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THE FLUX-PHASE PROBLEM ON PLANAR LATTICES

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Abstract. The problem is considered of determining the magnetic flux on various planar lattices that minimizes the ground state energy of free electrons. Several theorems are presented without proofs. Analogous results are also given for the Falicov-Kimball model with magnetic field.

There is a growing awareness that the quantum mechanical many-body problem is indeed complex, that correlations among electrons are of great importance in condensed matter physics, and that back-of-the-envelope mean-field calculations may not reveal everything of interest. In particular, a question of great subtlety is the interaction of electrons with magnetic fields. The most obvious question there concerns the existence of ferromagnetism, namely the fact that electron spins line up parallel to each other even though there is (essentially) no interaction term in the Hamiltonian that directly involves the spins. Neither the potential energy nor the kinetic energy (even with the Pauli principle included) favors spin alignment. In fact the kinetic energy favors $S = 0$. Nevertheless, there is a very subtle interplay between the two that causes a reversal from $S = 0$ to a ground state with a large value of S. To my mind a true resolution of this problem still remains as an important goal of condensed matter theory.

Electrons can also interact with a magnetic field through their orbital motion. Generally, one thinks of this effect as primarily diamagnetic, i.e., a magnetic field tends to raise the kinetic energy of an electron. This is indeed true for a single electron and can even be quantified via the well-known diamagnetic inequality. However, the simultaneous presence of many electrons (i.e. raising the density from zero to some positive value) can substantially alter the picture. A magnetic field might now *lower* the total electronic energy.

I am grateful to Paul Wiegmann for drawing my attention to the following model problem in which he and many others have recently been interested. It shows dramatically that the diamagnetic inequality can be reversed in certain circumstances. Although one is interested in interacting electrons, the version I shall mostly (but not solely) consider here contains only "free" electrons. The word "free" is, however, a misnomer, for the Pauli principle is a very strong kind of interaction. (There are some people who maintain that a "principle" is not an "interaction", but that is wrong in my view. Any mechanism by which the presence of one particle changes the state of others can justly be called an interaction.) The model, moreover, is a lattice model. Partly this simplifies things, but partly it seems

to be essential because the effect is most dramatic when there is a half-filled band, i.e., when the number of (spinless) electrons is half the number of sites (or vertices) in the lattice. This case entails studying the lower half of the spectrum of the one-body kinetic energy operator - a notion that has no simple analogue in the continuum (although the determinant, about which something will be said later, does have a continuum analogue). Despite the fact that there is no obvious continuum analogue of "the sum of the bottom half of the eigenvalues of the Laplacian on a manifold", it is difficult to escape the feeling that this problem - with its remarkably simplicity - has an underlying differential geometric significance.

The results reported here were obtained partly in collaboration with Michael Loss.

To be specific, we start with a finite lattice (or graph) Λ consisting of sites (or vertices) labelled by x. The number of sites is denoted by $|\Lambda|$. The lattice is not assumed, at the outset, to be planar. For each pair $x, y \in \Lambda$ that are connected by a bond (or edge) there is a complex number t_{xy}, called the hopping amplitude, satisfying

$$t_{xy} = t_{xy}^*. \tag{1}$$

If x and y are not connected by a bond, $t_{xy} = 0$. Otherwise, $|t_{xy}| \neq 0$ is given *a-priori* and our problem will be to determine the optimum choice for t_{xy}, given the constraint. Note that $t_{xx} = 0$. If we write

$$t_{xy} = |t_{xy}| \exp[i\theta_{xy}], \tag{2}$$

the real number θ_{xy} can be regarded, physically, as the line integral of the magnetic vector potential between the (physical) points x and y.

The Hamiltonian for the electrons on Λ is

$$H = \sum_{x,y \in \Lambda} t_{xy} c_x^\dagger c_y \tag{3}$$

with $c^\dagger$ and c being the usual spinless fermion creation and annihilation operators. (Spin is irrelevant here; its inclusion would merely double everything.)

The $|\Lambda| \times |\Lambda|$ matrix $T \equiv \{t_{xy}\}_{x,y \in \Lambda}$ is Hermitian by (1). Its eigenvalues are denoted by $\lambda_1(T) \leq \lambda_2(T) \leq \ldots \leq \lambda_{|\Lambda|}(T)$. The **ground state energy** of H for $N \leq |\Lambda|$ electrons is obtained by filling the N lowest levels, namely

$$E_N(T) \equiv \sum_{j=1}^{N} \lambda_j(T). \tag{4}$$

We shall primarily be interested in the **absolute ground state energy**,

$$E(T) \equiv \sum_{\lambda_j < 0} \lambda_j(T), \tag{5}$$

which we call the **energy of the half-filled band**. This appelation comes from the following fact. Suppose Λ is bipartite, i.e. $\Lambda = A \cup B$ with A and B disjoint sets of sites and with $t_{xy} = 0$ when $x \in A$ and $y \in A$ or when $x \in B$ and $y \in B$. The square and hexagonal planar lattices are bipartite; the triangular lattice is not. For bipartite lattices, $T = -UTU^{-1}$, where U is the diagonal unitary matrix $U_{xy} = \delta_{xy}$ if $x \in A$ and $U_{xy} = -\delta_{xy}$ if $x \in B$. Thus, the nonzero λ's come in pairs λ and $-\lambda$. Therefore, $E(T) = E_{|\Lambda|/2}(T)$ if Λ is bipartite and $|\Lambda|$ is even. T necessarily has $\big||A| - |B|\big|$ zero eigenvalues.

For all Λ (bipartite or not), $E(T)$ is given by the trace formula

$$E(T) = \tfrac{1}{2} Trace\ T - \tfrac{1}{2} Trace|T| = -\tfrac{1}{2} Trace\sqrt{T^2} = -\tfrac{1}{2} \sum_{j=1}^{|\Lambda|} |\lambda_j(T)|, \tag{6}$$

since $Trace\ T = 0$ and $|T| = \sqrt{T^2}$.

A **planar lattice** is one whose edges and vertices can be embedded with noncrossing edges in the plane. The embedding is generally not unique. Λ is then essentially defined by its elementary cells, or circuits, and each of these has an even number of edges and sites in case Λ is bipartite. With the $|t_{xy}|$'s given, it is easy to see that the $\lambda(T)$'s depend *only* on the *flux* Φ through each elementary cell, defined (modulo 2π) by

$$\exp[i\Phi] \equiv \prod_{\text{edges of cell}} t_{xy} \Big/ \prod_{\text{edges of cell}} |t_{xy}|. \tag{7}$$

The chief question is this:

What choice of the Φ's minimizes $E(T)$?

It is to be emphasized that we are not restricting ourselves to the case of constant flux or uniform shape of the elementary cells – although that is what is usually done in the literature on this subject. Also, there is no thermodynamic limit being considered.

The conjecture has been [1] that the energy minimizing choice for the *square lattice* $\mathbf{Z}^2$ is

$$\Phi = \pi \text{ in all cells}, \tag{8}$$

which is the antithesis of the diamagnetic inequality (because $\Phi = \pi$ is the largest possible flux). If the electron number N is constrained to satisfy $N = f|\Lambda|$ then the optimum flux is conjectured to be $2\pi f$, for large lattices, but we shall not consider this – except to note that for $N = 1$ the choice $\Phi = 0$ in all cells is optimum. (This, in fact, is the diamagnetic inequality and it follows in the lattice context from the Perron-Frobenius theorem.)

In this talk several theorems connected with the energy minimization, and related questions will be stated. Proofs will be given elsewhere. The related quantities to be considered are: *the gap, the determinant, and the free energy.*

The **gap**, $G(T)$ is defined for a bipartite lattice by

$$\begin{aligned} G(T) &= \min\{\lambda_j : \lambda_j \geq 0\} - \max\{\lambda_j : \lambda_j \leq 0\} \qquad \text{when } |A| = |B| \\ &= \text{ same, but not counting } \big||A| - |B|\big| \text{ zeros} \quad \text{when } |A| \neq |B| \end{aligned} . \tag{9}$$

The **determinant**, $\det(T)$, is, of course, given by $\Pi_j \lambda_j(T)$. For a bipartite lattice with $|A| = |B|$ and with $G(T) > 0$ we have

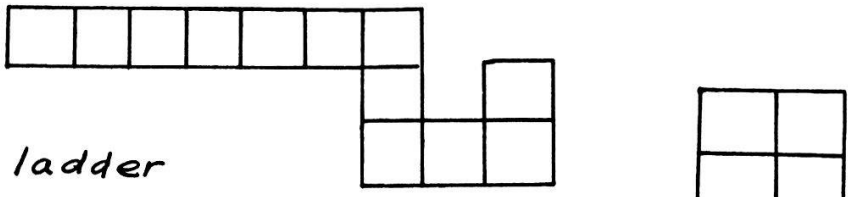
$$ln|\det(T)| = 2 \sum_{\lambda_j < 0} ln|\lambda_j|, \tag{10}$$

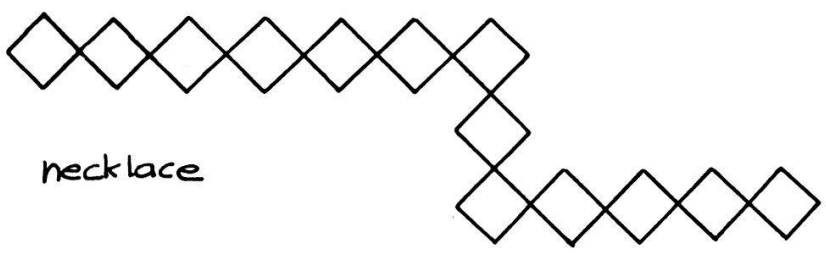
which is to be compared with $E(T)$ given by (5). Thus, the problem of maximizing $|\det(T)|$ is closely related to that of maximizing $G(T)$ and minimizing $E(T)$. We study $\det(T)$ for this reason and for the fact that it is much easier to deal with than $E(T)$ (since it is merely a polynomial in the t_{xy}'s). Another reason for studying $\det(T)$ is that it is a quantity of great interest in field theory. Because of the similarity of (5) and (10), one is tempted to conjecture that the minimum energy is achieved by the same flux that maximizes the determinant.

The **free energy**, $F(T)$, is well known. At inverse temperature β, and all Λ

$$\begin{aligned} -\beta F(T) &= Trace(ln\{1 + \exp(-\beta T)\}) \\ &= Trace(ln\{2\cosh(\tfrac{1}{2}\beta T)\}). \end{aligned} \tag{11}$$

There are two examples of finite subsets of $\mathbf{Z}^2$ about which much can be said: the **ladder** and the **necklace**. These are finite runs of boxes that can be bent at will (as shown below). Included in the ladder category is the special lattice consisting of four boxes as shown.





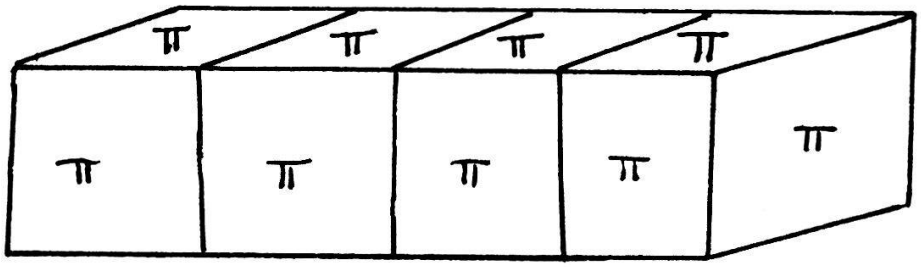
THEOREM 1. *For the ladder or necklace with* $|t_{xy}| = 1$ *on the bonds, the choice*

$$\Phi = \pi$$

in all cells uniquely gives the

(a) lowest energy, $E(T)$,
(b) largest gap, $G(T)$,
(c) largest $|\det(T)|$,
(d) lowest free energy $F(T)$ *for all temperatures.*

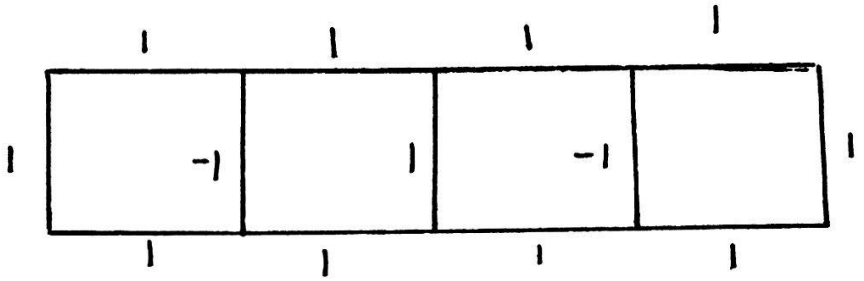
A similar theorem can be formulated for the 3-dimensional ladder consisting of cubes pictured below



THEOREM 2. *(a). The same four conclusions as in Theorem 1 hold for the 3-dimensional ladder.* $\Phi = \pi$ *in every face wins!*

(b). Suppose we replace $U(1)$ *by* $SU(2)$ *on each bond (i.e.,* T *is replaced by a* $|\Lambda| \times |\Lambda|$ *matrix of* 2×2 *unitary matrices). Then the same conclusions hold for the 2-dimensional lattices of Theorem 1 and for the 3-dimensional ladder, i.e., the product of the unitary matrices around each face must be* $-I$ *in order to achieve the results stated in Theorem 2.*

Note that in the usual $U(1)$ case the translational symmetry is broken down from period one to period 2.



In the $SU(2)$ case, however, this can be avoided by using the $SU(2)$ matrices $i\sigma_x, i\sigma_y$ and $i\sigma_z$ on every bond in the x, y and z directions respectively. Period one is thereby retained.

Remark: The conclusion that $\Phi = \pi$ in Theorems 1 and 2 for an arbitrary shape is remarkable for the absence of "boundary effects". While the proof is purely analytic, the strong conclusion suggests something more geometric.

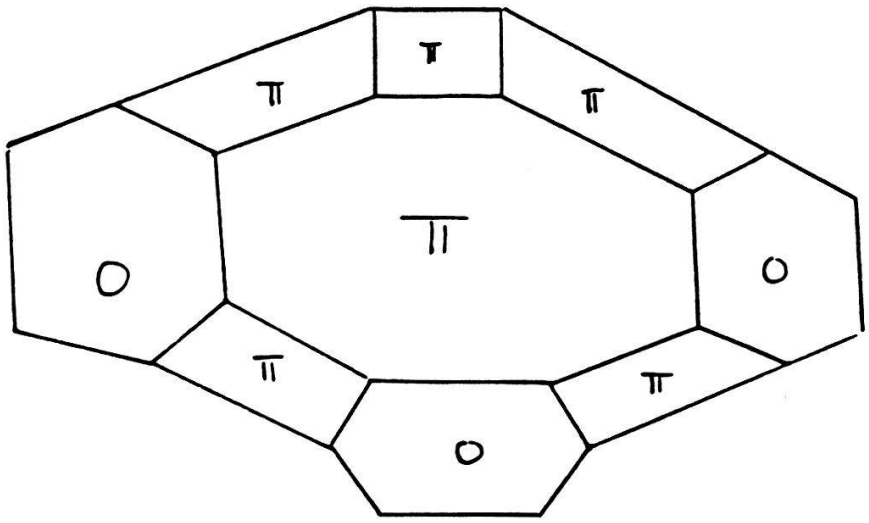
So far our theorems apply only to a limited class of Λ's. The following, about the determinant, is much more general. It was obtained in collaboration with Michael Loss.

THEOREM 3. *Let Λ be a planar lattice that is completely general except for the following requirements. (a). Λ is bipartite; (b). $|A| = |B|$. The number $|t_{xy}|$ is specified on each bond of Λ as before and we do not require $|t_{xy}| =$ constant.*

Then $|\det(T)|$ is maximized by the following choice of flux in each elementary cell of Λ (assuming Λ has no cut points; there is another rule if Λ has cut points):

(i) If the cell size is 4, 8, 12, 16, etc. then $\Phi = \pi$.
(ii) If the cell size is 6, 10, 14, etc. then $\Phi = 0$.

Since Φ is determined only modulo 2π, these conclusions can be rephrased as $\Phi = \pi(s-2)/2$ in a cell of size s. The conclusion agrees with generalized conjectures in [1] about the energy minimizing flux. Here is an example:



Remarks: (i). The requirement $|A| = |B|$ is really no restriction because $\det(T) = 0$ for every T when $|A| \neq |B|$. It is, of course, also possible that $\det(T) = 0$ for *every* choice of the fluxes, even if $|A| = |B|$.

(ii). It is truly remarkable that the conditions (i) and (ii) are totally local and that there are no "boundary effects". The determinant is certainly not a local quantity.

MAXIMIZING $E(T)$: We have concerned ourselves with minimizing $E(T)$ (or maximizing $G(T)$ and $|\det(T)|$). What about the opposite - maximizing $E(T)$? A natural conjecture would be that the choice $\Phi = 0$ achieves this for a square lattice, but this is

not always so. This somewhat surprising conclusion shows that the problem of minimizing $E(T)$ is somehow more natural than maximizing $E(T)$.

When Λ is a simple square consisting of four points it is indeed true that $\Phi = 0$ maximizes $E(T)$, and makes $G(T) = \det(T) = 0$. But the situation is quite different when Λ consists of two adjacent squares (i.e., Λ is a ladder with two cells and 6 sites). Here, the choice $\Phi = \pi/3$ in each cell gives the maximum $E(T)$ (which is -3.605) and gives $\det(T) = G(T) = 0$.

While there does not appear to be a simple rule for the ladder, the necklace is far more amenable. There, the choice $\Phi = 0$ in each square maximizes $E(T)$ and makes $G(T) = \det(T) = 0$.

NON-PLANAR LATTICES: The minimum energy problem is, of course, defined for an arbitrary lattice – although the Φ in eq. (7) cannot necessarily be interpreted as a physical magnetic flux. The problem is nevertheless interesting and the following theorem again hints at some underlying geometric mechanism.

Let Λ be any graph with some given hopping matrix T. This T may or may not be the T that minimizes $E(T)$. Since T is Hermitean it has orthonormal eigenvectors $\phi^1(x), \phi^2(x), \ldots, \phi^{|\Lambda|}(x)$, for $x \in \Lambda$, corresponding to the eigenvalues $\lambda_1(T), \ldots, \lambda_{|\Lambda|}(T)$. We can define a one-body density matrix ρ (or Green's function) corresponding to the half-filled band whose energy is given by (5). For x and $y \in \Lambda$ this is given by

$$\rho(x,y) = \sum_{\lambda_j < 0} \phi^j(x)\phi^j(y)^* + K(x,y). \tag{12}$$

The first term in (12) is clear, it is the contribution from the negative eigenvalues. The second term, $K(x,y)$, is ambiguous and can be present only if T has some zero eigenvalues. In that case K is a positive semidefinite Hermitean matrix composed of linear combinations of eigenvectors belonging to $\lambda = 0$. I.e., if $\lambda_n = \lambda_{n+1} = \ldots = \lambda_{n+m} = 0$ are the zero eigenvalues then

$$K(x,y) = \sum_{j=n}^{n+m} \sum_{k=n}^{n+m} C_{jk}\phi^j(x)\phi^k(y)^* \tag{13}$$

with C being some positive semidefinite $(m+1) \times (m+1)$ matrix. The choice of K is entirely a matter of taste and convenience.

THEOREM 4. *Suppose Λ is some bipartite lattice with T given and with ρ defined as in (12). Then there is a choice of K such that $Trace(\rho) = |\Lambda|/2$ and such that*

$$\rho(x,x) = 1/2 \quad \textit{for every } x \in \Lambda$$
$$\rho(x,y) = 0 \quad \textit{if } x \neq y \textit{ and if } x,y \in A \textit{ or if } x,y \in B.$$

This is rather surprising for it says that the density $\rho(x,x)$ is *exactly* $1/2$ on every site, no matter how bizarre Λ may be. Thus, long-range order, if it exists, has to be purely off-diagonal for a half-filled band. Furthermore, if $\rho(x,y)$ is regarded as some measure of correlation, then the $A-A$ and the $B-B$ correlations vanish.

INTERACTING ELECTRONS. Naturally, it is desirable to know whether any of the foregoing survives the introduction of normal interactions. Specifically, it would be nice to be able to study the Hubbard model with magnetic fields. I cannot achieve this goal but I can say something about the Falicov-Kimball model [2] (or what Kennedy and I, unaware of [2], called the static model [3]).

A one-body potential energy is added to the Hamiltonian in (3) and our new Hamiltonian is

$$H = \sum_{x,y\in\Lambda} t_{xy} c_x^\dagger c_y + U \sum_{x\in\Lambda} W(x) c_x^\dagger c_x. \tag{14}$$

Here $U > 0$ is fixed (we can also treat $U < 0$ by a simple hole-particle transformation) and $W(x)$ satisfies

$$0 \le W(x) \le 1 \qquad \text{for all } x \in \Lambda. \tag{15}$$

Note: (15) constitutes a generalization of the original model in [2] and [3]. There, the restriction $W(x) = 0$ or 1 was made. One could then make the following interpretation.

$W(x) = +1 \quad \Leftrightarrow$ a "nucleus" or an electron of "opposite spin" is is present at x

$W(x) = 0 \quad \Leftrightarrow$ an empty site.

We wish to find the ground state of H under the condition

$$\sum_{x\in\Lambda} W(x) + N_e \ge |\Lambda| \tag{16}$$

with $N_e \equiv \sum_{x\in\Lambda} c_x^\dagger c_x$. I.e., the band (including both kinds of "particles") is at least half full.

It was proved in [3] and in [4] that when we restrict to $W(x) = 0$ or 1 then the ground state for a *connected bipartite* lattice occurs precisely when $N_e = |A|$ and $W(x) = 1$ for $x \in B$, and the reverse. Thus, there are two ground states. The proof in [2] (and the conclusion) extends to the general case (15) and to an arbitrary choice of T (as long as Λ is connected).

Now I should like to discuss the same problem but with the addition of a magnetic field. Namely $|t_{xy}|$ is given but θ_{xy} has to be determined so as to minimize the ground state energy. The following is the relevant generalization of Theorems 1 and 2.

THEOREM 5. *Let Λ be a 2- or 3-dimensional ladder or a necklace with $|t_{xy}| = 1$ on all the bonds. Under conditions (15) and (16) there are precisely two ways to minimize the ground state energy of H in (14). In both*

$$\Phi = \pi$$

in all cells (or faces). The two choices of W and N_e are:

(i) $W(x) = 1$ *for* $x \in B, W(x) = 0$ *for* $x \in A$ *and* $N_e = |A|$.

(ii) The reverse, i.e., A and B are interchanged.

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REFERENCES

[1] Y. Hasegawa, P. Lederer, T.M. Rice and P.B. Wiegmann, Phys. Rev. Lett. **63**, 907 (1989).

[2] L.M. Falicov and J.C. Kimball, Phys. Rev. Lett. **22**, 997 (1969).

[3] T. Kennedy and E.H. Lieb, Physica **A138**, 320 (1986).

[4] U. Brandt and R. Schmidt, Z Phys. **B67**, 43 (1986).