PHYSICAL REVIEW B VOLUME 46, NUMBER 1 1 JULY 1992-I

Energy-level ordering in the one-dimensional t-J model: A rigorous result

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(Received 26 March 1992)

Two theorems about the spin properties of the ground state and the ordering of the energy levels for different spins of the one-dimensional t-J model are stated and proved. It is shown 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.

I. INTRODUCTION

In recent years the t-J model has attracted much attention as a model to describe the cuprate superconductors and as a model of highly correlated electron systems in general.[1] Notwithstanding its apparent simplicity, the rigorous results and exact solutions for the model, even in one dimension, are rather limited and still rare.[2-4] In this paper we state and prove two theorems about the spin properties of the ground state and the energy-level ordering with total spin S and applied boundary condition for the one-dimensional (1D) t-J model.

The t-J model we consider here is defined on the subspace of electrons without double occupancy. For a 1D chain with L sites, it takes the form

$$H=H_t+H_J,$$

$$H_t=-t\sum_{i=1}^{L-1}\sum_{\sigma}(\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{i+1\sigma}+\text{H.c.})-tb\sum_{\sigma}(\tilde{c}_{1\sigma}^{\dagger}\tilde{c}_{L\sigma}+\text{H.c.}), \tag{1}$$

$$H_J=J\sum_{i=1}^{L-1}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\tfrac{1}{4}n_in_{i+1})+J|b|(\mathbf{S}_1\cdot\mathbf{S}_L-\tfrac{1}{4}n_1n_L),$$

where $\tilde{c}_{i\sigma}=c_{i\sigma}(1-n_{i-\sigma})$, $\mathbf{S}_i=c_{i\alpha}^{\dagger}(\sigma/2)_{\alpha\beta}c_{i\beta}$, and n_i are the projected electron operator, spin-$\frac{1}{2}$ operator, and electron number at site i, respectively. H_t describes the hopping of an electron between nearest-neighbor sites with a hopping constant $-t$. [Without loss of generality, $t>0$ is assumed here. The case $t<0$ is obtained from the case $t>0$ using the local gauge transformation $c_{i\sigma}\rightarrow(-1)^{R_i}c_{i\sigma}$.] H_J denotes the antiferromagnetic exchange between electrons on neighboring sites ($J>0$). The hopping and spin exchange interaction terms between the two edge sites are explicitly identified in the Hamiltonian (1). Depending on the choice of the boundary conditions, the parameter b takes the following values: (1) $b=1$ with $c_{i+L,\sigma}=c_{i\sigma}$, if periodic boundary conditions (p.b.c.) are assumed; (2) $b=-1$ with $c_{i+L\sigma}=-c_{i\sigma}$, if antiperiodic boundary conditions (a.b.c.) are assumed; (3) $b=0$, if free boundary conditions (f.b.c.) are assumed.

The Hamiltonian H conserves the number of electrons N and the z component of the total spin S_z. Thus we can restrict our discussion to states within a subspace with a given value of S_z, say M, and a given value N. We choose the basis set of the Hilbert space of the N-electron states to consist of all distinct eigenfunctions of S_{iz} compatible with eigenvalue M, i.e.,

$$|\{x\}\{\sigma\}\rangle=c_{x_1\sigma_1}^{\dagger}\cdots c_{x_N\sigma_N}^{\dagger}|0\rangle, \tag{2}$$

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 eigenstates in this Hilbert subspace can be expanded in the basis set in terms of the amplitudes $f(\{x\}\{\sigma\})=f(x_1\sigma_1\cdots x_N\sigma_N)$:

$$\Phi=\sum_{\{x\}\{\sigma\}}f(\{x\}\{\sigma\})|\{x\}\{\sigma\}\rangle. \tag{3}$$

In this paper we study the ground state (or states if the ground state is degenerate) and the energy-level ordering in H. Of central importance is the total spin $\mathbf{S}$ which is a conserved quantity. If we denote by $E(S)$ the lowest eigenvalue of H for states with total spin S, then the following two theorems hold.

Theorem 1. (1) In the cases (a) $N=4n+2$ (n is an integer) with p.b.c. or (b) $N=4n$ with a.b.c., 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 a.b.c. or (b) $N=4n$ with p.b.c., $E(S)$ satisfies the inequality $E(2m+3)>E(2m+1)$.

Theorem 2. For arbitrary N with f.b.c., the ground state is unique and a spin singlet if N is even or twofold degenerate and a spin doublet if N is odd, and $E(S+1)>E(S)$.

These two theorems are extensions of a corresponding theorem proved by Lieb and Mattis for pure spin systems on bipartite lattices.[5] Their theorem is generally valid independent of the dimensionality and the geometry of the lattice provided the lattice can be divided into two sublattices which satisfy some constraints for the intrasublattice and the intersublattice spin couplings. However, for the t-J model, the mixing of the fermion degrees of freedom with the spin degrees of freedom makes the problem more complicated. Our extension of the Lieb-Mattis theorem to the t-J model only applies in 1D where, except for the edge contribution, H_t (electron hopping) does not change the order of the electrons along the chain.

The choice of the boundary conditions is important in our cases. First, when p.b.c. or a.b.c. are imposed, N must be even because our proof relies on the assumption that the antiferromagnetic coupling between two spins belonging to the same sublattice vanish (we denote all odd sites of the lattice as the A sublattice and the others as the B sublattice). Second, in 1D the hopping terms between the

two edge sites, i.e., $\tilde{c}^{\dagger}_{1\sigma}\tilde{c}_{L\sigma}+\text{H.c.}$, changes the order of electrons along the chain giving rise to an extra sign factor $(-1)^{N-1}$ in the matrix elements of these edge hopping terms. Our result, theorem 1, only applies when the boundary condition compensates for this extra sign factor.

Part of the result about the ground state in theorem 1 has already been found in the limit of $J\rightarrow 0$ (Ref. 3) (i.e., the limit of $U\rightarrow\infty$ of the Hubbard model) and also in the numerical calculation of the model on small lattices.[4] Our theorem provides the general statement and formal verification of these results.

II. THE LIEB-MATTIS THEOREM

To prove the theorem, we shall make use of a theorem which Lieb and Mattis used in their proof.[5] For convenience in our proof below, we restate and slightly rephrase it here and take it as a lemma without proof.

Lemma. 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.

Obviously this lemma cannot apply directly to the Hamiltonian (1). The matrix elements of the hopping terms (except for the edge hopping terms) are already seminegative in the basis (2). However, the matrix elements of the nondiagonal part (i.e., the spin-flipping terms $S_i^{+}S_{i+1}^{-}+\text{H.c.}$) in H_J are not seminegative if the basis set (2) is chosen. Naively, one might perform a local spin rotation transformation by letting

$$S_i^{\pm}\rightarrow -S_i^{\pm},\quad S_{iz}\rightarrow S_{iz} \tag{4}$$

for the spins on sublattice A but leaving the spins on sublattice B invariantly make the matrix elements negative. However, this local spin rotation transformation will bring an extra factor $\pm i\sigma$ to the hopping terms in H. Therefore the condition required for the lemma to apply will not be satisfied by this spin rotation.

To overcome this difficulty, we introduce a hole-dependent spin rotation transformation

$$U=\prod_{i=1}^{L}\exp\left[i\pi\left(\sum_{l\le i}n_l\right)S_{iz}\right]. \tag{5}$$

This is a canonical transformation. The spin exchange terms transform to

$$US_{iz}S_{i+1z}U^{\dagger}=S_{iz}S_{i+1z},$$

$$U(S_i^{+}S_{i+1}^{-}+S_i^{-}S_{i+1}^{+})U^{\dagger}=-(S_i^{+}S_{i+1}^{-}+S_i^{-}S_{i+1}^{+}),$$

$$US_{1z}S_{Lz}U^{\dagger}=S_{1z}S_{Lz},$$

$$U(S_1^{+}S_L^{-}+S_1^{-}S_L^{+})U^{\dagger}=(-1)^{N-1}(S_1^{+}S_L^{-}+S_1^{-}S_L^{+}).$$

These are the same as the transforms of the spin exchange terms under the transformation (4). The attraction of this transformation is that the hopping terms between two nearest-neighbor sites remain unchanged under the transformation as

$$U\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{i+1\sigma}U^{\dagger}=\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{i+1\sigma}.$$

The transform of the edge hopping terms is more subtle as it depends on both N and S_z:

$$U(\tilde{c}^{\dagger}_{1\sigma}\tilde{c}_{L\sigma}+\text{H.c.})U^{\dagger}=e^{i\pi(S_z-N/2\sigma)}(\tilde{c}^{\dagger}_{1\sigma}\tilde{c}_{L\sigma}+\text{H.c.}).$$

Clearly, after the transformation all the nondiagonal matrix elements except for those arising out of the edge terms are seminegative as required by the lemma. For the nondiagonal contribution of the edge terms, the nonvanishing matrix elements are

$$\langle 1\sigma_N,x_1\sigma_1\cdots x_{N-1}\sigma_{N-1}|U\left(-tb\sum_{\sigma}\tilde{c}^{\dagger}_{1\sigma}\tilde{c}_{L\sigma}\right)U^{\dagger}|x_1\sigma_1\cdots x_{N-1}\sigma_{N-1},L\sigma_N\rangle=e^{i\pi(M+N-N/2\sigma)}bt,$$

$$\langle x_2\sigma_2\cdots x_N\sigma_N,L\sigma_1|U\left(-tb\sum_{\sigma}\tilde{c}^{\dagger}_{L\sigma}\tilde{c}_{1\sigma}\right)U^{\dagger}|1\sigma_1,x_2\sigma_2\cdots x_N\sigma_N\rangle=e^{-i\pi(M+N-N/2\sigma)}bt,$$

$$\langle 1-\sigma,x_2\sigma_2\cdots x_{N-1}\sigma_{N-1},L\sigma|U(S_1^{+}S_L^{-}+S_1^{-}S_L^{+})U^{\dagger}|1\sigma,x_2\sigma_2\cdots x_{N-1}\sigma_{N-1},L-\sigma\rangle=e^{i\pi(N-1)}.$$

These are smaller than zero only in the following five cases:

(i) $N=4n+2$ (n is an integer),

$M=0,2,\ldots,2n$, $b=1$;

(ii) $N=4n+2$, $M=1,3,\ldots,2n+1$, $b=-1$;

(iii) $N=4n$, $M=0,2,\ldots,2n$, $b=-1$;

(iv) $N=4n$, $M=1,3,\ldots,2n-1$, $b=1$;

(v) $b=0$.

The first four cases correspond to the four itemized cases listed in the statement of theorem 1. The last case corresponds to theorem 2. In the following, we restrict our discussion to these five cases. Since all the nondiagonal matrix elements of $UHU^{\dagger}$ are smaller than or equal to zero in these cases, the lemma now applies.

III. PROOF OF THEOREMS

We consider only the cases of even N and p.b.c. or a.b.c.

Consider first a Hamiltonian which is defined on the same Hilbert space as H:

$$H'=H_t+H'_J,$$
$$H'_J=J\mathbf{S}_A\cdot\mathbf{S}_B, \tag{6}$$

where $\mathbf{S}_A$ and $\mathbf{S}_B$ are defined as the total spins belonging,

respectively, to the A and B sublattice in a squeezed spin lattice in which all holes are omitted,

$$\mathbf{S}_A=\sum_i \frac{1+\exp\left(i\pi\sum_{l\le i} n_l\right)}{2}\mathbf{S}_i\,,$$

$$\mathbf{S}_B=\sum_i \frac{1-\exp\left(i\pi\sum_{l\le i} n_l\right)}{2}\mathbf{S}_i\,.$$

It can be shown that $\mathbf{S}_A$ and $\mathbf{S}_B$ commute.

The Hamiltonian H' is exactly soluble. It is straightforward to check that H_J' commutes with all terms in H_t:

$$\left[H_J', \sum_\sigma \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+1\sigma}\right]=0\,,$$

$$\left[H_J', \sum_\sigma \tilde{c}_{1\sigma}^\dagger \tilde{c}_{L\sigma}\right]=0\,.$$

This implies that the charge and spin degrees of freedom are separated in H'. The eigenvalue of H' is therefore a sum of the electron hopping energy E_t and the spin-correlation energy E_J. Correspondingly, the eigenfunction of H' is a product of a function of electron space coordinates and a function of electron-spin coordinates

$$f(x_1\sigma_1,\ldots,x_N\sigma_N)=X(x_1,\ldots,x_N)Y(\sigma_1\cdots\sigma_N)\,, \quad (7)$$

where $X(x_1,\ldots,x_N)$ is an eigenfunction of H_t with all spin indices omitted (a Slater determinant of noninteracting spinless fermions here) and $Y(\sigma_1\cdots\sigma_N)$ is an eigenfunction of H_J'

The energy eigenvalues, E_J, of the spin Hamiltonian can be obtained by solving H_J'

$$E_J=\tfrac{1}{2}J[S(S+1)-S_A(S_A+1)-S_B(S_B+1)]\,, \quad (8)$$

where S is the total spin of the system and $S_{A(B)}$ is the value of $\mathbf{S}_{A(B)}$. When $S_z=M$, the minimum of E_J will be reached when $S=M$ and $S_A=S_B=N/4$ ($N/4$ is the maximum value S_A and S_B can take).

The eigenvalue of the kinetic part of the Hamiltonian, E_t, is a sum of the kinetic energy of the noninteracting spinless fermions:

$$E_t=-2t\sum_i \cos k_i\,,$$

where the electron momenta k_i are determined from the boundary conditions

$$X(x_1,\ldots,x_{N-1},L+1)Y(\sigma_1\cdots\sigma_N)$$
$$=(-1)^{N-1}bX(1,x_1,\ldots,x_{N-1})Y(\sigma_N\sigma_1\cdots\sigma_{N-1})\,. \quad (9)$$

The difference between $Y(\sigma_N\sigma_1\cdots\sigma_{N-1})$ and $Y(\sigma_1\cdots\sigma_N)$ corresponds just to a shift of the spins along the ring by one unit (in the squeezed spin lattice). It is equivalent to swapping $\mathbf{S}_A$ and $\mathbf{S}_B$. From the theory of angular momentum we know that

$$\frac{Y(\sigma_N\sigma_1\cdots\sigma_{N-1})}{Y(\sigma_1\cdots\sigma_N)}=(-1)^{N/2-M} \quad (10)$$

when $S_A=S_B=N/4$ and $S=M$. Substituting (10) into (9), we obtain

$$X(x_1,\ldots,x_{N-1},L+1)=(-1)^{N/2-M-1}$$
$$\times bX(1,x_1,\ldots,x_{N-1})\,. \quad (11)$$

In the cases of (i)-(iv) this gives

$$X(x_1,\ldots,x_{N-1},L+1)=X(1,x_1,\ldots,x_{N-1})\,. \quad (12)$$

This is equivalent to taking a.b.c. in a spinless fermion system. Since the ground-state energy of noninteracting fermions with a.b.c. is lower than the ground-state energy of the corresponding system with any other boundary condition when N is even, we see from the above argument that when $S=M$ and $S_A=S_B=N/4$ both E_J and E_t can simultaneously attain their respective minima. Thus the ground state of H' has total spin $S=M$ in the $S_z=M$ subspace.

Next we consider the properties of H' under the transformation (5). Since H_t is the same as the kinetic part of H, we need only consider the J term in H'. It is easy to show that

$$UH_J'U^\dagger=J[S_{Az}S_{Bz}-\tfrac{1}{2}(S_A^+S_B^-+S_A^-S_B^+)]\,. \quad (13)$$

Thus the nondiagonal matrix elements of $UH_J'U^\dagger$ are seminegative. Combining this result with that for H_t, we see that all the nondiagonal matrix elements for $UH'U^\dagger$ are also seminegative. According to the lemma all the coefficients of the ground state of $UH'U^\dagger$ are semipositive up to a common phase factor. More strictly, since the Hamiltonian H' cannot be divided into sets of noninteracting parts in the subspace $S_z=M$, all coefficients will be nonzero. This means that the ground state of H' is nondegenerate in the subspace $S_z=M$.

Now let us return to the Hamiltonian H. By the lemma, all the coefficients of the ground state of $UHU^\dagger$ are also positive in the $S_z=M$ subspace. The ground state of $UHU^\dagger$ and the ground state of $UH'U^\dagger$ will then be nonorthogonal (two vectors cannot be orthogonal if all their coefficients in some basis have the same sign), and therefore the ground state of H' and the ground state of H will also be nonorthogonal and the ground state of H in the $S_z=M$ subspace must have spin $S=M$.

Finally let us consider the ordering of the energy levels for different S. It is known that any eigenstate with spin S has a corresponding eigenfunction in the $|S_z|\le S$ subspace of eigenfunctions. Thus the energy of the lowest-energy state of a $S_z=M$ subspace will not be larger than the energy of a corresponding state of a subspace with $S_z>M$. Generally $E(S+1)\ge E(S)$. For H, since the lowest-energy state for a given S_z is nondegenerate in the cases (i)-(iv) as shown before, we immediately get that $E(S+2)>E(S)$, where S=even/odd if $N=4n+2$ and p.b.c./a.b.c. are imposed or if $N=4n$ and a.b.c./p.b.c. are imposed. Theorem 1 is therefore proved.

The proof for theorem 2 is similar to that for theorem 1. As f.b.c. are assumed, the edge terms in H vanish. So the theorem holds without the limit on N.

IV. CONCLUSION

In conclusion, two theorems 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 in the 1D t-J model have been stated and proved. In proving the theorems we have introduced a hole-dependent nonlocal gauge transformation. After this transformation all the nondiagonal matrix elements of the t-J model are seminegative provided proper boundary conditions are imposed. A possible major application of this transformed Hamiltonian will be in Monte Carlo simulations. As all the nondiagonal matrix elements of this Hamiltonian are nonpositive there will be no sign problem. Work on this aspect is in progress.

ACKNOWLEDGMENTS

One of the authors (T.X.) would like to thank Mr. D. P. Chu for many useful discussions. This work was supported by SERC Grant No. GR/E/79798.

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