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On the flux phase conjecture at half-filling: an improved proof

Nicolas Macris
Institut de Physique Théorique
Ecole Polytechnique Féderale de Lausanne
CH 1015 Lausanne
Switzerland
E-mail: macris@eldp.epfl.ch

Bruno Nachtergaele
Department of Physics
Princeton University
Princeton, NJ 08544-0708, USA
E-mail: bxn@math.princeton.edu

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Abstract

We present a simplification of Lieb's proof of the flux phase conjecture for interacting fermion systems — such as the Hubbard model —, at half filling on a general class of graphs. The main ingredient is a procedure which transforms a class of fermionic Hamiltonians into reflection positive form. The method can also be applied to other problems, which we briefly illustrate with two examples concerning the $t - V$ model and an extended Falicov-Kimball model.

Keywords: Hubbard model, Flux Phase, Reflection Positivity

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1 Introduction

The main purpose of this note is to give a simplified version of Lieb's proof of the flux phase conjecture in [1], which at the same time allows for some straightforward generalizations. Those readers who are mainly interested in the basic argument, rather than in learning about the more general description of it, are advised to think about a finite regular square lattice on a cylinder while reading this and the next section. Once the argument is properly understood the generalizations become straightforward.

The physical context where the first conjectures appeared [2] is reviewed in [3]. For a history and a more general formulation of the problem we refer to the first mathematical studies on the subject by Lieb [4] and Lieb and Loss [5].

Consider a system of spinless fermions (adding spin poses no problems) on a finite set of sites Λ, at half-filling, and with a Hamiltonian of the form

$$H = \sum_{x,y\in\Lambda} t_{xy} c_x^\dagger c_y + H_{\text{int}} \tag{1.1}$$

Here, t_{xy} is a hermitian matrix. We will explain later what kind of interactions H_{int} are allowed (see Section 2). For now, let us just say that the usual on-site Hubbard interaction is among them (i.e. for spin 1/2 fermions one takes $H_{\text{int}} = U\sum_{x\in\Lambda}(n_{x,\uparrow}-1/2)(n_{x,\downarrow}-1/2)$), and that only gauge invariant interactions will be considered.

Let Γ be the graph with set of vertices Λ and the set of edges $\{< x,y >|\ t_{xy}\neq 0\}$. A *circuit* in the graph Γ is a finite sequence $\gamma=(x_1,\ldots,x_k)$ of distinct vertices, with the property that $< x_i, x_{i+1} >$, for $i=1,\ldots,k-1$, and $< x_k, x_1 >$, are all edges in the graph. By representing the circuit as an ordered sequence we have implicitly given it one of the two possible orientations (for $k>2$).

The ground state energy of (1.1) depends on the, in general complex, parameters t_{xy} only through their modulus $|t_{xy}|$, and the flux variables Φ_γ, for circuits γ, which are defined as follows:

$$\Phi_\gamma = \sum_{i=1}^{n} \varphi_{x_i,x_{i+1}}, \quad \mathrm{mod} 2\pi \tag{1.2}$$

where $\gamma = (x_1, \ldots, x_n)$, and $t_{xy} = \exp(i\varphi_{xy})|t_{xy}|$. This follows from [5, Lemma 2.1] where it was proved that there is a unitary transformation relating any two Hamiltonians with phases $\{\varphi_{xy} \mid < xy > \in \Gamma\}$ that satisfy (1.2) with the same fluxes Φ_γ for all γ. This unitary transformation is of the form

$$c_x^\dagger \mapsto e^{i\theta_x} c_x^\dagger, \quad c_x \mapsto e^{-i\theta_x} c_x \tag{1.3}$$

and is called a gauge transformation. We will often write $\{\varphi_{xy}\}$ instead of $\{\varphi_{xy} \mid < xy > \in \Gamma\}$.

The *flux phase problem* can now be formulated as follows: for fixed values of the moduli $|t_{xy}|$, find the phases φ_{xy} (or, equivalently, the fluxes Φ_γ) for which the ground state energy of the Hamiltonian (1.1) attains its minimal value. We cannot solve this problem in general. In fact, we do not expect that there is a simple solution in general. We are looking for a solution in terms of a *basic set of circuits* $\mathcal{C}$ (e.g., the plaquettes of the square lattice). The set $\mathcal{C}$ should be not too large and consist only of "simple" circuits, so that the solution ($\equiv$ the values of the fluxes through the circuits in $\mathcal{C}$) can be easily described. On the other hand $\mathcal{C}$ should contain enough circuits so that their flux uniquely determines Φ_γ for all circuits γ.

Definition 1.1 *A set $\mathcal{C}$ of circuits in a graph Γ is called a basic set of circuits if for any two configurations of phases $\{\varphi_{xy}\}$ and $\{\varphi'_{xy}\}$ that produce the same fluxes $\{\Phi_\gamma \mid \gamma \in \mathcal{C}\}$, there exists a gauge transformation relating $\{\varphi_{xy}\}$ and $\{\varphi'_{xy}\}$, i.e. $\varphi'_{xy} = \varphi_{xy} + \theta_y - \theta_x$, for some real $\theta_x, x \in \Lambda$.*

Lieb and Loss showed in [5, Lemma 2.1] that the set of all circuits of a graph satisfies Definition 1.1. Often, it is more convenient to work with a rather small subset of the set of all circuits. For examples of good choices of the set $\mathcal{C}$ we refer to Section 3.

The class of models that we treat in this paper is described by the following two assumptions on the graph Γ together with the configuration of $|t_{xy}|$'s associated with the bonds:

A1. All circuits $\gamma = (x_1, \ldots, x_n)$ in Γ are of even length, i.e. $n = 2k$. This is equivalent to requiring that the graph Γ is bipartite, but we will not use explicitly a decomposition into two sublattices.

A2. There is a *basic set of circuits* $\mathcal{C}$ such that for each $\gamma \in \mathcal{C}$ there is an embedding of the graph in $\mathbf{R}^D$, for some D, such that there is a $D-1$-dimensional reflection hyperplane P not containing any vertex of Λ, with the following properties:

1. The whole graph Γ, together with the configuration of $|t_{xy}|$'s, is invariant under reflection through P.
2. All circuits $\gamma \in \mathcal{C}$ that are intersected by P (i.e. not all vertices are in one of the two halfspaces) are, up to orientation, invariant under reflection through P. In particular, γ is invariant under reflection through P.

The embedding of the graph in $\mathbf{R}^D$ used to describe Assumption A2 is not essential. We only introduce it in order to simplify the description.

Before we can state our main result we have to say what we mean by "flux configuration" and "canonical flux configuration".

Definition 1.2 (Flux configuration) *Let $\{\Phi_\gamma\}$ be a set of fluxes (i.e. real numbers mod 2π) through all circuits of the graph. We say that $\{\Phi_\gamma\}$ is a flux configuration, if there exist a set of phases $\{\varphi_{xy}\}$ such that (1.2) holds for all γ.*

Figure 1: Two different embeddings of a graph in the plane. The solid lines indicate the edges. The dashed lines show a triangulation. The Lieb-Loss flux through the circuit $(1, 2, 3, 4, 5, 6, 7, 8)$ is 0 for the first and π for the second embedding.

Definition 1.3 (Canonical flux configuration) *Assume that* Γ *satisfies the assumptions A1-2. A flux configuration* $\{\Phi_\gamma\}$ *is called canonical if there is a set* $\mathcal{C}$ *of basic circuits satisfying A2 and such that for all* $\gamma \in \mathcal{C}$, $\Phi_\gamma = 0$ *if* γ *has length* $2 \bmod 4$, *and* $\Phi_\gamma = \pi$ *if* γ *has length* $0 \bmod 4$.

Note that it is *not* true, in general, that in a canonical flux configuration *all* circuits satisfy $\Phi_\gamma = 0$ if γ has length $2 \bmod 4$, and $\Phi_\gamma = \pi$ if γ has length $0 \bmod 4$.

The arguments in Section 2 will show that, for graphs that satisfy the assumptions A1-2, there always exists a canonical flux configuration.

The definition of canonical flux configuration given here is different from the one put forward in [5] for planar graphs embedded in the plane. A planar graph embedded in the plane can be triangulated and Lieb and Loss [5] note that the number of triangles enclosed by a circuit is independent of the triangulation, and they define a flux configuration by putting a flux $\pi/2$ in each triangle. The resulting flux configuration for the original graph, however, depends on the embedding in the plane one starts from (see Figure 1 for an example). Our definition is restricted to graphs that have a basic set of circuits satisfying the assumptions A1 and A2. They need not be planar, but, on the other hand many planar graphs do not have a canonical flux configuration according to the definition given here. Also we do not know whether there are graphs for which different choices of $\mathcal{C}$ lead to different canonical flux configurations.

Our main result is the following theorem.

Theorem 1.4 *Under the assumptions A1 and A2 we have the following:*
i) There exists a configuration of phases $\{\varphi^{(c)}_{xy}\}$ *such that the corresponding configuration of fluxes is a canonical configuration.*
ii) For the Hamiltonians (1.1) we have

$$\inf_{\{\varphi_{xy}\}} \lambda_0(H(\{\varphi_{xy}\})) = \lambda_0(H(\{\varphi^{(c)}_{xy}\})) \tag{1.4}$$

where $\lambda_0(H)$ *denotes the smallest eigenvalue of* H*, i.e., canonical flux configurations minimize the ground state energy.*

Quite generally we expect the energy minimizing flux configuration to be unique up to gauge transformations, but we have not studied the question of uniqueness. Non-uniqueness could arise in two ways. If there is more than one canonical flux configuration the minimum will be attained in both. The other possibility is that there is a non-canonical minimizing flux configuration.

2 Proof of the Main Result

First, we only consider non-interacting spinless fermions. The Hamiltonian is (1.1) with $H_{\text{int}} = 0$. We will indicate at the end of this section how spin and certain interactions can be included.

Statement i) of the Theorem 1.4 , for the case of planar graphs, is a consequence of [5, Lemma 2.2]. For the more general situation considered here i) will be a byproduct of the proof of ii).

The main argument is an application of the Dyson-Lieb-Simon Lemma in the following form.

Lemma 2.1 *Let $A, B, C_1, \ldots, C_n$ be a collection of $d \times d$ complex matrices (n could be infinite) with the following properties: A and B are Hermitian, and for all i, C_i is real and $\sum_i C_i \otimes C_i$ is symmetric (as a $d^2 \times d^2$ matrix). Let $\lambda_0(A, B)$ denote the lowest eigenvalue of the matrix*

$$T(A,B) \equiv A \otimes \mathbb{1} + \mathbb{1} \otimes B \quad - \sum_i C_i \otimes C_i \tag{2.1}$$

Then

$$\lambda_0(A,B) \geq \frac{1}{2}\left(\lambda_0(A,\overline{A}) + \lambda_0(\overline{B},B)\right) \tag{2.2}$$

where $\overline{A}$ denotes the matrix obtained from A by complex conjugation of the matrix elements. In particular

$$\lambda_0(A,B) \geq \min\left(\lambda_0(A,\overline{A}), \lambda_0(\overline{B},B)\right) \tag{2.3}$$

In the formulation of this lemma in [6] the matrices A and B are required to have real matrix elements. It is crucial for our application that we consider complex matrices A and

B. This is a straightforward extension. For a proof of Lemma 2.1 in the zero-temperature form stated here see [7].

Before we can apply this lemma we have to bring the Hamiltonian into the form (2.1). This will be achieved in three steps each consisting of an elementary transformation.

Given a circuit of the set $\mathcal{C}$ we consider an embedding of the graph in $\mathbf{R}^D$ and a reflection plane P of the circuit (it exists by assumption). This defines a left part (L), a right part (R), and a set (M) of vertices which belong to edges $< x, y >$ with $x \in L$ and $y \in R$ or $x \in R$ and $y \in L$. The three steps are:

i) A *Jordan-Wigner* type transformation,

ii) A *particle-hole* transformation,

iii) A *gauge* transformation.

We know from experience that one easily gets confused while performing this sequence of transformations. Therefore, we now spell them out in detail and indicate the purpose of each of them.

Step i): We introduce new operators $d_x^\#$ defined by

$$d_x = (-1)^{N_L} c_x \ , \quad d_x^\dagger = c_x^\dagger (-1)^{N_L} \tag{2.4}$$

for all $x \in \Lambda$, and where N_L is the total particle number in the left half of the lattice, i.e., $N_L = \sum_{x\in L} c_x^\dagger c_x$. If one considers fermions with spin, N_L has to be the total particle number on the left, i.e., $N_L = \sum_{x\in L,\sigma} c_{x\sigma}^\dagger c_{x\sigma}$. In one dimension, the transformation defined in (2.4) is similar to the usual Jordan-Wigner transformation. Strictly speaking however, even in one dimension, it is different. A slightly different transformations was employed previously by several authors, e.g., in [9]. Note however that in [9] the paragraph about fermions contains a mistake. With the transformation employed there the hopping terms on the right acquire the *opposite* sign of the hopping terms on the left, and thus the Hamiltonian is *not* in reflection positive form.

Using the canonical anticommutation relations of the c operators, one easily finds that the d operators satisfy the following algebra:

$$\left.\begin{array}{rcl} \{d_x^\dagger, d_y\} & = & \delta_{xy} \\ \{d_x, d_y\} = \{d_x^\dagger, d_y^\dagger\} & = & 0 \end{array}\right\} \quad \text{if } x, y \in L \text{ or } x, y \in R$$

$$\left.\begin{array}{rcl} [d_x^\dagger, d_y] & = & 0 \\ [d_x, d_y] = [d_x^\dagger, d_y^\dagger] & = & 0 \end{array}\right\} \quad \text{if } x \in L, y \in R \text{ or } x \in R, y \in L$$

The operators $d_x^\#$ acting on Fock space (associated to Λ) can be identified with operators of the form

$$\begin{array}{ll} d_x^\# \otimes \mathbb{I} & \quad \text{for } x \in L \\ \mathbb{I} \otimes d_x^\# & \quad \text{for } x \in R \end{array}$$

acting on the tensor product space $\mathcal{H}_L \otimes \mathcal{H}_R$, where each factor corresponds to the Fock space associated to the left and right parts of the lattice. In terms of the $d_x^\#$ the Hamiltonian can be considered as acting on $\mathcal{H}_L \otimes \mathcal{H}_R$ and takes the form

$$\begin{aligned} H &= \sum_{x,y \in \Lambda} t_{xy} d_x^\dagger d_y && (2.5) \\ &= \sum_{x,y \in L} t_{xy} d_x^\dagger d_y + \sum_{x,y \in R} t_{xy} d_x^\dagger d_y + \sum_{x,y \in M} t_{xy} d_x^\dagger d_y && (2.6) \end{aligned}$$

The third term of (2.6) describes the interaction between the left and the right half of the lattice and is of the tensor product form as in (2.1).

Step ii): The second step is a simple particle-hole transformation on the right half of the lattice. i.e., for all $x \in R$

$$d_x \mapsto d_x^\dagger, \quad d_x^\dagger \mapsto d_x \tag{2.7}$$

while the $d_x^\#$ with $x \in L$ remain unchanged. The Hamiltonian becomes

$$\begin{aligned} H &= \sum_{x,y\in L} t_{xy} d_x^\dagger d_y + \sum_{x,y\in R} (-\overline{t_{xy}}) d_x^\dagger d_y &(2.8)\\ &+ \sum_{x\in L, y\in R} t_{xy} d_x^\dagger d_y^\dagger + \sum_{x\in R, y\in L} t_{xy} d_x d_y &(2.9)\end{aligned}$$

Step iii): Finally we perform a gauge transformation with the purpose of making the hopping matrix elements across the reflection plane all negative. A transformation that achieves this is the following:

$$\begin{aligned} d_y^\dagger &\mapsto -e^{-i\varphi_{xy}} d_y^\dagger \\ d_y &\mapsto -e^{i\varphi_{xy}} d_y \end{aligned} \tag{2.10}$$

for sites $y \in R$ which are connected to a site $x \in L$ (i.e. given $y \in R$ there exist an $x \in L$ such that $t_{xy} \neq 0$).

Therefore we have a new set of hopping matrix elements $\{t'_{xy}\}$ with *the same fluxes* as the original configuration $\{t_{xy}\}$, (because a gauge transformation does not change the fluxes) and $|t'_{xy}| = |t_{xy}|$, in terms of which the Hamiltonian is

$$\begin{aligned} H &= \sum_{x,y\in L} t'_{xy} d_x^\dagger d_y + \sum_{x,y\in R} (-\overline{t'_{xy}}) d_x^\dagger d_y &(2.11)\\ &- \sum_{x\in L, y\in R} |t'_{xy}| d_x^\dagger d_y^\dagger - \sum_{x\in R, y\in L} |t'_{xy}| d_x d_y &(2.12)\end{aligned}$$

We denote by Φ_L (respectively Φ_R) the set of fluxes through basic circuits which are entirely in L (respectively R), and by Φ_M the flux configuration for basic circuits which have the same reflection plane P. These fluxes refer to a particular orientation of the basic circuits: first orient in an arbitrary way all circuits on the left, and for the circuits on the right take the orientation opposite to the one obtained by reflection of the left part. For the ones in the middle choose an arbitrary orientation. For a fixed configuration of $|t_{xy}|$, the ground state energy depends on the phases φ_{xy} only through the fluxes and we will denote this energy by $E_0(\Phi_L, \Phi_M, \Phi_R)$.

We adopt the convention that the same set of fluxes Φ_L when it appears as the third argument of E_0, assigns the flux to a circuit on the right that is associated by reflection to the circuit on the left. We can now state the basic lemma.

Lemma 2.2 *Assume that the configuration $\{|t_{xy}|\}$ is invariant under reflections. Then*

$$E_0(\Phi_L, \Phi_M, \Phi_R) \geq \frac{1}{2}\left(E_0(-\Phi_R, \Phi_M^{(c)}, \Phi_R) + E_0(\Phi_L, \Phi_M^{(c)}, -\Phi_L)\right) \tag{2.13}$$

where $\Phi_M^{(c)}$ is the canonical flux configuration through the basic circuits intersecting P.

proof:

The proof is a direct application of Lemma 2.1 to the Hamiltonian in the form (2.12), while carefully keeping track of the flux configurations. The operator $T(A, B)$ of (2.1) is given by

$$\begin{aligned} A &= \sum_{x,y\in L} t'_{xy} d_x^\dagger d_y \\ B &= \sum_{x,y\in R} (-\overline{t'_{xy}}) d_x^\dagger d_y \\ \sum_i C_i \otimes C_i &= \sum_{x\in L, y\in R} |t'_{xy}| d_x^\dagger d_y^\dagger + \sum_{x\in R, y\in L} |t'_{xy}| d_x d_y \end{aligned}$$

and $\lambda_0(A, \overline{A})$ is the ground state energy of the Hamiltonian

$$\begin{aligned} T(A, \overline{A}) &= \sum_{x,y\in L} t'_{xy} d_x^\dagger d_y + \sum_{x,y\in L} \overline{t'_{xy}} d_{r(x)}^\dagger d_{r(y)} - \sum_{x\in L, y\in R} |t'_{xy}| d_x^\dagger d_y^\dagger - \sum_{x\in R, y\in L} |t'_{xy}| d_x d_y \\ &= \sum_{x,y\in L} t'_{xy} d_x^\dagger d_y + \sum_{x,y\in L} t'_{xy} d_{r(y)}^\dagger d_{r(x)} - \sum_{x\in L, y\in R} |t'_{xy}| d_x^\dagger d_y^\dagger - \sum_{x\in R, y\in L} |t'_{xy}| d_x d_y \end{aligned}$$

where $r(x)$ denotes the reflection of the site x through P. This can be written back in the form of (2.12) with a new configuration of hopping matrix elements t''_{xy} which do *not*, in general, have the same fluxes as the original hoppings. We now determine the new configuration of fluxes $(\Phi''_L, \Phi''_M, \Phi''_R)$.

First, take a circuit in the middle part $\gamma = (x_1, ..., x_{2n})$. We label the vertices such that $x_1, \ldots, x_n \in R$, and $x_{n+1}, \ldots, x_{2n} \in L$ (see Figure 2). The edges intersected by P are $< x_{2n}, x_1 >$ and $< x_n, x_{n+1} >$. The corresponding term in the transformed Hamiltonian is

$$\sum_{i=n+1}^{2n-1} t'_{x_i,x_{i+1}} d^\dagger_{x_i} d_{x_{i+1}} + \sum_{i=1}^{n-1} (-\overline{t'_{x_i,x_{i+1}}}) d^\dagger_{x_i} d_{x_{i+1}} \tag{2.14}$$

$$-|t'_{x_{2n},x_1}| d^\dagger_{x_{2n}} d^\dagger_{x_1} - |t'_{x_{n+1},x_n}| d^\dagger_{x_{n+1}} d^\dagger_{x_n} + \text{h.c.} \tag{2.15}$$

and the corresponding flux is the original one $\Phi_\gamma = \sum_{i=1}^{2n} \varphi_{x_i,x_{i+1}} = \sum_{i=n+1}^{2n-1} \varphi'_{x_i,x_{i+1}} + \sum_{i=1}^{n-1} \varphi'_{x_i,x_{i+1}}$ mod 2π. After reflection it becomes

$$\sum_{i=n+1}^{2n-1} t'_{x_i,x_{i+1}} d^\dagger_{x_i} d_{x_{i+1}} + \sum_{i=n+1}^{2n-1} t'_{x_i,x_{i+1}} d^\dagger_{r(x_{i+1})} d_{r(x_i)} \tag{2.16}$$

$$-|t'_{x_{2n},x_1}| d^\dagger_{x_{2n}} d^\dagger_{x_1} - |t'_{x_{n+1},x_n}| d^\dagger_{x_{n+1}} d^\dagger_{x_n} + \text{h.c.} \tag{2.17}$$

The new flux on γ is $\Phi''_\gamma = \sum_{i=n+1}^{2n-1} \varphi'_{x_i,x_{i+1}} + \sum_{i=n+1}^{2n-1} (\pi - \varphi'_{x_i,x_{i+1}})$ mod 2π, which is equal to $(n-1)\pi$, i.e., the canonical flux through the circuit γ.

Next, we consider a circuit on the left $\gamma = (x_1, ..., x_{2n})$, oriented from x_1 to x_{2n} (n is an integer), and its reflection $r(\gamma) = (r(x_1), ..., r(x_{2n}))$ on the right oriented from $r(x_{2n})$ to $r(x_1)$ (See Figure 2). After the transformations i)-iii) the corresponding terms in the Hamiltonian are (with the convention $x_{2n+1} = x_1$)

$$A = \sum_{i=1}^{2n} t'_{x_i,x_{i+1}} d^\dagger_{x_i} d_{x_{i+1}} + \text{h.c.} \tag{2.18}$$

$$B = \sum_{i=1}^{2n} (-\overline{t'_{r(x_{i+1}),r(x_i)}}) d^\dagger_{r(x_{i+1})} d_{r(x_i)} + \text{h.c.} \tag{2.19}$$

and the fluxes through γ and $r(\gamma)$ are respectively $\Phi_\gamma = \sum_{i=1}^{2n} \varphi_{x_i,x_{i+1}} = \sum_{i=1}^{2n} \varphi'_{x_i,x_{i+1}}$ and $\Phi_{r(\gamma)} = \sum_{i=1}^{2n} \varphi_{r(x_{i+1}),r(x_i)} = \sum_{i=1}^{2n} \varphi'_{r(x_{i+1}),r(x_i)}$. When we apply Lemma 2.1 we have to replace B by

$$\bar{A} = \sum_{i=1}^{2n} \overline{t'_{x_i,x_{i+1}}} d^\dagger_{r(x_i)} d_{r(x_{i+1})} + \text{h.c.} = \sum_{i=1}^{2n} t'_{x_i,x_{i+1}} d^\dagger_{r(x_{(i+1)})} d_{r(x_i)} + \text{h.c.} \tag{2.20}$$

The new corresponding flux through $r(\gamma)$ is $\Phi''_{r(\gamma)} = \sum_{i=1}^{2n}(\pi - \varphi'_{x_i,x_{i+1}})$, which is equal to $-\Phi_\gamma$. In particular if γ on the left has the flux 0 or π then $r(\gamma)$ on the right has the same flux.

One argues similarly for $\lambda_0(\overline{B}, B)$. This ends the proof of Lemma 2.2. ∎

Proof of Theorem 1.4 By assumption the configuration $\{|t_{xy}|\}$ is invariant under reflections through all reflection planes of the circuits in $\mathcal{C}$. The crucial property is that for each basic circuit there is a reflection plane that intersects it and for which the conditions of Lemma 2.2 are satisfied. The theorem is then proved as an application of Lemma 2.2. The Lemma yields the existence of a configuration of fluxes for which the ground state energy is at least as low, while at the same time the new flux configuration is produced from the old one by either

$$(\Phi_L, \Phi_M, \Phi_R) \mapsto (\Phi_L, \Phi_M^{(c)}, -\Phi_L), \text{ or } (\Phi_L, \Phi_M, \Phi_R) \mapsto (-\Phi_R, \Phi_M^{(c)}, \Phi_R) \tag{2.21}$$

In both cases the flux in all circuits intersected by P becomes canonical. By the same argument as in [6, Proof of Theorem 4.2] or [8], one can now prove that the minimum is attained in a canonical configuration by showing that, in an energy minimizing configuration, the maximum number of circuits in $\mathcal{C}$ with canonical flux must be the total number of circuits in $|\mathcal{C}|$. Let $\{\Phi_\gamma\}$ be a minimizing configuration with a given number $N_c(\{\Phi_\gamma\})$ of circuits (in $\mathcal{C}$) with canonical flux, and let $\gamma_0 \in \mathcal{C}$ be a circuit that does not have canonical flux in that configuration. Let P be a reflection plane leaving γ_0 invariant. After reflection the new configurations in (2.21) both have the same minimal energy. Then writing $\{\Phi_\gamma\} =$

(Φ_L, Φ_M, Φ_R)

$$N_c(\Phi_L, \Phi_M^{(c)}, -\Phi_L) + N_c(-\Phi_R, \Phi_M^{(c)}, \Phi_R) = 2\left(N_c(\Phi_L, \Phi_M, \Phi_R) + N_c(\Phi_M^{(c)}) - N_c(\Phi_M)\right)$$

As γ_0 is a circuit in M that does not have canonical flux in Φ_M while in $\Phi_M^{(c)}$ it does (just like any other circuit of $\mathcal{C}$ intersected by P) it is clear that $N_c(\Phi_M^{(c)}) - N_c(\Phi_M) \geq 1$. We conclude that at least one of the new minimizing configurations has strictly more circuits with canonical flux than $\{\Phi_\gamma\}$. This argument is then repeated until all $\gamma \in \mathcal{C}$ have canonical flux. ■

Remarks:

a) Finite temperatures. Lemma 2.1 holds with λ_0 replaced by $-\log \operatorname{tr} \exp(-\beta H)$. Thus Lemma 2.2 holds also with the ground state energy E_0 replaced by the free energy (at half filling), and of course its proof and the proof of theorem 1.4 is the same.

b) Interacting systems. It is straightforward to generalize the proofs to include spin and some class of interactions. One can accommodate for example a Hubbard term

$$\sum_{x \in \Lambda} h_x = \sum_{x \in L} h_x + \sum_{x \in R} h_x$$

where $h_x = U(n_{x\uparrow} - \frac{1}{2})(n_{x\downarrow} - \frac{1}{2})$, $n_{x\sigma} = c_{x\sigma}^\dagger c_{x\sigma}$, $\sigma = \uparrow, \downarrow$, U is an arbitrary real number. Another example is a nearest neighbor repulsive potential

$$\sum_{x,y \in \Lambda} h_{xy} = \sum_{x,y \in L} h_{xy} + \sum_{x,y \in M} h_{xy} + \sum_{x,y \in R} h_{xy}$$

where $h_{xy} = V(n_{x\uparrow} + n_{x\downarrow} - 1)(n_{y\uparrow} + n_{y\downarrow} - 1)$ with V a positive number. Longer range interactions, and spin dependent forces such as a Heisenberg antiferromagnetic exchange term can also be included. These cases are also discussed in [1]. Let us describe what happens in the transformations i)-iii). In the first step i) one has to replace (2.4) by

$$d_{x\sigma} = (-1)^{N_L} c_{x\sigma} \ , \quad d_{x\sigma}^\dagger = c_{x\sigma}^\dagger (-1)^{N_L}$$

with $N_L = \sum_{x\in L}(n_{x\uparrow} + n_{x\downarrow})$. In step ii) for $x \in R$, $n_{x\sigma} \to 1 - n_{x\sigma}$. The Hubbard term remains unchanged, but the nearest neighbor interaction becomes

$$\sum_{x,y\in\Lambda} h_{xy} = \sum_{x,y\in L} h_{xy} - \sum_{x,y\in M} h_{xy} + \sum_{x,y\in R} h_{xy}$$

Thus the interaction between the left and right parts of the lattice is of the form $\sum_i C_i \otimes C_i$ with the correct sign because $V > 0$. The third step iii) is a gauge transformation which does not affect the interaction terms. Summarizing we see that we can bring the Hamiltonians into the form (2.1). Then the proofs of Lemma 2.2 and Theorem 1.4 are unchanged.

We believe that these remarks are useful in other problems. We illustrate this by two examples: the $t - V$ model and a generalized Falicov Kimball model.

c) Spinless $t - V$ model. This model of spinless electrons has Hamiltonian 1.1 with the interaction part equal to $V \sum_{x,y\in\Lambda}(n_x - 1/2)(n_y - 1/2)$ where the sum is over nearest neighbors only and V is positive. The remarks above show that on a cubic lattice, i.e., $D = 3$, with periodic boundary conditions in all directions and a flux configuration through each square plaquette equal to π, and $|t_{xy}| = t$ for all bonds $< xy >$, it can be brought in a reflection positive form with respect to all reflection planes. Then it is an exercise to see that the methods of [6] used for the Heisenberg model can be used also in the present situation to prove that, when t/V is small enough there is long range order at low temperature β^{-1}. More precisely if $< \cdot >_\Lambda$ is the thermal average with periodic boundary conditions, one can prove $(-1)^{|x|+|y|} < (n_x - 1/2)(n_y - 1/2) >_\Lambda > c > 0$, for all x and y in Λ, for some strictly positive constant c independent of Λ. (We note that in the present case the uniform density theorem [10] applies, so in particular $< n_x >_\Lambda = 1/2$ for all β, t and V). In fact this result is true for any flux configuration and one can also add a small chemical potential term (see [11],[12] and [13] for recent rigorous results). Although our proof does not work in $D = 2$, the result is expected to hold also in two dimensions.

d) One can also consider the case of spin 1/2 electrons with attractive Hubbard interaction and a nearest neighbor repulsion, i.e., a $t-V-U$ model, and it can be shown that for low enough temperatures, in three or more dimensions, for t/V small enough, and $U+4V \leq 0$, the model has checkerboard long range order of the electron density by following the proof of [6] for the Heisenberg antiferromagnet. Here again, checkerboard long range order is expected to occur also in $D=2$, but the proof given here does not directly apply.

e) Extended Falicov- Kimball model. The extended Falicov-Kimball model we wish to mention has the Hamiltonian

$$H(\{w_x\}) = \sum_{x,y\in\Lambda,\sigma=\uparrow,\downarrow} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} + U \sum_{x\in\Lambda} h_x + V \sum_{x,y\in\Lambda} h_{xy} \tag{2.22}$$

$$+U' \sum_{x\in\Lambda} (n_{x\uparrow} + n_{x\downarrow} - 1)(2w_x - 1) \tag{2.23}$$

where $\{w_x\}$ is a configuration of random variables with values 0 or 1, describing the position of classical particles (say nuclei or fermions with a large effective mass, we refer to [14] for a discussion of the physical interpretations). The usual Falicov-Kimball model has $U=V=0$ and only one type of electron (say the spin up electrons). The energy of a nuclear configuration $\{w_x\}$ is $\lambda_0(H(\{w_x\}))$, the smallest eigenvalue of (2.23) in the total Fock space of the electrons. A theorem of Kennedy and Lieb [14] asserts that for the usual Falicov-Kimball model on a bipartite lattice $\Lambda = A \cup B$ union of two sublattices A and B, for all U' the minimum of $\lambda_0(H(\{w_x\}))$ is attained for one of the two configurations $(w_x = 0, x\in A, w_x = 1, x \in B)$ or $(w_x = 0, x\in B, w_x = 1, x\in A)$. This is true irrespective of the boundary conditions or the flux configuration (provided it exists). Many more detailed results are known but it is only this one that we will now generalize.

We take a D-dimensional hypercubic lattice with periodic boundary conditions in all directions and set the flux configuration to be equal to π in all square plaquettes, and also the canonical flux through the circuits created by the periodic boundary conditions. It is explained in the next section why this can be done and why it is the correct choice. We set $|t_{xy}| = t$. By performing the sequence of transformations i)-iii) the Hamiltonian is brought to a refection positive form. The only term we have not discussed so far is the last one in (2.23) (the one with coupling constant U'.) After the transformations i)-iii) it becomes the following:

$$U' \sum_{x \in L} (n_{x\uparrow} + n_{x\downarrow} - 1)(2w_x - 1) - U' \sum_{x \in R} (n_{x\uparrow} + n_{x\downarrow} - 1)(2w_x - 1) \tag{2.24}$$

where L and R refer to the left and right parts of the lattice with respect to some reflection plane P. Let $r(x)$ denote the site obtained by reflection of x through P. It is convenient to use the variables $s_x = 2w_x - 1$ and write $E_0(\{s_x\}_{x\in L}, \{s_x\}_{x\in R}) = \lambda_0(H(\{w_x\}))$. By applying Lemma 2.1 one obtains

$$E_0(\{s_x\}_{x\in L}, \{s_x\}_{x\in R}) \geq \frac{1}{2} \left(E_0(\{s_x\}_{x\in L}, \{s'_x\}_{x\in R}) + E_0(\{s''_x\}_{x\in L}, \{s_x\}_{x\in R})\right) \tag{2.25}$$

where for $x \in R$ $s'_x = -s_{r(x)}$ and for $x \in L$ $s''_x = -s_{r(x)}$. By repeated reflections (across all reflection planes in all D directions) one concludes that the minimum energy is attained in the checkerboard configurations of the variables s_x (or, equivalently, of the w_x). Note that this result holds for all U, U', and for all $V \geq 0$.

3 Examples and Discussions

In this section we comment and illustrate Theorem 1.4 by various examples. First let us consider several planar graphs.

1. Planar graphs. The most basic case is that of a square lattice with periodic boundary conditions in one direction and an even number of sites in that direction, say the horizontal one. Thus we have a cylinder (which can be embedded in the plane). A basic set of circuits $\mathcal{C}$

is constituted by the square plaquettes of length $n = 4$, and one big circle along a basis of the cylinder. We emphasize that if one takes only the square plaquettes then the flux through circuits that wind around the cylinder is not uniquely determined, and thus the set of square plaquettes alone is not a basic set of circuits. Obviously one can find reflection planes that satisfy our assumptions: these are the vertical planes that cut the cylinder in two equal halves. Furthermore in order to have $|t_{xy}|$ invariant under reflection across these planes we must require that $\{|t_{xy}|, < xy > \text{ horizontal}\}$ has period 2 in the horizontal direction, and $\{|t_{xy}|, < xy > \text{ vertical}\}$ is translation invariant in the horizontal direction. There is no constraint for $|t_{xy}|$ along the vertical direction. A canonical flux configuration can be described by putting a flux π through each square plaquette and $\pi(N-1)$ through the basis of length $2N$ of the cylinder. Theorem 1.4 states that this flux configuration minimizes the ground state energy.

As Lieb points out [1], one can obtain the optimal flux on other graphs simply by "erasing", that is, letting $|t_{xy}| \to 0$ on some edges in a way that preserves the assumptions. For example one can get the hexagonal lattice with periodic boundary conditions where the flux through each hexagon is 0 and $\pi(N-1)$ through the basis. Many planar graphs that cannot be obtained by this procedure satisfy our assumptions however. An example is given in Figure 3.

In all these examples one can also take periodic boundary conditions in both the vertical and horizontal directions. This wraps the graph on a torus, thus it is not planar any more. A new circuit has to be added to $\mathcal{C}$, namely a circuit winding around the torus in the "vertical" direction. The reason for this will become clear in the next paragraph.

2. Basic sets of circuits. Before discussing more general examples it is useful to indicate a way of checking that a set $\mathcal{C}$ is a basic set of circuits. We describe a sufficient condition. We start by representing any oriented circuit γ as a sum over all edges e_j of the graph

$$\gamma = \sum_j \varepsilon_j e_j$$

The edges have a fixed reference orientation and the ε_j are equal to 0 if e_j does not belong to γ, +1 ($resp.$ -1) if e_j occurs in γ with the same (respectively. opposite) orientation than γ. We require that any circuit γ can be decomposed as

$$\gamma = \sum_i a_i \gamma_i \tag{3.1}$$

with integer a_i and $\gamma_i \in \mathcal{C}$. We call such sets $\mathcal{C}$ generating.

If the flux configuration is specified for all $\gamma_i \in \mathcal{C}$ then using (3.1) we can compute the flux through γ, namely $\Phi_\gamma = \sum_i a_i \Phi_i$. Since the flux configuration through $\gamma_i \in \mathcal{C}$ corresponds to a set of phases, different decompositions of γ lead to the same flux. Once the flux is determined for all circuits, it follows from Lemma 2.1 in [5] that $\mathcal{C}$ is a basic set of circuits.

The property that $\mathcal{C}$ is generating can be expressed as a simple topological property of the surface (two-dimensional complex) consisting of the set of vertices Λ, the edges in Γ, and the set of triangles obtained by triangulation of all the circuits $\gamma \in \mathcal{C}$. The set $\mathcal{C}$ is generating if and only if the first homology group over the integers of this surface is trivial (see e.g. [15]). If one views the complex as a continuous two dimensional manifold this corresponds to the property that any closed curve can be contracted to a point.

3. Non planar examples. For non planar graphs it is not obvious that there exists phases which correspond to the canonical flux. Let us consider, e.g., a single D-dimensional hypercube. We show that in general for a given configuration of fluxes through the two dimensional squares, one cannot find corresponding phases for the t_{xy}. The number of k-dimensional subcubes is equal to $2^{D-k}D!/(D-k)!k!$. Indeed, a k dimensional subcube is determined by the set of points $(x_1, ..., x_D)$ with $0 \leq x_{i_1} \leq 1$, ..., $0 \leq x_{i_k} \leq 1$, and $x_j = 0$ or 1 for $j \neq i_1 ... i_k$.

So we have $D!/(D-k)!k!$ choices for $i_1...i_k$ and 2^{D-k} choices for the x_j's. Thus the number of flux variables through squares is $2^{D-3}D(D-1)$, and the number of phases on the edges is $2^{D-1}D$. In general one will have to solve a system of equations which is overdetermined if $2^{D-1}D < 2^{D-3}D(D-1)$, i.e. $D > 5$. However for the canonical flux configuration there always exist a solution of this system of equations. In fact our proof of the flux phase conjecture constructs such a solution, for any graph satisfying the assumptions of Theorem 1.4.

In particular the hypercubic lattice falls into our class of graphs. In order to satisfy the assumptions we have to take periodic boundary conditions in $D-1$ or D directions. A generating set of circuits is constituted by all the square plaquettes and $D-1$ circuits, that are the $D-1$ coordinate axis in the periodic directions. The canonical flux configuration is unique and equals π for each plaquette and $\pi(N_i - 1)$ through the $D-1$ circuits in the periodic directions of lengths $2N_i$, $i = 1, ..., D-1$. One can of course imagine many non-planar graphs satisfying the assumptions A1-A2.

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Figure 2: By assumption, when a circuit is intersected by the reflection plane, it is reflected into itself. Such circuits constitute the "middle part" of the graph. The figure also shows a circuit $(1, 2, 3, 4)$ in the left part of the graph and its reflection $(r(1), r(2), r(3), r(4))$ on the right.

Figure 3: A graph with non uniform optimal flux. Periodic boundary conditions are assumed in the horizontal direction.