Ferromagnetism in the Hubbard model on line graphs and further considerations

1991 J. Phys. A: Math. Gen. 24 3311

(http://iopscience.iop.org/0305-4470/24/14/018)

J. Phys. A: Math. Gen. 24 (1991) 3311-3321. Printed in the UK

Ferromagnetism in the Hubbard model on line graphs and further considerations

A Mielke

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

Received 11 March 1991

Abstract. Let $L(G)$ be the line graph of a graph $G=(V, E)$. The Hubbard model on $L(G)$ has ferromagnetic ground states with a saturated spin if the interaction is repulsive ($U>0$) and if the number of electrons N satisfies $N \geqslant M$. $M=|E|+|V|-1$ if G is bipartite and $M=|E|+|V|$ otherwise. We show that the ferromagnetic ground state is unique if $N=M$. Further we give a sufficient condition for the existence of other ground states if $N>M$. The results are valid also for a multi-band Hubbard model on a bipartite graph. In the case of a periodic lattice, the results are related to the existence of a flat energy band.

1. Introduction

Apart from the simple theory of Stoner, which is essentially a single-band mean-field approximation, and further developments in this direction, not too much is known about ferromagnetism of itinerant electrons. In general one does not know on what conditions a system of itinerant electrons has a ferromagnetic ground state. Only the one-dimensional case is relatively simple: the theorem of Lieb and Mattis [1] tells us *that the ground state of itinerant electrons on a line is never ferromagnetic. In more* than one spatial dimension the Hubbard model [2, 3] is a simple model to discuss such a question. It describes itinerant electrons on a lattice or more general on a graph with an on-site interaction. There are only some special cases in which the existence of a ferromagnetic ground state of the Hubbard model is known. If one has a hard-core repulsion between the electrons and if the dynamically allowed permutations are all even, there is one among the ground state that has a maximal spin $S=N/2$ (saturated ferromagnetism) [4]. There are two cases where this theorem applies. The first is the one-dimensional case with periodic boundary conditions and with an even number of electrons [5]. This model has a large symmetry and there are many other ground states. One may show that up to exponentially small corrections the system behaves as an *ideal paramagnet* [6]. If the lattice on the other hand obeys a certain connectivity condition [7] (which is not satisfied for example in the one-dimensional case) and if there is exactly one hole, the ferromagnetic ground state is unique apart from the degeneracy due to the global SU(2) invariance of the Hamiltonian. This is the well known theorem of Nagaoka [8, 9]. But this case is somewhat particular since it has been shown by Sütö [10] that such a system behaves in the thermodynamic limit and for any temperature $T>0$ as an ideal paramagnet.

A unique ground state (again apart from the degeneracy due to the global SU(2) invariance) that may have a macroscopic but not saturated value for the spin is obtained for the Hubbard model on a bipartite lattice if the number of electrons is equal to the

0305-4470/91/143311+11$03.50

number of sites [11]. This theorem of Lieb was the first proven example of itinerant-electron ferromagnetism in systems without unrealistic assumptions like a hard-core repulsion.

Very recently we have shown that the Hubbard model on a line graph (e.g. on the Kagomé lattice) has ferromagnetic (saturated) ground states if the number of electrons obeys a certain inequality (see below) [12]. The proof is very simple and uses some results of the theory of line graphs. But this result says nothing about the existence of other ground states. The question, whether there are other ground states, will be discussed in the following.

Our article is organized as follows. Section 2 contains a general introduction to some standard graph theoretical tools. They may be found in any standard textbook on graph theory (see e.g. [13]). We introduce the Hubbard model on a line graph and mention the result of [12]. In section 3 we will show that for a certain number of electrons the ferromagnetic ground state of the Hubbard model on a large class of line graphs (line graphs of twofold connected graphs) is unique apart from the usual SU(2) degeneracy. Further we give a sufficient condition for the existence of ground states with a spin below $S = N/2$. In section 4 we give some extensions of the theory presented so far to the case of a multi-band Hubbard model on some bipartite graphs. In section 5 we discuss the results and conclude with some possible future developments starting from the present investigations. We will see that the ferromagnetic ground states in our case as well as in the case of Lieb [11] occur together with a flat energy band in a multi-band Hubbard model. This fact allows for a discussion of the results within the framework of Stoner's criterion.

2. The Hubbard model on a line graph

Let $G = (V, E)$ be a finite simple graph. V is the set of vertices (sites) and E is the set of edges of G. An edge is a subset of V with two elements. Unless noted otherwise, we will always assume that a graph is simple and finite. Most of our results are valid for graphs with multiple edges as well. Two vertices x and y of a graph are called adjacent if the graph contains an edge $e = \{x, y\}$. The degree of x is the number of vertices being adjacent to x. A vertex x is called incident to an edge e if x is an element of e. A graph 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 (i.e. has exactly one element out of each vertex class).

We define the adjacency matrix of the graph G to be the matrix $A = (a_{xy})_{x,y \in V}$ where $a_{xy} = 1$ if the two vertices are adjacent and $a_{xy} = 0$ otherwise. Further we introduce 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. Details on these matrices may be found in [14].

A sequence $(x_1, e_1, x_2, e_2, \ldots, e_{n-1}, x_n)$ where $e_i = \{x_i, x_{i+1}\} \in E$ for all $1 \leq i \leq n-1$ is called a walk in G. If $x_1 = x_n$, the walk is closed. A walk is called a trail if all its edges are distinct and it is called a path if all its vertices are distinct. A cycle is a closed trail $(x_1, e_1, x_2, e_2, \ldots, e_{n-1}, x_n)$ with $n \geq 3$ whose vertices x_i, $1 \leq i < n$, are distinct. A graph G is connected if for each pair x, y of vertices of G there exists a path from x to y.

The line graph $L(G) = (V_L, E_L)$ of G is constructed as follows. Its vertex set is the edge set of G, $V_L = E$. Two vertices of V_L are adjacent if the corresponding edges in

G have a vertex in common. For instance one may take the hexagonal lattice (or a finite part of it e.g. with periodic boundary conditions). The line graph of it is the Kagomé lattice. Another example is the line graph of the square lattice with periodic boundary conditions, which is a square lattice with two diagonal edges on half of the squares. This graph may be represented by a regular lattice of corner-sharing tetrahedra. A similar line graph in three dimensions is the lattice of the octahedral sites of a spinel [15]. It is the line graph of the diamond lattice.

Some of the spectral properties of the adjacency matrix A_L of a line graph $L(G)$ may be found in [14]. A_L is easily constructed if one knows the incidence matrix of G. One has

$$B(G)^t B(G) = 2I_{|E|} + A_L \tag{2.1}$$

where B^t is the transposed of B and I_n denotes the n-dimensional unit matrix. Since $B^t B$ is a positive-semidefinite matrix it follows from (2.1) that each eigenvalue a of the adjacency matrix A_L obeys $a \geqslant -2$. The eigenspace corresponding to the eigenvalue -2 is the kernel of $B(G)$. It is easily constructed as shown in [12]. Each closed walk of even length $c = (x_1, e_1, x_2, e_2, \ldots, e_n, x_1)$ of G corresponds to a vector $v(c) = \Sigma (-)^i e_i$ out of the kernel of B and the kernel of B is spanned by all these vectors. In [12] we showed that the dimension of the kernel of B is $|E| - |V| + 1$ if $G = (V, E)$ is bipartite and $|E| - |V|$ otherwise. This number is thus the multiplicity $m(-2)$ of the eigenvalue -2 of A_L.

Let us now define the Hubbard model on a line graph. The Hamiltonian of the Hubbard model on a graph G has the form

$$H = -\sum_{x,y,\sigma} a_{xy} c^+_{x\sigma} c_{y\sigma} + U \sum_x n_{x+} n_{x-}. \tag{2.2}$$

where x, y are elements of V and σ denotes a spin degree of freedom which may be up $(+)$ or down $(-)$. a_{xy} are the entries of 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. They obey the usual anticommutation relations for fermions. $n_{x\sigma} = c^+_{x\sigma} c_{x\sigma}$, $n_x = n_{x+} + n_{x-}$ are occupation numbers. U is a positive real number, it describes the magnitude of the on-site repulsion of the electrons on the vertices. The interaction term represents the Coulomb repulsion between electrons on the same site. Due to the Pauli principle it acts only between electrons with different spins. The other matrix elements of the Coulomb interaction are completely neglected in the model.

In the following, N is the number of electrons and one has $N \leqslant 2|V|$ where $|V|$ denotes the numer 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

$$S^+ = \sum_x c^+_{x+} c_{x-} \qquad S^- = \sum_x c^+_{x-} c_{x+} \qquad S^z = \tfrac{1}{2}(N_+ - N_-). \tag{2.3}$$

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

$$S^2 = (S^z)^2 + \tfrac{1}{2}(S^+ S^- + S^- S^+). \tag{2.4}$$

This operator has the eigenvalues $S(S+1)$ and we call S the spin of the eigenstate. In the following we will deal with a particle–hole transformed version of the Hamiltonian. After a particle–hole transformation the sign of the kinetic energy is changed and neglecting a trivial constant $U(|V| - N)$ we obtain

$$H = \sum_{x,y,\sigma} a_{xy} c^+_{x\sigma} c_{y\sigma} + U \sum_x n_{x+} n_{x-}. \tag{2.5}$$

The spin of the eigenstates of the Hamiltonian is not changed by the particle-hole transformation. All the results derived below are valid for the Hamiltonian (2.5). Of course it is always possible to transform back to the original Hamiltonian (2.2). If H in (2.5) has a ground state for N electrons with a spin S and an energy E, the transformed ground state is a ground state of H in (2.2) for $2|V|-N$ electrons with a spin S and an energy $E+U(|V|-N)$.

We will discuss the Hamiltonian (2.5) on line graphs. The kinetic energy in (2.5) is simply the adjacency matrix of the line graph and as a consequence of the above mentioned properties the following theorem holds [12].

Theorem 1. Let $L(G)=(V_L, E_L)$ be a line graph of a connected graph $G=(V, E)$ and let $M=|E|-|V|+1$ if G is bipartite and $M=|E|-|V|$ otherwise. The Hamiltonian (2.5) on the line graph $L(G)$ in a system with $N \leq M$ electrons has ferromagnetic ground states with the saturated value $S=N/2$ for the spin and an energy $-2N$.

Unfortunately this theorem says nothing about the existence of other ground states. For instance, if N is much smaller than M the electrons can be seen as a dilute gas and one would expect the formation of a featureless paramagnetic liquid. In the following section we will try to clarify this point.

3. Ground states

Let us first introduce another graph theoretical notion. A vertex x of G is called a cutvertex if there exists a pair of vertices x', y' in G such that a path between x' and y' exists and each path between x' and y' contains x. Each connected graph G which does not contain a cutvertex is called twofold connected. In a twofold connected graph each vertex is an element of a cycle. We have

Proposition 1. Let G be a twofold connected graph and suppose that -2 is an eigenvalue of the adjacency matrix of $L(G)$ with a multiplicity $m(-2, G) \geq 2$. Let $P=(x, e_1, \ldots, e_n, y)$ be a path in G such that the degree of each vertex of P in G that is not an endvertex of P is two. Let $G'=(V', E')$ be the subgraph of G which is obtained from G by deleting all the edges and all the vertices of P except x and y. Let P be such that G' is bipartite if and only if G is bipartite. Then

(i) -2 is an eigenvalue of the adjacency matrix of $L(G')$ with a multiplicity $m(-2, G')=m(-2, G)-1$.

(ii) Let H and H' be the Hamiltonians (2.5) of the Hubbard model on $L(G)$ and $L(G')$ with $N=m(-2, G)$ and $N'=m(-2, G')$ electrons respectively. If the ground state of H' is unique, the ground state of H is unique (apart from the degeneracy due to the SU(2) invariance).

Proof. (i) We have $m(-2, G)=|E|-|V|+1$ if G is bipartite and $m(-2, G)=|E|-|V|$ otherwise. Deleting P except its endvertices means the deletion of n edges and $n-1$ vertices, since the degree of each deleted vertex is two. Therefore we have $m(-2, G')=m(-2, G)-n+(n-1)=m(-2, G)-1$. We mention that G' and $L(G')$ are connected, since G is twofold connected. This fact will be used later.

(ii) Due to theorem 1 a ground state of H has the energy $-2N$. Further we know that it is an eigenstate of the kinetic energy with an eigenvalue $-2N$. This means that it may be written as a linear combination of products of single particle states that are elements of the kernel of $B(G)$. Let us now notice that each element of the kernel of $B(G')$ is (apart from zero components on the new edges of G) an element of the kernel of $B(G)$. We may choose an orthonormal basis $\{v_1, v_2, \ldots, v_M\}$ in the kernel of $B(G)$ such that $\{v_1, v_2, \ldots, v_{M-1}\}$ is an orthonormal basis in the kernel of $B(G')$. Let $d^+_{M\sigma}$ ($d_{M\sigma}$) be the creation (annihilation) operator of an electron with spin σ in the state v_M,

$$d^+_{M\sigma} = \sum_{x \in V_L} v_M(x) c^+_{x\sigma}. \tag{3.1}$$

$v_M(x)$ is the component of v_M corresponding to the vertex x of $L(G)$. Any N-particle state Φ with a kinetic energy $-2N$ on $L(G)$ may be written as

$$\Phi = \Phi_1 + d^+_{M+}\Phi_2 + d^+_{M-}\Phi_3 + d^+_{M+}d^+_{M-}\Phi_4 \tag{3.2}$$

where Φ_i are multiparticle states on $L(G')$. Φ_1 has the kinetic energy $-2N$, Φ_2 and Φ_3 have the kinetic energy $-2(N-1)$ and Φ_4 has the kinetic energy $-2(N-2)$. We will now try to give necessary and sufficient conditions for Φ to be a ground state. Φ is a ground state if and only if it does not contain doubly occupied sites, i.e.

$$c_{x+}c_{x-}\Phi = 0 \qquad \text{for all } x \in V_L. \tag{3.3}$$

This means that $\Phi_4 = 0$ since the fourth term in (3.2) contains doubly occupied sites corresponding to the edges of P whereas these sites are occupied at most once in the other three terms. Condition (3.3) now reads

$$\begin{aligned} c_{x+}c_{x-}\Phi = {} & d^+_{M+}c_{x+}c_{x-}\Phi_2 + d^+_{M-}c_{x+}c_{x-}\Phi_3 + c_{x+}c_{x-}\Phi_1 \\ & - v_M(x)c_{x-}\Phi_2 + v_M(x)c_{x+}\Phi_3 = 0 \end{aligned} \tag{3.4}$$

where we used that

$$c_{x\sigma}d^+_{M\sigma} + d^+_{M\sigma}c_{x\sigma} = v_M(x). \tag{3.5}$$

The first term in the sum in (3.4) is the only term that contains an electron with spin + in the state v_M. It is therefore linearly independent of the other terms and must vanish separately. The same is true for the second term in (3.4) and we obtain

$$c_{x+}c_{x-}\Phi_2 = 0 \qquad c_{x+}c_{x-}\Phi_3 = 0 \tag{3.6a}$$

$$c_{x+}c_{x-}\Phi_1 - v_M(x)c_{x-}\Phi_2 + v_M(x)c_{x+}\Phi_3 = 0. \tag{3.6b}$$

(3.6a) shows that Φ_2 and Φ_3 are ground states of H'. Since the ground state of H' is supposed to be unique apart from the degeneracy due to the SU(2) invariance, Φ_2 and Φ_3 are ferromagnetic with a saturated value $S = N'/2$ for the spin due to theorem 1. We may now choose Φ to be an eigenstate of $\boldsymbol{S}^2$ and S^z with the condition $\boldsymbol{S}^2\Phi = S^z(S^z+1)\Phi$. This means

$$S^+\Phi = 0. \tag{3.7}$$

(3.2) then yields

$$\Phi_3 = -S^+\Phi_2 \qquad S^+\Phi_3 = 0 \qquad S^+\Phi_1 = 0. \tag{3.8}$$

Let Φ_0 be the Slater determinant of all the basis states in the kernel of $B(G')$, all electrons have a spin +. Because of the conditions (3.8) we have only two possibilities

for the z-component of the spin of Φ, namely $S^z\Phi = (N/2)\Phi$ or $S^z\Phi = (N/2-1)\Phi$. The first possibility yields a ground state of H with a saturated value for the spin and this state is unique. It is obtained if $\Phi_2 = \Phi_0$, i.e.

$$\Phi = d^+_{M+}\Phi_0. \tag{3.9a}$$

Φ is simply the Slater determinant of all single particle states in the eigenspace of -2 of the adjacency matrix of $L(G)$. There is no contribution of Φ_1 since Φ_1 obeys $S^z\Phi_1 = (N/2-1)\Phi_1$.

The second possibility is obtained if one puts $\Phi_3 = \Phi_0$ and $\Phi_2 = -S_-\Phi_0/N$, i.e.

$$\Phi = \Phi_1 - N^{-1}d^+_{M+}S_-\Phi_0 + d^+_{M-}\Phi_0. \tag{3.9b}$$

Since $S^z\Phi_1 = (N/2-1)\Phi_1$ and Φ_1 is a linear combination of products of elements out of the kernel of B, its general form is

$$\Phi_1 = \sum_x w(x)c^+_{x-}\Phi_0 \tag{3.10}$$

where w is an element of the kernel of $B(G')$. Using $c_{x-}\Phi_0 = 0$, (3.3), (3.4) may now be written as

$$[w(x) + (1+1/N)v_M(x)]c_{x+}\Phi_0 = 0 \qquad \text{for all } x \in V_L. \tag{3.11}$$

Since w and v_M are orthogonal and both different from 0, $w(x) + (1+1/N)v_M(x)$ is different from 0 for some $x \in V_L$. On the other hand, since Φ_0 is the Slater determinant of all the basis states of the kernel of $B(G')$ and since G' is connected, $c_{x+}\Phi_0$ is different from 0 whenever $w(x)$ is different from 0 or $v_M(x)$ is different from 0 and x is contained in a cycle of G'. Therefore the left-hand side of (3.11) does not vanish for all $x \in V_L$ and Φ in (3.9b) is not a ground state of H. The twofold connectivity of G is important here since otherwise $v_M(x)$ could be zero on the vertices corresponding to the edges of G' contained in a cycle, i.e. $v_M(x)w(x) = 0$ for all $w(x)$ in the kernel of $B(G')$. The only ground states of H are given by (3.9a) and the corresponding states that are constructed using the global SU(2) invariance of H. This completes the proof of proposition 1. □

A twofold connected graph may be constructed as follows. Let $G_0 = (V_0, E_0)$ be a cycle. We construct $G_1 = (V_1, E_1)$ from G_0 by adding a path $(x, e_1, x_1, e_2, x_2, \ldots, x_{n-1}, e_n, y)$. Here x, y are different elements of V_0 whereas the x_i, $i = 1, \ldots, n-1$, are not contained in V_0. In the same way we may add a path to G_1 to obtain G_2 and so on. Each of these graphs does not contain a cutvertex and each graph that does not contain a cutvertex may be constructed in this way. A non-bipartite graph may be constructed in this way starting with an odd cycle. If we want to construct a bipartite graph, we have to start with an even cycle and we have to make sure that a cycle of G_{i+1} that contains the path added to G_i (and therefore all cycles) is even.

Let $G = (V, E)$ be a twofold connected graph and suppose that -2 is an eigenvalue of the adjacency matrix of $L(G)$. Let $M = m(-2)$ be the multiplicity of this eigenvalue. Let G_0 be a subgraph of G and let M_0 be the multiplicity of the eigenvalue -2 of the adjacency matrix of $L(G_0)$. Let G_0 be bipartite if and only if G is bipartite. We choose G_0 such that $M_0 = 1$. Therefore the ground state of the Hubbard model on $L(G_0)$ with $N_0 = 1$ electron is unique apart from the degeneracy due to the SU(2) invariance. We now construct a sequence $(G_0, N_0), (G_1, N_1), \ldots, (G_i, N_i), \ldots, (G_{M-1} = G, N_{M-1} = M)$, where all the graphs G_i are subgraphs of G, G_i is constructed from G_{i-1} by adding

a path $(x, e_1, x_1, e_2, x_2, \ldots, x_{n-1}, e_n, y)$ as described above. Further, $N_i = N_{i-1}+1$. G_0 may be chosen twofold connected: as a consequence all the G_i are twofold connected. Then proposition 1 tells us that the Hubbard model on each $L(G_i)$ with N_i electrons has, apart from the trivial degeneracy, a unique ground state. This result may be formulated in the following theorem.

Theorem 2. Let $L(G) = (V_L, E_L)$ be a line graph of a twofold connected graph $G = (V, E)$ and let $M = |E| - |V| + 1$ if G is bipartite and $M = |E| - |V|$ otherwise. The ground state of the Hamiltonian (2.5) on the line graph $L(G)$ with $N = M$ electrons is unique apart from the degeneracy due to the SU(2) invariance.

As a remark we mention that the examples for line graphs discussed above, i.e. the Kagomé lattice (with periodic boundary conditions or a finite part of it) or the sublattice of the octahedral sites of a spinel, are both line graphs of twofold connected graphs so that theorem 2 applies.

The next important point is the existence of ground states for the Hubbard model (2.5) on a line graph if the number of electrons is smaller than M in theorems 1 or 2. Here we are only able to give a sufficient condition, namely

Theorem 3. Let G be a graph and let H be the Hubbard model (2.5) on $L(G)$ with $N \leqslant M$ electrons, M as given in theorem 2. If two edge disjoint subgraphs $G_+ = (V_+, E_+)$ and $G_- = (V_-, E_-)$ of G exist, such that $N = M_+ + M_-$, then H has a ground state with a spin $S = (M_+ - M_-)/2$. Here M_+ and M_- are defined as M in theorem 2.

Proof. This theorem is a simple consequence of theorem 1. If G_+ and G_- exist, we may construct the Φ_+ as the Slater determinant of a complete orthonormal set of single particle states of the eigenspace of -2 of the adjacency matrix of $L(G_+)$. All the electrons in Φ_+ should have a spin $+$. Similarly we construct Φ_- on $L(G_-)$ with spin $-$. Since G_+ and G_- are edge disjoint, the product $\Phi = \Phi_+\Phi_-$ has no doubly occupied sites on $L(G)$. It is a ground state of H with $M_+ + M_-$ electrons. It has a non-vanishing component in the subspace of the multiparticle states with spin $(M_+ - M_-)/2$. □

If G has a cutvertex, it is possible to construct such subgraphs G_+ and G_- even when $N = M$. Therefore G in theorem 2 must be twofold connected. If $N < M$ and G is twofold connected, there may be many possibilities to construct two such subgraphs. But since theorem 3 gives only a sufficient condition for the existence of ground states of H, we do not know whether it is possible to obtain a ground state with a minimal spin in this way.

Theorem 3 helps us to understand the magnetic behaviour of the Hubbard model on line graphs at small densities. Let us look at the special case of a line graph of a regular d-dimensional lattice. If $M - N \approx |E|^{(d-1)/d}$ or larger, it is easy to construct subgraphs G_+ and G_- with $M_+ = M_-$. Theorem 3 shows that H has in this case ground states with any value of the spin between 0 and $\frac{1}{2}$ and $N/2$ exist. This indicates that at sufficiently low densities the Hubbard model shows a paramagnetic behaviour. On the other hand, it is not clear whether for $N = M$ in the thermodynamic limit one obtains a ferromagnetic or a paramagnetic behaviour. The results of theorems 1 to 3 are valid only for finite graphs. But using the same argument theorem 3 suggests that in the limit of large valence (i.e. large d) the Hubbard model on a line graph shows a ferromagnetic behaviour even for small densities. As the simplest example one may

take the line graph of a complete graph K_n. $L(K_n)$ has $\frac{1}{2}n(n-1)$ sites and $M=\frac{1}{2}n(n-3)$. To obtain a ground state with a spin 0 (or $\frac{1}{2}$) using theorem 3, $M-N$ must be of the order $n^2/4\approx M/2$. Therefore one might expect a ferromagnetic behaviour in the limit of large n.

Transforming back to the original Hamiltonian (2.2) we obtain

Corollary. Let $L(G)$ be the line graph of $G=(V,E)$ and let H in (2.2) be the Hamiltonian on $L(G)$. Let $M=|E|+|V|-1$ if G is bipartite, $M=|E|+|V|$ otherwise. Then

(i) H has ground states with a saturated value $S=|E|-\frac{1}{2}N$ if $N\geqslant M$.

(ii) If G is twofold connected and $N=M$, the groundstate of H is unique apart from the degeneracy due to the SU(2) invariance.

(iii) For a subgraph G_σ of G let $M_\sigma=|E_\sigma|+|V_\sigma|-1$ if G is bipartite, $M_\sigma=|E_\sigma|+|V_\sigma|$ otherwise. If two edge disjoint subgraphs G_+ and G_- of G exist such that $N=M_++M_-$, then H has ground states with a spin $S=||E_+|-|E_-|-\frac{1}{2}M_++\frac{1}{2}M_-|$.

4. Results for the Hubbard model on bipartite graphs

The adjacency matrix of a bipartite graph may be written in the form

$$A=\begin{bmatrix}0_n & X\\ X^t & 0_m\end{bmatrix} \tag{4.1}$$

where $n=|V_1|$, $m=|V_2|$. 0_n is the $n\times n$ 0-matrix and X is an $n\times m$-matrix with entries 0 or 1. We will assume that $n\leqslant m$. Then $\operatorname{rank}(X)\leqslant n$ and $\dim(\operatorname{kernel}(X))\geqslant m-n$. We will now discuss the Hubbard model defined by

$$H=\sum_{x,y,\sigma} t_{xy}c^+_{x\sigma}c_{y\sigma}+U\sum_x n_{x+}n_{x-} \tag{4.2}$$

on the bipartite graph $G=(V,E)$ described by the adjacency matrix A in (4.1). The single particle operator is given by the matrix $T=(t_{xy})_{x,y\in V}$ which describes the kinetic energy of a single particle as well as a potential. Let us take

$$T=\begin{bmatrix}t_1XX^t+v_1I_n & tX\\ tX^t & t_2X^tX+v_2I_m\end{bmatrix}. \tag{4.3}$$

t is the hopping matrix element between nearest-neighbour sites, t_1 describes a hopping between next-nearest-neighbour sites in V_1, t_2 in V_2 respectively. Since XX^t and X^tX have non-vanishing diagonal entries, T contains also an on-site potential proportional to t_1 on V_1 and to t_2 on V_2. I_n is an $n\times n$ unit matrix and the terms proportional to v_1 and v_2 are further contributions to the on-site potential.

The Hamiltonian (4.2) has ferromagnetic ground states if the matrix T has a lowest eigenvalue with a large multiplicity. Let us make the following ansatz for an eigenvector of T

$$y=\begin{bmatrix}Xx\\ \beta x\end{bmatrix}\qquad \text{where } X^tXx=bx. \tag{4.4}$$

x is an eigenvector of X^tX with eigenvalue b and β is some unknown constant. If x is out of the kernel of X, $b=0$ and we may choose $\beta=1$. In this case y is an eigenvector

of T with the eigenvalue v_2. The multiplicity of v_2 is equal to the dimension of the kernel of X. If x is not out of the kernel of X, $b>0$ and we have

$$Ty=\begin{bmatrix}(t_1b+v_1+t\beta)Xx\\(tb/\beta+t_2b+v_2)\beta x\end{bmatrix}. \tag{4.5}$$

y is an eigenvector of T with the eigenvalue τ if and only if

$$\tau=t_1b+v_1+t\beta=tb/\beta+t_2b+v_2. \tag{4.6}$$

Let

$$s=(t_1b+v_1-t_2b-v_2)/t \tag{4.7}$$

then (4.6) leads to the quadratic equation $\beta^2+s\beta-b=0$ for β. This equation has two real solutions, each of them yielding an eigenvector y of T and the corresponding eigenvalue by equations (4.4) and (4.6). If for all eigenvalues b of X^tX

$$t_2\{s/2+(s^2/4+b)^{1/2}\}>t>0 \qquad \text{or} \qquad t_2\{s/2-(s^2/4+b)^{1/2}\}<t<0 \tag{4.8}$$

all the eigenvalues τ in (4.6) exceed v_2. In this case T has a lowest eigenvalue with a large multiplicity $m(v_2)\geqslant m-n=|V_2|-|V_1|$. The Hubbard model (4.2) has ferromagnetic ground states whenever $N\leqslant m(v_2)$. If, on the other hand,

$$t_2\{s/2+(s^2/4+b)^{1/2}\}<t<0 \qquad \text{or} \qquad t_2\{s/2-(s^2/4+b)^{1/2}\}>t>0 \tag{4.9}$$

v_2 exceeds all the eigenvalues τ in (4.6) and the Hubbard model (4.2) has ferromagnetic ground states if $N\geqslant|V_2|+|V_1|-m(v_2)$. Clearly, these two cases are related by a particle-hole transformation of (4.2).

In general X in (4.1) may be interpreted as the incidence matrix of a hypergraph H [13]. H may be a simple graph G', in this case $X=B(G')$. The graph G having the adjacency matrix (4.1) is obtained from G' by dividing each edge of G' by a new vertex into two new edges. In this case $V_1=V'$, $V_2=E'$ and $m(v_2)=|E'|-|V'|+1$ if G is bipartite, $m(v_2)=|E'|-|V'|$ otherwise. The ground states of the Hamiltonian (4.2) are completely equivalent to the ground states of the Hamiltonian (2.5) on the line graph $L(G')$ if condition (4.8) is fulfilled and theorems 1, 2 and 3 may be carried over. Let us illustrate this with the example where G' is a finite part of the quadratic lattice (compare [11]). Then G represents e.g. the Cu-O planes in the high-T_c superconductors. In the next section we will see that the Hubbard model on G is a model with three energy bands. After a particle-hole transformation of (4.2) we obtain a Hubbard model on G which has ferromagnetic ground states if $N\geqslant 5|V'|-1$. This means that two energy bands are entirely filled whereas the third energy band is partially filled (half filled if $N=5|V'|$).

5. Discusion

In order to give an interpretation of our results, we will restrict ourselves to the case of regular d-dimensional periodic lattices with periodic boundary conditions, i.e. on a d-dimensional torus. A lattice is regular, if the number of nearest neighboured sites is constant. It is useful to work in the momentum space. Let the graph $G=(V, E)$ be a regular d-dimensional lattice with periodic boundary conditions and let A_G be its adjacency matrix. Let z be the number of nearest neighbours in G. The eigenvalues

of A_G may be written as a_{ks} where k is a d-dimensional momentum vector and s is a band index, $s = 1, \ldots, n_G$. Since G is regular, we have

$$A_G = B(G)B(G)^t - zI_{|V|}. \tag{5.1}$$

Let now e_{ks}, $s = 1, \ldots, n_L$, be the eigenvalues of the adjacency matrix A_L of the line graph $L(G)$, which is also a regular lattice. Because of the representation (2.1) of A_L one has the following relation between the eigenvalues of the adjacency matrices of G and $L(G)$:

$$e_{ks} = z - 2 + a_{ks}. \tag{5.2}$$

To each energy band in G corresponds an energy band in $L(G)$. But A_L has at least one additional energy band that contains the eigenvalues -2 corresponding to the eigenstates that are elements of the kernel of $B(G)$. These energy bands are flat, e_{ks} do not depend on k. In the case of the Kagomé lattice, $L(G)$ has three energy bands and the hexagonal lattice G has two energy bands. The same is true for the sublattice of the octahedral sites of a spinel and the diamond lattice respectively.

Introducing the creation and annihilation operators for electrons with a momentum k and a spin σ in the bands $d^+_{ks\sigma}$ and $d_{ks\sigma}$, the Hamiltonian (2.5) takes the form

$$H = \sum_{k,s,\sigma} e_{ks} d^+_{ks\sigma} d_{ks\sigma} + U \sum_{k_1 \ldots k} \sum_{s_1 \ldots s_4} J^{s_1 s_2 s_3 s_4}_{k_1 k_2 k_3 k_4} d_{k_1 s_1} + d_{k_2 s_2} - d_{k_3 s_3} - d_{k_4 s_4} + \tag{5.3}$$

where J is a coupling constant that is easily calculated from the single particle states in the energy bands. In the framework of a mean field approximation, and neglecting inter-band scattering, (5.3) reduces for the lowest energy band to the model of Stoner. Since the band is flat, Hund's rule leads to ferromagnetic ground states. In fact, this corresponds to the results of Kanamori [3], who obtained ferromagnetic ground states for all $U > 0$ if the band width vanishes. Stoner's criterion for ferromagnetism is $n_F U > 1$ (see e.g. [2]), where n_F is the density of states at the Fermi level. In the case of a flat band, n_F is extremely large so that U may be very small. But it is clear that such a framework cannot be applied in our case, since the bands are not separated by gaps and the interband scattering cannot be neglected.

Nevertheless, the existence of a flat band seems to be interesting. The second theorem of Lieb [11] tells us that the Hubbard model on a bipartite graph with a half filled band has a unique ground state with a spin $S = \frac{1}{2}||V_2| - |V_1||$. Clearly S may be extensive so that the ground state is ferromagnetic. In this case the eigenvalue 0 of the kinetic energy (4.1) of a single particle is degenerate, its multiplicity $m(0) \geq ||V_2| - |V_1||$ and its eigenspace is the kernel of X in (4.1). This fact suggests that there may be a connection between this result and ours. Indeed, if we restrict ourselves again to periodic lattices, the adjacency matrix of a bipartite lattice with a macroscopic $m(0)$ has several energy bands. This may be seen if one recognizes that $-XX^t$ is (up to a constant) the Laplacian on the hypergraph described by the incidence matrix X ($-BB^t$ is up to a constant the Laplacian on a graph G, compare (5.1)). Each energy band of XX^t yields two energy bands of A in (4.1) and additional energy bands corresponding to the kernel of X occur. These energy bands are flat. For example, the two-dimensional lattice that corresponds to the CuO planes in a high temperature superconductor [11] has three energy bands. One of these bands is the flat band corresponding to the eigenstates out of the kernel of X. In the theorem of Lieb as well as in our results ferromagnetism occurs together with at least one flat energy band in a model with more than one energy band. This connection should be elaborated in order to obtain a deeper understanding of ferromagnetism in the Hubbard model.

Another important problem is the existence of ferromagnetism in the thermodynamic limit and for positive temperatures. As mentioned in the introduction, the ferromagnetism of Nagaoka breaks down in the thermodynamic limit for any temperature $T > 0$. We discussed already some of the problems that arise in our case due to theorem 3. As well as the flat energy band allows for a ferromagnetic ground state, it causes the problem that the single particle states in this band may be written in a Wannier basis as well and that all the Wannier states in the band are degenerate. The on-site interaction of the Hubbard model may be written in this basis and one may assume that the interaction between electrons in the Wannier states in the flat band is of short range. Therefore one may construct a ground state that has a different spin in different, well separated regions of the lattice such that its total spin is small. This is the situation described in theorem 3. Although no rigorous results are available, the same argument may be applied in the case of Lieb as well.

Acknowledgments

I wish to thank H Kunz and A Sütö for many useful discussions and suggestions.

References

[1] Lieb E H and Mattis D C 1962 *Phys. Rev.* **125** 164
[2] Hubbard J 1963 *Proc. R. Soc.* A **276** 238; 1964 *Proc. R. Soc.* A **277** 237
[3] Kanamori J 1963 *Prog. Theor. Phys.* **30** 275
[4] Aizenman M and Lieb E H 1990 *Phys. Rev. Lett.* **65** 1470
[5] Herring C 1975 *Phys. Rev.* B **11** 2056
[6] Mielke A 1991 *J. Stat. Phys.* **62** 50
[7] Tasaki H 1989 *Phys. Rev.* B **40** 9192
[8] Nagaoka Y 1966 *Phys. Rev.* **147** 392
[9] Thouless D 1965 *Proc. Phys. Soc.* **86** 893
[10] Sütö A 1991 *Phys. Rev.* B **43** 8779
[11] Lieb E H 1989 *Phys. Rev. Lett.* **62** 1201
[12] Mielke A 1991 *J. Phys. A: Math. Gen.* **24** L73
[13] Bergé C 1970 *Graphes et Hypergraphes* (Paris: Dunod)
[14] Biggs N 1974 *Algebraic Graph Theory* (Cambridge: Cambridge University Press)
[15] Anderson P W 1956 *Phys. Rev.* **102** 1008