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LETTER TO THE EDITOR

Ferromagnetic ground states for the Hubbard model on line graphs

A Mielke

Institut de Physique Théorique, Ecole Polytechnique Fédérale de Lausanne, PHB-Ecublens, CH-1015 Lausanne, Switzerland

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Abstract. We discuss some of the properties of the Hubbard model on a line graph with n vertices. It is shown that the model has ferromagnetic ground states if the interaction is repulsive ($U>0$) and if the number of electrons N satisfies $2n \geqslant N \geqslant M$. M is a natural number that depends on the line graph. For example, the Kagomé lattice is a line graph, it has $M=5n/3-1$.

The question which are the conditions for a system of itinerant electrons to have a ferromagnetic ground state, has long been discussed and a final answer is not within view. The Hubbard model [1] is a simple model to discuss such a question. It describes itinerant electrons on a lattice or more generally on a graph with an onside interaction. The Hamiltonian has the form

$$H=-\sum_{x,y,\sigma} a_{xy} c^+_{x\sigma} c_{y\sigma} + U \sum_x n_{x+} n_{x-}. \tag{1}$$

Let $G=(V,E)$ be a finite connected graph without loops (i.e. without an edge that connects a single vertex with itself). G may have multiple edges, V is the set of vertices and E is the set of edges of G. x, y in (1) are elements of V, a_{xy} is equal to the number of edges connecting x and y and in the case of a simple graph, a_{xy} is thus 0 or 1. (a_{xy}) is the adjacency matrix of G. $c^+_{x\sigma}$ $(c_{x\sigma})$ are the creation (annihilation) operators for electrons with spin σ on the vertex x and $n_{x\sigma}=c^+_{x\sigma}c_{x\sigma}$, $n_x=n_{x+}+n_{x-}$. They obey the usual anticommutation relations for fermions. U is a positive real number, it describes the magnitude of the on-side repulsion of the electrons on the vertices.

In the following N is the number of electrons and one has $N\leqslant 2|V|$ where $|V|$ denotes the number of elements of V. The Hamiltonian conserves the number of electrons with spin $+$ $(-)$, which we denote by N_+ (N_-). It commutes with the spin operators

$$S^+=\sum_x c^+_{x+}c_{x-} \qquad S^-=\sum_x c^+_{x-}c_{x+} \qquad S^z=\tfrac{1}{2}(N_+-N_-). \tag{2}$$

These operators generate a global SU(2) symmetry. We may choose the eigenstates of H to be also eigenstates of

$$S^2_{\mathrm{op}}=(S^z)^2+\tfrac{1}{2}(S^+S^-+S^-S^+). \tag{3}$$

This operator has the eigenvalues $S(S+1)$ and we call S the spin of the eigenstate.

There are only some special cases in which the existence of a ferromagnetic ground state of the Hubbard model is known. In the case of a hard-core repulsion between

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the electrons (i.e. $U=\infty$) and if the dynamically allowed permutations are all even, there is one among the ground states that has a maximal spin $S=N/2$ (saturated ferromagnetism) [2]. There are two cases where this theorem may be applied. The first is the one-dimensional case with an even number of electrons [3]. In this case there are many other ground states and one may show that up to exponentially small corrections the system behaves as an ideal paramagnet [4]. If the graph on the other hand obeys a certain connectivity condition [5] (which is not satisfied for example in the one-dimensional case) and if the number of electrons is $N=|V|-1$, the ferromagnetic ground state is unique up to the degeneracy due to the global SU(2) invariance of H. This is the theorem of Nagaoka [6, 7]. But this case is somewhat particular since it has been shown by Sütö [8] that such a system behaves in the thermodynamic limit and for any temperature $T>0$ as an ideal paramagnet.

A unique ground state (again up to the degeneracy due to the global SU(2) invariance) with a macroscopic but not saturated value for the spin is obtained if the graph G is bipartite and $N=|V|$. A graph G is called bipartite if it has two disjoint vertex classes V_1 and V_2 such that each vertex is either in V_1 or in V_2 and each edge joins a vertex of V_1 to a vertex of V_2. Lieb [9] has shown that in this case the ground state has a spin $S=\frac{1}{2}||V_1|-|V_2||$. It is clear that S may be macroscopic.

We will discuss the Hamiltonian (1) on graphs which belong to a certain class, namely on line graphs. The line graph $L(G)=(V_L, E_L)$ of a graph $G(V, E)$ is constructed as follows. Its vertex set is the edge set of G, $V_L=E$. Two vertices of V_L are connected by as many edges as the corresponding edges in G have vertices in common. Some of the spectral properties of simple line graphs may be found in [10] and most of them are valid for general line graphs without loops as well. The adjacency matrix A_L of the line graph $L(G)$ is easily constructed if one knows the incidence matrix $B(G)=(b_{xe})_{x\in V, e\in E}$ of G. b_{xe} is equal to 1 if the vertex x is incident to the edge e and zero otherwise. Then one has

$$B(G)^{t}B(G)=2I_{|E|}+A_L \tag{4}$$

where B^t is the transpose of B and I_n denotes the n-dimensional unit matrix. Since B^tB is a positive-semidefinite matrix it follows from (4) that each eigenvalue a of the adjacency matrix A_L obeys $a\geqslant -2$. Furthermore, if -2 is an eigenvalue of A_L, then its eigenspace is the kernel of $B(G)$ and its multiplicity $m(-2)\geqslant|E|-|V|$. In particular, the following proposition holds.

Proposition

(*a*) If G is a tree or a graph with only one cycle that is odd, then -2 is not an eigenvalue of A_L.

(*b*) If G is bipartite but not a tree, then -2 is an eigenvalue of A_L and its multiplicity is $m(-2)=|E|-|V|+1$.

(*c*) If G is not bipartite and not a graph with only one cycle that is odd, then -2 is an eigenvalue of A_L and its multiplicity is $m(-2)=|E|-|V|$.

Proof

(*a*) The edges and vertices of a tree T may always be ordered in such a way that the incidence matrix takes the form

$$B(\mathrm{T})=\begin{bmatrix} B'(\mathrm{T}) \\ b \end{bmatrix} \tag{5}$$

where b is a row with entries 0 or 1 and B' is a $|E|\times|E|$ matrix whose entries are 1 in the diagonal, 0 in the upper triangle and 0 or 1 in the lower triangle. B' is thus non-singular. Therefore the rank of B as well as the rank of B^tB is $|E|$. B^tB is non-singular and from (4) it follows that -2 is not an eigenvalue of A_L.

On the other hand, let G be a tree with an additional edge such that G contains one cycle of length l where l is odd. Then as above we may order the edges and vertices of G in such a way that its incidence matrix B takes the form

$$B=\begin{bmatrix} B_l & X \\ O & B'' \end{bmatrix} \tag{6}$$

where B_l is the incidence matrix of a cycle of length l, O is a $(|V|-l)\times l$ matrix whose entries are all equal to zero, B'' is a $(|V|-l)\times(|V|-l)$ matrix whose entries are 1 in the diagonal, 0 in the upper triangle and 0 or 1 in the lower triangle and X is a $l\times(|V|-l)$ matrix with entries 0 or 1. From this structure and the fact that l is odd it follows that B is non-singular and therefore B^tB is non-singular. So -2 is not an eigenvalue of A_L.

(b) Let V_1 and V_2 be the two vertex classes of the bipartite graph G. Each edge may be oriented from V_1 to V_2. Let $S=\mathrm{diag}(s_x)$ be the diagonal matrix with entries s_x in the diagonal where $s_x=1$ if $x\in V_1$ and $s_x=-1$ if $x\in V_2$. The matrix $D=SB$ is the oriented incidence matrix for this orientation. This matrix has rank $|V|-1$ and its kernel is called the circuit space of G (see e.g. [10]). The kernel of B is thus the circuit space with respect to this orientation and its dimension is $|E|-|V|+1$. From (4) it follows that it is also the eigenspace of the eigenvalue -2 of A_L.

(c) Let G' be a simple subgraph of G which is constructed from a spanning tree of G with an additional edge such that G' contains one cycle of length l where l is odd. In the proof of (a) it was shown that the incidence matrix B' of G' is non-singular. Therefore the incidence matrix $B(G)$ contains a $|V|\times|V|$ matrix that is non-singular. The rank of B and of B^tB is thus $|V|$ and the eigenspace of the eigenvalue -2 of A_L has the dimension $|E|-|V|$. The eigenspace itself may be constructed as in (b). Let $c_n=(e_1, e_2, \ldots, e_n)$ be an even cycle. Then we may associate a vector $v(c_n)=\Sigma(-)^ie_i$ with c_n. $v(c_n)$ is an element of the kernel of B. Using the subgraph G' it is easily seen that there are $|E|-|V|$ linear independent vectors of this kind each of them corresponding to an edge of G not contained in G'. These vectors span the kernel of B. □

Let us now assume that G contains at least one even or two odd cycles, as a consequence $m(-2)>0$. In general the multiplicity of -2 may be very large and this fact has a simple consequence for the eigenstates of the Hubbard Hamiltonian on a line graph. This may be seen after a particle hole transformation

$$b^+_{x\sigma}=c_{x\sigma} \qquad b_{x\sigma}=c^+_{x\sigma}. \tag{7}$$

Such a transformation replaces $n_{x\sigma}$ by $(1-n_{x\sigma})$. The transformed particle numbers are $N'=2|V|-N$, $N'_+=|V|-N_+$, $N'_-=|V|-N_-$ and the transformed Hamiltonian, after a shift of the energy scale by $-U(|V|-N')$, becomes

$$H'=\sum_{x,y,\sigma} a_{xy}b^+_{x\sigma}b_{y\sigma}+U\sum_x n_{x+}n_{x-}. \tag{8}$$

In comparison with (1) the sign of the kinetic energy has changed. In the same way the sign of the spin operators (2) is changed by this transformation whereas the total spin (3) is left invariant. Since the expectation value of the kinetic energy of a single particle is not less than -2 and the expectation value of the interaction is not less than 0, an eigenvalue of H' is not less than $-2N'$. If now $N' \leq m(-2)$, it is possible to construct eigenstates with $S = N'/2$. To do this, we choose an orthonormal basis in the eigenspace of the eigenvalue -2 of A_L. We let $N'_- = 0$ and build a multiparticle state that is a Slater determinant of N' basis states. Such a state is clearly an eigenstate of H' with the eigenvalue $-2N'$. Since the spin is not changed by the particle hole transformation (7) and the trace of the adjacency matrix is equal to zero, we arrive at the following theorem.

Theorem. Let $L(G) = (V_L, E_L)$ be a line graph of a finite connected graph $G = (V, E)$ and let $M = |V| + |E| - 1$ if G is bipartite and $M = |V| + |E|$ otherwise. The Hamiltonian (1) on the line graph $L(G)$ in a system with $N \geq M$ electrons has ferromagnetic ground states with the saturated value $S = \frac{1}{2}(2|V_L| - N)$ for the spin and an energy $U(|V_L| - N) - 2(2|V_L| - N)$.

This theorem may be illustrated by some interesting examples. For instance one may take the hexagonal lattice with periodic boundary conditions (or a finite part of it). The line graph of it is the Kagomé lattice and $m(-2) = |V_L|/3 + 1$. The Hubbard model on the Kagomé lattice has ferromagnetic ground states if $N \geq (5/3)|V_L| - 1$. Another example is the line graph of the square lattice with periodic boundary conditions (or a finite part of it), which is a square lattice with cross hoppings on half of the squares. This graph may be represented by a regular lattice of cornersharing tetrahedra. One has $m(-2) = |V_L|/2 + 1$ and therefore the Hubbard model on this graph has ferromagnetic ground states if $N \geq (3/2)|V_L| - 1$. A similar line graph in three dimensions is the lattice of the octahedral sites of a spinel [11]. It is in fact the line graph of the diamond lattice. As above the multiplicity of -2 is $m(-2) = |V_L|/2 + 1$ and therefore one again finds ferromagnetic ground states for the Hubbard model on this graph if $N \geq (3/2)|V_L| - 1$. It should be mentioned that a general line graph is a graph that consists of complete graphs K_n connected at the vertices such that two complete graphs have one vertex in common.

The theorem mentioned above is easily generalized to a larger class of graphs. In fact, it is true whenever the adjacency matrix satisfies (4) for some matrix B, and M is determined by the dimension of the kernel of B. The adjacency matrices of the hyperoctahedral graphs (sometimes called cocktail party graphs) H_b (see [10]) and of the generalized line graphs $L(G; b_1, \ldots, b_{|v|})$ introduced by Hoffmann [12] satisfy (4) as well. One has $m(-2) = b - 1$ in the case of the hyperoctahedral graph H_b, $m(-2) = |E| - |V| + \Sigma\, b_i + 1$ for the generalized line graphs of a bipartite graph $G = (V, E)$ and $m(-2) = |E| - |V| + \Sigma\, b_i$ for the generalized line graphs of a non-bipartite graph.

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