THE FLUX PHASE OF THE HALF-FILLED BAND

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Abstract: The conjecture is verified that the optimum, energy minimizing magnetic flux for a half-filled band of electrons hopping on a planar, bipartite graph is π per square plaquette. We require *only* that the graph has periodicity in one direction and the result includes the hexagonal lattice (with flux 0 per hexagon) as a special case. The theorem goes beyond previous conjectures in several ways: (1) It does not assume, a-priori, that all plaquettes have the same flux (as in Hofstadter's model); (2) A Hubbard type on-site interaction of any sign, as well as certain longer range interactions, can be included; (3) The conclusion holds for positive temperature as well as the ground state; (4) The results hold in $D \geq 2$ dimensions if there is periodicity in $D-1$ directions (e.g., the cubic lattice has the lowest energy if there is flux π in each square face).

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The flux phase conjecture states that the ground state (g.s.) energy minimizing magnetic flux through a square, planar lattice on which free electrons hop is π per plaquette when the electron filling factor is 1/2 [1-4]. (Zeeman terms are excluded.) This conjecture, along with extensions to positive temperature, higher dimensional geometries and allowance for some electron-electron interactions, will be proved here.

If the sites of the lattice are interpreted as atoms in a solid then flux π would correspond to magnetic fields available only on neutron stars. The significance of the flux phase is thus not primarily as a literal interpretation in terms of physical magnetic fields. One interesting interpretation concerns mean field calculations connected with superconductivity. The main interest, however, in the author's view, is that it shows that diamagnetism (which states that the optimal flux is zero — and which is correct when the electron density is very small) can be reversed when the density is high. Indeed, it can be maximally reversed, as in this case (since flux on a lattice is determined only modulo 2π). Thus, there is a peculiar, non-intuitive and poorly understood effect of the Pauli principle on the way in which orbital motion interacts with magnetic fields. It has been studied extensively [5-13]. See [10] for some history.

To define things precisely, we start with a general *finite graph* Λ, which is a collection of $|\Lambda|$ sites and certain bonds denoted by xy with x and y in Λ and $x \neq y$. A positive weight $|t_{xy}| = |t_{yx}|$ is specified in advance for each bond. By convention $t_{xx} = 0$. The hopping amplitude is then $t_{xy} = |t_{xy}| \exp[i\phi(x,y)]$, with $\phi(x,y) = -\phi(y,x)$ for hermiticity, and the problem is to find the numbers $\phi(x,y)$ that minimize the total electronic ground state energy (when $\beta = 1/kT = \infty$) or free energy (when $\beta < \infty$).

A *circuit* in Λ is a sequence of points $x_1, x_2, \ldots, x_n, x_1$ with $t_{x_i x_{i+1}} \neq 0$ for all i. The flux through this circuit is $\sum_{i=1}^{n} \phi(x_i, x_{i+1})$ (mod2π). It is a fact [10] that the spectrum of the hermitian matrix $T = \{t_{xy}\}_{x,y\in\Lambda}$ depends on the ϕ's *only* through the fluxes. This is also true of the Hamiltonians below. No a priori assumption is made that the flux need be the same in all plaquettes; indeed, the flux is not even assumed to be the same for up- and down-spin electrons. We allow different $|t_{xy}|$'s and $\phi(x,y)$'s for the up- and down-spin electrons. We denote these by $T^{\uparrow}, T^{\downarrow}$. Thus, our results apply to the Falicov-Kimball model (where $T^{\downarrow} = 0$), for example.

The *electronic kinetic energy operator*, in second-quantized notation, is

$$K = -\sum_{x,y\in\Lambda} t^{\uparrow}_{xy} c^{\dagger}_{x\uparrow} c_{y\uparrow} + t^{\downarrow}_{xy} c^{\dagger}_{x\downarrow} c_{y\downarrow}. \tag{1}$$

The c's satisfy the fermion anticommutation relations $\{c^{\dagger}_{x\sigma}, c_{y\tau}\} = \delta_{xy}\delta_{\sigma\tau}$, $\{c_{x\sigma}, c_{y\tau}\} = 0$. The electron number is $N = N_{\uparrow} + N_{\downarrow}$ and $N_\sigma = \sum_{x\in\Lambda} n_{x\sigma}$ with $n_{x\sigma} = c^{\dagger}_{x\sigma} c_{x\sigma}$. If the Hamiltonian H equals K, then the ground state energy E_0 would be $E_0 = \sum_{\lambda<0} \lambda(T^{\uparrow}) + \sum_{\lambda<0} \lambda(T^{\downarrow})$, i.e., the sum of the negative eigenvalues, $\lambda(T)$, of the matrices $T^{\uparrow}$ and $T^{\downarrow}$.

For *bipartite graphs* (i.e., $\Lambda = A \cup B$, $A \cap B = \emptyset$ and $t_{xy} = 0$ unless $x \in A$, $y \in B$ or $x \in B$, $y \in A$) E_0 is achieved when $N = |\Lambda|$, and hence the appelation half filled band, since $0 \leq N \leq 2|\Lambda|$ in general. In the Hubbard model $H = K + W^0$,

$$W^0 = \sum_{x\in\Lambda} U_x (n_{x\uparrow} - \tfrac{1}{2})(n_{x\downarrow} - \tfrac{1}{2}), \tag{2}$$

but we can also add certain longer range density-density interactions, W^d and spin-spin interactions W^s to be specified later, of the form (with $w^k_{xy} = w^{k*}_{xy} = w^k_{yx}$, $k = d, 1, 2, 3$ and S^j being Pauli matrices)

$$\begin{aligned} W^d &= \sum_{x,y\in\Lambda} w^d_{xy} (n_{x\uparrow} + n_{x\downarrow} - 1)(n_{y\uparrow} + n_{y\downarrow} - 1) \\ W^s &= \sum_{j=1}^{3} \sum_{x,y\in\Lambda} \sum_{\sigma,\tau,\mu,\lambda} w^j_{xy} (c^{\dagger}_{x\sigma} S^j_{\sigma\tau} c_{x\tau})(c^{\dagger}_{y\mu} S^j_{\mu\lambda} c_{y\lambda}). \end{aligned} \tag{3}$$

W^0, W^d and W^s are invariant under the unitary hole-particle (h-p) transformation τ, with $\tau c_{x\sigma}\tau^{-1} = c^\dagger_{x\sigma}$. The kinetic energy operator with complex T's satisfies

$$\tau K(T^\uparrow, T^\downarrow)\tau^{-1} = K(-T^{\uparrow *}, -T^{\downarrow *}) \tag{4}$$

where T^* denotes the complex conjugate matrix $t_{xy} \to t^*_{xy} = t_{yx}$.

The grand-canonical partition function of our system, which we want to maximize, is $Z = \mathrm{Tr}\exp[-\beta H]$ at inverse temperature β. By h-p symmetry, $\langle N\rangle \equiv \mathrm{Tr}Ne^{-\beta H}/Z$ is $|\Lambda|$, which is the half-filled band. The $\beta \to \infty$ limit is discussed at the end.

Henceforth, all graphs will be bipartite, in which case all elementary circuits contain an even number of sites and bonds. The original flux phase conjecture is that when $H = K$, $N = |\Lambda|$ and Λ is planar the optimum choice of fluxes is π in every circuit containing 0(mod4) sites and 0 in circuits with 2(mod4) sites.

Several cases of this were proved in [9, 10] and it was pointed out in [10] that the conjecture can not always hold for *arbitrary* values of $|t_{xy}|$. It depends on Λ. Despite this caveat, however, it was proved in [10] that log $[\det(T^2)] = \sum_j \log[\lambda_j(T)^2]$ is maximized when the fluxes accord with the conjecture. This is true for an *arbitrary* bipartite, planar graph with *arbitrary* $|t_{xy}|$'s. (On any bipartite graph, the nonzero eigenvalues of T come in opposite pairs $\lambda, -\lambda$.)

The *generalized flux phase conjecture* is that the above choice is also optimal for $H = K + W^0 + W^d + W^s$ and for all $\beta \leq \infty$. We shall prove this here for graphs that have a certain periodicity. The usual square lattice with periodic boundary conditions is included. The result holds also for higher dimensional, non-planar graphs. The type of graphs Λ considered here is illustrated in Fig. 1 for the planar case. Λ is wrapped on a cylinder, i.e., the sites at the right end are identified with the sites on the left. The $|t_{xy}|$'s on the vertical edges must be periodic, i.e., they are allowed to vary in an arbitrary way along each column, but all the columns must be identical. The horizontal $|t_{xy}|$'s can also vary as we move vertically but they are only required to have period 2 in the horizontal direction, i.e., every *second* column of horizontal edges must be the same. Thus, if we erase the horizontal edges 1, 3, 5, etc. from every second column and if we erase edges 2, 4, 6, etc. from the remaining columns in between, the hexagonal lattice is obtained. Our result includes this case, and flux π in each (imaginary) square then implies flux 0 in each hexagon. Octagons, decagons, etc. can also be included provided periodicity 2 is maintained. We can, if we wish, insert vertical edges connecting the bottom row to the top row, as indicated by the vertical arrows in Fig. 1. Λ will no longer be planar, but that does not matter.

An easier way to state the periodicity requirements is to cut Λ at the two dashed lines, called P in Fig. 1. The two half-cylinders (as well as the $|t_{xy}|$'s on the edges) are required to be mirror images of each other. The $|t_{xy}|$'s on the edges that intersect the dashed lines are arbitrary because each is its own mirror image. We then say that $|T|$ is *reflection symmetric* with respect to the cutting lines, P, through the bonds. Our theorem says that when $H = K$ the optimum flux is then π for those squares containing the cutting lines. If the $|t_{xy}|$'s are reflection symmetric w.r.t. *every* choice of cutting lines – which is equivalent to the above periodicity requirement – then flux π will be optimal in *every* square of Λ.

The periodicity of the $|t_{xy}|$'s mentioned above is *not* needed for the theorem below. Only reflection symmetry is needed. The periodicity comes in when we wish to insure flux π in *every* plaquette of Λ. This is achieved by repeated reflection in hyperplanes in the standard way [14-15]; indeed, one can easily derive the usual chessboard estimates [14].

In fact Λ could be built in a similar way out of D-dimensional (hyper)cubes instead of squares. Cutting lines become cutting $(D-1)$-dimensional hyperplanes, and reflection symmetry is generalized in an obvious way. Our theorem will then state that the optimal flux in each two-dimensional square plaquette of the (hyper)cubic lattice is π in every plaquette cut by the hyperplanes. As in the $D = 2$ case, flux π will be optimal in *every* plaquette if we have periodicity in $D - 1$ directions.

Returning to the two-dimensional situation (with obvious generalization to $D > 2$) we require only that the U_x's in W^0 be constant in the horizontal direction (as are the $|t_{xy}|$'s on vertical edges). As for w^k_{xy} in W^d and W^s, they are required to be reflection positive for reflection in vertical planes (the dashed lines, P, in Fig. 1), as explained below. The inclusion of W^d and W^s is mainly for completeness and nothing essential will be lost by setting $W^d = W^s = 0$.

In general, a Hamiltonian, H, can be written (with respect to a cutting hyperplane, P) as

$$H = H_L + H_R + H_{\rm int} \tag{5}$$

where H_L is all the terms involving sites in the left half-cylinder, H_R involves right half-cylinder sites and $H_{\rm int}$ involves both. The subscripts L, R, and *int* will also be used for the separate pieces, e.g. $K_L, K_R, K_{\rm int}$, etc. Associated with the left Hamiltonian H_L is a right Hamiltonian, $\Theta(H_L)$, which is obtained from H_L by three steps: *the unitary transformation $\mathcal{R}$ generated by geometric reflection through the plane P; hole-particle transformation τ; and complex conjugation $*$.* $\Theta(H_L) = (\tau\mathcal{R}(H_L)\tau^{-1})^*$. This notion of *operator reflection* can be applied to any operator, A_L in the left algebra (i.e., A_L is a polynomial in the operators $c_{x\sigma}, c^\dagger_{x\sigma}$ with x in the left half-cylinder). In particular $\theta(c_{l\sigma}) = c^\dagger_{r\sigma}$. A similar definition holds for the left Hamiltonian $\Theta(H_R)$ and, clearly, $\Theta(\Theta(H_L)) = H_L$. Note, from (4), that $\Theta(K_L) = -\mathcal{R}(K_L),\ \Theta(W^\alpha) = \mathcal{R}(W^\alpha),\ \alpha = 0, d, s$.

Reflection positivity of w_{xy} means that it is symmetric under reflections and, for x in the left and y in the right half-cylinder, w_{xy} can be written as a sum (or integral) of functions of the form $a(x)a(\mathcal{R}y)^*$. In other words, $W^d_{\rm int}, W^s_{\rm int}$ are sums (or integral) of operators of the form $-A_L\Theta(A_L)$, where the $(-)$ in $W^d_{\rm int}$ comes from $\tau(n_{x\uparrow}+n_{x\downarrow}-1)\tau^{-1} = 1-n_{x\uparrow}-n_{x\downarrow}$, and similarly for $W^s_{\rm int}$. An important example is $w_{xy}=w>0$ if x,y are nearest neighbors, $w_{xy}=0$ otherwise. Such a W^s is antiferromagnetic. See [14].

Concerning $K_{\rm int}$, we note that it is generally not invariant under the three operations. However, with l and r denoting a generic left, right image pair cut by P, we are at liberty to choose $\Theta(l,r)=0$, i.e., $t_{lr}=|t_{lr}|\geq 0$, and we do so. (Note: to simplify the notation the symbols, $\uparrow$ and σ, will not be indicated.) This is so because a simple gauge transformation $c_r\to\exp[-i\Theta(l,r)]c_r$ makes $t_{lr}>0$ without changing any fluxes. No circuits are involved. This choice of phase for t_{lr} is only a convention, for it does not change any physics, but it is important for (6) and (7) below.

With the foregoing convention for $H_{\rm int}$, the Hamiltonian is said to be *reflection symmetric* if $\Theta(H_L)=H_R$. The flux π theorem will be a corollary of the following lemma.

LEMMA (Reflection positivity). *With H as given in (5) with respect to some hyperplane, P, assume that $K_{\rm int}$ satisfies the above positivity convention. Assume also that $W^d_{\rm int}$ and $W^s_{\rm int}$ are reflection positive. Then, for each $\beta\geq 0$ and with $H_{\rm int}$ fixed,*

$$Z(H_L,H_R)^2\leq Z(H_L,\Theta(H_L))Z(\Theta(H_R),H_R), \tag{6}$$

where $Z(H_L,H_R)\equiv{\rm Tr}\exp[-\beta H]$. Moreover, if $H_R=\Theta(H_L)$ and if A_L (resp. A_R) is any even operator in the left (resp. right) algebra (e.g., A_L is a sum of monomials in $c^{\#}_{x\sigma}$ of even degree) then

$$|{\rm Tr}A_LA_Re^{-\beta H}|^2\leq {\rm Tr}A_L\Theta(A_L)e^{-\beta H}\,{\rm Tr}\Theta(A_R)A_Re^{-\beta H}\quad . \tag{7}$$

Proof: Use the Lie-Trotter formula to approximate $e^{-\beta H}$ as a product of $M\gg 1$ factors $V=V_{\rm int}V_LV_R$, i.e., $e^{-\beta H}=\lim_{M\to\infty}V^M$, where $V_{\rm int}=(1-\beta H_{\rm int}/M)$, $V_L=\exp[-\beta H_L/M], V_R=\exp[-\beta H_R/M]$. Notice that V_L contains only even polynomials in the $c^{\#}$'s, and so V_L commutes with every right operator (including odd operators). Likewise, V_R commutes with all left operators.

If the M factors of $V_{\rm int}$ are multiplied out we obtain for V^M a sum of terms, each having the form $X=a_1V_LV_Ra_2V_LV_Ra_3V_LV_R\cdots a_MV_LV_R$ and each a_i has one of three forms: (i) $A_L\Theta(A_L)$, with A_L an even operator or (ii) $c^\dagger_l c_r$ or (iii) $-c_l c^\dagger_r$. Our strategy is to move all the left operators to the left *without* changing the order either of the left operators among themselves or the right operators. The operators A_L commute with all the right operators and cause no difficulty. The difficult point is that the $c^{\#}_l$ operators have to move through the $c^{\#}_r$ operators to their left, and each such move gives rise to a -1 factor.

I claim that either $\mathrm{Tr}X = 0$ or else the number of -1 factors is even. To see this note that by particle conservation (and the particle conserving nature of V_L and V_R) the number of $c_l^\dagger c_r$ factors must equal the number of $c_l c_r^\dagger$ factors if $\mathrm{Tr}X \neq 0$. Call this common number J. The number of -1 factors is independent of the order of these $2J$ factors and their order relative to the $A_L\Theta(A_L)$ factors. The first $c_l^\#$ must move through zero $c_r^\#$'s. The second $c_l^\#$ moves through one $c_r^\#$, etc.. Thus, the number of -1 factors is $0+1+2+\cdots+(2J-1) = J(2J-1)$. On the other hand, each $c_l c_r^\dagger$ term carries a -1 factor and there are J of these. Altogether there are $J + J(2J-1) = 2J^2 = 0(\mathrm{mod}2)$ factors of -1, as claimed.

In brief, X can be brought into the form $X = X_L X_R$ with X_L and X_R even operators. Since $\mathrm{Tr}\mathbf{1} = 4^{|\Lambda|}$, we have $4^{|\Lambda|}\mathrm{Tr}X = \mathrm{Tr}X_L\mathrm{Tr}X_R$. Moreover, $(\mathrm{Tr}X_L)^* = \mathrm{Tr}\Theta(X_L)$ and thus $|\mathrm{Tr}X_L|^2 = \mathrm{Tr}X_L\Theta(X_L)$. Now, denoting the various X's by X^α, we have $|\mathrm{Tr}V^M|^2 = |\sum_\alpha \mathrm{Tr}X^\alpha|^2 = 4^{-2|\Lambda|}|\sum_\alpha \mathrm{Tr}X_L^\alpha \mathrm{Tr}X_R^\alpha|^2 \leq 4^{-2|\Lambda|}\sum_\alpha|\mathrm{Tr}X_L^\alpha|^2\sum_\alpha|\mathrm{Tr}X_R^\alpha|^2 = \sum_\alpha \mathrm{Tr}X_L^\alpha\Theta(X_L^\alpha)\sum_\alpha \mathrm{Tr}X_R^\alpha\Theta(X_R^\alpha) \to Z(H_L,\Theta(H_L))Z(H_R,\Theta(H_R))$. (7) is obtained in the same way. QED

THEOREM (Flux π is optimal). *Assume the $|t_{xy}^{\uparrow,\downarrow}|$ are reflection invariant w.r.t. P. Assume also that $\Theta(W_L^\alpha) = W_R^\alpha$ and W_{int}^α is reflection positive, $\alpha = 0, d, s$. Then Z is maximized by putting flux π in each square face of Λ that intersects P.*

Proof: We make the gauge transformation above so that K_{int} has $t_{lr} = |t_{lr}|$. From (6), we have that when H_L, H_R is optimal, so is $H_L, \Theta(H_L)$ and $\Theta(H_R), H_R$. But the statement $K_R = \Theta(K_L)$ implies the flux π condition by (4). QED

Remarks: (i). It is interesting to note that (6) can also be used to show that when the fluxes are fixed at π and one varies over the $|t_{xy}|$, the lowest energy is attained in a reflection symmetric configuration of $|t_{xy}|$. A one-dimensional version of the lemma was proved and used in [16] to study the Peierls instability for the Hubbard model on a ring.

(ii). The lemma and theorem say that flux π for $T^\uparrow$ and $T^\downarrow$ is optimal. If we fix $\phi^\uparrow(x,y)$, we are then free to choose $\phi^\downarrow(x,y) = \phi^\uparrow(x,y)$, since any other choice with flux π differs from $\phi^\uparrow(x,y)$ by a trivial gauge transformation, $c_{x\downarrow} \to e^{i\mu(x)}c_{x\downarrow}$. Thus, when $|t_{xy}^\uparrow| = |t_{xy}^\downarrow|$, the minimizer can have $T^\downarrow = T^\uparrow$, thereby preserving $SU(2)$ invariance.

(iii). To discuss the ground state we let $\beta \to \infty$. Do we get $N = |\Lambda|$ or does the g.s. belong to $N = |\Lambda| + m$ and $N = |\Lambda| - m$ with $m > 0$? In the Falicov-Kimball model, generally, the g.s. has $N = 2|A|$ and $N = 2|B|$, as the only choices [17] (but note that $2|A| = 2|B| = |\Lambda|$ in our case). In the following cases I can also prove that at least one g.s. has $N = |\Lambda|$.

First, assume reflection symmetry and positivity w.r.t. *all* hyperplanes parallel to P, so that we are now looking at a K with flux π in *every* plaquette of Λ. After a trivial gauge transformation, this condition can be realized with real T, which we assume henceforth.

Next, assume $T^\uparrow = T^\downarrow$, so that $SU(2)$ invariance holds. Third, assume $W^d = W^s = 0$, i.e., the Hubbard model. As is well known, we can then construct another set of $SU(2)$ generators — the *pseudospin.* (See [18] and, for more details, [19].) By using the spin and pseudospin raising operators $\sum_x c^\dagger_{x\uparrow} c_{x\downarrow}$, $\sum_x (-1)^x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow}$, (with $(-1)^x = +1$ for $x \in A$, -1 for $x \in B$) and their adjoints, one can conclude that the absolute ground state belongs to $N = |\Lambda|$ or $N = |\Lambda| \pm 1$.

Finally, to show that the g.s. has $N = |\Lambda|$, assume either that $U_x \leq 0$ for all x or $U_x \geq 0$ for all x. We can then use spin-space reflection positivity [17] in *Fock space*, together with the evenness of $|\Lambda|$ in our case, to infer $N = |\Lambda|$. (This reflection positivity tells us that if a g.s. has numbers $N_\uparrow = \lambda, N_\downarrow = \mu$ then there are ground states with (λ, λ) and (μ, μ). Thus, if $|\Lambda| = 2m$ and $N = |\Lambda| - 1$, so that $N_\uparrow = m,\ N_\downarrow = m - 1$, then there is also an (m, m) g.s..) If all $U_x \neq 0$, the g.s. is unique [18].

Extensions: The flux phase for the half-filled band has been proved here for a large class of Hamiltonians, including the ones common in the physics literature. The proof is sufficiently simple that it obviously applies to many other models.

One generalization is to fermions with $n \neq 2$ colors, i.e. from $SU(2)$ to $SU(n)$.

Certain specialized forms of electron-phonon interactions can be included.

Another generalization is to $SU(2)$ instead of $U(1)$ gauge fields [15, 20]. Thus, $t_{xy} \sum_\sigma c^\dagger_{x\sigma} c_{y\sigma}$ is replaced by $|t_{xy}| \sum_{\sigma\tau} c^\dagger_{x\sigma} U^{\sigma\tau}_{xy} c_{y\tau}$ with $|t_{xy}|$ given, as before, and with $U_{xy} \in SU(2)$ to be determined. (Even more generally, we can replace $t^\uparrow_{xy} c^\dagger_{x\uparrow} c_{y\uparrow} + t^\downarrow_{xy} c^\dagger_{x\downarrow} c_{y\downarrow}$ by $\sum_{\sigma\lambda\tau} c^\dagger_{x\sigma} M^{\sigma\lambda}_{x;xy} |t^\lambda_{xy}| M^{\lambda\tau}_{y;xy} c_{y\tau}$ where $M_{x;xy} \in SU(2)$ and $|t^\lambda_{xy}|$ is given; in this case the $SU(2)$ matrix associated with xy is $U_{xy} = M_{x;xy} M_{y;xy}$.) Again, we will find that the energy is minimized by flux π in each plaquette, i.e., the product of the four matrices around a plaquette satisfies $U_{xy} U_{yz} U_{zw} U_{wx} = -1$.

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FIGURE CAPTION

FIG. 1. Typical 2D lattice with horizontal periodic boundary conditions (left boxes = right boxes). Different bond weights illustrate the requirement of horizontal periodicity 2. Dashed lines (P) are a reflection plane. A generic left-right pair of sites is indicated by l, r.