Theorem on the one-dimensional interacting-electron system on a lattice

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A theorem about the spin properties of the ground state and the ordering of the energy levels for different spins of an interacting-electron model including an arbitrary diagonal interacting potential, an antiferromagnetic exchange, and an electron pair-hopping term for particles on a one-dimensional lattice is stated and proved. We show that when the number of electrons $N=4n+2$ (n an integer) with periodic boundary conditions or $N=4n$ with antiperiodic boundary conditions, the ground state is a nondegenerate singlet. This theorem generalizes a similar theorem Lieb and Mattis proved for the one-dimensional interacting electron system.

I. INTRODUCTION

The properties of the ground states of interaction-electron systems have been studied for many decades. However, rigorous results for them, even in one dimension are still rare. In 1962, Lieb and Mattis[1] showed that for a one-dimensional (1D) electron system with a diagonal interaction potential which conserves the total spin (either on a lattice or in the continuum limit) the ground state is a spin singlet and the lowest energy level belonging to each Hilbert subspace of a total spin S is ordered in a special way. In 1989, Lieb[2] showed that for the attractive Hubbard model in any dimension the ground state is a spin singlet. He also proved that for the repulsive Hubbard model on a bipartite lattice with A and B sites on each sublattice the ground state has the total spin $S=|A-B|/2$ at half filling. Ueda, Tsunetsugu, and Sigrist have recently extended this work of Lieb to the periodic Anderson model and shown that the ground state of the periodic Anderson model is also a singlet at half filling.[3] More recently, the authors have shown that the ground state of the 1D t-J model is a spin singlet and nondegenerate for any even number of electrons with applied boundary conditions.[4]

In one dimension, some of the interacting-electron models, for instance, the Hubbard model,[5] the single impurity Kondo model,[6] and the supersymmetric t-J model,[7] can be solved using the Bethe ansatz. However it is generally hard to obtain the value of the total spin and degeneracy of the ground state from the solution of the Bethe ansatz alone.

In this paper we generalize the theorem Lieb and Mattis proved in 1962[1] and the theorems we proved recently for the 1D t-J model.[4] We show that the theorem of Lieb and Mattis for the 1D electron system on a lattice[1] is still valid in the presence of an antiferromagnetic exchange interaction and/or some other nondiagonal interaction terms (the model Hamiltonian will be defined precisely later). We will also consider the effect of the boundary conditions which was ignored in the proof of Lieb and Mattis.[1]

The 1D interacting-electron system we consider here is defined on a lattice of L sites by the Hamiltonian

$$
\begin{aligned}
&H=H_t+H_V+H_J+H_P\ ,\\
&H_t=-\sum_{i\sigma} t_i c^{\dagger}_{i+1\sigma}c_{i\sigma}+\text{H.c.}\quad (t_i>0)\ ,\\
&H_V=V(n_1,\ldots,n_N)\ ,\\
&H_J=\sum_i J_i \mathbf{S}_i\cdot\mathbf{S}_i+1\quad (J_i\geq 0)\ ,\\
&H_P=-\sum_i T_i c^{\dagger}_{i+1\uparrow}c^{\dagger}_{i+1\downarrow}c_{i\downarrow}c_{i\uparrow}+\text{H.c.}\quad (T_i\geq 0)\ ,
\end{aligned}
\tag{1}
$$

where $c_{i\sigma}(c^{\dagger}_{i\sigma})$, $n_i=\sum_\sigma c^{\dagger}_{i\sigma}c_{i\sigma}$, and $\mathbf{S}_i=c^{\dagger}_{i\alpha}(\sigma/2)_{\alpha\beta}c_{i\beta}$ are, respectively, the electron annihilation (creation) operator, the electron number, and the electron spin operator at site i. $V(n_1,\ldots,n_N)$ is an arbitrary real function of $n_1,\ldots,n_N$ with N the total number of electrons. H_t describes the hopping of an electron between nearest-neighbor sites with a site-dependent hopping constant $-t_i$. $t_i>0$ has been assumed here. However, a global phase factor can be added to t_i, in which case the theorem we shall prove later is still valid, provided that the boundary condition is suitably amended. t_i (same as for J_i and T_i) can also be a function of electron configurations; generally, it can be represented as $t_i(n_1,\ldots,n_N)$. H_J describes the antiferromagnetic exchange between electrons on neighboring sites. H_P denotes the hopping of an electron pair between nearest neighbors.

The Hamiltonian H conserves the number of electrons and the total spin of the system. Thus we can restrict our discussion to states within a subspace with a given value of the z component of the total spin S_z, say M, and a given value N. We choose the basis set of this Hilbert subspace to be

$$
|\{x_\uparrow\}\{x_\downarrow\}\rangle=c^{\dagger}_{x_{1\uparrow}}\cdots c^{\dagger}_{x_{M_1\uparrow}}c^{\dagger}_{x_{1\downarrow}}\cdots c^{\dagger}_{x_{M_2\downarrow}}|0\rangle\ ,
\tag{2}
$$

where $\{x_\uparrow\}=\{x_{1\uparrow},\ldots,x_{M_1\uparrow}|x_{1\uparrow}<\cdots<x_{M_1\uparrow}\}$ and $\{x_\downarrow\}=\{x_{1\downarrow},\ldots,x_{M_2\downarrow}|x_{1\downarrow}<\cdots<x_{M_2\downarrow}\}$; $M_1(M_2)$ is the total number of up (down) spins, $N=M_1+M_2$, and $M=(M_1-M_2)/2$. The eigenstate of H can be expanded

in this basis in terms of the amplitudes $f(\{x_\uparrow\}\{x_\downarrow\})$:

$$\Phi=\sum_{\{x_\uparrow\}\{x_\downarrow\}} f(\{x_\uparrow\}\{x_\downarrow\})|\{x_\uparrow\}\{x_\downarrow\}\rangle \ . \tag{3}$$

Three kinds of boundary conditions will be considered in this paper: (1) periodic boundary conditions (PBC); (2) antiperiodic boundary conditions (ABC); (3) free boundary conditions (FBC). If the lowest energy level belonging to a total spin S is defined by $E(S)$, then the following theorem holds.

Theorem (1) In the cases (a) $N=4n+2$ (n=integer) with PBC or (b) $N=4n$ with ABC, the ground state is unique and a spin singlet, and $E(S)$ satisfies the inequality $E(2m+2)>E(2m)$, where m is an integer.

(2) In the cases (a) $N=4n+2$ with ABC or (b) $N=4n$ with PBC, $E(S)$ satisfies the inequality $E(2m+3)>E(2m+1)$.

(3) For arbitrary N with FBC, the ground state is unique and a spin singlet if N is even or twofold degenerate and a spin if N is odd, and $E(S+1)>E(S)$.

The content of this theorem is the same as the theorem we proved for the 1D t-J model.[4] However, it is valid for a much wider class of models. The theorem covers many of the interacting-electron models which are physically interesting in one dimension. If $t_i=t$ and $H_J=H_P=0$, it reproduces the result of Lieb and Mattis.[1] The theorem we proved recently for the 1D t-J model is also included in this theorem since the 1D t-J model is only a special limit of the Hamiltonian (1) with $t_i=t$, $J_i=J$, $H_P=0$, and $H_V=U\sum_i n_{i\uparrow}n_{i\downarrow}-(J/4)\sum_i n_i n_{i+1}$ in the limit of $U\to\infty$.

The choice of the boundary condition is important in the theorem. When PBC or ABC are imposed, N must be even because it is only in this case that all off-diagonal matrix elements of the hopping terms and the exchange terms between the two edge sites are seminegative and the theorem can be proved. However, if different boundary conditions are allowed for the up- and down-spin electrons and ABC are imposed for the spin operators, then an analogous theorem can be proved for the case when N is odd if either of the following two boundary conditions are assumed for the electrons: (1) PBC for the up-spin electrons and ABC for the down-spin electrons; (2) ABC for the up-spin electrons and PBC for the down-spin electrons. In both cases, the ground state of the system can be shown to be twofold degenerate and a spin doublet.

To prove the theorem, we shall make use of a theorem which was first used by Lieb and Mattis in their proofs.[1,4,8] That theorem says that: If, for a Hilbert space with a given basis set, all the off-diagonal matrix elements of a Hamiltonian H are real and seminegative, then to within a common phase factor all the coefficients of the ground-state wave function are positive or zero. If the Hilbert space cannot be divided into two subspaces such that all the matrix elements of H between vectors belonging to different subspaces vanish, then to within a common phase factor all the coefficients of the ground-state wave function will be positive and the ground state is unique. In the following we shall call this theorem the Lieb-Mattis (LM) theorem.

II. PROOF OF THE THEOREM

We first consider the case of FBC.

A proper choice for the basis set is important if we are to make use of the LM theorem in our proof. Previously[4] we used the LM theorem to prove a similar theorem for the 1D t-J model, but we chose the vectors

$$|\{x\}\{\sigma\}\rangle=c^\dagger_{x_1\sigma_1}\cdots c^\dagger_{x_N\sigma_N}|0\rangle \tag{4}$$

as the basis states, where $\{x\}=\{x_1,x_2\cdots x_N|1\le x_1<x_2<\cdots<x_N\le L\}$ and $\{\sigma\}=\{\sigma_1\sigma_2\cdots\sigma_N|\sum_i\sigma_i=M\}$. The off-diagonal matrix elements of the antiferromagnetic exchange term are not seminegative in this basis. In Ref. 4 we had to introduce a gauge transformation to remedy this defect.[4] However, a better and simpler choice for the basis states is that of Eq. (2). It is simple to check that all nondiagonal matrix elements of H in the basis set (2) are seminegative and that the Hamiltonian H cannot be divided into sets of noninteracting parts in the subspace of M_1 up spins and M_2 down spins. Thus the gauge transformation we introduced in Ref. 4 for the 1D t-J model is no longer needed. According to the LM theorem, all the coefficients of the lowest energy state of H in this subspace can be chosen positive and this lowest energy state is nondegenerate. We denote this state as $\Phi_0(M_1,M_2)$.

The value of the spin of the state $\Phi_0(M_1,M_2)$ can be found by noting that $\Phi_0(M_1,M_2)$ is not orthogonal to the ground state of a noninteracting electron system, i.e., $H_V=H_J=H_P$ and $t_i=t$, in the same subspace, because they both contain all the basis states (2) with no changes of signs in the amplitudes. The ground state for the noninteracting electron system with a uniform hopping constant t is easily found. It is easy to prove that it has total spin $S=|M_1-M_2|/2=|M|$. Thus the lowest energy state of H in this subspace also has total spin $S=|M|$. Furthermore, since any eigenstate with spin S has a corresponding eigenfunction in the $|S_z|<S$ subspace of eigenfunctions (N fixed), $E(S)<E(S+1)$ is immediately obtained. (The strict inequality follows by virtue of the uniqueness of the lowest energy state.) Obviously, the ground state of H is unique and a spin singlet when $N=$ even and twofold degenerate and a spin doublet when $N=$odd.

The case of PBC or ABC is more complicated since in this case the nondiagonal matrix elements of the boundary terms in H are not always smaller than or equal to zero. Generally, the nonzero nondiagonal matrix elements of these edge terms are functions of M_1 and M_2. But it can be shown that they become negative in the following four cases:

(i) $M_1=$odd, $M_2=$odd, $N=4n+2$ (n an integer), with PBC imposed;

(ii) $M_1=$even, $M_2=$even, $N=4n$, with ABC imposed;

(iii) $M_1=$even, $M_2=$even, $N=4n+2$, with ABC imposed;

(iv) $M_1=$odd, $M_2=$odd, $N=4n$, with PBC imposed.

These four cases correspond to the four itemized cases in (1) and (2) of the theorem. If we restrict our discussion to these four cases, then following the same steps as for

the case of FBC we find that clauses (1) and (2) of the theorem are true.

The theorem is therefore proved.

III. CONCLUSION

In conclusion, a theorem concerning the value of the total spin and the degeneracy of the ground state and the ordering of the energy levels for different total spins of 1D interacting-electron model has been stated and proved. This theorem generalizes a similar theorem proved by Lieb and Mattis for 1D electron models to include the antiferromagnetic exchange and other nondiagonal interaction terms in the Hamiltonian. The theorem shows that the ground state of 1D electron systems is generally boundary-condition dependent. Although the effect of boundary conditions is only of order $1/L$ in the thermodynamic limit, it is important for a system on a finite lattice.[9] Our theorem should be useful in guiding the choice of boundary conditions in studies of the Hamiltonian H on a finite lattice.

As seen from the proof of the theorem, all coefficients of the ground state of H in the subspace spanned by the basis set (2) have the same sign as those for the ground state of a noninteracting electron system with equal hopping constant. Thus if the interactions, H_V, H_J, and H_P are increased adiabatically from zero then the ground state will evolve within the relevant subspace from the noninteracting ground state without any level crossings. (Any level crossings would require some coefficients to change sign).

The LM theorem plays an important role in our proof. In some special cases this theorem can be also used in two or higher dimensions. The Nagaoka theorem[10] for the one-hole Hubbard model in the limit of $U\rightarrow\infty$, for example, can be simply proved by using this LM theorem. However, this theorem cannot in general be used in the case of electron systems in two or higher dimensions owing to the "minus sign" problem associated with the swapping of two electrons in these systems.[11] This is the reason why our theorem is valid only in one dimension.

So far, only the properties of the total spin of the system governed by H has been considered. However, the properties of other physical quantities which are conserved by H can also be studied by using LM theorem. For a homogeneous system (i.e., setting $t_i=t$, $J_i=J$, and $T_i=T$ in H), for example, it can be shown that the lowest energy state of H in each Hilbert space with M_1 up spins and M_2 down spins has total momentum zero[12] in the above-mentioned four cases (i)-(iv) using the LM theorem.

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[11]It is the same "minus sign" problem encountered in the quantum Monte Carlo simulations of electron systems in two or higher dimensions.

[12]The total momentum is defined as a summation $\sum_{k\sigma}kc^{\dagger}_{k\sigma}c_{k\sigma}$, where $c_{k\sigma}$ is the Fourier transform of $c_{i\sigma}$, $k=(2\pi/L)n$ (n an integer) if PBC are imposed and $=2\pi/L(n+\frac{1}{2})$ if ABC are imposed.