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Exact ground states for the Hubbard model on the Kagomé lattice

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Abstract. We give a complete and rigorous description of the ground states of the Hubbard model on the Kagomé lattice for electron densities $n \geq \frac{5}{3}$ and $U > 0$. If $\frac{11}{6} > n \geq \frac{5}{3}$ the system shows a ferromagnetic behaviour at zero temperature. If n is above $\frac{11}{6}$ the system is paramagnetic. The proof of these results uses some graph-theoretic methods. The results are applicable to all line graphs of planar lattices, of which the Kagomé lattice is an example.

1. Introduction

In two previous papers [1, 2] we investigated the Hubbard model on a special class of lattices (or more general graphs), namely on lattices that are line graphs. The Kagomé lattice in two dimensions or the lattice of the octahedral sites of a spinel in three dimensions, already mentioned in [1], are well known lattices, which are line graphs. The Hubbard model [3, 4] is defined by the Hamiltonian

$$H = -\sum_{x,y,\sigma} t_{xy} c^{+}_{x\sigma} c_{y\sigma} + U \sum_{x} n_{x+} n_{x-}. \tag{1.1}$$

We assume that t_{xy} is equal to $t > 0$ if the lattice sites x and y are nearest neighbours, 0 otherwise. $c^{+}_{x\sigma}$ and its adjoint $c_{x\sigma}$ are electron creation and annihilation operators for electrons with spin σ on the lattice sites. They satisfy the usual fermion anticommutation relations. The main result of [1, 2] was that this Hamiltonian on a line graph has ferromagnetic ground states with a saturated value for the spin if the number of particles $N \geq M$ and $U > 0$. M is a natural number that depends on the underlying lattice. For the Kagomé lattice $M = \frac{5}{3}N_s - 1$ where N_s is the number of lattice sites. We showed that if $N = M$, the ferromagnetic ground state is unique up to the usual degeneracy due to the SU(2) symmetry of the model. On the other hand, if $N > M$ the ground state is no longer unique. If e.g. for the Kagomé lattice the density is above $\frac{5}{3}$, the degeneracy of the ground state grows exponentially with the system size.

In the present paper we give a complete description of the ground states of the Hubbard model (1.1) on a line graph for all $N \geq M$. Unfortunately, this is only possible for the two-dimensional case. A typical and perhaps the most important example is the Kagomé lattice. We calculate upper and lower bounds on the ground state degeneracy. Using these bounds we are able to estimate the average spin of the ground states. We shall show that for the Hubbard model on the Kagomé lattice the average spin of the ground states is an extensive quantity if the density is between $\frac{5}{3}$ and $\frac{11}{6}$ (and for all $U > 0$). The model has a ferromagnetic behaviour at zero temperature. To

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our knowledge, this is the first rigorous result which gives ferromagnetism for the Hubbard model in a finite density range. Clearly such a result is only possible for finite systems or at zero temperature. At any $T>0$ and in the thermodynamic limit, there is no ferromagnetic long range order in two dimensions [5]. If the density is above $\frac{11}{6}$, the Hubbard model on the Kagomé lattice shows a paramagnetic behaviour in the sense that the average spin of the ground states in no longer extensive.

The general plan of this paper is as follows. In section 2 we give some preliminary definitions and state the main theorem. Section 3 contains the proof of the theorem. It is followed by some remarks concerning generalizations to line graphs of non-planar graphs. The reader who is mainly interested in the consequences may skip section 3. In section 4 we discuss the question whether the Hubbard model on a line graph shows a ferromagnetic behaviour at $T=0$ in some finite density range using results from percolation theory. Section 5 contains some final remarks.

2. Definitions and results

By a graph we mean a collection of vertices (sites) and edges (bonds) between them. We exclude the possibility of multiple edges between a pair of vertices. Each finite part of a lattice is a graph. (We refer to an edge as a line between two nearest neighboured sites of the lattice.) A graph will be denoted by $G=(V, E)$ where V is the set of vertices and E is the set of edges. $|V|$ is the number of vertices and $|E|$ is the number of edges. The line graph $L(G)$ has the edges of G as vertices and two vertices are connected by an edge, if the corresponding edges in G have a vertex in common. As an example it is shown in figure 1 that the Kagomé lattice is the line graph of the hexagonal lattice.

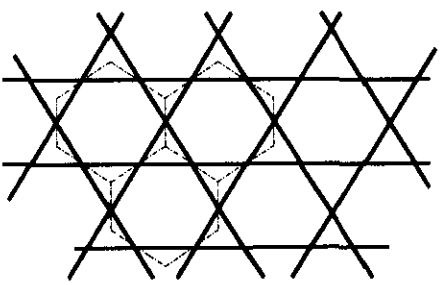

Figure 1. The hexagonal lattice (dashed lines) and its line graph, the Kagomé lattice.

We use some standard graph theoretical notions, which may be found in every standard textbook on graph theory, e.g. [6]. The words 'walk', 'path', and 'cycle' have the obvious meaning. A walk of length n is a sequence $c=(x_1, e_1, x_2, e_2, \ldots, e_{n-1}, x_n)$ where e_i is an edge joining x_i to x_{i+1}. A path is a self avoiding walk and a cycle is a self avoiding closed walk. A graph is 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. A bipartite graph has only cycles of even length. A graph is planar, if it has a representation in the plane and the representation is referred to as a plane graph. The vertices and edges of a plane graph divide the plane into a set of connected components, called faces. Each plane graph has exactly one unbounded

face. Let $F(G)$ be the set of bounded faces, then by Euler's formula $|F|=|E|-|V|+1$. The boundary of each bounded face is called a facial cycle. Usually $f\in F(G)$ will denote either the face or the facial cycle. A graph G is k-connected ($k\geqslant 1$) if any two vertices of G can be joined by k disjoint paths. A 1-connected graph is connected. If G is not connected, it consists of different connected components. In a 2-connected graph each edge is contained in a cycle. Further we need the adjacency matrix of the graph G $A=(a_{xy})_{x,y\in V}$ and the incidence matrix $B(G)=(b_{xe})_{x\in V,e\in E}$ of G. $a_{xy}=1$ if the two vertices are adjacent and $a_{xy}=0$ otherwise, b_{xe} is equal to 1 if the vertex x is incident to the edge e ($x\in e$) and zero otherwise. An induced subgraph of G is constructed by a subset of V and all the edges in G joining the vertices in this subset. From a given graph G we may construct new graphs by subdividing some of the edges of G by new vertices. Such a graph will be called a subdivision of G.

In the following we will not deal directly with the Hamiltonian (1.1), but with its particle-hole transformed version. Such a transformation may be introduced using the operator

$$I=\prod_{x\sigma}(c^{+}_{x\sigma}+c_{x\sigma}). \tag{2.1}$$

One has immediately

$$II^{+}=1 \tag{2.2a}$$

$$Ic_{x\sigma}=c^{+}_{x\sigma}I \tag{2.2b}$$

$$Ic^{+}_{x\sigma}=c_{x\sigma}I. \tag{2.2c}$$

After a particle-hole transformation the sign of the kinetic energy is changed. One obtains with $t_{xy}=ta_{xy}$

$$IHI^{+}=H'=t\sum_{x,y,\sigma}a_{xy}c^{+}_{x\sigma}c_{y\sigma}+U\sum_{x}n_{x+}n_{x-}+U(|V|-N). \tag{2.3}$$

In the following we take $t=1$ and neglect the trivial constant $U(|V|-N)$. Further we omit the prime in (2.3), our Hamiltonian will be

$$H=\sum_{x,y,\sigma}a_{xy}c^{+}_{x\sigma}c_{y\sigma}+U\sum_{x}n_{x+}n_{x-}. \tag{2.4}$$

Since I is a unitary transformation, every result derived for H in (2.4) may be carried over to the original Hamiltonian in (1.1). Only the particle number N is replaced by $2N_s-N$.

Further we introduce the spin operators

$$S_{+}=\sum_{x}c^{+}_{x+}c_{x-},\quad S_{-}=\sum_{x}c^{+}_{x-}c_{x+},\quad S_z=\tfrac{1}{2}(N_{+}-N_{-}). \tag{2.5}$$

They generate the global SU(2) spin symmetry of the Hamiltonian. The eigenstates of the Hamiltonian are assumed to be eigenstates of S_z and S^2 defined as usual

$$S^2=(S_z)^2+\tfrac{1}{2}(S_{+}S_{-}+S_{-}S_{+}). \tag{2.6}$$

The eigenvalues of S^2 are $S(S+1)$ and S will be called the spin of the eigenstate. In what follows we will make use of the main result of [2], namely:

Theorem 0. Let $L(G)$ be the line graph of $G=(V,E)$ and let H in (2.4) be the Hamiltonian on $L(G)$ with N electrons. Let $C=|E|-|V|+1$ if G is bipartite, $C=|E|-|V|$ otherwise. Then

(i) H has ferromagnetic ground states with a saturated value $S=N/2$ if $N\leqslant C$.

(ii) If G is 2-connected and bipartite and $N = C$, the ground state is unique apart from the degeneracy due to the SU(2) invariance†.

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

The result (i) follows from the fact that the adjacency matrix of the line graph $L(G)$ has the form $A = B(G)^+ B(G) - 2$. The lowest eigenvalue of A is -2 and each element of the kernel of $B(G)$ is an eigenstate to this eigenvalue. C in theorem 0 is simply the multiplicity of the eigenvalue -2 and the eigenstates mentioned in the theorem are constructed as Slater determinants from some single particle eigenstates of the eigenvalue -2 of the kinetic energy.

A basis of the kernel of $B(G)$ may be constructed as follows. Since G is bipartite with vertex classes V_1 and V_2 each edge in G may be oriented from V_1 to V_2. Furthermore, each facial cycle $f \in F(G)$ will be oriented clockwise. We now define

$$\begin{aligned} d_f(e) &= 1 \quad \text{if } f \text{ contains } e \text{ and } e \text{ and } f \text{ have the same orientation} \\ d_f(e) &= -1 \quad \text{if } f \text{ contains } e \text{ and } e \text{ and } f \text{ have opposite orientation} \\ d_f(e) &= 0 \quad \text{if } f \text{ does not contain } e. \end{aligned} \tag{2.7}$$

The set $\{d_f, f \in F(G)\}$ is a basis (not orthonormal) of the kernel of $B(G)$ [6, 7].

Let G_σ be a subgraph of the bipartite plane graph G. Clearly, G_σ is a bipartite plane graph as well. Let F_σ be a subset of the facial cycles of G_σ and let $\Phi_\sigma(F_\sigma)$ be the Slater determinant of all the states d_f, $f \in F_\sigma$ with electrons with a spin σ. We mention that a facial cycle of G_σ is a cycle of G, but not necessarily a facial of G. On the other hand, each $f \in F_\sigma$ is a sum of some elements of $F(G)$. Now let G_+ and G_- be a pair of edge disjoint subgraphs of G and let F_+ and F_- be of subsets of the facial cycles of G_+ and G_- respectively. Then we define

$$\Phi(F_+, F_-) = \Phi_+(F_+)\Phi_-(F_-) \tag{2.8}$$

$\Phi(F_+, F_-)$ is an eigenstate of the z-component S_z of the spin, $S_z = |F_+| - |F_-|$, but it is not an eigenstate of S^2. It contains components for all spins $S \geqslant ||F_+| - |F_-||$. Let P_s be the projector onto the subspace of given spin S, then we define

$$\Phi_{s,m}(F_+, F_-) = S_\pm^n P_s \Phi(F_+, F_-) \tag{2.9}$$

where n and the sign are chosen such that the state is an eigenstate of S_z with the eigenvalue m. The states mentioned in (iii) of theorem 0 are constructed in this way. We are now able to state the main result of this paper.

Theorem 1. Let H be the Hamiltonian (2.4) of the Hubbard model with N electrons on a line graph $L(G)$ where $G = (V, E)$ is a 2-connected, bipartite plane graph. Let $N \leqslant |E| - |V| + 1$. The eigenspace of the ground states of H for fixed S and $S_z = m$ is spanned by the states (2.9).

† We should mention that (ii) was formulated for non-bipartite graphs as well in [2]. But the proof as given in [2] is only valid for the case of bipartite graphs and in the case of a non-bipartite graph one needs an additional assumption which is mainly technical. (For instance, (ii) is true for a non-bipartite graph G that is a 3-connected graph or a subdivision of a 3-connected graph.) Here we will treat the case of bipartite graphs only.

G_+ and G_- are not necessarily connected, but it is possible to restrict the set of pairs G_+ G_- to such subgraphs G_+ or G_- that have only 2-connected components. Theorem 1 is in some sense the inverse of part (iii) of theorem 0. The proof of this theorem uses some elements of graph theory and will be presented in the subsequent section. The reader who is mainly interested in the consequences of this theorem may directly pass to section 4.

3. Proof of theorem 1

Let G be a 2-connected, bipartite plane graph and let

$$s_{fg} = -\sum_{e \in E} d_f(e) d_g(e) \qquad f, g \in F(G) \tag{3.1}$$

The matrix $S = (s_{fg})_{f,g \in F(G)}$ is regular and we denote by S^{-1} the inverse, which has the components $(S^{-1})_{fg}$. Let us now define the operators

$$d^+_{f\sigma} = \sum_{e \in E} d_f(e) c^+_{e\sigma} \tag{3.2}$$

where $c^+_{e\sigma}$ is the creation operator of an electron with a spin σ on the vertex e of the line graph $L(G)$, which is also an edge e of G. Furthermore we introduce

$$d_{f\sigma} = -\sum_{g \in F} \sum_{e \in E} (S^{-1})_{fg} d_g(e) c_{e\sigma} \tag{3.3}$$

where $c_{e\sigma}$ is the usual annihilation operator of an electron. d is not the adjoint operator of d^+, but its dual. They obey the usual anticommutation relations for fermions

$$d_{f\sigma} d^+_{g\sigma'} + d^+_{g\sigma'} d_{f\sigma} = \delta_{\sigma,\sigma'} \delta_{f,g}. \tag{3.4}$$

A basis of N-particle states constructed with the operators d^+ is not an orthonormal basis, so it is not identical to its dual basis. Due to (3.4) the dual basis may be formed using the operators d. Each N-particle state with kinetic energy $-2N$ may be written as

$$|\Phi\rangle = \sum \Phi(f_1, \ldots, f_N; \sigma_1, \ldots, \sigma_N) d^+_{f_1\sigma_1} \ldots d^+_{f_N\sigma_N} |0\rangle \tag{3.5}$$

Any state $|\Phi\rangle$ is a ground state of the Hamiltonian (2.4) with $N \leqslant |F|$ on $L(G)$ if and only if there is no doubly occupied site, i.e.

$$c_{e+} c_{e-} |\Phi\rangle = 0 \qquad \text{for all } e \in E. \tag{3.6}$$

If we restrict ourselves to states of the form (3.5), the condition (3.6) may be written as

$$a^d_{fg} (d_{f+} - d_{g+})(d_{f-} - d_{g-}) |\Phi\rangle = 0 \qquad \text{for all } f, g \in F(G) \tag{3.7a}$$

and

$$a^d_{0f} d_{f+} d_{f-} |\Phi\rangle = 0 \qquad \text{for all } f \in F(G) \tag{3.7b}$$

where

$$\begin{aligned} a^d_{ff} &= 0 && \text{for all } f \\ a^d_{fg} &= 1 && \text{if } f \text{ and } g \text{ have one edge in common} \\ a^d_{fg} &= 0 && \text{if } f \text{ and } g \text{ have no edge in common.} \end{aligned} \tag{3.8}$$

f and g are facial cycles of G, the cycle of the unbounded face is denoted by 0. We note that (a^d_{fg}) is the adjacency matrix of the dual graph of G.

From the conditions (3.7) it follows that if theorem 1 is true for some G, it is true for each bipartite subdivision of G, since the algebra of the operators d and d^+ and the matrix (a^d_{fg}) are the same for both. Furthermore it is clear that theorem 1 holds for all bipartite, 2-connected graphs with less than eight edges. These graphs are presented in figure 2. G_1 and G_2 contain only one facial cycle and N has to be one. In these cases the theorem is trivial. G_3 and G_4 contain two facial cycles and N may be one or two. In the case $N=2$ we have only the unique ferromagnetic ground state due to theorem 0, the case $N=1$ is trivial. So theorem 1 holds for all these graphs. We now have to introduce the concept of a bridge of a cycle [7]. A bridge K of a cycle c in G is either an edge of G not belonging to c that is incident to two vertices of c or a component of $G-c$ (this is the graph obtained from G by deleting all the vertices of c and all the edges incident to these vertices) together with all the vertices of G adjacent to K and all the edges of G incident to K. The facial cycles of G_3 and G_4 have one bridge, the bridge of the cycle of the unbounded face of G_4 consists of a single edge only. Now it is clear that theorem 1 holds for all G with the property that there is no cycle with more than one bridge. In fact, if G has no cycle with more than one bridge, it must be one of the graphs G_1 to G_4 or a subdivision of one of these graphs (see lemma 1.6.4 in [7]). Let G be a graph with a cycle with at least two bridges. Then G has two facial cycles f and g such that the cycle $c=f+g$ has exactly two bridges. One of them is $f\cap g$. Let G' be the subgraph of G obtained by deleting the edges and the inner vertices of $f\cap g$ from G. G' is 2-connected, bipartite and planar if G has these properties. Each ground state of H on $L(G)$ with N electrons may be written as

$$|\Phi\rangle=|\Phi_1\rangle+(d^+_{f+}-d^+_{g+})|\Phi_2\rangle+(d^+_{f-}-d^+_{g-})|\Phi_3\rangle \tag{3.9}$$

where $|\Phi_i\rangle$ are states of the form (3.5) on $L(G')$. Since $|\Phi\rangle$ is a ground state, there is no term with a double occupancy on $f-g$. This follows also from (3.7). Let now

$$d^+_{\pm\sigma}=d^+_{f\sigma}\pm d^+_{g\sigma},\ d_{\pm\sigma}=\tfrac{1}{2}(d_{f\sigma}\pm d_{g\sigma}). \tag{3.10}$$

using these operators we obtain from (3.7)

$$\begin{aligned}
&a^d_{fh}[(d_{++}-d_{h+})(d_{+-}-d_{h-})|\Phi_1\rangle+(d_{++}-d_{h+})|\Phi_3\rangle-(d_{+-}-d_{h-})|\Phi_2\rangle]=0\\
&a^d_{gh}[(d_{++}-d_{h+})(d_{+-}-d_{h-})|\Phi_1\rangle+(d_{++}-d_{h+})|\Phi_3\rangle-(d_{+-}-d_{h-})|\Phi_2\rangle]=0\\
&a^d_{f0}[d_{++}d_{+-}|\Phi_1\rangle+d_{++}|\Phi_3\rangle-d_{+-}|\Phi_2\rangle]=0\\
&a^d_{g0}[d_{++}d_{+-}|\Phi_1\rangle+d_{++}|\Phi_3\rangle-d_{+-}|\Phi_2\rangle]=0\\
&a^d_{kh}(d_{k+}-d_{h+})(d_{k-}-d_{h-})|\Phi_i\rangle=0\\
&a^d_{0h}d_{h+}d_{h-}|\Phi_i\rangle=0
\end{aligned} \tag{3.11a-f}$$

where h and k are facial cycles of G' not equal to c and $i=1,2,3$. From these conditions it follows that $|\Phi_2\rangle$ and $|\Phi_3\rangle$ are ground states of H on $L(G')$ with $N-1$ electrons. The equations for $|\Phi_1\rangle$ may be solved with the ansatz

$$|\Phi_1\rangle=\sum(a^d_{fh}-a^d_{gh})(d^+_{h+}|\Phi_2\rangle+d^+_{h-}|\Phi_3\rangle)+|\Phi^1_1\rangle \tag{3.12}$$

where the sum runs over all $h\in F(G')$, h not equal to c. To formulate the conditions obtained for $|\Phi^1_1\rangle$, let us now define the distance of two facial bounded cycles h and k as the smallest integer $n\geqslant 0$ such that the matrix element of the nth power of S $(S^n)_{hk}$ is not zero. This integer is called $d(h,k)$. Further we introduce

$$\begin{aligned}
&a^{(n)}_{hk}=1 \qquad \text{if } d(h,k)=n\\
&a^{(n)}_{hk}=0 \qquad \text{otherwise}
\end{aligned} \tag{3.13}$$

and

$$\begin{aligned} &w^{(n)}_{f_1,\ldots,f_{n+1}} = 1 \qquad \text{if } s_{f_i,f_{i+1}} \text{ is non-zero for all } i = 1,\ldots,n \\ &w^{(n)}_{f_1,\ldots,f_{n+1}} = 0 \qquad \text{otherwise.} \end{aligned} \tag{3.14}$$

With these quantities we may write the conditions for $|\Phi^1_1\rangle$ in the form

$$\begin{aligned} &(a^d_{fh} + a^d_{gh})(d_{++} - d_{h+})(d_{+-} - d_{h-})|\Phi^1_1\rangle = 0 \\ &(w^{(2)}_{fhk} + w^{(2)}_{ghk})(d_{h+} - d_{k+})(d_{h-} - d_{k-})|\Phi^1_1\rangle + \\ &(w^{(2)}_{fhk} - w^{(2)}_{ghk})[(d_{h+} - d_{k+})|\Phi_3\rangle - (d_{h-} - d_{k-})|\Phi_2\rangle] = 0 \\ &a^d_{hk}(1 - w^{(2)}_{fhk})(1 - w^{(2)}_{ghk})(1 - w^{(2)}_{fkh})(1 - w^{(2)}_{gkh})(d_{k+} - d_{h+})(d_{k-} - d_{h-})|\Phi^1_1\rangle = 0 \end{aligned} \tag{3.15}$$

where h and k are elements of $F(G')$ not equal to c. As before, these equations can be solved with the ansatz

$$|\Phi^1_1\rangle = \sum (a^{(2)}_{fh} - a^{(2)}_{gh})(d^+_{h+}|\Phi_2\rangle + d^+_{h-}|\Phi_3\rangle) + |\Phi^2_1\rangle \tag{3.16}$$

where the sum is over all $h \in F(G')$, h not equal to c. The conditions obtained for $|\Phi^2_1\rangle$ using (3.15) are

$$\begin{aligned} &(a^d_{fh} + a^d_{gh})(d_{++} - d_{h+})(d_{+-} - d_{h-})|\Phi^2_1\rangle = 0 \\ &(w^{(2)}_{fhk} + w^{(2)}_{ghk})(d_{h+} - d_{k+})(d_{h-} - d_{k-})|\Phi^2_1\rangle = 0 \\ &(w^{(3)}_{fhkl} + w^{(3)}_{ghkl})[(d_{k+} - d_{l+})(d_{k-} - d_{l-})|\Phi^2_1\rangle + \\ &(w^{(3)}_{fhkl} - w^{(3)}_{ghkl})[(d_{k+} - d_{l+})|\Phi_3\rangle - (d_{k-} - d_{l-})|\Phi_2\rangle] = 0 \\ &a^d_{hk} \prod_l (l - w^{(3)}_{flhk})(1 - w^{(3)}_{glhk})(1 - w^{(3)}_{flkh})(1 - w^{(3)}_{glkh}) \\ &(d_{h+} - d_{k+})(d_{h-} - d_{k-})|\Phi^2_1\rangle = 0 \end{aligned} \tag{3.17}$$

This process may be iterated. Let $d(G)$ be the largest distance between two facial bounded cycles of G, then it terminates after at least $d(G)$ steps. The final result is

$$|\Phi_1\rangle = \sum_{k=1}^{d(G)} \sum_h (a^{(k)}_{fh} - a^{(k)}_{gh})(d^+_{h+}|\Phi_2\rangle + d^+_{h-}|\Phi_3\rangle) + |\Phi^{d(G)}_1\rangle \tag{3.18}$$

where the sum over h excludes c as before. The final conditions for $|\Phi^{d(G)}_1\rangle$ are

$$a^d_{hk}(d_{h+} - d_{k+})(d_{h-} - d_{k-})|\Phi^{d(G)}_1\rangle = 0 \tag{3.19}$$

where h and k are not equal to c. Since

$$\sum_{k=1}^{d(G)} a^{(k)}_{fh} = \sum_{k=1}^{d(G)} a^{(k)}_{gh} \tag{3.20}$$

we obtain

$$|\Phi_1\rangle = |\Phi^{d(G)}_1\rangle \tag{3.21}$$

The representation of G in the plane may now be chosen such that $a^d_{f0} - a^d_{g0} = 0$. This is always possible. Then it follows from (3.11), (3.19) and (3.21) that $|\Phi_1\rangle$ is a ground state of the Hamiltonian H on $L(G')$ as it was shown for $|\Phi_2\rangle$ and $|\Phi_3\rangle$ before. But, if $|\Phi_1\rangle$ is a ground state of H on $L(G')$, the conditions (3.11*a–d*) read

$$\begin{aligned} &(a^d_{fh} + a^d_{gh})[(d_{++} - d_{h+})|\Phi_3\rangle - (d_{+-} - d_{h-})|\Phi_2\rangle] = 0 \\ &(a^d_{f0} + a^d_{g0})(d_{++}|\Phi_3\rangle - d_{+-}|\Phi_2\rangle) = 0. \end{aligned} \tag{3.22}$$

This shows that the expression

$$|\Phi\rangle - |\Phi_1\rangle = d^+_{-+}|\Phi_2\rangle + d^+_{--}|\Phi_3\rangle \tag{3.23}$$

has no singlet on the cycles $f+g$ or $f-g$ and a neighboured cycle h. The only singlet that is allowed (only if $a^d_{f0} = a^d_{g0} = 0$) is a singlet on $f+g$ or $f-g$ and $f+g+\Sigma h$ where the sum is over all neighboured cycles of f and g. But this cycle has no edges with $f+g$ or $f-g$ in common. This result may be used to prove theorem 1 by induction on the number of edges of the graphs. Theorem 1 is true for all bipartite 2-connected plane graphs with at most seven edges. Suppose theorem 1 to be true for all bipartite 2-connected plane graphs with at most m edges. Let now G be a graph with $m+1$ edges. If G has only cycles with at most one bridge, we know already that theorem 1 is fulfilled. Let us therefore consider a graph G with at least one cycle with two bridges. From the construction above we know that each ground state of H on $L(G)$ may be written in the form (3.9) where the $|\Phi_i\rangle$ are ground states on $L(G')$. By our induction hypotheses these states are linear combinations of the states (2.9), since G' has at most m edges. We already know that the electrons on $f \pm g$ in $|\Phi\rangle - |\Phi_1\rangle$ do not form a singlet with electrons on other cycles having an edge with $f \pm g$ in common. Therefore, it is possible to write the right hand side of (3.23) as a linear combination of the states (2.9) as well. Then $|\Phi\rangle$ is a linear combination of these states. This proves theorem 1.

A straightforward generalization of theorem 1 to non-planar graphs is not possible. From the theorem of Kuratowski we know that a graph is planar if and only if it does not contain a subgraph that is a subdivision of the complete graph K_5 or of the complete bipartite graph $K_{3,3}$ (see e.g. [6, 7]). The diagonalization of the Hubbard model on the line graph of $K_{3,3}$ or on the line graph of a bipartite subdivision of K_5 is easily done numerically. One finds that the Hubbard model (2.4) on $L(K_{3,3})$ has a ground state with $S=0$ for $N=2$, but it is not possible to find two edge disjoint subgraphs G_+ and G_- as needed to construct a ground state of the form (2.9) with $S=0$ for $N=2$. The same problem occurs for the line graph of a bipartite subdivision of K_5. The construction of the states and especially the proof of theorem 1 uses the possibility to construct a basis of the kernel of $B(G)$ using the facial cycles of G. In fact, this basis has the property that each edge of G belongs to at most two elements it. S MacLane proved in 1937 the well-known result that a graph is planar if and only if such a basis exists [7]. Therefore, we may understand why our result holds only in the case of line graphs of plane graphs.

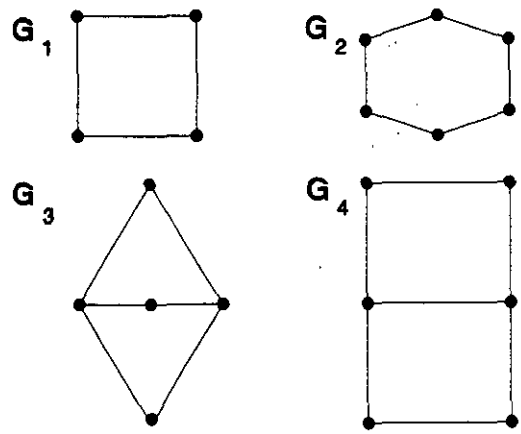

Figure 2. The 2-connected bipartite plane graphs with at most seven edges.

4. Ferromagnetic versus paramagnetic behaviour

Theorem 1 gives us a complete description of the ground states of the Hamiltonian (2.4). Since the ground states are degenerate, it is not clear whether the model shows a ferromagnetic behaviour or not, although there are some ferromagnetic ground states amongst them. In the following we will study the magnetic behaviour of the model (2.4). For simplicity we restrict ourselves to the case of regular lattices. In the following G will be a sufficiently large but finite part of a two-dimensional regular periodic lattice. As a typical case we take the hexagonal lattice, $L(G)$ will be (a large but finite part of) the Kagomé lattice in this case. To decide the question of the ferromagnetic behaviour, we will look at the ground state expectation value of S^2 given by

$$\langle S^2\rangle = \sum_S d(N,S)(2S+1)S(S+1) \Big/ \sum_S d(N,S)(2S+1) \tag{4.1}$$

where $d(N,S)$ is the degeneracy of the ground state of (2.4) for fixed N, S_z and S. We say that the system is ferromagnetic if $\langle S^2\rangle/N^2$ tends to a finite value for large system sizes (finite size effects are assumed to be negligible). Otherwise the system is paramagnetic.

The set formed by the states (2.9) is not necessarily linearly independent. In fact, if N is well below $|F|$, there are many linearly dependent states. Therefore, it is difficult to calculate $d(N,S)$. But we are able to give some upper and lower bounds on $d(N,S)$. A lower bound is obtained by choosing a suitable subset of linearly independent states of the form (2.9). This may be done as follows. Let G_0 be the graph obtained from the dual graph of G by deleting the vertex corresponding to the unbounded face of G and the edges incident to this vertex. The vertices of G_0 are the elements of $F(G)$. Let $V_{0\sigma}$ be the set of vertices of some induced subgraph $G_{0\sigma}$ of G_0. We define the states $\Phi_\sigma(V_{0\sigma})$ as the Slater determinant of the single particle states $d_f, f\in V_{0\sigma}$ with electrons with a spin σ. Let now G_{0+} and G_{0-} be a pair of induced subgraphs of G_0 such that no vertex of G_{0+} is adjacent to a vertex of G_{0-}. Then we let $\Phi(V_{0+}, V_{0-}) = \Phi_+(V_{0+})\Phi_-(V_{0-})$ and

$$\Phi_{s,m}(V_{0+}, V_{0-}) = S_\pm^n P_s \Phi(V_{0+}, V_{0-}) \tag{4.2}$$

as before. The states (4.2) form a set of linearly independent states, but not necessarily a basis of the space spanned by the states (2.9). Let $d_0(N,S)$ be the manner of states (4.2) for fixed N, S_z and S, then

$$d_0(N,S) \leqslant d(N,S). \tag{4.3}$$

On the other hand, the states (2.9) which are not linear combinations of the states (4.2) are states where F_+ (or F_-) contains a cycle c such that some elements of F_- (or F_+) and thus a component of G_- (G_+) lies inside c. Clearly, such a cycle c contains more edges than a facial cycle of the lattice G. Due to the construction of the states (2.9) it is not possible to place an electron with spin $-$ (or $+$) on a facial cycle that has an edge in common with c. The number of facial cycles that have an edge in common with c is much larger than the number of facial cycles that have an edge in common with a given facial cycle. Therefore, the number of linearly independent states that contain such a larger cycle is smaller than $d_0(N,S)$. This shows that

$$d(N,S) < 2d_0(N,S). \tag{4.4}$$

As a simple consequence of the two inequalities (4.3), (4.4) we obtain

$$\langle S^2\rangle_0/2 \leqslant \langle S^2\rangle \leqslant 2\langle S^2\rangle_0 \tag{4.5}$$

where

$$\langle S^2\rangle_0 = \sum_S d_0(N,S)(2S+1)S(S+1) \Big/ \sum_S d_0(N,S)(2S+1). \tag{4.6}$$

Therefore, instead of $\langle S^2\rangle/N^2$ we may study the behaviour of $\langle S^2\rangle_0/N^2$ for large system sizes. A pair of subgraphs G_{0+}, G_{0-} may be constructed as follows: We choose a set P of N vertices of G_0 at random. Then we take the subgraph of G_0 induced by P. This induced subgraph has several connected components. We form G_{0+} and G_{0-} out of these components such that the union of G_{0+} and G_{0-} is the induced subgraph. Each pair of subgraphs is obtained in this way. This means that we have to study the site percolation problem on G_0 (for a review see e.g. [8]). With probability $p = N/|F|$ we choose some vertices from G_0. If p is above the critical value p_c, we have with probability 1 an infinite component on the lattice, the percolation cluster. All the other components are finite. Therefore $\langle S^2\rangle_0/N^2$ tends to some finite value if the density of electrons is above $p_c(|F|/N_s)$. If the probability p is below p_c the situation changes drastically. There is no infinite component and the system becomes paramagnetic. The value of p_c is well-known for various lattices. If $L(G)$ is the Kagomé lattice, G is the hexagonal lattice and G_0 is the triangular lattice. In this case $p_c = \frac{1}{2}$ and $|F|/N_s = \frac{1}{3}$. Therefore, we conclude that the Hubbard model (2.4) on the Kagomé lattice behaves ferromagnetic at $T = 0$ for densities between $\frac{1}{3}$ and $\frac{1}{6}$.

Transforming back to the original Hamiltonian (1.1), the density n has to be replaced by $2-n$. Therefore the Hubbard model (1.1) shows a ferromagnetic behaviour on the Kagomé lattice for densities between $\frac{5}{3}$ and $\frac{11}{6}$. Instead of the Kagomé lattice, we may take any line graph of a planar bipartite lattice. Then p_c will be different, nevertheless one finds a ferromagnetic behaviour in some finite density range as well. The line graph of e.g. the square lattice is a square lattice with cross hoppings on half of the squares. We have $|F|/N_s = \frac{1}{2}$. Its dual lattice is the square lattice as well and $p_c = 0.593$ [8]. The ferromagnetic behaviour occurs if $1.703 > n \geqslant 1.5$.

5. Final remarks

Theorem 1 and the result of section 4 show that the Hubbard model (1.1) on a lattice that is a line graph behaves ferromagnetic for $N \geqslant M = 2N_s - |F|$ as long as N is not too large. On the other hand, if $N > M$, the ground state degeneracy is very large and small perturbations will be important. Therefore, a realistic system on e.g. the Kagomé lattice will certainly not show the ideal behaviour of the Hubbard model. There are mainly two perturbations which may be discussed. The first is an interaction with some longer range. The effect of such contributions in a single-band model has been investigated by Hirsch [9]. The results seem to indicate that an interaction of longer range favours ferromagnetism. Although rigorous results are not available, this may be the case in models with more than one band as well. The second perturbation that may be important is a single particle operator that perturbs the kinetic energy of the Hamiltonian. Such a perturbation will lift the degeneracy of the highest energy band on a line graph. Therefore, ferromagnetism will be disturbed for small U. But one may hope that above some critical interaction strength ferromagnetism persists.

In [1, 2] possible generalizations of the results for the Hubbard model on line graphs have been discussed. Similarly theorem 1 may be carried over to these cases as well. We mention especially the case of the graph $S(G)$ which is constructed from

$G=(V, E)$ by subdividing each edge by a new vertex into two new edges. An example is the two-dimensional CuO_2 sublattice in the high-temperature superconductors, in this case G is simply the square lattice formed by Cu. If one introduces the Hubbard model on $S(G)$ with nearest and next nearest neighbour hoppings and on-site potentials, the different parameters of the model may be chosen such that the single particle part of the Hamiltonian has a highest energy band, which is flat [2]. In this case we have a complete analogy between the ground states of (1.1) on $L(G)$ discussed above and the ground states of this model.

As a consequence of a theorem of Lieb [10], the Hubbard model (1.1) on $S(G)$ (without next-nearest neighbour hopping!) has a ferromagnetic ground state if $N=N_s$. In [2] we pointed out the relation between his result and ours. It would be interesting to see, whether one has a ferromagnetic behaviour in this case in a finite density range around half filling. One may hope that in this case there is no large ground state degeneracy and that one has only some ferromagnetic ground states.

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