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FLUXES, LAPLACIANS AND KASTELEYN'S THEOREM

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Abstract: The following problem, which stems from the "flux phase" problem in condensed matter physics, is analyzed and extended here: One is given a planar graph (or lattice) with prescribed vertices, edges and a weight $|t_{xy}|$ on each edge (x, y). The flux phase problem (which we partially solve) is to find the real phase function on the edges, $\theta(x, y)$, so that the matrix $T := \{|t_{xy}|\exp[i\theta(x, y)]\}$ minimizes the sum of the negative eigenvalues of $-T$. One extension of this problem which is also partially solved is the analogous question for the Falicov-Kimball model. There one replaces the matrix $-T$ by $-T + V$, where V is a diagonal matrix representing a potential. Another extension of this problem, which we solve completely for planar, bipartite graphs, is to maximize $|\det T|$. Our analysis of this determinant problem is closely connected with Kasteleyn's 1961 theorem (for arbitrary planar graphs) and, indeed, yields an alternate, and we believe more transparent proof of it.

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I. INTRODUCTION

The genesis of this paper was an attempt to understand a problem in condensed matter physics related to questions about electron correlations, superconductivity and electron-magnetic field interactions. The basic idea, which was proposed a few years ago is that a magnetic field can lower the energy of electrons when the electron density is not small. Certain very specific and very interesting mathematical conjectures about eigenvalues of the Laplacian were made and the present paper contains a proof of some of them. Furthermore, those conjectures lead to additional natural conjectures about determinants of Laplacians which we both present and prove here. It is not clear whether these determinantal theorems have physical applications but they might, conceivably in the context of quantum field theory. Some, but not all, of the results given here were announced earlier in [LE].

The setting is quantum mechanics on a graph or lattice. (All our terminology will be defined precisely in the sequel.) Physically, the vertices of our graph Λ can be thought of either as a discretization of space (i.e. replace the Laplacian by a finite difference operator) or they can be seen as locations of atoms in a solid. There are $|\Lambda|$ vertices. In the atomic interpretation the edges become electron bonds joining the atoms, and the model is known as the tight-binding model or Hückel model. The natural Laplacian $\mathcal{L}$ associated with Λ is a $|\Lambda| \times |\Lambda|$ matrix indexed by the vertices of Λ and whose diagonal elements satisfy $-\mathcal{L}_{xx}$ = number of attached edges (or valency) of vertex x. The other elements are $\mathcal{L}_{xy} = 1$ if x and y are connected by an edge, and zero otherwise.

For us it is more convenient to consider the matrix $\widehat{\mathcal{L}}$ which is the Laplacian without the diagonal term, i.e., $\mathcal{L}_{xx}$ is replaced by zero. In the context of graph theory $\widehat{\mathcal{L}}$ is also known as the adjacency matrix. There are three excuses for this: (i) in the solid state context $\widehat{\mathcal{L}}$ is the natural object because atoms do not bond to themselves; (ii) most of the graphs that are considered in the physics literature have constant valency, so $\widehat{\mathcal{L}}$ and $\mathcal{L}$ have the same spectrum modulo a constant which is equal to this valency; (iii) mathematically $\widehat{\mathcal{L}}$ seems to be the more natural object — from our point of view, at least — because its spectrum on a bipartite graph is always a union of pairs λ and $-\lambda$ (when $\lambda \neq 0$), as explained in Sect. II. The spectrum of $\mathcal{L}$ generally does not have any such symmetry.

We label the eigenvalues of $\widehat{\mathcal{L}}$ by $\lambda_1(\widehat{\mathcal{L}}) \geq \lambda_2(\widehat{\mathcal{L}}) \geq \ldots$. The Hamiltonian for a single electron is $-\mathcal{L}$ or $-\widehat{\mathcal{L}}$, and we take it to be $-\widehat{\mathcal{L}}$ here. If our system has M *free* electrons the rule of quantum mechanics is that the eigenvalues of our system are all the possible sums of M of the $(-\lambda_i)$'s in which each $-\lambda_i$ is allowed to appear at most twice in the sum. There are $\binom{2|\Lambda|}{M}$ eigenvalues. In particular, if $M = 2N$ the smallest eigenvalue is

$$E_0^{(N)} = -2\sum_{j=1}^{N} \lambda_j(\widehat{\mathcal{L}}). \tag{1.1}$$

A (spatially varying) magnetic field is now added to the system in the following way. $\widehat{\mathcal{L}}_{xy}$ is replaced by $T_{xy} = \widehat{\mathcal{L}}_{xy} \exp[i\theta(x,y)]$, with θ real and with $\theta(x,y) = -\theta(y,x)$ so that T is Hermitian. The function $\theta(x,y)$ is interpreted physically as the integral of a magnetic vector potential from the point x to the point y. This T is the discrete analogue of replacing the Laplacian on $\mathbb{R}^n$ by $(\nabla - iA(x))^2$ (with $\nabla =$ gradient), which is the Laplacian on a $U(1)$ bundle.

The central question that we address is this: *What choice of θ minimizes $E_0^{(N)}$ for a given N?*

In order to appreciate this question, consider the $N = 1$ case. Then, $\theta \equiv 0$ is an answer because (with ϕ being the normalized largest eigenvector of T) $\lambda_1(T) = \sum \overline{\phi}_x \phi_y \widehat{\mathcal{L}}_{xy} \exp[i\theta(x,y)] \leq \sum |\phi_x||\phi_y| \widehat{\mathcal{L}}_{xy} \leq \lambda_1(\widehat{\mathcal{L}})$. This proof that $\theta \equiv 0$ is optimum also works in a more general setting, namely for the lowest eigenvalue of the "Schrödinger operator" $-T + V$, where V is any real diagonal matrix. Again, $T = \widehat{\mathcal{L}}$, or $\theta \equiv 0$, minimizes $-\lambda_1(T - V)$. The same is true in $\mathbb{R}^n$ for $-(\nabla - iA(x))^2 + V(x)$; the minimum occurs when $A(x) \equiv 0$. This conclusion is known as the *diamagnetic inequality* and states, physically, that "a magnetic field raises the energy".

It was discovered by [AM] and [KG] that the situation can be quite different when N is close to $\frac{1}{2}|\Lambda|$. (When $N = |\Lambda|, E_0^{(N)} = \mathrm{Tr} T = 0$ for all θ; hence $N = \frac{1}{2}|\Lambda|$ is the most extreme case.) Since then, the problem has been investigated for various lattices and N's by several authors such as [BR], [BBR], [HLRW], [RD], [WP], [WWZ] some of whom consider it to be important in the theory of high temperature superconductivity. [HLRW], for example, start with the square lattice $\mathbf{Z}^2$, take Λ to be a large rectangular subset of $\mathbf{Z}^2$, and then let $|\Lambda| \to \infty$ and $N \to \infty$ with $N/|\Lambda|$ fixed. They also take the magnetic flux (which is the sum of the θ's around the edges of a face, and which is defined in Sect. II) to have the *same value* in each square box of $\mathbf{Z}^2$. On the basis of their numerical evidence they proposed that flux/box $= 2\pi N/|\Lambda|$ is the optimal choice. In [AM] the term "flux phase" was introduced to describe this state in which the presence of a magnetic field lowers the energy.

It should be pointed out that the spectrum of $\widehat{\mathcal{L}}$ for $\mathbf{Z}^2$ as a function of constant flux/box was discussed by many authors for many years; it was Hofstadter [HD] who grasped the full beauty of this object — which is anything but a continuous function of the flux and which is full of gaps — and called it a "butterfly". The spectrum can be found by solving a one-dimensional difference equation, due to Harper [HP], which is a discrete analogue of , but more complicated than, Mathieu's equation. The spectrum is such a complicated function of the flux that it is difficult to decide on the optimum flux for a given N.

The most striking case is $N/|\Lambda| = \frac{1}{2}$, or $M = |\Lambda|$, which is called the **half-filled band**. The optimal flux is supposed to be π, which is the maximum possible flux since flux is determined only modulo 2π and since flux and $-$flux yield identical spectra. It is this case that we investigate in this paper in an attempt to verify the rule just stated and which appears in [AM], [HLRW], [RD]. We are completely successful only in some special cases, but we have been able to generalize the problem in several interesting directions. For example, one of our main results is Theorem 3.1. It completely solves the problem for determinants (i.e. for products of eigenvalues instead of sums of eigenvalues) on bipartite planar graphs.

Our determinant theorem turns out to be closely related to Kasteleyn's famous 1961 theorem about planar graphs, which allowed him to solve (in principle) the dimer problem and Ising model for all planar graphs. Our route, via fluxes, gives an alternative proof of Kasteleyn's theorem and, we believe, a more transparent one. This is presented in the Appendix.

The setting we adopt is a general graph Λ, with no particular symmetry such as $\mathbf{Z}^2$ enjoys, and an *arbitrary*, but *fixed* amplitude $|t_{xy}| > 0$ given on each edge ($|t_{xy}| = 1$ in the case of $\widehat{\mathcal{L}}$). The problem is to determine θ and $T := \{t_{xy}\}_{x,y\in\Lambda}$ with $t_{xy} = |t_{xy}| \exp[i\theta(x,y)]$ so as to minimize the (absolute) **ground state energy**

$$E_0(T) := -\mathrm{Tr}|T| - \mathrm{Tr}T = -\mathrm{Tr}|T|, \tag{1.2}$$

with Tr = Trace. The right side of (1.2) is twice the sum of the negative eigenvalues of $-T$. For a bipartite graph this is the sum of the $|\Lambda|/2$ or $(|\Lambda|-1)/2$ lowest eigenvalues of $-T$.

A word has to be said here about different definitions of ground state energy. Electrons have two spin states available to them and the Pauli exclusion principle states that each eigenstate of $-T$ can be occupied by at most one electron of each kind. Thus, each eigenstate can be occupied by 0 or 1 (twice) or 2 electrons. That explains the factor of 2 in (1.1): there the lowest N eigenstates of $-T$ are each occupied by two electrons. Our definition of $E_0(T)$ in (1.2) is the absolutely lowest ground state energy and corresponds to the electron number being twice the number of negative eigenvalues. On the other hand, the half-filled band would have the electron number equal to $|\Lambda|$ by definition. If $|\Lambda| = 2N$ is even, then the half-filled band ground state energy is given by (1.1) with $N = |\Lambda|/2$. If $|\Lambda| = 2N+1$, the half-filled band ground state energy is $-2\sum_{j=1}^{N}\lambda_j - \lambda_{N+1}$. It is this half-filled band energy that is mostly considered in the physics literature. However, we regard our definition (1.2) as mathematically more natural and physically as interesting as the strict half-filled band definition. *For bipartite graphs $E_0(T)$ and $E_0^{(N)}$ with $N = |\Lambda|/2$ or $(|\Lambda|-1)/2$ agree with each other.* (Note that if Λ is bipartite and $|\Lambda| = 2N+1$ then $\lambda_{N+1} = 0$.)

The two definitions can produce strikingly different conclusions, however, in special cases. In [RD] the ground state energy $E_0(T)$ of N electrons (including spin) hopping on a ring of N sites is considered. By Theorem 4.1 we know that for a ring with N odd (and which is therefore not bipartite), the expression (1.2) is minimized by flux π and flux 0. However it has been shown in some cases (see [RD]) that the half-filled band energy for such a ring is minimized by the flux $\pi/2$ (which, incidentally, we call the canonical flux in this paper).

There is an important difference between our minimization problem and the one in [HLRW] and some other papers in the physics literature. For a regular structure like $\mathbf{Z}^2$ we allow *different fluxes in different boxes.* In the physics literature the problem is sometimes stated with *constant fluxes* or with periodic fluxes. We find our formulation (with arbitrary fluxes) to be more natural mathematically and we believe it to be more natural in those physical problems where this theory might be applicable.

Besides the ground state energy problem we consider other functions of T, such as $\ln|\det T| = \mathrm{Tr}\ln|T|$. A particularly important one, physically, is $\ln\Xi$ where Ξ is the **grand canonical partition function** with chemical potential μ and inverse temperature β, given by

$$\Xi = \sum_{m_1}\cdots\sum_{m_{|\Lambda|}}\sum_{n_1}\cdots\sum_{n_{|\Lambda|}}\exp\left[\beta\sum_{j=1}^{|\Lambda|}\lambda_j(n_j+m_j)+\beta\mu\right] = \prod_{j=1}^{|\Lambda|}\left\{1+\exp[\beta(\lambda_j+\mu)]\right\}^2, \tag{1.3}$$

where the sum on each n_i and m_i is over the set $\{0,1\}$. The physical **free energy** is defined by $\mathcal{F} = -\beta^{-1}\ln\Xi$. We consider only $\mu = 0$ here because that corresponds to a half-filled band in the bipartite case (see (4.5) and footnote).

Another important quantity is the **gap**, $G(T)$, which is *not* defined by a trace. We define it to be

$$G(T) = -\lambda_{N+1} + \lambda_N, \tag{1.4}$$

where N is the number of negative eigenalues of $-T$, i.e., the smallest number such that $E_0^{(N)} = E_0(T)$. Clearly $G(T)$ is the energy needed to add one more electron to the system from the absolute ground state. For the half-filled band on a bipartite graph with $|\Lambda| = 2N$, $G(T) = 2\lambda_N$. This, however, may not be mathematically interesting because λ_N may be automatically zero for dimensional reasons. That is, if $|A|$ and $|B|$ are the two subsets of vertices of Λ that define the bipartite structure, then T always has at least $\big||B|-|A|\big|$ zero eigenvalues. For this reason we define $\widetilde{G}(T)$ for a *bipartite* Λ (with $|\Lambda|$ odd or even) to be

$$\widetilde{G}(T)=\lambda_{|A|}-\lambda_{|B|+1}, \tag{1.5}$$

assuming $|B|\geq|A|$. We can then ask the question: *Which flux maximizes $G(T)$ or $\widetilde{G}(T)$ in the bipartite case?*

So far we have discussed free — or noninteracting — electrons. The same questions can be asked for interacting electrons and very much less is known in that case. In Sect. VIII, however, we are able to carry over our techniques to one example — the Falicov-Kimball model.

Many of these results were announced in [LE]. We thank P. Wiegmann for bringing this problem to our attention and along with I. Affleck, D. Arovas, J. Bellissard and J. Conway, for helpful discussions.

II. DEFINITIONS AND PROPERTIES OF FLUXES

A **graph** Λ is a finite set of **vertices** (or **sites**), usually denoted by lower case roman letters x,y,z etc., together with **edges** (or **bonds**), which are certain unordered pairs of *distinct* sites and are denoted by (x,y), equivalently (y,x). Thus there will be at most one edge between two vertices. The set of sites or vertices will be denoted by V or $V(\Lambda)$ and the number of them by $|\Lambda|$. The set of edges will be denoted by E or $E(\Lambda)$. If $(x,y)\in E$ the sites x and y are said to be **end points** of the edge (x,y).

A graph Λ is connected if for every pair of sites x and y there is a **path** P in Λ connecting x and y, i.e., there is a sequence of points $x=x_0,x_1,x_2,\ldots,x_n=y$ such that (x_i,x_{i+1}) is an edge for every $0\leq i<n$. Although Λ is not just the set of vertices, but also contains the edges, we shall nevertheless sometimes write $x\in\Lambda$ where x is a site in Λ.

A **hopping matrix** T associated with a graph Λ is a Hermitian $|\Lambda|\times|\Lambda|$ matrix indexed by the sites of Λ, with elements denoted by $t_{xy}=\overline{t_{yx}}$ for $x,y\in\Lambda$, and with the important property that $t_{xy}\neq 0$ only if $(x,y)\in E$, i.e., if x and y are connected by an edge. In particular, $t_{xx}=0$ for all $x\in V$. The T matrix is the important object here. For that reason if $t_{xy}=0$ for any edge (x,y) we might as well delete this edge from the graph Λ. Thus, without loss of generality we can assume that every t_{xy} is nonzero and that the corresponding graph Λ is connected. If it is not connected T breaks up into blocks which can be considered separately. We call $|t_{xy}|$ the **hopping amplitudes**. No other assumption is made about t_{xy} unless explicitly stated otherwise. The eigenvalues of T are usually denoted by λ, and sometimes by $\lambda(T)$ to be more specific.

A **circuit** C of length ℓ in Λ is an ordered sequence of *distinct* sites $x_1, \ldots, x_\ell$ with the property that (x_i, x_{i+1}) is an edge for $i = 1, \ldots, \ell$ with $x_{\ell+1} \equiv x_1$. We explicitly *include* $\ell = 2$. Note that $x_2, \ldots, x_\ell, x_1$ is the same circuit as C, but $x_\ell, x_{\ell-1}, \ldots, x_1$ is different.

If C is a circuit then we can define the **flux** Φ_C **of** T **through** C, which is a number in $[0, 2\pi)$, as

$$\Phi_C \equiv \arg\left(\prod_{i=1}^{n} t_{x_i, x_{i+1}}\right) \equiv \arg\left(\prod_C T\right). \tag{2.1}$$

The symbol $\prod\limits_C T$ has an evident meaning.

A **gauge transformation** is a diagonal unitary transformation U with elements, $u_{xy} = \exp[i\phi_x]\delta_{xy}$, where $\phi_x : V \to \mathbb{R}$ is a function on the sites. Obviously a gauge transformation $T \to U^*TU$ leaves the spectrum of T and all the fluxes unchanged.

2.1. LEMMA (Fluxes determine the spectrum). *Let T and T' be two hopping matrices which have the same hopping amplitudes and the same flux through each circuit C of the graph Λ. Then there is a gauge transformation U such that $T' = U^*TU$.*

Proof: By our convention the t_{xy} and t'_{xy} are never zero. Thus $W_{xy} \equiv t_{xy}/t'_{xy}$ satisfies $|W_{xy}| = 1$ for all edges (x, y), and the flux of W through each circuit of Λ is zero. Let x_0 be an arbitrary but henceforth fixed site in Λ. For any x we can pick a path P connecting x_0 and x and define $\phi_x = \arg\left(\prod\limits_P W\right)$. The value of ϕ_x does not depend on the choice of the path because, if P' is another path connecting x_0 and x, we have that $\arg\left(\prod\limits_P W\right) = \arg\left(\prod\limits_{P'} W\right)$ since the flux through the circuit given by connecting x_0 to x along P and then connecting x to x_0 along P' is zero. If x and y are arbitrary sites in Λ with $(x, y) \in E$, and if we take P_x to be a path connecting x_0 to x and P_y a path connecting x_0 to y we observe that $1 = \prod\limits_{P_x} W \, W_{xy} \prod\limits_{P_y} \overline{W}$ since P_x followed by (x, y) is a path from x_0 to y. But this equals $\exp[i(\phi_x - \phi_y)]W_{xy}$ and hence $W_{xy} = \exp[-i(\phi_x - \phi_y)]$. Thus $t'_{xy} = \exp[i\phi_x]t_{xy}\exp[-i\phi_y]$, which proves the lemma. ■

Up to now a graph has been regarded as an abstract object consisting of vertices and edges. Now we wish to regard graphs as embedded either in $\mathbb{R}^2$ or $\mathbb{R}^3$. This means that the sites of Λ can be regarded as distinct fixed points in $\mathbb{R}^3$ and each edge (x, y) will be identified with exactly one piecewise linear curve between x and $y \in \mathbb{R}^3$. It is convenient to *exclude* the end points x and y in the definition of an edge. We require that any one edge does not intersect the other edges or the sites. Circuits are then identified with simple, oriented closed curves.

Obviously any graph can be embedded in $\mathbb{R}^3$ but only some graphs, called **planar graphs**, can be embedded in $\mathbb{R}^2$. It is these graphs that will mostly concern us in this paper.

The set of edges E and sites V of a planar graph, regarded as a set in $\mathbb{R}^2$, is closed. Its complement is therefore open and this complement has a finite number of connected components which we label $F_0, F_1, F_2, \ldots$. We define F_0 to be the open set that contains the point at infinity, (i.e. the exterior of the graph). The others we call the **faces** of the graph Λ. Each face has a boundary and this boundary is composed of a subset of the edges and sites of Λ. For later purposes we call **elementary circuits** those circuits which are entirely contained in the boundary of a single face.

If the graph is planar a circuit, C, of length greater than 2 will have an inside and an outside. The interior, which is an open set, is then the union of a certain number of faces, edges and vertices called **interior faces, interior edges** and **interior vertices**. We denote their numbers by f, e, v. We can speak of the **orientation** of C as being either positive (anticlockwise) or negative (clockwise) according as the winding number with respect to a point in its interior is either $+1$ or -1.

In general, an arbitrary specification of fluxes through the circuits of Λ may be inconsistent in the sense that there may not exist a choice of T with the prescribed fluxes. Some kind of divergence – or closedness condition is needed. In two dimension, however, the following lemma shows how fluxes can be specified in a consistent way.

2.2. LEMMA (Construction of phases from fluxes). *Let Λ be a planar graph and let $F_1, F_2, \ldots F_f$ be its faces. Let $\Phi^1, \Phi^2, \ldots, \Phi^f$ be any given numbers in $[0, 2\pi)$. (We call Φ^j the* **flux through** *F_j.) Then there is a function $\theta(x,y) : E(\Lambda) \to [0, 2\pi)$ so that the fluxes defined by (2.1) with $t_{xy} := \exp[i\theta(x,y)]$ satisfy $\Phi_C = \sum_{interior\ faces\ of\ C} \Phi^j$ for every positively oriented circuit C on Λ.*

Proof: Pick a point $z_j = (z_j^1, z_j^2) \in \mathbb{R}^2$ in each face F_j and consider the vector (really, a one-form) field on $\mathbb{R}^2$, $\vec{A}(x) = \vec{A}(x^1, x^2)$, with singularities at the z_j's given by

$$\vec{A}(x) = \sum_{\text{all faces } F_j \text{ of } \Lambda} \Phi^j \vec{a}(x - z_j)$$

with $\vec{a}(x) = (2\pi)^{-1}[(x^1)^2 + (x^2)^2]^{-1}(-x^2, x^1)$. For each pair $x, y \in V(\Lambda)$ with $(x,y) \in E(\Lambda)$ define $\theta(x,y) = \int_x^y \vec{A}$, i.e., the integral from x to y along the curve representing the edge (x,y). The flux Φ_C through any circuit C on Λ is given by $\oint_C A$. By Cauchy's integral formula (or Stokes' theorem), this integral equals Φ_C given above. ■

Remark: A more practical and direct way to construct phases $\theta(x,y)$ satisfying the conclusion of Lemma 2.2 is to concentrate the vector field $\vec{a}(x - z_j)$ along a line. More precisely, let L_j denote some semi-infinite line starting from z_j and extending to infinity, but which does not intersect any of the sites of Λ and whose intersection with an edge is always transverse, i.e., nontangent. We orient L_j from z_j outwards. For each *ordered* pair of sites (x,y), with $(x,y) \in E$, first orient the curve representing (x,y) in the direction from $x \in \mathbb{R}^2$ to $y \in \mathbb{R}^2$. Call this oriented curve ε. Then let $\mu_j(x,y) \equiv \Sigma_{L_j \cap \varepsilon}(\pm 1)$, where the sum is over all the points of intersection of L_j with this curve ε and where the $+$ sign (resp. $-$ sign) is taken if the (counterclockwise) angle from L_j to ε is less than (resp. more than) π. Finally, we set $\theta(x,y) = \Sigma_{j=1}^{f} \Phi^j \mu_j(x,y)$.

It is a fact that every planar graph, Λ, can be **triangulated**, i.e., that there is a planar graph Λ' with precisely the *same* vertices as Λ and whose edges E' (which are now sets of curves) contain E, the edge-set of Λ, and with the property that Λ' is **triangular**.The concept of a planar graph Λ' being triangular means that every one of the faces of Λ' has as its boundary the union of three edges and three vertices. We say that Λ' is a **triangulation** of Λ. It is easy to check that the three edges must always form a circuit. Note that, in general, a graph Λ can be triangulated in several ways.

2.3. LEMMA (Number of triangles in a circuit). *Let Λ be a triangular planar graph and let C be a circuit in Λ of length $\ell \geq 2$. Let f and v denote the number of interior faces and interior vertices of C. Then*

$$\ell - f + 2v = 2. \tag{2.2}$$

For $\ell = 2$, (2.2) is clearly true (with $f = v = 0$). Therefore we need consider only $\ell > 2$.

First proof: Let β be one of the ℓ edges in C. This edge must be part of the boundary of exactly one of the inner triangles, which we call τ. The boundary of τ contains 3 edges, $\beta_1, \beta_2, \beta_3$. There are two cases.

(a) $\beta_1 = \beta$ and β_2, β_3 are interior to C.

(b) $\beta_1 = \beta$, β_2 is an edge of C, β_3 is interior to C.

In case (a) we consider the circuit C' whose edges are the same as those of C except that β is replaced by the two edges β_2, β_3. In case (b) we remove β_1 and β_2 from C and replace them with β_3. It is easy to check that $\ell' - f' + 2v' = \ell - f + 2v$ and that $f' = f - 1$. By successively removing triangles in this way we eventually have only one triangle left, in which case $\ell = 3, f = 1, v = 0$.

Second proof: Euler's formula says that (total number of vertices) + (total number of faces) $-$ (total number of edges) $= 1$. Since ℓ also equals the number of vertices in C, we have that $1 = (v + \ell) + (f) - (\ell + e)$, where e is the number of interior edges. Each edge in C lies in the boundary of precisely one interior triangle, while each interior edge lies in the boundary of two such triangles. Since each triangle has three edges in its boundary, and since C has ℓ edges, we have $3f = 2e + \ell$. Therefore $e = 3f/2 - \ell/2$ and $1 = v + f - e = v - f/2 + \ell/2$. ■

2.4. COROLLARY (f is independent of triangulation). *Let Λ be an arbitrary planar graph and let Λ' denote a triangulation of Λ. For each circuit C in Λ the number of triangular faces of Λ' that are interior to C is independent of the triangulation Λ'.*

Proof: The result follows from (2.2) since ℓ and v do not depend on the chosen triangulation Λ'. ■

With the aid of triangulation we can describe the **canonical flux distribution** for *any* planar graph Λ. Choose any triangulation Λ' and place flux $\pi/2$ in every triangular face. By Lemma 2.2, this defines phases $\theta(x,y)$ on $E(\Lambda')$ and hence on $E(\Lambda)$. *A-priori*, these phases might depend on the triangulation but, by Corollary 2.4, all triangulation give rise to the same set of fluxes through the circuits of Λ. By Lemma 2.1 the $\theta(x,y)$'s are uniquely defined up to a gauge transformation, i.e., $\theta(x,y) \to \theta(x,y) + \phi_x - \phi_y$ with the function ϕ_x being the only quantity that might depend on the triangulation. Since the flux distribution is invariant under gauge transformations, the canonical flux distribution is well defined!

Of special interest to us are bipartite planar graphs. In general a **bipartite graph** is a graph Λ whose vertex set V is the union of two disjoint sets A and B with the property that (x,y) is never an edge of Λ if $x \in A$ and $y \in A$ or $x \in B$ and $y \in B$. We shall assume $|B| \geq |A|$. If Λ is a planar bipartite graph the canonical flux will always be π through every elementary square, zero through every elementary hexagon etc. However one has to be cautious about this because one could have, for instance, a square with vertices a, b, c, d and a fifth vertex g inside the square connected by an edge only to a. In this case our rule says that the canonical flux through the circuit a, b, c, d is zero and not π.

A special feature of bipartite graphs, planar or otherwise, is that the nonzero eigenvalues of any hopping matrix T come in opposite pairs, i.e., if λ is an eigenvalue of T then so is $-\lambda$. This follows from $T = -U^*TU$ where U is the diagonal unitary matrix with $+1$ on the A-sites and -1 on the B-vertices. T itself can be written in the form $\begin{pmatrix} 0 & M \\ M^* & 0 \end{pmatrix}$, where M contains the matrix elements between A and B sites.

III. DETERMINANTS FOR PLANAR GRAPHS

One of the main theorems of this paper is Theorem 3.1 about determinants of bipartite graphs, and one of the concepts needed there is that of the **dimer partition function** $D(T)$ of the graph Λ with hopping matrix T. A **dimer covering** (or matching) of Λ is a subset $\{e_1, e_2, \ldots, e_n\}$ of E such that every site in Λ is an end point of precisely one of the e_i's. In general, Λ has many dimer coverings, but it may have none at all. In particular, if $|\Lambda|$ is odd or if Λ is bipartite and $|A| \neq |B|$ then there are no dimer coverings.

We define the **dimer partition function** to be

$$D(T) = \sum_{\text{dimer coverings}} \prod_i |t_{x_i,y_i}|, \tag{3.1}$$

where the product is over all the edges $e_i = (x_i, y_i)$ that constitute a particular dimer covering. If $|t_{xy}| = 1$ then $D(T)$ is just the number of dimer coverings of Λ. Note that $D(T)$ depends only on the $|t_{xy}|$'s and is therefore independent of the fluxes. In particular, $D(T)$ is determined by the upper triangular array $\{t_{xy}\}_{x\leq y}$. (See the appendix.)

3.1. THEOREM (Canonical flux counts dimers and maximizes bipartite graph determinants). *Let Λ be a planar graph and let $|t_{xy}|$ be given positive numbers for all edges (x,y) in Λ. For the canonical flux distribution*

$$\det T = (-1)^{|\Lambda|/2} D(T)^2. \tag{3.2}$$

If, in addition, Λ is bipartite the canonical flux distribution maximizes $|\det T|$ among all flux distributions.

Before proving the theorem we make a series of remarks:

(i). Unless $|A| = |B|$ in the bipartite case, $D(T) = 0$ and $\det T = 0$ for *every* choice of flux. In the general case, $D(T) = 0$ unless $|\Lambda|$ is even. More generally, we could consider non-bipartite graphs with T of the form $T_K = \begin{pmatrix} 0 & M \\ M^* & K \end{pmatrix}$, with K selfadjoint. This means that edges are added between B-vertices but not between A-vertices. It is then an easy exercise in linear algebra to prove that $\det T_K = 0$ unless $|B| \geq |A|$, and that if $|B| = |A|$ then $\det T_K$ is independent of K, i.e., $\det T_K = \det T_0$. As an example, start with the simple square, i.e., $|\Lambda| = 4$ and (1,2), (2,3), (3,4), (4,1) are the edges. Theorem 3.1 says that the determinant is maximized by flux $= \pi$ through the square. Now add a diagonal edge (1,3) with some hopping amplitude $|t_{1,3}|$ on this new edge. We now have a graph that consists of two triangles. The observation just made says that the determinant is independent of the individual fluxes through the two triangles and depends only on their sum. The canonical flux distribution, which is $\pi/2$ in each triangle, is optimal, but is by no means the unique optimizer.

(ii). In the bipartite case, the sign of the determinant as given in (3.2) is correct for any T, not just the canonical T. This follows from the $\lambda, -\lambda$ pairing of the eigenvalues which holds for a bipartite lattice.

We can go further and define the elementary symmetric functions

$$e_k(T) = \sum_{i_1<i_2<\ldots<i_k} \prod_{j=1}^{k} \lambda_{i_j}(T) \tag{3.3}$$

for $1 \le k \le |\Lambda|$ and with $e_0(T) = 1$. They are the coefficients in the characteristic polynomial

$$\det(T+z) = \sum_{k=0}^{|\Lambda|} e_k(T) z^{|\Lambda|-k}. \tag{3.4}$$

Here, the $\lambda_i(T)$'s are the eigenvalues of T. For the same reason (the $\lambda, -\lambda$ pairing) we see that for a bipartite graph

$$\begin{aligned} e_k(T) &= 0, && k \text{ odd} \\ e_k(T) &= (-1)^{k/2}|e_k(T)|, && k \text{ even.} \end{aligned} \tag{3.5}$$

In fact, $e_k(T)$ is a sum of determinants of principal submatrices of T in which $|\Lambda| - k$ columns and corresponding rows are removed. Each such submatrix is naturally associated with a subgraph of Λ — which is necessarily bipartite as well. Therefore, we can conclude that the sign of the determinant of every principal submatrix of even order, k, is $(-1)^{k/2}$. For odd k, such determinants are always zero. Warning: The canonical flux distribution need not maximize $|e_k(T)|$ for $k \neq |\Lambda|$. The reason is that the canonical flux distribution for a subgraph might differ from the one for the full graph Λ. See Theorem 5.1, however.

(iii). The canonical flux distribution maximizes $\det T$ in the bipartite case. It fails, generally, to do so in the non-bipartite case; nevertheless, it does have a "maximum property" which is given in Theorem A.2 in the appendix.

(iv). In the Appendix it is shown that Theorem 3.1 is one of the two key ingredients in a proof of Kasteleyn's theorem.

Proof: By definition, the determinant is a sum over permutations of monomials in the matrix elements of T, each of which is a product of the kind $\varepsilon(\pi)t_{1,\pi(1)}\cdots t_{|\Lambda|,\pi(|\Lambda|)}$. Here, $\varepsilon(\pi) = \pm 1$ is the signature of π. Using the cycle decomposition of the permutation π we see that the above monomial can be written as $\prod_{j=1}^{k}(-1)^{\ell_j - 1}\prod_{C_j} T$, where $C_1, \ldots, C_k$ is a family of circuits with the property that every vertex of the graph is in precisely one circuit. Here ℓ_j denotes the length of the circuit C_j. By the definition of the canonical flux distribution, $\prod_{C_j} T = \prod_{C_j} |t_{xy}| \exp[\pm i\pi f_j/2]$, where f_j is the number of interior triangles of C_j, and the sign in the exponent indicates the orientation of C_j. Thus, the determinant is now a sum over all circuit decompositions of terms of the form $\prod_{j=1}^{k}\prod_{C_j}|t_{xy}|(-1)^{\ell_j-1}\cos(\pi f_j/2)$. Note that the factor 2 is counted by distinguishing circuits of different orientations.

By Lemma 2.3, $f_j = \ell_j + 2v_j - 2$. Thus, $(-1)^{\ell_j - 1}\cos(\pi f_j/2) = (-1)^{\ell_j-1}\cos(\pi\ell_j/2 + \pi v_j - \pi) = (-1)^{\ell_j}\cos(\pi\ell_j/2 + \pi v_j)$. If ℓ_j is odd, the cosine vanishes. Hence, *only even circuits contribute to the determinant.* This is a crucial property of the canonical flux distribution! Moreover, since every vertex must belong to a circuit, and every circuit has even length, v_j is also even for all j and hence $2v_j \equiv 0 \pmod 4$ and does not contribute to the sign of the monomial. Therefore the monomial equals $\prod_{j=1}^{k}\cos(\pi\ell_j/2)\prod_{C_j}|t_{xy}| = \prod_{j=1}^{k}(-1)^{\ell_j/2}\prod_{C_j}|t_{xy}| = (-1)^{|\Lambda|/2}\prod_{C_j}|t_{xy}|$ since $\sum_{j=1}^{k}\ell_j = |\Lambda|$. Note that when $|\Lambda|$ is odd there is at least one circuit of odd length in every circuit decomposition, and hence $\det T = 0$.

The last step is to derive relation (3.2), which is geometrically "obvious". It suffices to note in our case that $D(T)\cdot D(T)$ is a sum of terms, each of which is of the form $\mathcal{D}_1\mathcal{D}_2$, where $\mathcal{D}_1$ (likewise $\mathcal{D}_2$) denotes a single term in (3.1) corresponding to a single dimer covering. If we superimpose the two coverings we get a collection of disjoint circuits $C_1, \dots, C_k$ on Λ. Each site of Λ is in exactly one of these circuits. Additionally, each circuit will have an *even* length. This "circuit covering" of Λ corresponds to a term in $\det T$. Conversely, each term in $\det T$ corresponds to a "circuit covering". (Note: it is here that we use the fact that only circuits of even length contribute to $\det T$, for otherwise some terms in $\det T$ might give rise to "circuit coverings" that contain circuits of odd length.) All that is needed is to check that the weights in $D(T)^2$ correspond to those in $\det T$. The weight of a "circuit covering" in $\det T$ is 2^n, where $n \le k$ is the number of circuits whose length exceeds 2. The factor of 2 comes from the two possible orientations of the circuit or, in other words, the contribution of a cyclic permutation and its inverse. The same factor 2^n arises in $D(T)^2$ because each circuit can be decomposed into a dimer covering of the circuit in exactly two ways. ■

IV. RINGS WITH ARBITRARY WEIGHTS

We begin our study of the problem of maximizing eigenvalue sums of T with respect to fluxes by considering the simplest possible case. In the process some notation and identities will be established that will prove useful in later sections of this paper.

A **ring** of $R > 2$ vertices (or R edges) is a graph Λ with $|\Lambda| = R$ vertices labeled 1 up to R and with edges $(1,2),(2,3),\dots,(R-1,R),(R,1)$. The hopping matrix is then determined by R complex numbers $t_{12},\dots,t_{R1}$ with magnitudes given a priori as $|t_{i,i+1}|$. Note that Λ is not necessarily bipartite, i.e., $R = |\Lambda|$ does not have to be even.

Although the spectrum of T is easy to compute explicitly if $|t_{i,i+1}|$ is independent of i, and hence one might think that our main theorem here, 4.1, is without content, we draw the reader's attention to the fact that we shall consider all possible T's. In other words, we shall be dealing with the "random one-dimensional Laplacian" whose spectrum is the object of much current research. From this point of view, it is somewhat surprising that some physical quantities of this random system can easily be maximized with respect to the flux.

While our goal is to compute $E_0(T)$ in (1.2), we shall consider more general functions of the eigenvalues of T. Let $f : \mathbb{R}^+ \to \mathbb{R}$ be a real valued function defined for nonnegative reals, and define F by

$$F(T) = \mathrm{Tr} f(T^2) = \sum_{j=1}^{|\Lambda|} f(\lambda_j^2), \tag{4.1}$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{|\Lambda|}$ are the eigenvalues of T. The f needed for E_0 is

$$f_1(x) = \sqrt{x} \tag{4.2}$$

while for $\ln|\det T|$ it is

$$f_2(x) = \tfrac{1}{2} \ln x. \tag{4.3}$$

Still another physically important function is

$$f_3(x) = \ln \cosh \sqrt{x}. \tag{4.4}$$

appropriate to the free energy, $\mathcal{F} = -\beta^{-1} \ln \Xi$, in the grand canonical ensemble† (1.3):

$$\begin{aligned} \mathcal{F} &= -2\beta^{-1} \mathrm{Tr} \ln(e^{-\beta T} + 1) = -2\beta^{-1} \mathrm{Tr}\{\ln[\cosh(\beta T/2)] + \ln 2 - \beta T/2\} \\ &= -2\beta^{-1} \mathrm{Tr} f_3(\beta^2 T^2/4) - 2\beta^{-1} |\Lambda| \ln 2 \end{aligned} \tag{4.5}$$

since $\mathrm{Tr}\, T = 0$. Here, β^{-1} = (Boltzmann's constant) $\times$ (temperature).

All these functions have the property of being *concave*, i.e., $f(\lambda x + (1-\lambda)y) \geq \lambda f(x) + (1-\lambda) f(y)$ for all $x \geq 0, y \geq 0$ and $0 < \lambda < 1$. (In fact they are *strictly* concave, i.e., equality implies that $x = y$.)

These three functions also belong to a more restricted class of functions which we call **integrated Pick functions**. These are functions with the integral representation

$$f(x) = c \ln x + \int_0^\infty \ln\left(1 + \frac{x}{s}\right) \mu(\mathrm{d}s) \tag{4.6}$$

† In (4.5) we have set the chemical potential μ equal to zero. For a bipartite lattice this yields an average particle number $M = 2N = |\Lambda|$, which follows from $M = 2\sum_{j=1}^{|\Lambda|} \exp(-\beta\lambda_j)[1 + \exp(-\beta\lambda_j)]^{-1}$ together with the $(\lambda, -\lambda)$ pairing.

where $c \geq 0$ and where μ is a nonnegative measure on $[0, \infty)$ such that this integral is finite. For the functions in (4.2)-(4.4) we have this integral representation with $\mu(\mathrm{d}s) = (\text{const.}) s^{-1/2}\ \mathrm{d}s$ and $c = 0$ for (4.2), $\mu(\mathrm{d}s) \equiv 0$ and $c = 1$ for (4.3) and $\mu(\mathrm{d}s) =$
$\sum_{k=0}^{\infty} \delta(s - [\pi(k + \frac{1}{2})]^{-2})\mathrm{d}s$, and $c = 0$ with $\delta =$ Dirac's δ-function. See [KL, eqs. (3.12), (3.16)]. Combining (4.1) with (4.6) yields

$$F(T) = c \ln \det T^2 + \int_0^\infty \ln \det(1 + T^2/s)\mu(\mathrm{d}s), \tag{4.7}$$

and we see that the problem of maximizing $F(T)$ is reduced to that of maximizing various determinants with respect to the flux.

The function $G(T)$ given in (1.4) cannot be represented in the form (4.7); nevertheless we shall also be able to maximize $G(T)$.

4.1. THEOREM (Maximizing flux for the ring). *Consider a hopping matrix T with arbitrary, but fixed amplitudes $|t_{xy}|$ on a ring of R sites, let f be an integrated Pick function given by (4.6) and let $F(T)$ be as in (4.1). Then the canonical flux*
$\pi(R+2)/2 \ (\mathrm{mod} 2\pi)$ *maximizes both $F(T)$ and the gap $G(T)$ if R is even. If R is odd, $F(T)$ and $G(T)$ are maximized by both of the choices 0 and π.*

Remark: When R is odd the canonical flux is always $\pi/2$ or $3\pi/2$ and never 0 or π.

Proof: For $F(T)$ it suffices, by formula (4.7), to show that the flux described above maximizes $\det(c^2 + T^2) = |\det(ic + T)|^2$ for all real numbers c.

As a first step we observe that for the invariants (or elementary symmetric functions) we have that $e_k(T) = 0$ for k odd and $1 \leq k \leq R - 1$. This follows directly from remark (ii) after Theorem 3.1 when R is even. When R is odd it also follows from remark (ii) together with the observation that every proper subgraph of a ring is bipartite. We also see, from remark (ii), that the sign of $e_{2m}(T)$ is $(-1)^m$.

With this information about the signs of the e_k's, we can write, from (3.4) with $z = ic$,

$$\det(c^2 + T^2) = \begin{cases} \left(\sum\limits_{m=0}^{|\Lambda|/2} |e_{2m}(T)| c^{|\Lambda| - 2m} \right)^2, & |\Lambda| \text{ even} \\ \left(\sum\limits_{m=0}^{(|\Lambda|-1)/2} |e_{2m}(T)| c^{|\Lambda| - 2m} \right)^2 + (\det T)^2, & |\Lambda| \text{ odd} \ . \end{cases} \tag{4.8}$$

For future use we remark that both parts of (4.8), hold for *any bipartite graph* Λ, not just a ring with an even number of sites.

As a second step we shall show that in the expression (3.4) for $\det(T+z)$, with $z \in \mathbb{C}$, the invariants $e_k(T)$ are *independent of the flux* if $k < R$. This is true only for a ring. Note that the invariants are real since T is Hermitian. Recall that the number $e_k(T)$ can be computed from T by calculating the subdeterminants of T with any $R-k$ columns and corresponding rows removed, and then summing these numbers over all possible removals. The result is a sum of monomials of the form $\prod\limits_j(-1)^{\ell_j-1}\prod\limits_{C_j} T$ where the product is taken over all circuits C_i that cover the subgraph obtained by removing k vertices and the corresponding edges. But for $k < R$ the only circuits that cover this subgraph form a dimer covering; their contribution does not depend on the flux but only on the numbers $|t_{i,i+1}|$. Thus the only term in (3.4) that depends on the flux is $e_{|\Lambda|}(T) = \det T$.

In both cases in (4.8), the problem of maximizing $\det(c^2+T^2)$ is seen to be the same as maximizing $|\det T|$. If R is even this problem is solved in Theorem 3.1. If R is odd there are precisely two circuits that contribute to $\det T$. These are the circuits that traverse the entire ring (in either direction) and correspond to an even permutation. Thus, for a ring of odd length

$$\det T = 2Re\left\{\prod_{i=1}^{R} t_{i,i+1}\right\} = 2(\cos\Phi)\prod_{i=1}^{R}|t_{i,i+1}|, \tag{4.9}$$

from which we see that $\Phi = 0$ or $\Phi = \pi$ maximizes $|\det T|$, and hence also $F(T)$. This completes the proof for $F(T)$.

To compute $G(T)$ we return to (4.7) and write $Q_\Phi(\lambda) \equiv \det(T-\lambda) = P(\lambda) + \det T$, with P being a polynomial of order R whose coefficients are *independent* of the flux Φ. P is even if R is even and P is odd if R is odd. We note that as $\det T$ varies between its maximum and minimum values, Q_Φ always has R roots. We leave it to the reader to verify the following with the aid of a graph of $Q_\Phi(\lambda)$. Even R: The maximum separation between $\lambda_{R/2}$ and $\lambda_{R/2+1}$ is achieved by making $|Q_\Phi(0)|$ as large as possible. Since $Q_\Phi(0) = \det T$, this means choosing Φ to make $|\det T|$ as large as possible — as stated in our theorem. Odd R: If $\det T = 0$, the eigenvalues of Q_Φ are paired (because P is odd). Then $-\lambda_{(R-1)/2} = \lambda_{(R+3)/2}$ and $\lambda_{(R+1)/2} = 0$. Thus $G_+ := [\lambda_{(R+1)/2} - \lambda_{(R+3)/2}] = [\lambda_{(R-1)/2} - \lambda_{(R+1)/2}] =: G_-$ when $\det T = 0$. As $|\det T|$ increases, either G_+ increases, G_- decreases and $\lambda_{(R+1)/2} > 0$ or vice versa and $\lambda_{(R+1)/2} < 0$. Thus $G = \max(G_+, G_-)$ and this increases with $|\det T|$. By (4.9) we see that $\Phi = 0$ or $\Phi = \pi$ maximizes $|\det T|$. ■

V. TREES OF RINGS

Most of the results in Theorem 4.1 for bipartite rings with arbitrary hopping amplitudes $|t_{xy}|$ can be extended to a much larger class of planar graphs. Two special cases of this class are the ladders and the necklaces; they are discussed in detail in the next section because even stronger results can be obtained for them. It was those two classes, in fact, that were the origin of this work and that were reported in [LE].

A planar graph Λ is said to be a **tree of rings** if and only if Λ has an embedding in $\mathbb{R}^2$ such that every circuit in Λ has no interior vertices.

The simplest example consists of two rings which have exactly one vertex in common. Another example consists of two rings that have exactly one edge (i.e., two neighboring vertices) in common. More generally, one can have a "tree of rings" in which two successive rings share either one edge or one vertex. The canonical flux distribution for a tree of rings would have flux $(\pi/2)[(\ell-2)(\text{mod}4)]$ in each circuit of length ℓ.

5.1. THEOREM (Maximizing flux for bipartite trees of rings). *Let Λ be a bipartite, planar graph that is a tree of rings and let $|t_{xy}|$ be arbitrary given hopping amplitudes. For f an integrated Pick function, let $F(T)$ be as in (4.1). Then the canonical flux distribution maximizes $F(T)$. Moreover, it also maximizes the magnitude of each elementary symmetric function $e_k(T)$ defined in (3.3).*

Proof: As in the proof of Theorem 4.1 (*cf.* eq. (4.8)) we have that $\det(c^2+T^2)$ will be maximized if we can *simultaneously* maximize all the $|e_k(T)|$'s and if they all have the sign $(-1)^{k/2}$. The latter question was dealt with in the remark (ii) just after Theorem 3.1.

Each $e_k(T)$ can be evaluated as a sum of determinants of principal submatrices of T of order k. In terms of graphs, a particular term in the sum is the determinant of T restricted to a subgraph Λ' with $|\Lambda'|=k$. The important point is that the circuits of Λ' are (i) a subset of the circuits of Λ and (ii′) they have no interior points. The canonical flux distribution for Λ' is the same as for Λ; this means that if C is a circuit that is both in Λ and in Λ' then $\Phi_C=\Phi'_C=0$ or π where Φ_C is the canonical flux through C (in Λ) and Φ'_C is the canonical flux (in Λ'). (Note: The only way in which Φ_C could differ from Φ'_C is if C had some interior vertices that were removed in passing from Λ to Λ'. But C had no interior vertices to start with.) Hence each subdeterminant appearing in $e_k(T)$ is maximized (in absolute value) by the original canonical flux distribution in Λ. Since the signs of all these subdeterminants are the same, in fact they depend only on k (see remark (ii) after Theorem 3.1), we see that $|e_k(T)|$ is maximized. ∎

VI. LADDERS AND NECKLACES

Most, but not all the graphs considered in this section are special cases of those discussed in Section 5. Here we consider certain graphs that are finite subsets of the infinite lattice $\mathbf{Z}^2$, which is the infinite embedded graph whose vertices are points in the plane with integer coordinates and whose edges are the horizontal and vertical line segments joining vertices a unit distance apart. Of particular importance are **boxes**, which are the subgraphs of $\mathbf{Z}^2$ with 4 vertices and 4 edges forming a circuit. In general, our graphs need not be subgraphs of $\mathbf{Z}^2$, i.e., they need not contain *all* the edges of $\mathbf{Z}^2$ that connect the vertices V in our graph. (Example: Λ contains the 4 vertices of a box but only 3 of its edges.) Evidently, all our graphs are bipartite — with the A — B decomposition of their vertices being the one inherited from $\mathbf{Z}^2$. Before describing them in detail, a few remarks are needed.

If T is a hopping matrix of a *bipartite* graph Λ, the matrix T^2 is evidently block diagonal, i.e. $T^2 = \begin{pmatrix} \alpha_T & 0 \\ 0 & \beta_T \end{pmatrix}$, where α_T is $|A| \times |A|$, β_T is $|B| \times |B|$ and both are positive semidefinite. Assuming that $\nu := |B| - |A| \geq 0$, we have that the eigenvalues satisfy

$$\operatorname{spec}(\beta_T) = \operatorname{spec}(\alpha_T) \cup \{\nu \text{ zeros}\}. \tag{6.1}$$

This is a simple consequence of the fact that $T = \begin{pmatrix} 0 & M \\ M^* & 0 \end{pmatrix}$, so that $\alpha_T = MM^*$ and $\beta_T = M^*M$. Since the eigenvalues of T come in pairs, and there are $|\Lambda|$ of them, we conclude that

$$\operatorname{spec}(T^2) = \{\operatorname{spec}(\alpha_T) \text{ with double multiplicity}\} \cup \{\nu \text{ zeros}\}, \tag{6.2}$$

$$\operatorname{spec}(T) = \operatorname{spec}\left(\sqrt{\alpha_T}\right) \cup \operatorname{spec}\left(-\sqrt{\alpha_T}\right) \cup \{\nu \text{ zeros}\}. \tag{6.3}$$

Thus $\operatorname{spec}(T)$ is determined by *either* α_T or β_T alone.

The matrix α_T has diagonal elements, $(\alpha_T)_{aa} = \sum_{b\in B} |t_{ab}|^2$ for $a \in A$. The off-diagonal elements of α_T can be thought of as a hopping matrix of a new graph Λ_A, which need not be planar. The vertices of Λ_A are the A-vertices of Λ. A necessary condition for the pair (a, a') to be an edge of Λ_A is that there is a B-vertex, b, such that (a, b) and (b, a') are edges in Λ. There may be more than one such b for a given pair (a, a') and it is important to note that since $(\alpha_T)_{aa'} = \sum_b t_{ab}t_{ba'}$, it can happen that $(\alpha_T)_{aa'} = 0$, in which case (a, a') is *not* an edge of Λ_A, in conformity with our earlier convention. Similar remarks hold for $(\beta_T)_{bb'}$ and Λ_B.

There are special edges in Λ_A or Λ_B which we call **interior diagonals**. These are edges (a, a') or (b, b') in which a and a' (or b and b') belong to some (same) box S that is a subgraph of Λ. This set of edges is denoted by D_A. Since circuits of length 4 can only be the edges of boxes, it follows that the interior diagonals are the *only* edges that can possibly disappear from Λ_A because of the equality $\sum_b t_{ab}t_{ba'} = 0$. Likewise for Λ_B and D_B.

The graphs we shall consider here can be described as follows. Let $\Lambda'_A = \Lambda_A \sim D_A$, i.e., the vertices of Λ'_A are those of Λ_A but the edges are those of Λ_A *without* the interior diagonals. Analogously, Λ'_B is defined. We say that Λ is a **hidden tree** if either Λ'_A or Λ'_B is a tree (i.e., does not contain any circuits).

Two important examples introduced in [LE] are **ladders** and **necklaces**. Each is a connected union of n boxes, labelled $1, 2, \ldots, n$, forming a one-dimensional array. In the ladder the boxes are joined along (parallel) edges, with box j connected to $j+1$. In the necklace, boxes j and $j+1$ have only a single vertex in common, and these vertices are either all A or all B. In both examples, boxes j and k are disjoint if $|j-k|>1$. With the usual orientation of $\mathbf{Z}^2$, ladders are either horizontal or vertical, while a necklace runs at 45° to either of these directions.

One can generalize the ladder by allowing occasional 90° bends, while still keeping the one-dimensional character. Now, squares j and k can now have a vertex (but not an edge) in common if $|j-k|=2$; squares 1 and n are disjoint. The bends cannot be completely arbitrary, however, because the "hidden tree" condition must be maintained. It can never be maintained for a necklace with 90° bends.

Another, not so trivial example is that in which Λ is the union of 4 squares, all of which have a vertex in common and which together form a square of side length 2. Here $|A|=4$ and $|B|=5$. Although Λ'_A is a tree, Λ'_B is *not* a tree. (6.1) notwithstanding, it is somewhat surprising, when viewing the graphs for Λ_A and Λ_B, that they have the same spectrum — except for one zero eigenvalue. Another example in this vein is the Λ that resembles a (3,2) Young diagram, i.e. 3 squares in a horizontal row and 2 squares, also in a horizontal row, directly beneath them. The simplest case that is not a hidden tree, and for which none of our theorems apply, is two rows of three squares each.

Finally, we make some remarks about the next theorem.

(i). Ladders and necklaces are trees of rings, but the last three examples (two rows of squares) are not. Thus, for ladders and necklaces, the fact that the canonical flux distribution maximizes $\mathrm{Tr}|T|$, $\mathcal{F}$ and $|\det T|$ is already covered by Theorem 5.1. The statement about the gap is new, however, as is the method of proof.

(ii). The concave function $F(T^2)$ is definitely a generalization of the function in (4.1). Not all concave functions (even those that are invariant under unitary transformations) are eigenvalue sums as in (4.1). In particular, the sum of the k lowest eigenvalues of T^2 is not such a function and it is needed, in fact, to prove the theorem about the gap.

6.1. THEOREM (Canonical flux maximizes concave functions on hidden trees). *Let Λ be a graph that is a subset of $\mathbf{Z}^2$ and suppose that Λ'_A (resp. Λ'_B) is a tree. Let F be a concave function on the cone of positive definite matrices of order $|A|$ (resp. $|B|$) with the property that $F(U^*PU)=F(P)$ for every $P>0$ and every gauge transformation U (restricted to Λ_A, of course). Finally, let $\{|t_{xy}|\}$ be unit hopping amplitudes on Λ, i.e. $|t_{xy}|=1$ if $(x,y)\in E(\Lambda)$.*

Our conclusion is that among all hopping matrices T with this unit hopping amplitude, $F(\alpha_T)$ (resp. $F(\beta_T)$) is maximized by the canonical flux.

Proof: We shall assume Λ'_A is a tree. The proof for Λ'_B is similar. Assume T maximizes $F(\alpha_T)$. Let $U = \{u_x\delta_{xy}\}_{x,y\in V(\Lambda)}$ be the following gauge transformation: If $x = (n,m)$ with $n,m \in \mathbf{Z}$, then $u_x = (-1)^n$. Let $Y = U^*TU$. By concavity and gauge invariance, the block diagonal matrix $P^2 := \frac{1}{2}(T^2 + Y^2)$ satisfies $F(\alpha_P) \geq \frac{1}{2}F(\alpha_T) + \frac{1}{2}F(\alpha_Y) = F(\alpha_T)$. This inequality proves our theorem if we can show that the matrix α_P can be achieved by the canonical flux distribution, i.e. if there is a gauge such that $C :=$ (T with the canonical flux distribution) satisfies $\alpha_C = \alpha_P$.

Now note that T^2 and $Y^2 = U^*T^2U$ are related as follows:

$$(Y^2)_{xy} = -(T^2)_{xy} \qquad \text{if } (x,y) \text{ is an interior diagonal}$$
$$(Y^2)_{xy} = (T^2)_{xy} \qquad \text{otherwise.}$$

Therefore, $(P^2)_{xy} = 0$ for $(x,y) \in D_A \cup D_B$ and $(P^2)_{xy} = (T^2)_{xy}$ otherwise.

For any gauge, $(C^2)_{xy} = 0$ if (x,y) is an interior diagonal. This is so because the flux through each box in Λ is π, and if we label the four vertices 1, 2, 3, 4 (counterclockwise) with 1 and 3 $\in V_A$ we have $(C^2)_{13} = C_{12}C_{23} + C_{14}C_{43}$. But $C_{12}C_{23}C_{34}C_{41} = -1$ and $C_{14} = \overline{C}_{41} = 1/C_{41}, C_{43} = 1/C_{34}$ (since, e.g., $|C_{14}|^2 = 1$), so $(C^2)_{13} = 0$, as required. As for the diagonal elements, they are clearly equal, i.e., $(C^2)_{xx} = (P^2)_{xx}$.

Finally we have to compare the other matrix elements of C^2 and P^2 on Λ_A. In fact, they are both nonzero only on Λ'_A, in which case they satisfy $|(C^2)_{aa'}| = |(P^2)_{aa'}| = 1$ because there is precisely one path (i.e., B-vertex) between a and a'. Therefore $(C^2)_{aa'} = \exp[i\theta(a,a')](P^2)_{aa'}$ for each edge in $\Lambda_{A'}$. The relevant question is then the following: Is there a gauge transformation U such that $(U^*C^2U)_{aa'} = (P^2)_{aa'}$? In other words, can we find $u_x = \exp[i\phi_x]$ such that $\phi_a - \phi_{a'} = \theta(a,a')$ for every edge (a,a') in Λ'_A? Since Λ'_A is a tree, the answer is trivially, yes. All one-forms on a tree are exact. ∎

Applications: For a graph with hopping amplitudes satisfying the hypotheses of Theorem 6.1 the canonical flux distribution yields:

(a) The lowest ground state energy $E_0(T)$ and free energy $\mathcal{F}(T)$ for all temperatures.

(b) The largest $|\det T|$ and gap $\widetilde{G}(T)$.

The functions $-E_0(T), -\mathcal{F}(T)$ and $\log|\det T|$ are concave since they are integrated Pick functions, which are concave in T^2 as mentioned in Section IV. The gap $\widetilde{G}(T)$ can be computed from the matrices α_T and β_T. Assuming that $\nu \equiv |B| - |A| \geq 0$ we see that $\widetilde{G}(T) = 2(\inf\operatorname{spec}\alpha_T)^{1/2}$ and that $\widetilde{G}(T) = 2\left(\sum_{i=1}^{\nu+1}\gamma_i\right)^{1/2}$, where γ_i denote the eigenvalues of β_T arranged in increasing order. Of course we used that $\gamma_1 = \gamma_2 = \ldots = \gamma_\nu = 0$. Now the sum of the first k eigenvalues of a Hermitian matrix H is a concave function of H. Moreover since $x \mapsto \sqrt{x}$ is concave and increasing, we see that $\widetilde{G}(T)$ is a concave function of α_T (resp. β_T). Moreover it is gauge invariant and hence satisfies the assumptions of Theorem 6.1. Note that we had to discuss the above two formulas for $\widetilde{G}(T)$ since both possibilities (Λ'_A is a tree or Λ'_B is a tree) have to be considered.

In the case of ladders and necklaces the result about $E_0(T), \mathcal{F}(T)$ and $|\det T|$ were covered by Theorem 5.1, but the examples with two rows of boxes, cited above, were not covered. (In fact, the two-rowed examples *cannot* be extended to the full generality of Theorem 5.1; see Section VIIB.) For ladders and necklaces, the result about the gap is not covered by Theorem 5.1. In [LE] it was mistakenly asserted in Theorem 1 that (a) and (b) hold for *fully* generalized ladders and necklaces in which *arbitrary* $90°$ bends are allowed. Indeed, for $E_0(T), \mathcal{F}(T)$ and $|\det T|$ this is correct (by Theorem 5.1). For the gap, however, we must use Theorem 6.1 and this fails for bent necklaces and for ladders with arbitrary bends. It does hold, however, for generalized ladders that are hidden trees.

Additional remarks and examples: There are two more cases where the concavity argument in the proof of Theorem 6.1 is applicable but where the graph is not necessarily a hidden tree, or even planar.

(i) Row of cubes: Instead of a row of squares as in the ladder, take Λ to be a row of cubes joined on their faces, i.e., neighboring cubes have four edges and one face in common. Such a graph is, in fact, bipartite and planar, but it is not a hidden tree. If there are n cubes then Λ is the $4 \times n$ planar, square lattice with "periodic boundary conditions" in one direction. [Indeed, we can even make the row of cubes into a torus (i.e., attach the first cube to the last), which is the same thing as the $4 \times (n+1)$ planar, square lattice with periodic boundary conditions in both directions; the following argument will continue to work in this case provided n is odd.]

We assume, as in Theorem 6.1, that $|t_{xy}| = 1$ for every edge. The flux in every face can easily be arranged to be π in the following way. Start with the face that cube 1 and cube 2 have in common and put flux π through it by making $t_{xy} = 1$ on three edges and -1 on the fourth. Then use the negative of this on the corresponding edges that cube 2 and cube 3 have in common — and so on alternately. Finally, set $t_{xy} = +1$ on the remaining edges, i.e., those edges that are perpendicular to the faces between the cubes. A first application of the concavity argument shows that we get an upper bound in terms of T^2, but without interior diagonals on the faces common to all the cubes. In a second, similar application of the argument we can get an upper bound in terms of a matrix that has no interior diagonals on any of the other faces of the cubes as well. In fact the only nonzero elements of T^2 that remain will consist of four independent one-dimensional chains (or else, in the case of the torus, four independent rings of length $n+1$ with zero flux through each ring). Theorem 4.1 says that if $n+1 \equiv 2 (\mathrm{mod}\ 4)$ the optimizing flux for such rings is zero and hence the above concavity argument shows that our choice of fluxes cannot be improved. If $n+1 \equiv 0 (\mathrm{mod}\ 4)$ the optimum choice for such a ring is flux π. This can be achieved by a slight modification of our initial choice of the t_{xy}'s along the edges perpendicular to the inter-cube faces. Initially we chose them all to be $+1$ but now we choose them all to be $+1$ *except* for the n^{th} cube. There we choose $t_{xy} = -1$ along the four perpendicular edges.

(ii) $SU(2)$-valued fields: We have considered the case that $t_{xy} = |t_{xy}| \exp[i\theta(x,y)]$ with $e^{i\theta}$ the unknown variable. It is also amusing to replace $e^{i\theta}$, which is in $U(1)$ by a 2×2 matrix U_{xy} in $SU(2)$. In other words, T becomes a $2|\Lambda| \times 2|\Lambda|$ Hermitian matrix in which each t_{xy} (for $x,y \in V(\Lambda)$) equals a given number $|t_{xy}|$ times an (x,y)-dependent element of $SU(2)$. We require $t_{xy} = t_{xy}^*$. Theorem 6.1 goes through in this case when $|t_{xy}| = 1$. We do not know whether Theorem 3.1, for instance, can be generalized to the $SU(2)$ case.

There is, however, an interesting special feature of $SU(2)$. For the ladder or row of cubes, we had to break the translation invariance from period one to period two in order to achieve flux π in each face, i.e., T could not be made the same in every box but we had to translate by two boxes (or cubes) in order to recover T. With $SU(2)$ fields we can achieve the optimal flux distribution with period one. This means the following. We require that the product of the four t_{xy}'s around a square face (which is now a matrix product, of course) is the matrix $-I \in SU(2)$. This can be achieved by placing $i\sigma^1$ along all horizontal edges, $i\sigma^2$ along all vertical edges and (in the case of cubes) $i\sigma^3$ along all the edges in the remaining direction. Here $\sigma^1, \sigma^2, \sigma^3$ are the Pauli matrices. We then have $-I$ in every face because, for example $(i\sigma^1)(i\sigma^2)(-i\sigma^1)(-i\sigma^2) = -I$.

VII. SOME CONJECTURES AND COUNTEREXAMPLES.

(A). The smallest determinant: A natural question, to be compared with Theorem 3.1, is "Which flux distribution *minimizes* $|\det T|$ for a bipartite lattice?" Since the canonical flux distribution maximizes $|\det T|$ and since it places flux π in each square face (which is the maximum possible flux), it might be supposed that the answer to the question is zero flux, i.e. set $t_{xy} = |t_{xy}|$ for every edge in E. In the case where Λ is a simply connected net of boxes on $\mathbf{Z}^2$ and $|t_{xy}| = 1$ the determinant was computed by Deift and Tomei [DT] to have the three possible values $0, -1$ or $+1$. Despite this supportive example *the above conjecture is wrong*. In the case of two boxes with one common edge and $|t_{xy}| = 1$, the determinant *vanishes* when the flux in each square is $\pi/3$. On the other hand, $\det T = -1$ when the flux is zero.

(B) The smallest energy: In Section V we have seen examples of some graphs whose energy is minimized by the canonical flux distribution *for arbitrary* hopping amplitudes. Moreover, $|\det T|$

is always maximized by that flux distribution for *every* bipartite, planar graph with $|A| = |B|$. For such an arbitrary graph it is therefore natural to conjecture that $E(T)$ is also always minimized by the canonical flux distribution. Alas, this conjecture is also false for arbitrary $|t_{xy}|$, as we how show by an example.

In $\mathbf{Z}^2$ consider the graph consisting of four boxes arranged in a square, i.e. Λ has the nine vertices $o = (0,0), a = (1,0), b = (0,1), c = (-1,0), d = (0,-1)$ and $(\pm 1, \pm 1)$. If the conjecture were true for arbitrary amplitudes then $E_0(T)$ would always be minimal if the flux in each square is π. If we now let $|t_{oa}|, |t_{ob}|, |t_{oc}|$ and $|t_{od}|$ tend to zero, $E_0(T)$ becomes that of a ring of eight sites for which $E_0(T)$ is minimized by flux π (not $0 \equiv 4\pi$), as we saw in Theorem 4.1. Indeed, to see that 0 and π do not give the same value for $E_0(T)$ in general, for this ring, assume that the t's on the ring all have amplitudes equal to one. If the flux is zero then $E_0(T) = -\mathrm{Tr}|T|$ is easily computed to be $-2(1+\sqrt{2})$ and for flux π it equals $-2^{5/4}(\sqrt{1+\sqrt{2}} + \sqrt{\sqrt{2}-1})$ which is more negative.

VIII. THE FALICOV-KIMBALL MODEL

So far all our models concerned hopping matrices on a graph Λ. It is likely that the results obtained do not hold if we add a diagonal term to T, i.e., if we replace T by the matrix

$$H = -T + 2UW. \tag{8.1}$$

Here W is a real diagonal matrix satisfying $0 \leq W_x \leq 1$ for each x and U is a given real number called the coupling constant.

The eigenvalues of H can be interpreted as the possible energy levels of a single electron hopping on a graph Λ with kinetic energy $-T$ and potential energy $2UW$. This model, with W_x restricted to be 0 or 1, was introduced in [FK] as a model for a semiconductor-metal transition, and it was studied extensively in [KL], where it was called the "static model", and in [BS]. Our generalization to $W_x \in [0,1]$ for each x is a mild one that we include here primarily because it can be handled without extra complication. The points of view taken in [KL] were different from that in [FK]. There, the model was considered either as a simplified version of the Hubbard model in which electrons of one sign of spin are infinitely massive and therefore do not hop, or else as a model of independent electrons interacting with static nuclei. In the first view, $U > 0$ and $U < 0$ are both relevant. In the second, $U < 0$ is the physically relevant sign, and $W_x = 1$ (resp. 0) denotes the presence (resp. absence) of a nucleus at x.

The eigenvalues of H in (8.1) are denoted by $-\nu$ (not $-\lambda$) which, as usual, are ordered $\nu_1 \geq \nu_2 \geq \ldots \geq \nu_{|\Lambda|}$. The ground state energy of a system of N *spinless* electrons, interacting with a magnetic field and with the nuclei, is given, as usual, by

$$E_0^{(N)} = -\sum_{i=1}^{N} \nu_i. \tag{8.2}$$

(There is no 2 here, as in (1.1), because there is no spin.) Notice that the spectrum of (8.1) is still invariant under gauge transformations. Thus the energy $E_0^{(N)}$ depends on N, the flux distribution and, of course on W.

As mentioned before, minimizing the energy over all fluxes with a fixed W is presumably a hopeless endeavor but the situation becomes easier if one tries to minimize the energy with respect to the fluxes *and* W. It is clear that the minimum is attained when $W = 0$ if $U > 0$ or when $W = I$ if $U < 0$, which is uninteresting both mathematically and physically. If, however, we introduce $N_n := \sum_{x\in\Lambda} W_x =$ (total charge of the static particles), then the half-filled band condition (from the Hubbard model point of view — at least) is that $N_n + N = |\Lambda|$. This is the case that parallels the restriction in the previous parts of this paper, since it means that on the average each lattice site is occupied by one particle. In fact we shall be a bit more general in the $U > 0$ case, and will treat a slightly different case when $U < 0$. We shall optimize the energy over all flux distributions and all potentials W and all choices of N subject to one of the following three constraints.

$$\sum_{x\in\Lambda} W_x + N \leq 2|A| \qquad \text{if } U < 0 \tag{8.3a}$$

$$\sum_{x\in\Lambda} W_x + N \leq 2|B| \qquad \text{if } U < 0 \tag{8.3b}$$

$$\sum_{x\in\Lambda} W_x + N \geq \ |\Lambda| \qquad \text{if } U > 0. \tag{8.3c}$$

Theorem 2.1 in [KL] says that in these three cases we can easily compute the minimum of $E_0^{(N)}$ with respect to W and M — regardless of the flux distribution. This result requires only one particular structure of the graph, namely that it is bipartite. Nothing else is required. As we shall see in Theorem 8.2 the result is that the nuclei want to occupy only the A sites or the B sites in order to minimize the total energy. We emphasie again that this fact is *independent* of the magnetic field.

Lemma 8.1 and Theorem 8.2 are really a transcription to the $W_x \in [0,1]$ case of Lemma 2.2 and Theorem 2.1 in [KL]. Since they are short we give them here. It is convenient to introduce the matrix $S = 2W - I$, so S is diagonal with $S_x \in [-1,1]$. Thus $H = h + UI$ with

$$h = -T + US. \tag{8.4}$$

The matrix h has eigenvalues $-\mu_1 \leq -\mu_2 \leq \ldots \leq -\mu_{|\Lambda|}$, with $\mu_j = \nu_j + U$.

8.1. LEMMA (Maximization with respect to the nuclear configuration). *Let Λ be a bipartite (not necessarily planar) graph and T a prescribed hopping matrix on Λ. We consider all functions S on the vertices of Λ satisfying $-1 \leq S_x \leq 1$ for all x. Let F be a concave, nondecreasing function from the set of Hermitian positive semidefinite matrices into the reals. Assume also that F is gauge invariant, $F(U^*PU) = F(P)$ when U is a gauge transformation.*

Then $F(h^2)$ is maximized with respect to S at $S = V$ and at $S = -V$, where

$$V_x = \begin{cases} +1 & \text{for } x \in A \\ -1 & \text{for } x \in B \end{cases} . \tag{8.5}$$

If F is strictly concave and strictly increasing then these are the only maximizers.

Proof: The matrix $V = V^*$ is a gauge transformation and hence h and $h' := VhV$ satisfy $F(h^2) = F(h'^2)$. Now $h^2 = T^2 + U^2S^2 - U(TS + ST)$ and, since $VTV = -T$ and $VSV = S$, $h'^2 = T^2 + U^2S^2 + U(TS + ST)$. By concavity

$$F(h^2) = \tfrac{1}{2}[F(h^2) + F(h'^2)] \leq F(T^2 + U^2S^2) \leq F(T^2 + U^2I), \tag{8.6}$$

since F is nondecreasing and $S^2 \leq I$. Note that $T^2 + U^2I = h^2$ when S is chosen to be $+V$ or $-V$. If F is strictly increasing and strictly concave we can have equality in (8.6) only if $TS + ST = 0$ and $S^2 = I$. The former implies that $t_{xy}(S_x + S_y) = 0$, which implies (since Λ is connected) that $S = (\text{constant})V$. The latter implies that $(\text{constant}) = \pm 1$. ■

8.2. THEOREM (Energy minima with respect to nuclear configurations). *Let Λ be a bipartite graph (not necessarily planar) and let T be a prescribed hopping matrix. We consider functions W on the vertices of Λ satisfying $0 \leq W_x \leq 1$.*

For the three cases given in (8.3) the minimum value of $E_0^{(N)}$ with respect to W and N is uniquely achieved as follows

$$N = |A| \quad \text{and} \quad W = W_A := \tfrac{1}{2}(I + V), \qquad U < 0 \tag{8.7a}$$

$$N = |B| \quad \text{and} \quad W = W_B := \tfrac{1}{2}(I - V), \qquad U < 0 \tag{8.7b}$$

$$N = |B| \quad \text{and} \quad W = W_A \text{ or } N = |A| \text{ and } W = W_B, \quad U > 0. \tag{8.7c}$$

For each of these three cases, the minimum $E_0^{(N)}$ is given by

$$E_0^{(N)} = -\tfrac{1}{2}\mathrm{Tr}|h| + \tfrac{1}{2}\mathrm{Tr}h + UN, \tag{8.8}$$

where $h = -T + U(2W - I)$.

Proof: By (8.2) and (8.4) we have that $E_0 = -\sum_{j=1}^N \nu_j \geq -\frac{1}{2}\mathrm{Tr}|h| + \frac{1}{2}\mathrm{Tr}h + UN =: A(h)$. By Lemma 8.1, $\mathrm{Tr}|h| = \mathrm{Tr}\sqrt{h^2}$ is maximal precisely at $W = W_A$ or $W = W_B$ since $x \to \sqrt{x}$ is a strictly increasing and strictly concave function. Also, $\frac{1}{2}\mathrm{Tr}h + UN = U\{\sum_x W_x - |\Lambda|/2 + N\} =: B(h)$. If $U > 0, B(h) \geq |\Lambda|/2$. If $U < 0$ $B(h) \geq U(2|A| - |\Lambda|/2)$ for (8.3a) and $B(h) \geq U(2|B| - |\Lambda|/2)$ for (8.3b). These three lower bounds in $B(h)$ are attained (under conditions (8.3)) if N and W satisfy (8.7).

To complete the proof, we have to show that the lower bound on $-\frac{1}{2}\mathrm{Tr}|h| =: C(h)$, given in Lemma 8.1, is compatible with the condition on N given in (8.7) (when W is also that given in (8.7)). For example, we have to show that if $W = W_A$ and $U < 0$ then the sum of the negative eigenvalues of h (namely $-\sum_{\mu_j \geq 0} \mu_j = -\frac{1}{2}\mathrm{Tr}|h| + \frac{1}{2}\mathrm{Tr}h$) equals the sum of the lowest $|A|$ eigenvalues of h. In other words, we have to show that h has exactly $|A|$ negative eigenvalues. We do so now with a proof different from the one in [KL]. First note that for $t \in [0,1], h_t = -tT + UV$ has no zero eigenvalues when $U \neq 0$ since $h_t^2 = t^2T^2 + U^2I \geq U^2I > 0$. Second, the matrix $h_0 = UV$ has precisely $|A|$ negative eigenvalues because $U < 0$. Since the eigenvalues of h_t are continuous functions of t and because no eigenvalue can cross zero, h also has precisely $|A|$ negative eigenvalues. The other two cases (8.7b) and (8.7c) are treated in the same fashion. ■

The next theorem is our main result about the FK model in a magnetic field.

8.3. THEOREM (Canonical flux minimizes energy on trees of rings). *Let Λ be a bipartite tree of rings, T a hopping matrix with arbitrarily prescribed amplitudes, $|t_{xy}|$. As in Theorem 8.2 we consider functions W on the vertices of Λ satisfying $0 \leq W_x \leq 1$.*

For the three cases given in (8.3) the minimum value of $E_0^{(N)}$ with respect to the flux distribution, N and W is achieved by the canonical flux distribution together with the N and W given by (8.7).

Proof: Minimizing first with respect to N and W, we can assume, by Theorem 8.2, that (8.7) is satisfied. In these cases we have that $E_0 = -\frac{1}{2}\mathrm{Tr}|h_{A,B}| +$ constant, where the constant depends on the case but *not* on the flux distribution. In each case, $W = W_A$ or W_B and we denote the two choices of h by h_A and h_B. Note that N no longer enters the discussion. Our only goal now is to maximize $\mathrm{Tr}|h_{A,B}|$ with respect to the flux distribution. But $\mathrm{Tr}|h_{A,B}| = \mathrm{Tr}\sqrt{h_{A,B}^2}$ and $h_{A,B}^2 = T^2 + U^2I$ since $S_{A,B}^2 = I$. The function $x \mapsto \sqrt{x}$ is an integrated Pick function, i.e., $\sqrt{x} = d\int_0^\infty \ln(1 + x/s)s^{-1/2}ds$ for some constant $d > 0$ (see. 4.6). Hence maximizing $\mathrm{Tr}|h_{A,B}|$ is reduced to maximizing $\det(c^2 + h_{A,B}^2) = \det(c^2 + U^2 + T^2)$ for all constants c. That this is achieved by the canonical flux distribution on trees of rings is precisely the content of Theorem 5.1. ■

APPENDIX: KASTELEYN'S THEOREM

We give here a different, and we believe more transparent proof of a deep theorem due to Kasteleyn [KP], which is one of the main tools for counting dimer configurations on planar graphs. Let us emphasize that Λ is now a finite graph that is *not necessarily bipartite.*

Historically, the motivation behind Kastelyn's theorem was an attempt to calculate efficiently the partition function $D(T)$ in (3.1) for large planar graphs— by reducing the problem to the calculation of a determinant. This was accomplished by Temperley and Fisher [TF] in special cases, but independently and in full generality by Kasteleyn [KP]. The starting point was Pfaff's theorem for an *antisymmetric matrix* A (of even order): $\det A = \mathrm{Pf}(A)^2$. Here $\mathrm{Pf}(A)$ is the **Pfaffian** of A (more precisely, the Pfaffian of the upper triangular array of $A = \{a_{xy}\}_{1\le x<y\le N}$), defined by

$$\mathrm{Pf}(A) = \sum_{\pi} \varepsilon(\pi) a_{\pi(1),\pi(2)} a_{\pi(3),\pi(4)} \cdots a_{\pi(N-1)}, a_{\pi(N)} \tag{A.1}$$

where the sum is over all permutations $\pi \in S_N$ with $\pi(1) < \pi(3) < \pi(5) < \ldots$ and with $\pi(i) < \pi(i+1)$ for odd i. Also, $\varepsilon(\pi)$ is the signature of π.

Each term in $\mathrm{Pf}(A)$ corresponds to a dimer covering of the graph Λ with N vertices and with edges corresponding to the nonzero elements of A.

The Kasteleyn, Temperley-Fisher idea is to set $a_{xy} = \exp[i\theta(x,y)]|t_{xy}|$ for $x < y$, with $\theta(x,y)$ chosen so that all terms in (A.1) have a common argument θ. Then, trivially, $D(T) = e^{i\theta}\mathrm{Pf}(A)$ for some θ and $|\det A| = D(T)^2$.

In Theorem 3.1 we solved the $D(T)$ problem, from a different perspective, by using the canonical flux distribution: $|\det T| = D(T)^2$. Moreover, we gave a very simple rule (in the proof of Theorem 3.1 and in the remark following Lemma 2.2) for an explicit construction of $\exp[i(\theta(x,y)]$. We did *not* try to construct an antisymmetric matrix, but it is a fact that among the gauge equivalent T's with canonical flux distribution, there *is* one that is antisymmetric. This is Theorem A.1 below. We note here that $\det T$ is a gauge invariant quantity, but $\mathrm{Pf}(T)$ is not.

Theorem A.1, together with Theorem 3.1 yields *Kasteleyn's theorem*, namely that there is always a real, antisymmetric matrix A such that $T = iA$ and $\mathrm{Pf}(A) = D(T)$. To see this implication, note that Theorem (3.1) says $\det A = \det(iT) = (-1)^{|\Lambda|/2}(-1)^{|\Lambda|/2}D(T)^2$. On the other hand $\det A = \mathrm{Pf}(A)^2$. We can then make $\mathrm{Pf}(A) = +D(T)$ by multiplying the first row and column of A by -1, if necessary. One way in which our proof is a little simpler than Kasteleyn's is that graphs with cut-points do not require special treatment, in either of Theorems A.1 or 3.1.

Theorem A.2 is another corollary of Theorem A.1. It answers the question: For which class of matrices (in the non-bipartite case) does the canonical flux distribution maximize $|\det T|$? Clearly the canonical flux cannot maximize $|\det T|$ in general. (A simple counterexample is provided by the triangle, $|\Lambda| = 3$ where $|\det T|$ is maximized by flux 0 or π (Theorem 4.1) but the canonical flux is $\pi/2$.)

A.1. THEOREM (Canonical flux and antisymmetry). *Let Λ be a finite planar graph with given hopping amplitudes $|t_{xy}|$. There exists a gauge such that the Hermitian hopping matrix T defined by the canonical flux distribution has purely imaginary elements, i.e., $T = iA$ with $A^T = -A$ and A real.*

Proof: We can assume Λ is triangulated and we can start with the remark following Lemma 2.2 which states (indeed, gives an explicit rule) that there is a matrix T° whose fluxes are canonical and such that $t^\circ_{xy} \in \{i, -i, 1, -1\}$ for all $(x, y) \in E$. Edges for which $t^\circ_{xy} = \pm i$ will be called "good" and those for which $t_{xy} = \pm 1$ will be called "bad". Our goal is to find a gauge transformation $U_{xy} = u_x \delta_{xy}$ with $u_x \in \{i, 1\}$ for all $x \in V$, such that U^*TU has no bad edges. We shall do so by showing that if T is *any* matrix with canonical fluxes and with $t_{xy} \in \{i, -i, 1, -1\}$ and with at least one bad edge then we can find a gauge transformation U with $u_x \in \{i, 1\}$ such that U^*TU has at least one less bad edge than T has. Since the number of edges of Λ is finite, the theorem is proved by induction.

Let $(a, b) \in E$ be a bad edge. Consider the set of sites $S = \{y \in V :$ there is a path from a to y whose edges are all good $\}$; by definition $a \in S$. Set $u_x = i$ if $x \in S$ and $u_x = 1$ if $x \notin S$. Clearly, if $(c, d) \in E$ was a good edge for T it remains a good edge for U^*TU (because either $u_c = u_d = 1$ or $u_c = u_d = i$).

To complete the proof we have only to show that the edge (a, b) has become a good edge. Since $a \in S$, we have to show that $b \notin S$. Indeed, suppose $b \in S$. Then there is a circuit $C = a, x_1, x_2, \ldots, x_n b$, of length greater than 2, such that the edges $(a, x_1), (x_1, x_2) \ldots, (x_{n-1}, x_n)$ are good while (x_n, b) is bad. We claim that this is impossible; in fact *every* circuit must have an *even* number of bad edges. To see this, use eq. (2.2) in Lemma 2.3, which says that $f = \ell$ (mod2). Here, f is the number of (triangular) faces inside C. We have $\Phi_C =$ flux through $C = \pm\pi f/2$ (by the definition of the canonical flux distribution). On the other hand, $\Phi_C = (\pi/2)\sum_G(\pm 1)$. Here, the sum is over the good edges and $+1$ or -1 is taken according to the direction in which the edge is traversed when C is traversed in an anticlockwise sense. In any event, $\Phi_C = (\pi/2)\{|G|(\mathrm{mod}2)\}$ where $|G|$ is the number of good edges in C. Thus, $f = |G|(\mathrm{mod}2)$, which proves our assertion. ■

A.2. THEOREM (Canonical flux maximizes antisymmetric determinants). *Let Λ be a planar (not necessarily bipartite) graph with hopping amplitudes $|t_{xy}|$ given. The canonical flux distribution maximizes $|\det T|$ among all flux distributions such that T is both Hermitian and antisymmetric.*

Proof: If T is antisymmetric, $\det T = \mathrm{Pf}(T)^2$. But, as we see easily from the definition (3.1), $|\mathrm{Pf}(T)| \leq D(T)$. By Theorem 3.1, $|\mathrm{Pf}(T_c)| = D(T)$, where T_c has the canonical flux distribution. By Theorem A.1, the gauge can be chosen so that T_c is antisymmetric. ■

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