Pair formation of hard core bosons in flat band systems

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Hard core bosons in a large class of one or two dimensional flat band systems have an upper critical density, below which the ground states can be described completely. At the critical density, the ground states are Wigner crystals. If one adds a particle to the system at the critical density, the ground state and the low lying multi particle states of the system can be described as a Wigner crystal with an additional pair of particles. The energy band for the pair is separated from the rest of the multi-particle spectrum. The proofs use a Gerschgorin type of argument for block diagonally dominant matrices. In certain one-dimensional or tree-like structures one can show that the pair is localised, for example in the chequerboard chain. For this one-dimensional system with periodic boundary condition the energy band for the pair is flat, the pair is localised.

1 Introduction

Strongly correlated bosons on lattices have attracted lots of interest in the past few years. One of the main reasons is the recent experimental progress to study such systems in optical lattices, see [9, 1, 2] and the references therein. Theoretically, interacting bosons on a lattice are described by the Hubbard model, proposed first to describe correlated fermions in condensed matter theory [12, 13, 11]. Even before it was used in theoretical chemistry to study correlated π-electron systems [23, 20]. The bosonic Hubbard model was to our knowledge first introduced by Fisher et al. [8]. It is expected to show a rich phase diagram including a Mott insulator and a superfluid phase.

It is well accepted that in the bosonic Hubbard model repulsively bound pairs occur [34, 24]. They appear for a sufficiently strong repulsive interaction as dynamically stable excited states. More recently, pair formation was proposed in the ground state of the bosonic Hubbard model in some special one-dimensional lattice structures [29, 32, 25, 27, 10, 6]. The pair formation occurring here is a collective effect and is caused by the interplay between the repulsive interaction and the movement of the particles in these lattice structures. The common feature of these one-dimensional lattices is that they have a flat band at the bottom of the single particle spectrum.

In the present paper we give a rigorous proof for pair formation in a large class of flat band structures. The class contains as examples the chequerboard chain [27, 6] and its two-dimensional analogue, the chequerboard lattice. To our knowledge this is the first proof of pair formation in two-dimensional lattice structures with flat bands. But the results are more general. The class contains infinitely many different structures, also including tree-like or fractal structures; examples for the latter are line graphs of some

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Vicsek fractals or Sierpinsky carpets (see e.g. [4] and the references therein). The definition of the class uses some graph theoretical conditions which we introduce later.

Whereas the bosonic Hubbard model with flat bands has been studied only recently, the fermionic case has been investigated since 1989, starting with a pioneering work by Lieb [16]. Many rigorous results have been obtained, for a review see [17, 31, 21] and the references therein. Flat band models are of special interest since in a flat band a very small interaction can yield strong correlation effects. Independent of the work on the Hubbard model, flat bands have been studied as well in spin systems, see e.g. [28, 5] and the references therein. Standard examples of flat band systems are the kagomé lattice or the chequerboard lattice in two dimensions or similar analogues in one dimension. But the class of models with flat bands is very large and such lattices can be constructed in any dimension. Experimentally, it is possible to build flat band systems using e.g. optical lattices [14] or exciton-polaritons [18].

For bosons at low temperature, one is interested in flat band systems where the flat band is the lowest band in the single particle spectrum. There are two main classes of flat band systems with that property: Line graphs of bipartite graphs, see e.g. [19, 20], which have no gap between the flat band and the rest of the single particle spectrum, and other decorated lattices, e.g. the ones proposed by Tasaki [30], which often have a gap between the flat band and the rest of the spectrum. If one is interested in obtaining rigorous results, the existence of a gap often simplifies the proofs. In the present paper we introduce a class of models which interpolate between these two cases. We investigate line graphs with modified hoppings. In these models the hopping is reduced on a subset of the edges. On one subset it is $t'$ with $0 < t' \leq t$. The models still have a lowest flat band for all $t'$. A detailed description is given below. The important point here is that the model contains a tunable parameter $t'$. The lattices have a gap above the lowest flat band for sufficiently small $t'$ and no gap for $t' = t$.

Whereas for fermionic systems, many rigorous results are available, rigorous results for bosons in flat band systems are rare. For line graphs of two-connected, bipartite plane graphs, Motruk et al. [22] showed that below a critical density the multi particle ground states of the bosonic Hubbard model with repulsive interaction can be completely classified. At the critical density, the bosons form a Wigner crystal, a fact which was already mentioned in [13] for few special lattices of this class like the kagomé lattice. To our knowledge, there are up to now no general rigorous results above the critical density for this class of lattices. The aim of the present paper is to start filling this gap. We investigate what happens if one adds one additional particle to the system. Further, we take the limit of a hard core repulsion between the particles, since for weak interaction pair formation is not expected [13]. Technically, the hard core repulsion reduces the Hilbert space dimension and thereby simplifies the proofs. We show rigorously that in the flat band systems of our class a pair is formed if one adds one particle. The pair states form a band that is separated from the rest of the spectrum. In special one-dimensional lattices or tree-like structures, the pair is localised and the effective band is flat except at the boundary. Whether this true for other lattices or in higher dimensions remains open.

The interesting case, namely the one where $t' = t$ or at least close to $t$ cannot be reached with the approach used here. We need a small but finite value for $t'/t$. Nevertheless, we believe that our model is helpful for a better understanding of the pair formation at larger values of $t'$, eventually also for $t' = t$. To support that view we compare our results with other findings for the class of lattices discussed here, esp. those from [6].

The paper is organised as follows. In the next section we provide, simply for illustrational purpose, a simple example, which we use to explain the basic concepts and ideas and the main results. In Sect. 3 we define the class of graphs we discuss and the model. We also present some basic results which are valid at or below the critical density, based on the rigorous work in [22]. In Sect. 4 we discuss the lower part of the spectrum for a particle number of one particle above the critical density. The proof is based on a Gerschgorin type of argument. In Sect. 5 we use this result to prove some properties of the corresponding eigenstates. It is shown that the low lying eigenstates are linear combinations of localised pair states. A
subclass of one-dimensional or tree-like systems have a local reflection symmetry. For those, the low lying eigenstates are degenerate except at the boundaries of the system and contain a localised pair. In the last section, we discuss possible generalisations of our results.

2 A simple example: the chequerboard chain

The present section explains the basic concepts used in the following sections within a simple example, the chequerboard chain. The class of lattices we construct later is quite large, the chequerboard chain is the most simple example. It is depicted in Fig. 1. It consist of cycles, shown with solid lines in the figure, and additional lines shown as dashed lines connecting neighboured cycles.

We consider a tight binding model on this lattice with hopping matrix elements $t$ on the edges belonging to a cycle and $t'$ on the edges connecting two cycles. We denote the lattice sites by $e, e'$. The Hamiltonian of a single particle moving on this lattice has the form

$$H_1 = \sum_{\{e, e'\}} t_{ee'} b_{e}^\dagger b_{e'}.$$  \hfill (1)

where

$$t_{ee'} = \begin{cases} t & \text{if } e, e' \text{ are connected by a line on a cycle;} \\ t' & \text{if } e, e' \text{ are connected by a line between two cycles;} \\ 0 & \text{otherwise} \end{cases}$$

We let $t \geq t' > 0$. Consider now a single particle state $\psi_C$ which is strictly localised to a single cycle $C$, i.e. $\psi_{C,e} = 0$ if the site $e$ does not belong to $C$. For sites $e$ on $C$ the modulus of $\psi_{C,e}$ shall be the same on all sites and the sign shall alternate. It is easy to see that this state is an eigenstate of $H$ with the eigenvalue $-2t$. Take a site $e''$ on a neighbouring cycle. It is always connected to two sites on $C$. Denote the two sites $e$ and $e'$, the hopping yields a contribution $t'(\psi_{C,e} + \psi_{C,e'})$ to this site. Since by definition, $\psi_{C,e}$ and $\psi_{C,e'}$ have the same modulus but opposite sign, the contribution vanishes. Therefore $H\psi_C$ vanishes on lattice sites outside $C$. On $C$, a factor $-2t$ is picked up. Since this construction is possible for each cycle of the lattice, the eigenvalue $-2t$ of $H_1$ is highly degenerate. The degeneracy is the number of cycles, which is one quarter of the number of lattice sites. One can show, this will be done in Sect. 3.3, that $-2t$ is the ground state of $H_1$. Since the lattice has four lattice sites in a unit cell, the energy spectrum consists of four bands. The lowest band contains the degenerate eigenvalues $-2t$, it is flat.

Note that the chequerboard chain has a local reflection symmetry. A reflection of the cycle $C$ which exchanges the upper and lower vertices does not change the Hamiltonian. This was already mentioned and used in [6]. We do not use this local reflection symmetry in our proofs since it is a special property of the chequerboard chain and some treelike structures we mention later.

For $t' = 0$, the Hamiltonian $H_1$ consists of disconnected cycles. For each cycle, the eigenvalues are $-2t$, 0 (twofold degenerate), and $2t$. Turning on $t'$, the coupling of the cycles lifts the degeneracy in the upper
three bands whereas due to the special structure of the hopping the lowest band remains flat. As long as \( t' < t \), there is a gap between the lowest band and the other three bands. The gap closes for \( t' = t \).

Let us now move to the multi-particle problem by adding a local repulsive interaction \( U \) to the Hamiltonian. The particles shall be bosons. The Hamiltonian is

\[
H = \sum_{\{e,e'\}} t_{ee'} b^\dagger_e b_{e'} + U \sum_e n_e (n_e - 1).
\]  

(2)

For a sufficiently low density of bosons, we can construct multi-particle ground states simply by putting at most one particle on each cycle \( C \) into the single particle state \( \psi_C \) of the lowest flat band. Such a state is clearly a ground state of the hopping part of the Hamiltonian, since all particles are sitting in single particle ground states. It minimises also the interaction, because no site \( e \) contains more than one particle. One can show, this was done in \([22]\) for a more general class of lattices, that the eigenstates constructed that way form a basis of the ground state space of \( H \) when the number of particles is less or equal to the number of sites. For the present example this is almost trivial.

The question we want to answer in this paper is what happens if we add an additional particle to the system so that the number of particles exceed the number of cycles by one. Since the particles are bosons, we can put the additional particle in one of the states \( \psi_C \) and thereby minimise the hopping part of the Hamiltonian. It is clear that thereby we generate a multi-particle state with doubly occupied sites and the interaction becomes important. We can also spread the additional particle on all sites. This lowers the interaction energy but increases the hopping energy. A third possibility is to put a pair of particles on the same cycle in such a way that they avoid each other. Then, the interaction energy of the multi-particle state would be zero but the hopping energy would be higher. This is the favourable option if the interaction energy is large. But it is clear that due to the presence of \( t' \) this is not an exact multi-particle eigenstate of \( H \). The question is therefore: Can we characterise the multi-particle ground states of \( H \) for large \( U \).

Our main result, the proof is given in Sect. \([4]\) states that for sufficiently small \( t' \) the low lying multi-particle states contain indeed a localised pair of bosons. The pair is mainly localised on a cycle, but not strictly localised. For the chequeboard chain with periodic boundary conditions, the local reflection symmetry mentioned above together with the translational invariance guaranties that the multi-particle ground state is degenerate. The degeneracy is the number of cycles. It can be understood as the original ground state, in which the added particle forms a pair with one of the other particles. The pair states are degenerate and can be interpreted as an effective flat band for the pair. This was already discussed in \([6]\) based on numerical calculations.

For the proof, we use the limit of a hard core repulsion \( U \to \infty \). Further, for the proof we need a sufficiently small \( t' \). But we expect our result to be true for all \( t' \leq t \). This is supported by the numerical results in \([6]\).

We now proceed as follows. The next section contains a complete description of the class of lattices the chequeboard chain is an example of. We use a graph theoretical language to construct this class. We also state the basic results for the case where the number of particles is less or equal to the maximal number which was the number of cycles in our example. The remaining part of the paper is about the low lying part of the spectrum and the properties of the corresponding eigenstates we obtain when we add a particle. The physical picture is exactly the one proposed above. The additional particle forms a pair with one of the other particles and the two avoid each other because of the hard core interaction. The effective pair state is localised, but not strictly localised.

For the proofs we use a Gerschgorin type argument. The generalised Gerschgorin theorem we use makes a statement about a matrix with a block structure where the off-diagonal blocks are sufficiently small. It can be applied if there is a gap between the ground state and the rest of the spectrum. If the off-diagonal part is small enough, the gap remains finite. This is the case if \( t' \) is small.
3 Definition of the model and basic properties

We consider hard core bosons on a class of graphs which form a subclass of line graphs of planar graphs. To define the class of lattices we require some basic notions of graph theory that can be found in the introductory chapters of the books of Bolobas [3] and Voss [33]. The same construction has been used for fermionic Hubbard models in [19, 20], where more details are presented. A graph can be drawn as a set of points, called vertices, and a set of lines, called edges, connecting vertices. A graph is uniquely defined by the vertex set and the edge set.

3.1 The class of lattices

Let \( G = (V(G), E(G)) \) be a graph with a vertex set \( V(G) \) and an edge set \( E(G) \). An edge \( e \in E(G) \) is a subset of \( V(G) \) with exactly two elements, the two vertices connected by the edge. We consider finite graphs, \( V(G) \) is a finite set.

A walk of length \( n \) is a sequence \( w = (e_1, e_2, \ldots, e_n) \) of edges \( e_i \in E(G) \) where subsequent edges have exactly one vertex in common, i.e. \( |e_i \cap e_{i+1}| = 1 \) for all \( i = 1, \ldots, n-1 \) and \( e_i \cap e_{i+1} \cap e_{i+2} = \emptyset \) for all \( i = 1, \ldots, n-2 \). The first condition also excludes that two subsequent edges are the same. The second condition assures that the walk passes through the edge, i.e. the preceding edge connects to one vertex of the edge, the succeeding edge connects to the second vertex. A path is a self-avoiding walk which means that no edge is passed more than once by the path, i.e. \( e_i \neq e_j \) for \( i \neq j \). Vertices can be met more than once by a path. A path which is closed, i.e. \( |e_1 \cap e_n| = 1 \) is called a cycle.

The graph \( G \) shall be a planar graph, which means that it can be drawn in a plane in such a way that no two edges intersect. If, in the plane representation of \( G \), we omit all edges and vertices from the plane, the plane is decomposed into connected components called faces. For a finite graph, there is exactly one unbounded face. Let \( F(G) \) be set of bounded faces of the graph. Due to Euler’s theorem, \( |F(G)| = |E(G)| - |V(G)| + 1 \).

By \( C \in F(G) \) we denote a face and also the boundary of that face. This is clearly possible since each face has a unique boundary. The boundary \( C \) is a cycle. If a cycle is the boundary of a face we also call it an elementary cycle. Each elementary cycle \( C \in F(G) \) itself is a subgraph of \( G \) and we denote the vertex set and the edge set of \( C \) by \( V(C) \) and \( E(C) \) respectively.

Further, we assume that \( G \) is two-connected and bipartite. Two-connected means that the graph remains connected, i.e. does not fall into two unconnected parts, if an arbitrary edge is removed from \( E(G) \). In other words, each edge belongs to a cycle \( C \). Bipartite means that \( V(G) = V_1 \cup V_2 \) with \( V_1 \cap V_2 = \emptyset \) and \( |e \cap V_i| = 1 \) for all \( e \in E(G) \) and \( i = 1, 2 \). If two vertices are connected by an edge, they are not in the same subset. In a bipartite graph, all cycles are of even length.

Let us consider colourings of the faces \( F(G) \). Note that the colouring of the faces of \( G \) is equivalent to the vertex colouring of the dual graph of \( G \), see [3] for details on colourings. Two faces \( C \) and \( C' \) can be coloured with the same colour if they have no edge in common, \( E(C) \cap E(C') = \emptyset \). \( \chi(G) \) is the chromatic number, it is the minimal number of colours needed to colour the faces of \( G \). Since \( G \) is planar, \( \chi(G) \leq 4 \), at most four colours are needed. Let \( F_1(G) \subseteq F(G) \) be the largest set of faces that can be coloured with one colour. If there are several sets of the same size, \( F_1(G) \) shall be one of them. Let \( E_1(G) = \cup_{C \in F_1(G)} E(C) \subseteq E(G) \) be the set of edges contained in the cycles of \( F_1(G) \). By \( G_1 \) we denote the graph obtained by collecting all the vertices and edges from all the cycles \( C \) in \( F(G) \), regarding vertices from different cycles \( C \) as distinct even when they correspond to a single vertex in \( G \). Note that \( E(G_1) = E_1(G) \) since each edge in \( E_1(G) \) belongs to exactly one cycle. Note that \( V(G_1) \neq \cup_{C \in F_1(G)} V(C) \) since two cycles in \( G \) may contain the same vertex in \( V(G) \) but not in \( V(G_1) \).

If the faces of \( G \) including the unbounded one can be coloured by two colours, each edge of \( G \) belongs to exactly one cycle \( C \in F_1(G) \) and therefore \( E_1(G) = E(G) \). Otherwise, \( E(G) \setminus E_1(G) \) is not empty. The
elements of $E(G) \setminus E_1(G)$ are called interstitials. If the faces in $F_1(G)$ can be coloured with two colours, interstitials appear only at the boundary of $G$. Otherwise, interstitials may be everywhere in $G$.

The set of graphs we deal with are line graphs of bipartite planar graphs. The line graph $L(G) = (V(L(G)), E(L(G)))$ of $G$ is constructed as follows: $V(L(G)) = E(G)$, $E(L(G)) = \{\{e, e'\} : e, e' \in E(G) \text{ and } |e \cap e'| = 1\}$. To draw the line graph, we put a new vertex onto each edge of the original graph and we connect two new vertices by a new edge, if the corresponding old edges have a vertex in common. Note that although the original graph $G$ shall be planar, $L(G)$ is not necessarily planar. We illustrate the construction below using an example where $L(G)$ is not planar.

We also need the line graph $L(G_1)$ of $G_1$. Since $G_1$ consists of unconnected cycles, $G_1$ and $L(G_1)$ are isomorphic.

The construction is illustrated in Fig. 2. On the left the graph $G$ with its set of bounded faces $F(G) = \{C_1, C_2, C_3, C_4, C_5\}$ is shown. Each $C_i$ is an elementary cycle. The faces including the outer face can be coloured with two colours. We have $F_1(G) = \{C_1, C_2, C_4, C_5\}$. $L(G_1)$ on the right hand side consists of the disconnected cycles $C_1, C_2, C_4, C_5$ of $L(G)$. $L(G_1)$ has the same vertex set as $L(G)$. There are no interstitials in this example. It becomes clear that even though $G$ is a planar graph, $L(G)$ in this example is not a planar graph. Whenever $G$ has a vertex with coordination number larger than 3, the line graph $L(G)$ contains a complete graph $K_4$ as a subgraph, which is not planar. For our construction we only need that $G$ is planar.

Any bipartite connected planar graph can be used as a starting point. Therefore, the class of line graphs we are looking at is large. It contains some well known examples, for instance the kagomé lattice and the chequerboard lattice. The latter is the line graph of the square lattice. For the square lattice, two colours are enough to colour the bounded faces $F(G)$. Possibly except for some edges at the boundary, every edge in $E(G)$ belongs to a cycle in $F_1(G)$. The example $G$ depicted in Fig. 2 is a cutout of the square lattice. For the honeycomb lattice, three colours are needed and as a consequence there is a large number of interstitials. The kagomé lattice is the line graph of the honeycomb lattice.

### 3.2 The Hamiltonian

The Hamiltonian of the bosonic Hubbard model on $L(G)$ is defined as

$$H = \sum_{\{e, e'\} \in E(L(G))} t_{ee'} b^\dagger_e b_{e'} + \sum_{e \in V(L(G))} U_e n_e (n_e - 1).$$

We denote the vertices of the line graph $L(G)$ by $e, e'$ because they are the edges of the original graph $G$. We use the usual notation with creation operators $b^\dagger_e$ and annihilation operators $b_e$ for bosons on the lattice sites $e \in V(L(G)) = E(G)$ with the usual bosonic commutation relations $[b_e, b_{e'}] = [b^\dagger_e, b^\dagger_{e'}] = 0$.
Figure 3: The hoppings for the example in Fig. 2.

The hoppings are defined as follows:
\[ t_{ee'} = \begin{cases} 
  t & \text{if } \{e, e'\} \in E(L(G)) \\
  t' & \text{if } \{e, e'\} \in E(L(G)) \setminus E(L(G_1)) \\
  0 & \text{otherwise} 
\end{cases} \quad (5) \]

and we assume \( t \geq t' > 0 \). Fig. 3 illustrates the hoppings for the line graph from Fig. 2.

The case \( t = t' \) is the usual nearest neighbour hopping on \( L(G) \). The model with \( t = t' \) has been treated e.g. in [22]. With this definition of the hopping matrix we write the Hamiltonian in the form
\[ H = tP_{\leq 1} \sum_{C \in F_1(G)} H_C P_{\leq 1} + t'P_{\leq 1} \sum_{C \neq C' \in F_1(G)} H_{C, C'} P_{\leq 1} + t'P_{\leq 1} H'P_{\leq 1}. \quad (6) \]

The first part is the Hamiltonian on \( L(G_1) \). \( H_C \) contains the hopping on the edges of \( C \in F_1(G) \) with amplitude 1. \( H_{C, C'} \) contains the hoppings from \( C' \) to \( C \) on the edges connecting the two cycles, also with amplitude 1. \( H' \) is only present if there are interstitials, it contains all hoppings on paths from some \( C \) to some other \( C' \) which contain exactly one vertex in \( C \), one vertex in \( C' \) and one or more interstitials, again with amplitude \( t' \).

3.3 Basic properties

To state some basic properties of the model, we introduce few matrices often used in graph theory. The most important is the adjacency matrix \( A(G) = (a_{xy})_{x, y \in V(G)} \) where \( a_{xy} = 1 \) if \( \{x, y\} \in E(G) \), \( a_{xy} = 0 \) otherwise. A second important matrix is the vertex-edge incidence matrix \( B(G) = (b_{xe})_{x \in V(G), e \in E(G)} \)
where \( b_{x e} = 1 \) if \( x \in e \), \( b_{x e} = 0 \) otherwise. The adjacency matrix of \( L(G) \) is \( A(L(G)) = B(G)^t B(G) - 2 \). Since \( B(G)^t B(G) \) is positive semi-definite, \( A(L(G)) \) is bounded from below by \(-2\). The eigenstates of \( A(L(G)) \) with eigenvalue \(-2\) are the elements of the kernel of \( B(G) \). They can be constructed as follows.

Each bounded face \( C \in F(G) \) is bounded by a cycle of even length. The cycle \( C \) can be oriented clockwise. Since \( G \) is bipartite, each edge of \( G \) can be oriented to point from one of the two disjoint subsets of \( V(G) \) to the other, e.g. from \( V_1 \) to \( V_2 \). Now let \( v_C = (v_{C e})_{e \in E(G)} \) be defined for a face \( C \) of \( G \) as follows: \( v_{C e} = 1 \) if \( e \in C \) and \( e \) and \( C \) have the same orientation, \( v_{C e} = -1 \) if \( e \in C \) and \( e \) and \( C \) have the opposite orientation, \( v_{C e} = 0 \) otherwise. It is easy to see that the \( v_C \) form a basis of the kernel of \( B(G) \), see e.g. \cite{19}. Since by assumption \( |F(G)| > 0 \), the kernel of \( B(G) \) is not empty. We introduce the creation operator \( b_C^+ = \frac{1}{\sqrt{|C|}} \sum_{e \in E(C)} v_{C e} b_e^+ \) and the corresponding annihilation operator \( b_C = \frac{1}{\sqrt{|C|}} \sum_{e \in E(C)} v_{C e} b_e \).

**Proposition.** For \( t \geq t' > 0 \) the ground state eigenvalue of the single particle Hamiltonian is \(-2t\) and is \( |F(G)|\)-fold degenerate. The ground states are \( v_C \) and their eigenvalues do not depend on \( t' \).

**Proof.** We have \( H + 2t = t'(\sum_C H_C + \sum_{C,C'} H_{C,C'} + H' + 2) + (t - t')(\sum_C H_C + 2) \). The first part is, for a single particle, just \( t'(A(L(G)) + 2) \geq 0 \). The second part is non-negative as well and is \((t - t')(A(L(\bigcup_{C \in F_1(G)} C)) + 2) \). Both are adjacency matrices of line graphs and \( F(\bigcup_{C \in F_1(G)} C) \subseteq F(G) \). The states \( v_C \) minimise both parts and are the only states that minimise the second part. Thus, by a simple variational argument, those states are the only single particle ground states of \( H \).

**Remarks.** The creation operators \( b_C^+ \) and the annihilation operators \( b_C \) commute with \( H_{C,C'} \) and with \( H' \). They do not commute with \( P_{\leq 1}(\sum_{C,C'} H_{C,C'} + H') P_{\leq 1} \).

For \( t \geq t' > 0 \), both parts of \( H + 2t \) are positive semi-definite. Therefore, the eigenvalues of \( H + 2t \) are monotonously increasing functions of \( t' \) and \( t' > t \). They are not monotonously increasing functions of \( t' \) for fixed \( t \).

For small values of \( t' \) the eigenvalue \(-2t\) is separated from the rest of the single particle spectrum by a gap if \( G \) is a sufficiently large lattice. For \( t' = t \), there is no gap.

**Proposition.** For \( t > t' > 0 \) and \( N \leq |F_1(G)| \), the ground states of \( H \) are the same as the ones for \( t' = 0 \) and the ground state energy is \(-2tN\).

**Proof.** Let \( H + 2tN = t'P_{\leq 1}(\sum_C H_C + \sum_{C,C'} H_{C,C'} + H' + 2N) P_{\leq 1} + (t - t')P_{\leq 1}(\sum_C H_C + 2N) P_{\leq 1} \). As before, the two parts are positive semi-definite. Again, we use a simple variational argument. This first part describes hard core bosons on \( L(G) \) with the hopping \( t' > 0 \). For this part, the result in \cite{22} applies. The second part describes hard core bosons on \( L(\bigcup_{C \in F_1(G)} C) \). Each of the cycles is disconnected from the others, the ground states are obtained by putting at most one particle in a state \( v_C \). Since \( N \leq |F_1(G)| \), this is possible. These states form a subset of the ground states of the first part and are the only states which minimise the second part. Therefore, they are the only ground states of \( H + 2tN \) with eigenvalue \( 0 \). Since they can be obtained by acting with a product of \( b_C^+ \) on the vacuum, they do not depend on \( t' \).

**Remark.** We exclude \( t' = t \) here because in that case the Hamiltonian may have more ground states than the Hamiltonian for \( t' = 0 \), since in that case the second part of \( H + 2tN \) vanishes and all the states described in \cite{22} become ground states.

4 **Lower part of the spectrum for** \( N = |F_1(G)| + 1 \)

The results stated in Sect. \cite{3.3} show that for \( N \leq |F_1(G)| \) all ground states of the Hamiltonian can be constructed. Essentially, the results from \cite{22} carry over to the case \( t' \leq t \). For \( t' < t \), the set of ground
states is even more simple. The question is what happens for \( N > |F_1(G)| \). Clearly, all eigenvalues obey \( E \geq -2tN \).

There is no general answer to that question. The reason is the following. Consider a graph with exactly two cycles \( C_1 \) and \( C_2 \), both of length 4, and a long enough chain of interstitials between them. Let \( N = |F(G)| + 1 = 3 \). The ground states of \( HC_1 + HC_2 \) contain one particle with energy \(-2\) on one cycle and two particles on the other one. The lowest energy of two hard core bosons on a cycle with length 4 is \(-2\sqrt{2}\). Consider now the full Hamiltonian. We can construct a variational state which contains one particle in each cycle with energy \(-2t\) and one on the chain. For a very long chain, the lowest energy for a particle on that chain comes close to \(-2t'\). For \( t' > (\sqrt{2} - 1)t \) it therefore becomes favourable to put the additional particle on the interstitials. A second point are long cycles. If a cycle is very long, it is possible to put two particles on it with only a very small loss of energy. Further, the energies lie very close to each other.

Therefore, we first restrict ourselves to a class of graphs without interstitials and where all cycles \( C \in F_1(G) \) have length 4. The chequerboard lattice and the chequerboard chain fall into this class. Generalisations are discussed in Sect. 6.

On a cycle with length 4 it is easy to construct all eigenstates with arbitrary particle number between 0 and 4. Since there are only few different eigenvalues, the eigenstates of \( H \) in \([1]\) with \( N > |F_1(G)| \) are highly degenerate for \( t' = 0 \). For a finite \( t' \), the degeneracy may split and the states will mix. As a consequence, even for very small \( t' > 0 \) it may be difficult to tell how the spectrum looks like. In the present case, due to the special structure of the lattice and the fact that \( b_C^\dagger \) commute with \( H_{C,O} \), it is possible to make use of a variant of Gerschgorin’s theorem to describe the lower part of the spectrum.

**Theorem 1** Let \( G \) be a connected bipartite planar graph with \( \cup_{C \in F_1(G)} E(C) = E(G) \) and \( |C| = 4 \) for all \( C \in F_1(G) \). Additionally we assume that all edges of \( G \) belong to a cycle \( C \in F_1(G) \). The Hamiltonian \( H \) in \([4]\) with \( N = |F_1(G)| + 1 \) hard core bosons on \( L(G) \) has exactly \( |F_1(G)| \) eigenstates with an energy at or below \(-2t(|F_1(G)| - 1) - 2\sqrt{2}t + \frac{1}{2\sqrt{2}}c(G)t'\) for \( t' < \frac{0.14025}{c(G)}t \) where \( c(G) \) is the largest number of cycles in \( F_1(G) \) connected to some cycle of \( F_1(G) \). These eigenvalues are separated from the rest of the spectrum by a finite gap.

Note that \( c(G) \) is a local quantity. It is not proportional to the number of lattice sites. For the chequerboard chain in Fig. 1 and for the example in Fig. 2 we have \( c(G) = 2 \), for the chequerboard lattice, \( c(G) = 4 \), independently of the size of the lattice.

The bound for \( t' \) obtained using the Gerschgorin type of argument is far from being optimal. The reason is that the special structure of the matrix does not enter. The argument does not take into account which eigenstates for \( t' = 0 \) can be reached from one of the ground states at \( t' = 0 \). Since in a perturbational treatment of \( t' \) the first order contribution to the ground state energy vanishes and the second order yields a negative contribution, we may expect that the lowest \( |F_1(G)| \) eigenstates have an energy below \(-2t(|F_1(G)| - 1) - 2\sqrt{2}t\). This is confirmed by the numerical or variational results in \([27, 6]\) for special lattices. Further, the class of graphs is still quite large. For special graphs in this class, e.g. the chequerboard chain in one dimension or the chequerboard lattice in two dimensions numerical results suggest that the result is even true for \( t' = t \).

Note that we only require that the boundaries of the faces in \( F_1(G) \) have length 4. \( G \) may have faces with longer boundaries. Therefore, line graphs of Vicsek fractals and Sierpinsky carpets \([4]\) formed of squares can be treated as well provided they obey the condition that all edges of \( G \) belong to \( F_1(G) \).

If \( t' \) is smaller than the bound given in the theorem there is a gap between the Gerschgorin cycle around \(-2t(|F_1(G)| - 1) - 2\sqrt{2}t\) and the rest of the spectrum. We therefore expect that using the continuity of the eigenvalues of the Hamiltonian as a function of the parameters of the Hamiltonian, the fact that there are \( |F_1(G)| \) low lying eigenstates separated from the rest of the spectrum remains true for sufficiently large values of \( U \). The main reason is that all quantities we are dealing with are local.
4.1 Proof of Theorem 1

The eigenstates of $P_{\leq 1} \sum_{G \in F_1(G)} H_C P_{\leq 1}$ can be constructed from the eigenstates on the cycles of length 4. For one or three particles, the eigenstates on a single cycle have the eigenvalues $-2$, $0$, $2$ and $0$ is twofold degenerate. For two particles, the eigenstates on a single cycle have the eigenvalues $-2\sqrt{2}$, $0$, $2\sqrt{2}$, $0$ is fourfold degenerate. Four particles on a single cycle have the eigenvalue $0$. The eigenvalues of $P_{\leq 1} \sum_{G \in F_1(G)} H_C P_{\leq 1}$ are therefore $E(n_1, \bar{n}_1, n_2, \bar{n}_2, n_3, \bar{n}_3) = -2(n_1 + n_3 - \bar{n}_1 - \bar{n}_3) - 2\sqrt{2}(n_2 - \bar{n}_2)$. $n_i$ are the number of cycles with $i$ particles in the lowest eigenvalue and $\bar{n}_i$ are the number of cycles with $i$ particles in the highest eigenvalue. All other eigenvalues on a single cycle vanish and therefore do not contribute to the eigenvalues of $P_{\leq 1} \sum_{G} H_C P_{\leq 1}$. The numbers $n_i$, $\bar{n}_i$ are subject to the additional condition $n_1 + \bar{n}_1 + 2n_2 + 2\bar{n}_2 + 3n_3 + 3\bar{n}_3 \leq N$. We choose all these states as the basis of the Hilbert space.

We now fix the particle number to $N = |F_1(G)| + 1$. The ground states of $P_{\leq 1} \sum_{G} H_C P_{\leq 1}$ have the eigenvalue $-2(N - 2) - 2\sqrt{2}$, there are exactly $|F_1(G)|$ of them, corresponding to one doubly occupied cycle and $N - 2$ singly occupied cycles, each in its ground state. States with higher energies have less singly occupied cycles in their ground state. The second lowest eigenvalue is $-2(N - 4) - 4\sqrt{2}$. The lowest state with $N - n$ singly occupied cycles in their ground state has the eigenvalue $-2(N - n) - 2\sqrt{2}[\frac{n}{2}]$. The second lowest eigenvalue with $N - 2$ singly occupied cycles in their ground state is $-2(N - 2)$.

The idea of the proof is to use a Gerschgorin type of argument. We actually use the generalisation of the Gerschgorin circle theorem by Feingold and Varga [7]. They showed the following. Let $A_1, ..., A_N$ are square matrices acting on the subspace $\Omega_i$ of order $n_i$ and $A_{j,i}$ are $n_j \times n_i$ matrices. They show among other things that each eigenvalue $\lambda$ of $A$ satisfies

$$ (\|(A_{i,i} - \lambda I_i)^{-1}\|)^{-1} \leq \sum_{k=1, k \neq i}^{N} \|A_{i,k}\|. \quad (8) $$

for at least one $i$, $1 \leq i \leq N$. Here, $I_i$ is the unit matrix of the same dimension as $A_{i,i}$. The matrix norm $\|A_{i,j}\|$ taken here is derived from an arbitrary vector norm on the subspaces $\Omega_i$ and $\Omega_j$ by

$$ \|A_{i,j}\| = \sup_{x \in \Omega_j, x \neq 0} \frac{\|A_{i,j}x\|}{\|x\|}. \quad (9) $$

One may even choose different norms in the different subspaces $\Omega_i$. We apply this result to our Hamiltonian [7].

Let us first consider the ground states of $P_{\leq 1} \sum_{G} H_C P_{\leq 1}$. Let $p_C^\dagger$ be the creation operator of the ground state of two particles on the cycle $C$. The ground state of $P_{\leq 1} \sum_{G} H_C P_{\leq 1}$ with two particles on $C$ is

$$ \psi_C = p_C^\dagger \prod_{G \in F_1(G) \setminus \{C\}} b_G^\dagger |0\rangle. \quad (10) $$

We estimate the matrix elements of $P_{\leq 1} \sum_{G} H_{C,C'} P_{\leq 1}$ between this state and other states.

$$ p_{\leq 1} \sum_{C,C'} H_{C,C'} \psi_C = p_{\leq 1} \prod_{C' \in F_1(G) \setminus \{C\}} b_{C'}^\dagger \sum_{C} H_{C,C} P_{\leq 1} b_C^\dagger |0\rangle $$

$$ = \sum_{C} \prod_{C' \in F_1(G) \setminus \{C,C\}} b_{C'}^\dagger P_{\leq 1} b_{C}^\dagger H_{C,C} P_{\leq 1} b_C^\dagger |0\rangle. \quad (11) $$
The second expression in (11) holds because the cycles do not overlap. The state $P_{\leq 1} b_C^\dagger H_{C,\bar{C}} P_C^\dagger |0\rangle$ can easily be calculated using the explicit form of the operators $b_C^\dagger$, $p_C^\dagger$, and $H_{C,\bar{C}}$, see Fig. 4. In this representation we have

$$H_{C,\bar{C}} = (b_3^\dagger + b_5^\dagger)(b_5 + b_6),$$

(12)

$$p_C^\dagger = \frac{1}{2} (b_3^\dagger b_7^\dagger + b_6^\dagger b_8^\dagger) - \frac{1}{2\sqrt{2}} (b_3^\dagger b_6 + b_6^\dagger b_3 + b_7^\dagger b_8 + b_8^\dagger b_7),$$

(13)

and

$$b_C^\dagger = \frac{1}{2} (b_1^\dagger - b_2^\dagger + b_3^\dagger - b_4^\dagger).$$

(14)

With the explicit form of these operators we obtain

$$P_{\leq 1}[H_{C,\bar{C}}; P_C^\dagger] b_C^\dagger P_{\leq 1} = \frac{1}{2} (b_1^\dagger - b_2^\dagger)(b_3^\dagger + b_4^\dagger) \left( \frac{1}{2} (1 - \frac{1}{\sqrt{2}})(b_3^\dagger + b_4^\dagger) - \frac{1}{2\sqrt{2}}(b_5^\dagger + b_6^\dagger) \right)$$

(15)

and therefore $\|P_{\leq 1} H_{C,\bar{C}} \psi_C\|_2 / \|\psi_C\|_2 \leq (1 - 2^{-1/2})^{1/2} < 0.5412$ for the standard norm $\|.\|_2$. But we may take instead the maximum norm in the basis of the eigenstates of $P_{\leq 1} \sum_C H_CP_{\leq 1}$. The last factor on the right hand side of (15) is a sum of three generators of eigenstates of $H_C$ with one particle. The largest prefactor is $\frac{1}{2}$. The other factors yield a sum of two generators of eigenstates of $H_C$ with two particles, each with prefactor $\frac{1}{\sqrt{2}}$. Therefore we obtain

$$\|P_{\leq 1} H_{C,\bar{C}} \psi_C\|_\infty / \|\psi_C\|_\infty \leq \frac{1}{2\sqrt{2}},$$

(16)

which yields a slightly better estimate. This holds for every cycle $C$ connected to $\bar{C}$. Let $c(\bar{C})$ be the number of cycles connected to the cycle $\bar{C}$. Then we obtain

$$\|P_{\leq 1} \sum_C H_{C,\bar{C}} \psi_C\|_\infty / \|\psi_C\|_\infty < \sum_C \|P_{\leq 1} H_{C,\bar{C}} \psi_C\|_\infty / \|\psi_C\|_\infty < \frac{1}{2\sqrt{2}} c(\bar{C}).$$

(17)

Using (8) this finally yields

$$| - 2(N - 2)t - 2\sqrt{2}t - \lambda | \leq \frac{1}{2\sqrt{2}} c(G)t'$$

(18)

where $c(G) = \max_{C \in F_1(G)} c(C)$. The centre of all the intervals is the same, since the eigenvalues of $P_{\leq 1} \sum_C H_CP_{\leq 1}$ in theses states are all the same, and all the intervals are contained in the largest one, which has $c(G)$ on the right hand side.

We now construct subspaces to obtain a suitable block structure of $H$. For any subset $F \subset F_1(G)$ we introduce the subspace $\Omega_F$ which is spanned by the eigenstates of $P_{\leq 1} \sum_C H_CP_{\leq 1}$ which are not ground
states and which are of the form $\prod_{C\in F} b^\dagger_C |\psi\rangle$ where $|\psi\rangle$ is any state with $N - |F|$ particles which are distribute on the remaining cycles in $F_1(G) \setminus F$. Further we introduce the particle number distribution $\bar{n} = \{ n_C \}_{C \in F_0(G)}$ where $n_C$ is the number of particle on the face $C$ in the eigenstate of $P_{\leq 1} \sum_C H_C P_{\leq 1}$. Let $\Omega_{F,\bar{n}} \subset \Omega_F$ be the subspace with a particle number distribution $\bar{n}$. Let $H_{F,\bar{n};F',\bar{n}'}$ be the matrix formed by the full Hamiltonian (4) restricted to the subspace $\Omega_{F,\bar{n}}$ and let $H_{F,\bar{n};F';\bar{n}'}$ be the matrix connecting the two subspaces $\Omega_{F,\bar{n}}$ and $\Omega_{F',\bar{n}'}$. In our basis, $H_{F,\bar{n};F',\bar{n}'}$ is diagonal and the lowest eigenvalue of $H_{F,\bar{n};F',\bar{n}'}$ is $-2|F| - 2\sqrt{2t}[\frac{1}{2}(N - |F|)]$, because we can put $\frac{1}{2}(N - |F|)$ pairs into states with the energy $-2\sqrt{2t}$. Let us now look at $H_{C,C'}$ acting on a state out of $\Omega_{F,\bar{n}}$. The important point is that $H_{C,C'}$ acts only on the cycles $C'$ and $C' \in F_1(G) \setminus F$. We get a non-zero result only if the cycle $C'$ is occupied by some particles in $|\psi\rangle$. We use a similar representation as in Fig. 4 but we allow for an arbitrary state on $C'$. Further, we have hard-core bosons, the projector eliminates doubly occupied sites. This yields the rather rough estimate

$$||P_{\leq 1} H_{C,C'} \prod_{C'' \in F} b^\dagger_{C''} \psi||_2 \leq 2 ||\psi||_2$$

(19)

for $\psi \in \Omega_F$ if $C' \notin F$ and $||H_{C,C'}\psi|| = 0$ for $\psi \in \Omega_F$ if $C' \in F$.

Since there are at most $N - |F|$ occupied cycles in states $\psi$, we obtain $||P_{\leq 1} \sum H_{C,C'} P_{\leq 1}||_2 \leq 2(N - |F|) c(G)$ for states in $\Omega_F$. This yields an estimate for the lower boundary of the Gerschgorin intervals (8) $-2|F| - 2\sqrt{2t}[\frac{1}{2}(N - |F|)] - 2t'(N - |F|) c(G)$, which can be used if $N - |F| > 2$. The length of the Gerschgorin intervals grows, its centre moves to higher energies $\sim (N - |F|)$. For $2t'(c(G)) > (2 - 2\sqrt{2}) t$, the lower boundary of the intervals moves to lower energies with growing $N - |F|$. To avoid that we need

$$t' < \frac{2 - \sqrt{2}}{2c(G)} t = 0.2928 \frac{t}{c(G)}.$$ 

(20)

The first Gerschgorin interval (18) is separated from all others if

$$-2(N - 2)t - 2\sqrt{2t} + \frac{1}{2\sqrt{2}} c(G) t' < -2t|F| - 2\sqrt{2t} \left[\frac{1}{2}(N - |F|)\right] - 2t'(N - |F|) c(G).$$

(21)

This is fulfilled for all $N - |F| > 2$ if

$$t' < \frac{4 - 2\sqrt{2}}{(8 + \frac{1}{2\sqrt{2}} c(G))} t = 0.14025 \frac{t}{c(G)}.$$ 

(22)

holds. The states with $N - |F| = 2$ must be treated separately. For that case, the lowest diagonal element is $-2t|F|$ and we obtain $t' < 0.649t/c(G)$ which is clearly fulfilled if (22) holds.

### 5 Eigenstates

Let $\Omega_0$ be the space spanned by the ground states $\psi_C$ of $P_{\leq 1} \sum C H_C P_{\leq 1}$ with $N = |F_1(G)| + 1$ particles in (10). The dimension of $\Omega_0$ is $|F_1(G)|$. Let $P_0$ be the projector onto this subspace and let $\bar{P}_0 = 1 - P_0$ be the projector onto the orthogonal subspace. We write the Hamilton $H$ in (4) in the form

$$H = \begin{pmatrix} H_0 & H_{01} \\ H_{10} & H_1 \end{pmatrix} = \begin{pmatrix} P_0 H P_0 & P_0 H \bar{P}_0 \\ \bar{P}_0 H P_0 & \bar{P}_0 H \bar{P}_0 \end{pmatrix}. $$

(23)

By construction $H_0 = [-2(N - 2) - 2\sqrt{2} t] P_0$. The Gerschgorin interval corresponding to $\Omega_0$ calculated with the norm $||.||_2$ is $I_0 = \{ \lambda : -2(N - 2)t - 2\sqrt{2t} - \lambda \leq (1 - 2^{-1/2})c(G)t' \}$. Further, let $I_1$ be the Gerschgorin interval corresponding to $P_0$. 


Theorem 2. Under the assumptions above and if the two Gerschgorin intervals do not overlap, i.e. \( I_0 \cap I_1 = \emptyset \), the eigenstates \( \psi \) of \( H \) with eigenvalue \( \lambda \) out of \( I_0 \) have the property \( ||P_0 \psi||_2 > ||\bar{P}_0 \psi||_2 \).

To show this, we start with \( H_{10} P_0 \psi + H_1 \bar{P}_0 \psi = \lambda \bar{P}_0 \psi \). Putting the part acting on \( \bar{P}_0 \psi \) to the left hand side yields \( \bar{P}_0 \psi = (\lambda P_0 - \bar{P}_0 H \bar{P}_0)^{-1} \bar{P}_0 H P_0 \psi \). Taking \( ||.||_2 \) on both sides yields

\[
(||(\lambda P_0 - \bar{P}_0 H \bar{P}_0)^{-1}||_2)^{-1} ||\bar{P}_0 \psi||_2 \leq ||\bar{P}_0 H P_0||_2 ||P_0 \psi||_2.
\]

Now assume that \( ||P_0 \psi||_2 \leq ||\bar{P}_0 \psi||_2 \). Then we would get

\[
(||(\lambda P_0 - \bar{P}_0 H \bar{P}_0)^{-1}||_2)^{-1} \leq ||\bar{P}_0 H P_0||_2
\]

which is exactly the condition \([3]\) for the Gerschgorin interval corresponding to the subspace given by \( \bar{P}_0 \). Therefore, \( \lambda \in I_1 \) which contradicts our assumptions \( \lambda \in I_0 \) and \( I_0 \cap I_1 = \emptyset \). Therefore we must have \( ||P_0 \psi||_2 > ||\bar{P}_0 \psi||_2 \). This is the statement in Theorem 2.

The proof works as well if \( H \) in \([23]\) is split into more than two blocks.

This theorem means that the eigenstates with eigenvalues in the lowest Gerschgorin interval are dominated by the ground states of \( P_{\leq 1} \sum_C H_C P_{\leq 1} \). The ground states of \( P_{\leq 1} \sum_C H_C P_{\leq 1} \) are degenerate and contain localised pairs. Due to the coupling between the cycles \( \propto t' \), two effects occur. First, we can get arbitrary linear combinations of these states in a low lying eigenstate of the full Hamiltonian. Second, other states contribute to the low lying eigenstates as well. But the \( |F_1(G)| \) low lying eigenstates are dominated in the above sense by the linear combination of localised pair states, which may be localised or extended. In this sense, we can speak of pair formation. The physical interpretation is that the low lying multi-particle states can be described by a Wigner crystal of \( |F_1(G)| \) particles in which one particle is replaced by a quasi-particle, the pair, for which we obtain an effective narrow band that is separated from the rest of the multi-particle spectrum. The pairs in the eigenstates are localised in the usual sense if the eigenvalues in the lowest Gerschgorin interval are degenerate, but this is not a necessary, only a sufficient condition. This result can in principle be used to improve the variational states used in \([6]\) by taking linear combinations of the pair states.

An example where the degeneracy and the localisation of the states in the lowest Gerschgorin interval can be proven is the chequerboard chain. As discussed in \([3]\), the chequerboard chain has a local reflection symmetry. Fig. 4 shows a part of such a chain. Exchanging the sites 1 and 2 and the sites 3 and 4, the Hamiltonian remains invariant. In the chain, this holds for each cycle \( C \in F_1(G) \). The reflection operator \( S_C \) that performs this reflection on the cycle \( C \) has the eigenvalues \( s_C = \pm 1 \). A singly occupied cycle in the ground state has \( s_C = -1 \), a doubly occupied cycle in the ground state has \( s_C = 1 \). Therefore, the ground state \( \psi_C \) of \( \sum_C H_C \) with \( N = |F_1(G)| + 1 \) particles, two on \( \bar{C} \) and one on all the other cycles has a signature \( s_{\bar{C}} = 1, s_C = -1 \) for all \( C \in F_1(G) \backslash \{ \bar{C} \} \). Since the entire Hamiltonian preserves that symmetry, we can restrict the Hilbert space to all states with that signature. In that Hilbert space, all the above arguments can be repeated. The only difference is that the lowest Gerschgorin interval contains only one eigenvalue that is not degenerate. The corresponding eigenstate, applying Theorem 2, has a localised pair on \( \bar{C} \). This holds true for all cycles \( \bar{C} \in F_1(G) \), therefore we obtain \( |F_1(G)| \) eigenstates with localised pairs. If the chequerboard chain has periodic boundary conditions, these states are degenerate. For open boundary conditions we have \( c(\bar{C}) = 1 \) for the two cycles at the boundary, \( c(\bar{C}) = 2 \) otherwise and therefore we get different eigenvalues for states close to the boundary. This argument yields a rigorous proof for the statements in \([3]\) for \( t' < 0.065t \). The numerical results in \([6]\) for \( t' = t \) can be repeated for arbitrary \( t' < t \) and indicate that the result can be expected to be true for \( t' \leq t \).

The argument can be readily generalised to tree like structures with local reflection symmetries. Fig. 5 shows an example of a treelike graph \( G \) with local reflection symmetries for each cycle \( C \in F_1(G) \). The local symmetry holds for the line graph \( L(G) \) as well. The only differences is that \( c(C) > 2 \) for some
cycles so that $c(G)$ is larger and the value of $t'$ needs to be smaller in order to have the lowest Gerschgorin interval separated from the rest of the spectrum.

For the two dimensional checkerboard lattice, \[27, 6\] yield arguments on the basis of variational states, extended and localised ones. The authors show that the localised ones have a lower energy, which may indicate that in two dimensions localised pairs occur as well. But we have no rigorous proof for that statement so far.

6 Generalisations

There are two possibilities to generalise the above results. The first is to consider lattices with cycles of length larger than 4 or with interstitials. The second is to consider $N = |F_1(G)| + n$ with some small $n > 1$.

Let us start with larger cycles. For cycles of length 6 one has six eigenstates with one particle. The two lowest eigenvalues are $-2$, $-1$ and the eigenvalue $-1$ is twofold degenerate. For two particles on a cycle, the lowest eigenvalue is $-2\sqrt{3}$, the second lowest is $-\sqrt{3}$. In principle, the technique above is still applicable, but since the gaps between the states are smaller, the bound for $t'$ becomes smaller as well.

Unfortunately, this result, although interesting, is not applicable to the most interesting lattice with cycles of length 6, which is the kagomé lattice. For the kagomé lattice, we have in addition interstitials, which means that in (6) the third term on the right hand side appears. For the kagomé lattice, each interstitial is only connected to two different cycles. This means that the third term $P_{\leq 1} H' P_{\leq 1}$ can be decomposed in the form of the second term $P_{\leq 1} \sum_{C,C'\in F_1(G)} H_{C,C'} P_{\leq 1}$. This helps a bit, but we would have to take into account that $H_{C,C'}$ contains additional lattice sites and therefore in addition to the states formed by cycles further states occur. But the important ingredient of our proof, namely the fact that in the ground states of $P_{\leq 1} \sum_{C} H_{C} P_{\leq 1}$ only particles from the doubly occupied cycles can hop, remains valid. Thus we may hope that the proof can be generalised to the kagomé lattice. At least the numerical results for the kagomé chain treated in \[6\], which has a local reflection symmetry as in the case of the checkerboard chain, indicate that there the results hold true for $t' \leq t$.

As mentioned before, general graphs with chains of interstitials cannot be treated and we have good
arguments that for those the result is not valid, see the discussion of Sect. [4].

The next question is what happens if we add some more particles. Drescher et al. [6] discussed that question for the chequerboard chain. Based on their numerical results and based on the exact local reflection symmetry they argued that for \( n = 2 \) two localised pairs occur which are well separated from each other. In principle it should be possible to extend the above method to that case. The lowest Gerschgorin interval then contains \( \frac{1}{2} |F_1(G)|(|F_1(G)| - 1) \) states corresponding to two doubly occupied cycles and \( |F_1(G)| - 2 \) singly occupied cycles. The estimates are a bit more complicated but still possible. The upper value for \( t' \) to separate the lowest Gerschgorin cycle from the rest will be lower. We can also use the local reflection symmetry in this case. This allows to treat a subspace of the entire Hilbert space in which the lowest Gerschgorin cycle contains only one eigenvalue. As a consequence, if the lowest Gerschgorin cycle is separated form the rest of the spectrum, Theorem 2 immediately shows that the two pairs are localised.

Beside line graphs other flat band systems derived from bipartite graphs have been proposed [19], which contain tunable parameters. In these systems, the parameters can be tuned such that the flat band lies at the bottom of the spectrum and that there is a gap. These systems are also candidates where the above considerations can eventually be applied.

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