{a'} \delta_{\sigma_{j+a'}, \sigma'_{j'+a'}} \tag{B.1}$$

Due to the last factor, one gets a contribution only if the two spin configurations are the same. The second term in H_1' may be calculated from

$$\langle r, k_1 \cdots k_N, \sigma_1' \sigma_N' | \sum_{x,\sigma,\sigma'} a^+_{x+1\sigma} a^+_{x\sigma'} a_{x\sigma} a_{x-1\sigma'}$$
$$+ \text{h.c.} | r, k_1 \cdots k_N, \sigma_1 \cdots \sigma_N \rangle$$
$$= L^{-N} (n_{\{\sigma\}} n_{\{\sigma'\}})^{1/2} N^{-2} \sum_P (-)^P \sum_{P'} (-)^{P'} \sum_{j,j'} \exp[2\pi i r(j-j')/N]$$
$$\times \sum_{x_1 < \cdots < x_N} \exp\left[i \sum_{a'} x_{a'} (k_{P_{a'}} - k_{P'_{a'}}) \right] \sum_a \delta_{x_a+1, x_{a+1}}$$
$$\times 2 \cos(k_{P_a} + k_{P_{a+1}}) \prod_{a'} \delta_{\sigma_{j+a'}, \sigma'_{j'+a'}} \tag{B.2}$$

As in (B.1), one gets a contribution only if the two spin configurations are the same. This is due to the fact that H_1' has the same symmetry as H_0. The situation is different for H_2'. For the first term in H_2' one obtains

$$\langle r, k_1 \cdots k_N, \sigma_1' \cdots \sigma_N' | \sum_{x,\sigma,\sigma'} a^+_{x+1\sigma} a^+_{x\sigma'} a_{x\sigma} a_{x+1\sigma'} | r, k_1 \cdots k_N, \sigma_1 \cdots \sigma_N \rangle$$
$$= L^{-n} (n_{\{\sigma\}} n_{\{\sigma'\}})^{1/2} N^{-2} \sum_P (-)^P \sum_{P'} (-)^{P'} \sum_{j,j'} \exp[2\pi i r(j-j')/N]$$
$$\times \sum_{x_1 < \cdots < x_N} \exp\left[i \sum_{a'} x_{a'} (k_{P_{a'}} - k_{P'_{a'}}) \right] \sum_a \delta_{x_a+1, x_{a+1}}$$
$$\times \delta_{\sigma_{j+a+1}, \sigma'_{j'+a}} \delta_{\sigma_{j+a}, \sigma_{j'+a+1}} \prod_{a' \neq a, a+1} \delta_{\sigma_{j+a'}, \sigma'_{j'+a'}} \tag{B.3}$$

Finally, the second term of H_2' may be written as

$$\langle r, k_1 \cdots k_N, \sigma_1' \cdots \sigma_N' | \sum_{x,\sigma} a_{x+1\sigma}^{+} n_x a_{x-1\sigma} + \text{h.c.} | r, k_1 \cdots k_N, \sigma_1 \cdots \sigma_N \rangle$$

$$= L^{-N} (n_{\{\sigma\}} n_{\{\sigma'\}})^{1/2} N^{-2} \sum_{P} (-)^{P} \sum_{P'} (-)^{P'} \sum_{j,j'} \exp[2\pi i r(j-j')/N]$$

$$\times \sum_{x_1 < \cdots < x_N} \exp\left[i \sum_{a'} x_{a'} (k_{P_{a'}} - k_{P_{a'}'}) \right] \sum_{a} \delta_{x_a+1, x_{a+1}} 2\cos(k_{P_a} + k_{P_{a+1}})$$

$$\times \delta_{\sigma_{j+a+1}, \sigma_{j'+a}'} \delta_{\sigma_{j+a}, \sigma_{j'+a+1}} \prod_{a' \neq a, a+1} \delta_{\sigma_{j+a'}, \sigma_{j'+a'}'} \tag{B.4}$$

Up to prefactors, we have calculated all the contributions to the matrix elements of H'. The matrix elements of H' are now given by (4.4). If one takes the tJ-model, only the (B.1) and (B.3) must be taken into account and one finds (4.15).

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