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LETTER TO THE EDITOR

The Marshall–Lieb–Mattis theorem for a class of $t-J$ model

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Abstract. We consider a class of $t-J$ model on a bipartite lattice characterised by negative hopping matrix elements within the same sublattice. When there are one or two (one in each sublattice) holes, we extend the theorems by Marshall and by Lieb and Mattis which determines the basic structure of the ground state. When the two sublattices contain the same number of electrons, the ground state is unique, is spin singlet, and satisfies the Marshall sign rule.

It is known rigorously that the ground state of a Heisenberg antiferromagnet on a finite bipartite lattice satisfies rather strong constraints. When two sublattices are identical, Marshall's classical result [1] implies that the ground state is non-degenerate, is spin singlet, and satisfies the so-called Marshall sign rule. Lieb and Mattis [2] derived stronger results for an arbitrary bipartite lattice. Recently Lieb [3] proved similar results for the exactly half-filled Hubbard model.

During the recent intensive study of the Heisenberg antiferromagnet, it has become clear that such rigorous constraints are quite important even in a heuristic or a numerical analysis of the problem. In the RVB (resonating-valence-bond) approaches [4], the Marshall rule is used to determine the signs of the coefficients in the valence-bond states. It was also found that [5], by making full use of the Marshall condition, one can reduce the dimensionality of the matrix to be diagonalised in calculating the exact ground state of a finite system. In some cases this reduction is so efficient that one only has to diagonalise a 3×3 matrix to get the ground state of a 10-spin system [5].

In an electron system which is not exactly half-filled, however, there is no apparent reason for the Marshall-Lieb-Mattis conditions to be satisfied. The famous Nagaoka theorem [6] and the recent exact results in the large-n $t-J$ model [7] provide concrete examples where the conditions are violated by the dynamical freedom of holes. Although being exact, both examples are limited to special cases, namely, $U=\infty$ and precisely one hole in the former, and $n=\infty$ in the latter. (Here n is the 'flavour' of electron, and $n=2$ is the standard system.) We must conclude that our knowledge on the general structures of the ground states of doped electron systems is rather incomplete.

In the present letter, we show that, in a special class of $t-J$ model, the strict extensions of the Marshall-Lieb-Mattis theorem can be proved. The $t-J$ model is probably the simplest model for strongly electron systems including dynamical holes. It describes electrons hopping around the lattice interacting with each other through infinitely large on-site Coulomb repulsion and nearest-neighbour antiferromagnetic interaction.

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The model is defined on a finite bipartite lattice, and is characterised by negative hopping matrix elements within the same sublattice. The proof works when there are one or two holes, but in the latter case we require that each sublattice contain one hole. Unfortunately such models may not be very realistic as models for the existing materials. However we believe that the present example sheds some light on the basic nature of the doped electron systems and, perhaps more importantly, provides textbook examples where the effect of doping can be studied by efficient diagonalisation algorithm in the spirit of [5].

Consider a finite lattice which can be divided into two sublattices A and B, which consist of $|A|$ sites and $|B|$ sites, respectively. For convenience we associate an integer with each lattice site, so that $i=1,\ldots,|A|$ are in the A sublattice and $i=|A|+1,\ldots,|A|+|B|$ are in the B sublattice. We put N electrons on the lattice without allowing any double occupancy. A site without an electron is said to be occupied by a hole. We denote by N_A and N_B the number of electrons on the A and B sublattices, respectively.

We consider the following $t-J$ Hamiltonian.

$$H=-\sum_{i,j} t_{ij}(c_{i\uparrow}^{\dagger}c_{j\uparrow}+c_{i\downarrow}^{\dagger}c_{j\downarrow})+\sum_{i,j} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j. \tag{1}$$

The anticommuting operators $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ creates and annihilates, respectively, an electron at site i with spin σ. The second summation is taken over sites i, j occupied by electrons where the spin operator $\boldsymbol{S}_i=(S_i^x, S_i^y, S_i^z)$ is defined by

$$S_i^x=\frac{1}{2}(c_{i\uparrow}^{\dagger}c_{i\downarrow}+c_{i\downarrow}^{\dagger}c_{i\uparrow}) \qquad S_i^y=\frac{1}{2\mathrm{i}}(c_{i\uparrow}^{\dagger}c_{i\downarrow}-c_{i\downarrow}^{\dagger}c_{i\uparrow})$$

$$S_i^z=\frac{1}{2}(c_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\downarrow}).$$

Here we consider a class of models which satisfy the following.

(i) $t_{ij}=t_{ji}\leqslant 0$ where i and j belong to the same sublattices. $t_{ij}=t_{ji}=0$ when i and j belong to the different sublattice. Therefore electrons hop only within one of the sublattices. Note that both N_A and N_B become conserved quantities under this condition.

(ii) $J_{ij}\geqslant 0$ (antiferromagnetic) when i and j belong to the different sublattices. $J_{ij}\leqslant 0$ (ferromagnetic) when i and j belong to the same sublattice.

(iii) All the sites are connected by non-vanishing J_{ij}, and all the sites in each sublattice are connected by non-vanishing t_{ij}.

(iv) There are one or two holes. In the latter case, there is one in each sublattice. In other words, $N_A=|A|$, $|A|-1$ and $N_B=|B|$, $|B|-1$.

Note that the most standard $t-J$ model with nearest-neighbour hoppings does not satisfy our condition (i). An example of the model which meets our conditions is a special (and an artificial) case of the so-called $t-t'-J$ model [8] (see figure 1) for the Cu—O plane in the high-T_c superconductors. The model is characterised by negative nearest-neighbour hoppings t, negative next-nearest-neighbour hoppings t', t'', as well as nearest-neighbour antiferromagnetic couplings J. By setting $t=0$ in the $t-t'-J$ model we get a model which satisfies our conditions. It is natural to expect that adding sufficiently small positive t in this model does not change our conclusions. But we have no rigorous estimates.

Before stating our result we specify the basis states we work with. When there is only one hole, the basis state is given by

$$|i;\sigma\rangle=(-1)^{i+\alpha(\sigma)}c_{1\sigma_1}^{\dagger}c_{2\sigma_2}^{\dagger}\ldots c_{i-1\sigma_{i-1}}^{\dagger}c_{i+1\sigma_{i+1}}^{\dagger}\ldots c_{N+M\sigma_{N+M}}^{\dagger}|0\rangle \tag{2a}$$

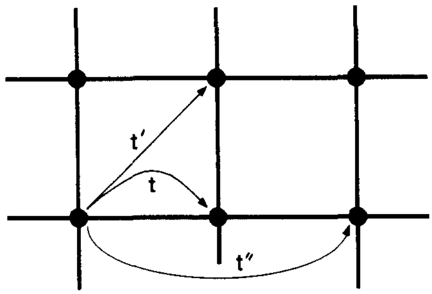

Figure 1. The $t-t'-J$ model [8] falls into our class when $t=0$ and t', $t''<0$.

where i is the position of the hole, $\sigma=\{\sigma_1,\ldots,\sigma_{N+M}\}$ represents the spin of electrons, and $\alpha(\sigma)$ is the number of electrons with downward spin on the A sublattice. The vacuum $|0\rangle$ is the state with no electrons. When there are two holes, i.e. one in each sublattice, the basis state is

$$|i,j;\sigma\rangle=(-1)^{i+j+\alpha(\sigma)}c^\dagger_{1\sigma_1}c^\dagger_{2\sigma_2}\ldots c^\dagger_{i-1\sigma_{i-1}}c^\dagger_{i+1\sigma_{i+1}}\ldots c^\dagger_{j-1\sigma_{j-1}}c^\dagger_{j+1\sigma_{j+1}}\ldots c^\dagger_{N+M\sigma_{N+M}}|0\rangle \tag{2b}$$

where i, j are the positions of the holes.

As usual we denote the eigenvalue of the operator $\boldsymbol{S}^2$ (where $\boldsymbol{S}=\Sigma_i\boldsymbol{S}_i$) as $S(S+1)$, and define the total S^z operator as $\Sigma_i S_i^z$. Then we have the following theorem.

Theorem. Consider a $t-J$ model which satisfies (i)-(iii). We restrict ourselves to a sector with fixed N_A and N_B allowed in (iv). Then the ground state (of this sector) has total spin $S=|N_A-N_B|/2$, and is unique up to the trivial $(2S+1)$-fold degeneracy. Moreover when the ground state is also an eigenstate of the total S^z, it is a linear combination of all the basis states (2) which have given S^z, and all the coefficients are strictly positive.

Proof. The proof is easy after finding out what should be proved. The first thing we should note is that, for arbitrary distinct basis states $|s\rangle$, $|s'\rangle$ of the form (2), we always have that $\langle s|H|s'\rangle\leq 0$. The proof of the inequality for the antiferromagnetic interaction part is elementary, and is the same as that in [1, 2]. To prove the inequality for the hopping part, we note that there is an identity

$$\begin{aligned}(c^\dagger_{i\uparrow}c_{k\uparrow}+c^\dagger_{i\downarrow}c_{k\downarrow})(-1)^{i+j}(c^\dagger_{1\sigma_1}c^\dagger_{2\sigma_2}\ldots c^\dagger_{i-1\sigma_{i-1}}c^\dagger_{i+1\sigma_{i+1}}\ldots c^\dagger_{N+M\sigma_{N+M}})\\ =-(-1)^{k+j}(c^\dagger_{1\sigma_1}c^\dagger_{2\sigma_2}\ldots c^\dagger_{k-1\sigma_{k-1}}c^\dagger_{k+1\sigma_{k+1}}\ldots c^\dagger_{N+M\sigma_{N+M}})\end{aligned}$$

(where we set $\sigma_i=\sigma_k$ on the right-hand side) and the similar one with i and j exchanged, which follow from the anticommuting nature of the electron operators. We also note that all the basis states with common N_A, N_B, and S^z are connected to each other through a sequence of non-vanishing matrix elements of H. Then it follows from the Perron–Frobenius theorem† (or the 'node counting argument') that, in each sector

† Let $M=\{M_{ij}\}$ be an $n\times n$ matrix with $M_{ij}\leq 0$ for $i\neq j$. We assume that M is indecomposable in the sense that, for any i, j, there is a sequence $\{i_1,i_2,\ldots,i_K\}$ with $i=i_1$, $j=i_K$, and $M_{i_ki_{k+1}}\neq 0$ for all $k<K$. Then the Perron–Frobenius theorem states (among other things) that the eigenstate of M with the minimum eigenvalue is unique (up to normalisation), and can be written as a linear combination of all the basis vectors with strictly positive coefficients.

with fixed N_A, N_B, and S^z, the lowest energy state is unique, and is a linear combination of all the basis states (in the sector) with strictly positive coefficients. This proves the half of the theorem.

Now it remains to determine the total spin of the ground state. This could be done in a way exactly the same as in [2], but here we take a short cut. If we set $t_{ij} = 0$ for all i, j, then the model reduces to a standard Heisenberg antiferromagnet, and Lieb and Mattis' theorem [2] determines the ground states. The ground states are degenerate up to the positions of the static holes, but they all have the value of total spin claimed in our theorem. Adding sufficiently small negative t_{ij} (which satisfy our criterion) will lift the degeneracy, but does not change the total spin. Since the ground state is known to be unique for *any* negative t_{ij} which satisfy our criterion, the total spin is unchanged and is equal to the value claimed in the theorem.

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