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Exact results for the $U = \infty$ Hubbard model

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Abstract. We investigate the $U = \infty$ Hubbard model on a large class of lattices which are line graphs. The most interesting lattices in this class are line graphs of regular bipartite lattices with N_s sites and coordination number $k \geq 4$. The ground state energy and some ground states are given. If the number of electrons N satisfies $N_s \geq N \geq 2N_s/k - 2$, the ground state energy is $-4|t|(N_s - N)$. The ground states have no magnetic ordering, they are projections of the ground states at $U = 0$ onto the subspace of states without doubly occupied sites.

1. Introduction

The Hubbard model is the simplest interesting model for itinerant electrons. It describes electrons moving on a lattice, and it covers the essential properties of itinerant electrons, namely the repulsive interaction, the spin and the Fermi statistics. The motion of the electrons is described by a hopping process, the interaction is taken to be local. The Hubbard model has been used to study many of the interesting problems in condensed matter physics.

Disregarding the solution of the model in one dimension [1], there are only a few exact results. Most of them concern the magnetic properties of the model. The well known theorem of Nagaoka [2] with Tasaki's extension [3] states that on a finite lattice with N_s lattice sites for hard-core interaction (and by continuity for very strong interaction), if the number of electrons is $N_e = N_s - 1$, and if the hopping matrix elements are non-negative, the model has a ferromagnetic ground state with a maximal spin $S = N_e/2$. By symmetry this result holds also for non-positive hopping matrix elements (this is the usual case) if the lattice is bipartite. On the other hand, other exact results show that the spin of the ground state is not maximal in some cases. Already Nagaoka [2] pointed out that his theorem is not valid on non-bipartite lattices with the usual negative hopping matrix elements. Furthermore, in many cases the theorem of Nagaoka is not true if $N_e < N_s - 1$, see e.g. Sütö [4]. In most of these cases the ground state is not known. An exception is the recent work of Brandt and Giesekeus [5]. They gave the ground-state energy and exact ground states of the Hubbard model with hard-core repulsion in a density range below half filling on some special decorated hypercubic or 'Perovskite-like' lattices. These lattices are in fact line graphs of cubic lattices with periodic boundary conditions. One of the periods has to be odd, so that the cubic lattice is not bipartite. They obtained non-trivial results if the dimension $d \geq 3$.

In the present paper we generalize the results of Brandt and Giesekeus to a larger class of lattices that are line graphs. This larger class includes the line graphs of all

bipartite regular lattices with a coordination number or valency $k \geq 4$ and of some non-bipartite regular lattices with $k > 4$, especially the line graphs of hypercubic lattices with periodic boundary conditions for dimensions $d \geq 2$ and the lattice of the octahedral sites of a spinel, which is the line graph of the diamond lattice. We give the ground-state energy and some ground states. These ground states have no magnetic order; they are paramagnetic. They are projections of the ground states of the system without interaction onto the subspace without doubly occupied sites.

For a wide range of density, we proved the existence of ferromagnetic ground states on lattices that are line graphs [6, 7]. This result is valid for any interaction strength, as long as the interaction is repulsive. It holds for negative hopping matrix elements if the density is well above half filling or, by symmetry, for positive hopping matrix elements and densities well below half filling. We will compare these results with the results obtained in the present paper. In both cases the fact that the lattice is a line graph is essential for the construction of the states and the proofs of the results use graph-theoretic methods.

Our paper will be organized as follows. The next section contains a description of the Hubbard model and a discussion of some of its symmetries. Furthermore we give some lower bounds of the Hamiltonian of the Hubbard model with hard-core repulsion. In section 3 some graph-theoretic notions are introduced. The construction of the ground states is shown and some sufficient conditions for the underlying lattices are presented. We give several examples of lattices that satisfy one of these conditions. Section 4 contains some concluding remarks.

2. The model

The Hubbard model is defined by the Hamiltonian

$$H_U = \sum_{x,y,\sigma} t_{xy} c_{x\sigma}^\dagger c_{y\sigma} + U \sum_x n_{x+} n_{x-}. \quad (2.1)$$

We assume that t_{xy} is equal to t (usually negative) if the lattice sites x and y are nearest-neighbours, and 0 otherwise. $c_{x\sigma}^\dagger$ and its adjoint $c_{x\sigma}$ are electron creation and annihilation operators for electrons with spin σ on the lattice site x . They satisfy the usual fermion anticommutation relations. $n_{x\sigma} = c_{x\sigma}^\dagger c_{x\sigma}$, $n_x = n_{x+} + n_{x-}$ 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 $N \leq 2N_s$ where N_s denotes the number of lattice sites. The Hamiltonian conserves the number of electrons with spin $+$ ($-$), which we denote by N_+ (N_-). It commutes with the spin operators

$$S^+ = \sum_x c_{x+}^\dagger c_{x-}, \quad S^- = \sum_x c_{x-}^\dagger c_{x+}, \quad S^z = \frac{1}{2}(N_+ - N_-) \quad (2.2)$$

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

$$S^2 = (S^z)^2 + \frac{1}{2}(S^+ S^- + S^- S^+). \quad (2.3)$$

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

With the help of a particle-hole transformation, the model with $t < 0$ may be transformed to one with $t > 0$. Such a transformation may be introduced using the operator

$$I = \prod_{x\sigma} (c_{x\sigma}^\dagger + c_{x\sigma}). \tag{2.4}$$

One has immediately

$$II^\dagger = 1 \tag{2.5a}$$

$$Ic_{x\sigma} = c_{x\sigma}^\dagger I \tag{2.5b}$$

$$Ic_{x\sigma}^\dagger = c_{x\sigma} I. \tag{2.5c}$$

After a particle-hole transformation the sign of the kinetic energy is changed. One obtains

$$IH_U I^\dagger = H'_U = - \sum_{x,y,\sigma} t_{xy} c_{x\sigma}^\dagger c_{y\sigma} + U \sum_x n_{x+} n_{x-} + U(N_s - N). \tag{2.6}$$

The last term is a trivial constant, which will be neglected. The particle number is transformed from N to $N' = 2N_s - N$. This transformation may be used to enforce $N \leq N_s$, but one has in turn to consider the two cases $t < 0$ and $t > 0$. This was already mentioned by Nagaoka [2].

In the following we will treat only the case $U = \infty$ and $N < N_s$. This simply means that the interaction term of (2.1) or (2.6) has to vanish; no site is doubly occupied. The projector onto the states without doubly occupied sites is

$$P_d = \prod_x (1 - n_{x+} n_{x-}) \tag{2.7}$$

and our Hamiltonian takes the form

$$H_\infty = P_d H_0 P_d = P_d \sum_{x,y,\sigma} t_{xy} c_{x\sigma}^\dagger c_{y\sigma} P_d. \tag{2.8}$$

We will now give some lower bounds on H_∞ . Let $t_i, i = 1, \dots, N_s$, be the eigenvalues of the matrix $T = (t_{xy})$, $t_i \leq t_{i+1}$. Let $\Phi_i(x)$ be the corresponding eigenvectors, which we choose to be real. Then

$$t_{xy} = \sum_i t_i \Phi_i(x) \Phi_i(y). \tag{2.9}$$

Let us introduce the operators

$$\Phi_{i\sigma}^\dagger = \sum_x \Phi_i(x) c_{x\sigma}^\dagger \quad \Phi_{i\sigma} = \sum_x \Phi_i(x) c_{x\sigma}. \tag{2.10}$$

Then H_∞ may be written as

$$H_\infty = P_d \sum_{i\sigma} t_i \Phi_{i\sigma}^\dagger \Phi_{i\sigma} P_d \tag{2.11}$$

or

$$H_\infty = -P_d \sum_{x,y,\sigma} t_{xy} c_{x\sigma} c_{y\sigma}^\dagger P_d \tag{2.12a}$$

$$= -P_d \sum_{i\sigma} t_i \Phi_{i\sigma} \Phi_{i\sigma}^\dagger P_d. \tag{2.12b}$$

These two expressions lead to the following two lower bounds.

$$H_\infty \geq t_1 N \quad (2.13)$$

$$H_\infty \geq -2t_{N_s}(N_s - N). \quad (2.14)$$

The first lower bound is not only valid for $U = \infty$, but for all $U > 0$. It was used to prove the existence of ferromagnetic ground states for the Hamiltonian (2.8) with $t > 0$ on a line graph [6]. The second lower bound is only valid if $U = \infty$. It can be improved by a factor $\frac{1}{2}$ in the case of a bipartite lattice. In the case of a regular bipartite lattice, the improved bound can be used to prove the theorem of Nagaoka. In the following we will discuss line graphs. Lattices that are line graphs are not bipartite. In this case, the ground-state energy is given by the right-hand side of (2.14) for some N , so that the bound (2.14) is best possible. This was used in the construction of Brandt and Giesekeus [5]. We will make use of it in the following treatment of the Hubbard model (2.8) on line graphs with $t < 0$.

Let us now recall the definition of a line graph (see e.g. [6, 8]). First a graph is a collection of sites (or vertices) with bonds (or edges) between them. A graph will be denoted by $G = (V, E)$, where V is the set of vertices and E is the set of edges. $|V|$ and $|E|$ denote the numbers of vertices and edges of G , respectively. Each lattice is a graph, where we refer to an edge as a line between two nearest-neighbouring sites. We deal only with connected graphs. A line graph is constructed from a given graph (or lattice) by putting new vertices on the edges of the graph and by connecting these new vertices with new edges, if the old edges have a vertex in common. A line graph of a graph G will be denoted by $L(G)$. In [6, 7] several examples of lattices that are line graphs have been discussed.

Let us now introduce the adjacency matrix $A(G) = (a_{xy})_{x,y \in V}$ and the incidence matrix $B(G) = (b_{xe})_{x \in V, e \in E}$ of a graph 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 and zero otherwise. Some of the spectral properties of the adjacency matrix $A_L = A(L(G))$ of a line graph $L(G)$ may be found in [8]. A_L is easily constructed if one knows the incidence matrix of G . One has

$$A_L = B(G)^t B(G) - 2I_{|E|} \quad (2.15)$$

where B^t is the transpose of B and I_n denotes the n -dimensional unit matrix. Since $B^t B$ is a positive-semidefinite matrix it follows from (2.15) that each eigenvalue of the adjacency matrix A_L is greater than or equal to -2 . The eigenspace corresponding to the eigenvalue -2 is the kernel of $B(G)$. The dimension of the kernel of $B(G)$ is $|E| - |V| + 1$ if G is bipartite (i.e. if it has two vertex classes, such that there are no edges between the vertices of the same class), and is $|E| - |V|$ if G is not bipartite (see e.g. [6]). This large degeneracy of the lowest eigenvalue has been used to obtain some exact, non-trivial results for the Hubbard model using the inequalities (2.13), (2.14).

3. Eigenstates

In the following we will discuss the Hamiltonian (2.8) on a line graph $L(G)$ and we will denote the vertices of the line graph by e, e', f , etc, as the corresponding edges of G . We have

$$t_{ef} = t a_{ef} \quad t < 0 \quad (3.1)$$

where a_{ef} are the matrix elements of the adjacency matrix (2.15) of the line graph and consequently

$$t_{N_s} = -2t. \tag{3.2}$$

Let us introduce the multiparticle state

$$|\Omega\rangle = P_d \prod_{\substack{\sigma, i \\ t_i < -2t}} \Phi_{i\sigma}^\dagger |0\rangle. \tag{3.3}$$

Since

$$P_d \Phi_{i\sigma}^\dagger P_d \Phi_{i\sigma}^\dagger = 0 \tag{3.4}$$

then $|\Omega\rangle$ is an eigenstate of H_∞ (2.12b) with the eigenvalue $-4|t|(N_s - N)$, or $|\Omega\rangle$ vanishes. Due to (2.14) and (3.2) $|\Omega\rangle$ is a ground state of H_∞ if it does not vanish. We therefore have to discuss the conditions for $|\Omega\rangle$ not to vanish.

The state $|\Omega\rangle$ is the projection of a state $|\Omega_0\rangle$, which is a product of two Slater determinants, each of the states $\{\Phi_i(e), t_i < -2t\}$. $|\Omega_0\rangle$ is the ground state of H_0 for the same number of electrons. The space spanned by the states $\{\Phi_i(e), t_i < -2t\}$ is the image of B^t , it has the dimension $|V| - 1$ if G is bipartite, $|V|$ if not.

A rather trivial necessary condition for $|\Omega\rangle$ not to vanish is obtained as follows. $N_s = |E|$ in our case, and $|\Omega\rangle$ contains $2(|V| - 1)$ electrons if G is bipartite or $2|V|$ electrons if not. Consequently, $|\Omega\rangle$ vanishes if G is bipartite and $2(|V| - 1) > |E|$ or if G is non-bipartite and $2|V| > |E|$. Below we will show that in the case of bipartite graphs or lattices where each site has the same valency $k \geq 4$ this condition is sufficient.

In the following we will present some sufficient conditions for $|\Omega\rangle$ not to vanish. In the proof we will always construct a non-vanishing multiparticle state that has a non-vanishing overlap with $|\Omega\rangle$. To construct such states, we will need some graph theoretic notions. These notions may be found in any standard textbook on graph theory, e.g. [9]. The degree or valency $d(x)$ of a vertex x is the number edges incident to x . If each vertex in G has the same degree k , G is called the regular of degree k or k -regular. In the case of regular lattices, the valency is usually called the coordination number. In a colouring of the edges of graph, the edges incident to a vertex get distinct colours. The edge chromatic number $c(G)$ is the minimal number of colours needed to colour the edges of G . A connected graph without any cycle is a tree. A subgraph of a graph $G = (V, E)$ is defined by a subset of V and a suitable subset of E . A subgraph is a spanning subgraph, if its vertex set is V . A spanning tree of G is a spanning subgraph of G that is a tree.

Instead of the basis $\{\Phi_i(e), t_i < -2t\}$, we may use a different basis of the image of B^t . A basis of this space is given by $\{b_{xe}, x \in V\}$ if G is not bipartite and $\{b_{xe}, x \in V \setminus \{x_0\}\}$ if G is bipartite, x_0 being any vertex of G . This may be seen as follows. It is clear that these states span the image of B^t ; we have to show they are linearly independent. If G is non-bipartite, the dimension of the image of B^t is equal to $|V|$, and therefore $\{b_{xe}, x \in V\}$ is a basis. On the other hand, if G is bipartite, the dimension of the image of B^t is equal to $|V| - 1$. In fact, let s_x be equal to 1 on one of the two vertex classes of the bipartite graph, -1 on the other vertex class. We have

$$\sum_x s_x b_{xe} = 0. \tag{3.5}$$

This is the only linear dependence of the b_{xe} , therefore $\{b_{xe}, x \in V \setminus \{x_0\}\}$ is a set of

linearly independent vectors for any x_0 and thus a basis. With

$$b_{x\sigma}^\dagger = \sum_e b_{xe} c_{e\sigma}^\dagger \quad (3.6)$$

we have up to a normalizing constant

$$|\Omega\rangle = P_d \prod_{x \neq x_0, \sigma} b_{x\sigma}^\dagger |0\rangle \quad \text{if } G \text{ is bipartite} \quad (3.7a)$$

and

$$|\Omega\rangle = P_d \prod_{x, \sigma} b_{x\sigma}^\dagger |0\rangle \quad \text{if } G \text{ is non-bipartite.} \quad (3.7b)$$

This representation is used to formulate the first and the second sufficient condition for $|\Omega\rangle \neq 0$.

Theorem 1. If G is bipartite and has a connected, k -regular spanning subgraph H , $k \geq 4$, $|\Omega\rangle$ does not vanish and is thus a ground state of the Hamiltonian H_∞ on $L(G)$.

Proof. If H is k -regular and bipartite, $c(H) = k$ (see e.g. [9, ch V, section 2]). This means that the edges of H may be coloured with k different colours. Let E_i , $i = 1, \dots, k$, be the corresponding edge classes. Each of these classes contains $|E|/k = |V|/2$ edges. Let now $E_+ = E_1 \cup (E_2 \setminus \{e \in E, e \text{ incident to } x_0\})$, $E_- = E_3 \cup (E_4 \setminus \{e \in E, e \text{ incident to } x_0\})$. $|E_+| = |E_-| = |V| - 1$. Then we define

$$|E_+, E_-\rangle = \prod_{e \in E_+} c_{e+}^\dagger \prod_{e \in E_-} c_{e-}^\dagger |0\rangle. \quad (3.8)$$

$|E_+, E_-\rangle$ contains no doubly occupied site and we have

$$\langle \Omega | E_+, E_- \rangle \neq 0. \quad (3.9)$$

Consequently, $|\Omega\rangle$ does not vanish.

Similarly we obtain:

Theorem 2. Let G have a non-bipartite k -regular spanning subgraph H with $c(H) = k \geq 4$. Then $|\Omega\rangle$ does not vanish and is a ground state of H_∞ on $L(G)$.

Examples of graphs that fall into these classes are k -regular bipartite graphs, $k \geq 4$, e.g. the square lattice with periodic boundary conditions, all periods being even, and the cubic or hypercubic lattices in $d \geq 3$ with periodic boundary conditions. If one of the periods is odd the hypercubic lattice is non-bipartite and theorem 2 applies. This special case has already been shown by Brandt and Giesekeus. The line graph of the square lattice is a two-dimensional lattice of tetrahedra, connected at the vertices such that each vertex belongs to exactly two tetrahedra. Another example is the diamond lattice with periodic boundary conditions (again all periods even), its line graph is the lattice of the octahedral sites of a spinel (see e.g. [10]). It may be viewed as a lattice of tetrahedra connected as described above, the centres of the tetrahedra forming the diamond lattice.

There is another sufficient condition for bipartite graphs.

Theorem 3. Let G be a bipartite graph. If G has two edge-disjoint spanning trees, $|\Omega\rangle$ does not vanish and is a ground state of H_∞ on $L(G)$.

Proof. If G is bipartite, each edge of G may be assumed to be oriented from V_1 to V_2 , which are the two vertex classes of G . The matrix $S = \text{diag}(s_x)$ has s_x as its diagonal entries, all the other entries are vanishing. Let T be a spanning tree of G and let $e = (x, y)$ be an edge of T . Then, for fixed $e = (x, y)$, let V_x (V_y) be the set of vertices of T that may be reached from x (y) without passing the edge e . Now, let $d_e(e') = 1$ if e' connects a vertex of V_x with a vertex of V_y and is oriented from V_x to V_y ; $d_e(e') = -1$ if e' connects a vertex of V_x with a vertex of V_y and is oriented from V_y to V_x ; $d_e(e') = 0$ otherwise. The set $D_T = \{d_e(e'), e \text{ is an edge of } T\}$ is the basis of the so-called cutspace of G (see e.g. [9]). The cutspace is the complement of the kernel of $SB(G)$, which is the kernel of $B(G)$. D_T is therefore a basis of the image of B^\dagger . Given two edge-disjoint spanning trees T_+ and T_- , we may introduce

$$d_{e\sigma}^\dagger = \sum_{f \in E} d_e(f) c_{f\sigma}^\dagger \quad e \text{ an edge of } T_\sigma. \tag{3.10}$$

Up to a normalizing constant we have

$$|\Omega\rangle = P_d \prod_{e \in T_+} d_{e+}^\dagger \prod_{e \in T_-} d_{e-}^\dagger |0\rangle. \tag{3.11}$$

On the other hand, let

$$|T_+, T_-\rangle = \prod_{e \in T_+} c_{e+}^\dagger \prod_{e \in T_-} c_{e-}^\dagger |0\rangle. \tag{3.12}$$

$|T_+, T_-\rangle$ contains no doubly occupied site. Now

$$\langle \Omega | T_+, T_- \rangle \neq 0. \tag{3.13}$$

Consequently, $|\Omega\rangle$ does not vanish.

A corresponding result for non-bipartite graphs is not true. It is possible to construct all bipartite graphs with two edge-disjoint spanning trees. First, let us notice that we may add an edge to a bipartite graph G such that the new graph is still bipartite. If G has two edge-disjoint spanning trees, the same is true for the new graph. Therefore it is sufficient to start from minimal graphs with two edge-disjoint spanning trees. If an edge is deleted from such a graph, it no longer has two edge-disjoint spanning trees. Each minimal graph with two edge-disjoint spanning trees may be obtained from the union of two trees that have the same vertex set. On the other hand, given a bipartite graph G , the existence of two edge-disjoint spanning trees is not obvious. It may be shown that a cubic lattice in dimension $d \geq 2$ with periodic boundary conditions has two edge-disjoint spanning trees. But it is not clear whether or not each k -regular, bipartite graph ($k \geq 4$) has two edge-disjoint spanning trees.

The results obtained so far may be somewhat generalized. Instead of $|\Omega\rangle$, we may take the state

$$|\Omega_F\rangle = P_d \prod_{\substack{\sigma, i \\ t_i < -2t}} \Phi_{i\sigma}^\dagger |F\rangle \tag{3.14}$$

where $|F\rangle$ is a state with some electrons in the single-particle states, which are eigenstates of T with the eigenvalue $-2t$. In our cases, these states are elements of the kernel of B . The kernel of B is called the cycle space of G , in fact, if a given cycle contains the edges e_1, e_2, \dots, e_n (n even), the vector $\Sigma(-1)^i e_i$ is an element of the kernel of B [6]. The conditions in the theorems above are such that each edge of G is contained in a cycle. Let E_0 be the subset of the edges of G not contained in E_+ or E_- in (3.8) or in

T_+ or T_- in (3.12). We choose $|F\rangle$ as a state made up of single-particle states on cycles that contain at least one edge of E_0 and different cycles contain different edges of E_0 . As long as the number of electrons is less than $|E|$, such a state $|F\rangle$ exists. $|\Omega_F\rangle$ does not vanish and is a ground state of H_∞ , if $|\Omega\rangle$ does not vanish. It is clear that $|\Omega_F\rangle$ contains more electrons than $|\Omega\rangle$. Since the product in (3.14) is a product of singlets, the spin of $|\Omega_F\rangle$ is the spin of $|F\rangle$, $|\Omega\rangle$ has a spin 0. Let N_0 be the number of electrons in $|\Omega\rangle$, $N < |E|$ the number of electrons in $|\Omega_F\rangle$. $|F\rangle$ has $N - N_0$ electrons and may have any spin $S \leq \frac{1}{2}(N - N_0)$.

4. Conclusions

We have shown that exact ground states of the Hubbard model with $U = \infty$ and $t < 0$ on line graphs may be obtained under several conditions. The most important examples of lattices which satisfy these conditions are line graphs of bipartite lattices with valency $k \geq 4$. In this case the ground-state energy is $E = -4|t|(N_s - N)$ if $N_s \geq N \geq N_0 = 4N_s/k - 2$. Unfortunately we were not able to show whether the ground state is unique if $N = N_0$, but it is degenerate if $N > N_0$. We obtained ground states for all spins $S \leq \frac{1}{2}(N - N_0)$. If $k > 4$, some of these states have an extensive spin. Nevertheless, due to the degeneracy of the ground state, the behaviour of the system is paramagnetic.

We may contrast the result obtained in this paper with known results for the Hubbard model at $U = \infty$ and $t > 0$. In this case, on the same lattices the theorem of Nagaoka is valid [3] and we have a unique (up to the $(2S + 1)$ -fold degeneracy due to the spin symmetry) ferromagnetic ground state if $N = N_s - 1$. Furthermore, we have a ferromagnetic ground state if $N \leq N_1 = (k - 2)N_s/k - 1$. The ferromagnetic ground state is unique if $N = N_1$ [7]. To our knowledge, this is the first case where, for the same model but in a different parameter regime, the existence of ferromagnetic and paramagnetic ground states has been rigorously proven. Unfortunately nothing is known about excited states or about the behaviour at non-zero temperatures.

It is perhaps interesting to see that for large k , or high space dimension (for a review see [11, 12]), where N_0 tends to 0 or N_1 tends to N_s , the ground-state energy and the ground states on the line graphs (of e.g. hypercubic lattices) are determined for almost all densities. But in contrast to the usual hypercubic lattices, it is not possible to find a scaling of t with some power of k such that the density of states for the non-interacting case is well defined and non-trivial. The limit of infinite dimension cannot be discussed for line graphs.

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