SPECTRAL AND STOCHASTIC SOLUTIONS TO BOUNDARY VALUE PROBLEMS ON MAGNETIC GRAPHS

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ABSTRACT. A magnetic graph is a graph G equipped with a signature structure σ on its edges. The discrete magnetic Laplace operator Δ_G^σ has been an interesting and useful tool in discrete analysis and computational physics for over twenty years. Its role in the study of quantum mechanics has been examined closely for decades. In this paper, we pose some boundary value problems associated to this difference operator, and adapt two classic techniques to the setting of magnetic graphs to solve them. The first technique utilizes random walks and the second uses the spectral properties of the operator. Throughout, we will prove some useful results concerning a Green's identity, a mean value-type characterization of harmonic functions, and extensions of the spectral solution technique to product graphs.

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1. INTRODUCTION

The study of discrete Laplace operators on graphs is rich and active. Applications are manifold in the world of geometry processing and computer graphics, to name but two examples. In the classic papers by Chung [7, 6], one finds an accessible introduction to the subject, detailing some theory and results related to the classical combinatorial Laplacian, the rich spectral theory it produces, and many interesting stochastic and geometric problems. In the spirit of both [6] and [12], we state and solve some boundary value problems associated to the discrete *magnetic* Laplace operator for so-called *magnetic* or *signed* graphs. By a *magnetic* graph, we simply mean a combinatorial graph equipped with what we shall call a *signature*, to be defined explicitly in the sequel, which associates with each oriented edge of the graph a unit complex number. The notion of a signature structure has been around for a long time and has gone by many names, dependent on the context. For instance, in [5, ch. 19] one finds combinatorial graphs equipped with 'K-chains,' a structure which is algebraically identical to what we call signature. In the early paper [12], one may find an early and concrete realization of a magnetic graph as a discrete analogue of a spatial region with the presence of a magnetic field; in this case, the signature structure is realized as the discrete analogue of a vector potential function associated to the magnetic field. The use of the discrete magnetic Laplacian as a tool

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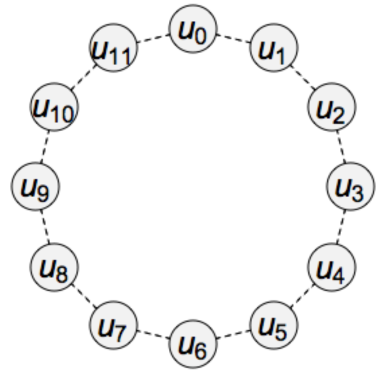

FIGURE 1. The circular path of the molecule Q.

to model magnetic fields in discrete space is well-studied, for instance, in the papers [15, 10, 2, 8] to name but a few. It is this particular application which appears to be the principal interest of applied researchers studying this topic. In this paper, we will solve a Poisson-type problem adapting spectral theoretic methods due to Chung, then solve a Dirichlet-type problem using random walks. The probabilistic interpretation of the Dirichlet problem associated to the classical combinatorial Laplace operator on connected graphs is well-known; for detailed descriptions, see [11, 14]. The introductory section of this paper will begin with two short expository sections which will motivate the concepts in this paper, first using an example problem, and then through some exposition on what exactly is meant by a 'discrete Laplacian.' In the second part of this paper, we will cover the formulation and solution of the Dirichlet problem using the random walk techniques; in addition, we will also discuss what is known as a 'magnetic lift.' The third part of this paper will mostly concern the Poisson-type problem: its formulation, solution, and the notion of a discrete Green's function it yields.

1.1. **A motivating example.** Let us begin by studying an example problem concerning the movement of a molecule Q. Let us suppose that Q is moving along a circular path in space, which we will model with the graph illustrated in Figure 1. By a graph, we mean a collection of vertices $\{u_0, u_1, ..., u_{11}\}$ and a collection of edges joining them. Formally, edges are considered as pairs of vertices $\big\{\{u_0, u_1\}, \{u_1, u_2\}, ..., \{u_{11}, u_0\}\big\}$ taken without any particular ordering. The graph we are considering is an example of what is often called a cycle graph.

In our basic model, we will suppose that Q begins its movement at the uppermost vertex u_0, and moves randomly between adjacent vertices. In particular, the probability that Q moves from a vertex u_i to one of its neighbors u_{i+1}, u_{i-1} is $1/2$ in each case. Furthermore, we will suppose that as Q moves between vertices, it is also subject to some rotational force; induced, for example, by a magnetic field. Specifically, we will imagine Q begins with an angular orientation pointing directly east, and if Q moves from the vertex u_i to its clockwise neighbor u_{i+1}, we will suppose it rotates through an angle of $\frac{\pi}{2}$ in the counterclockwise direction. Similarly, if Q moves from a vertex u_i to its counterclockwise neighbor u_{i-1}, it will rotate in the other way: $\frac{\pi}{2}$ in the clockwise direction.

We now ask the following question. Knowing both the initial position and initial angular orientation of Q, can we formulate and study a function which predicts the angular orientation of the molecule at any one of its possible positions?

To answer this question, we will model the rotation of the molecule in the following manner. Consider the following set $\widehat{E}$, which we will call the *oriented edges* of our cycle:

$$\widehat{E} := \big\{(u, v), (v, u) : \ u, v \text{ are adjacent vertices on the circular path}\big\}.$$

Next, let us define a function ω on $\widehat{E}$, by specifying it on the *clockwise* oriented neighbors:

$$\omega((u_i, u_k)) = \begin{cases} j & \text{if } 0 \leqslant i \leqslant 10, \ k = i+1 \\ j & \text{if } i = 11, k = 0 \end{cases} .$$

where in this example and throughout the rest of the paper, we understand j to be the unit complex number $\sqrt{-1}$. Verbally, ω gives the clockwise oriented edges a value of j. Let us now extend ω to the rest of $\widehat{E}$ according to this relation:

$$\omega((u_k, u_i)) = \overline{\omega((u_i, u_k))}.$$

That is, along the *counterclockwise* oriented edges, ω takes the complex conjugate of the associated oriented edge in the reverse order. Suppose for instance that the movement of the molecule Q begins at u_0 with angular orientation directly east, and moves directly along the cycle in the clockwise direction to the lowermost vertex u_6. The initial angular orientation can be modeled by the number 1, and as Q moves along the first edge in the clockwise direction, its angular orientation can be modeled by $1 \cdot j = j$, which when viewed in the complex plane, can be seen as a vector pointing north. The next step in its path would give an orientation $1 \cdot j \cdot j = -1$, which can be seen as a vector pointing west. Extending in a similar manner, the angular orientation of Q at the vertex u_6 becomes $j^6 = -1$, or directly west.

Let us generalize this notion to the case where Q has moved along an arbitrary path P through m steps, described by a sequence of m oriented edges: $((u_{k_0}, u_{k_1}), (u_{k_1}, u_{k_2}), ..., (u_{k_{m-1}}, u_{k_m}))$ where it is understood that, contrary to our model assumption and in the interest of generality, u_{k_0} need not equal u_0; that is, Q might start anywhere. As in [12], we define the *flux* of the path P, denoted $\mathrm{flux}(P)$ to be such a product as described previously:

$$\mathrm{flux}(P) := \prod_{i=0}^{m-1} \omega((u_{k_i}, u_{k_{i+1}})).$$

We interpret this notion of flux to mean the angular orientation of Q once it reaches the terminal vertex along the path P, having started with an initial angular orientation of 1. Notice that we may also interpret the complex conjugate $\overline{\mathrm{flux}(P)}$ as the angular orientation of the molecule which began a walk instead at the terminal vertex of the path u_{k_m}, with initial orientation 1, and proceeded in the opposite direction as before, stopping at u_{k_0}.

Let us now return to the original question concerning the prediction of the angular orientation of Q, once again recalling that its movements are at random. For $t \geqslant 0$, let $(S_t) = (S_0, S_1, ..., S_t)$ represent a random walk on the circular path, described by an ordered list of vertex positions which starts at S_0. Eventually, we know that (S_t) will approach the position u_0 with probability 1. The reasoning for this observation, which is somewhat technical, concerns the fact that our graph of interest has a connectedness property; a precise explanation be deferred until the second section of the paper, *cf* 2.1. That is, if we let $T = \min\{t : S_t = u_0\}$, then $\mathbb{P}[T < \infty] = 1$, where according to the standard notation of the area, $\mathbb{P}$ is the probability that the event in brackets occurs in the random process (S_t). Hence it is well defined to construct a slightly modified random walk

$$(\widetilde{S}_t) := (S_t)_{0 \leqslant t \leqslant T}$$

which we interpret as the same process S_t, which 'stops' once it reaches the vertex u_0. Now, let us define a function F on the vertex set of the circular path, as follows:

$$F(u) := \mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S}_t)} : S_0 = u\big]$$

where the flux of $\widetilde{S}_t$ is understood as being taken along the oriented edges of the random walk in the obvious sense, and S_0 is the initial position of the process. The symbol $\mathbb{E}$ is the standard notation for the 'expectation' of the random quantity in the brackets subject to the condition following the colon. Later in this introduction section, the reader will be supplied with some useful details and references to better inform these notions if she is unfamiliar with the terminology. The complex conjugate has been taken since the flux of the random walk is slightly different from the quantity we want to measure. We wish the quantity F to represent the angular orientation of Q at the initial vertex of the walk S_0, having started at the vertex u_0 and which proceeded along the vertices $(\widetilde{S}_t)$ in the reverse of their ordered formulation. We will finish this example with a computation that illustrates a fundamental relation that will appear throughout this research paper. Let us observe that for each vertex u,

$$\begin{aligned} F(u) &= \mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S}_t)} : S_0 = u\big] \\ &= \mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S_{t+1}})\omega((u, S_1))} : S_0 = u\big] \\ &= \sum_{v \sim u} \mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S_{t+1}})\omega((u, v))} : S_1 = v\big]\mathbb{P}[S_1 = v : S_0 = u] \\ &= \sum_{v \sim u} \overline{\omega((u, v))}\mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S_{t+1}})} : S_1 = v\big]\mathbb{P}[S_1 = v : S_0 = u] \\ &= \frac{1}{2} \sum_{v \sim u} \overline{\omega((u, v))}\mathbb{E}\big[\overline{\mathrm{flux}(\widetilde{S}_t)} : S_0 = v\big] \\ &= \frac{1}{2} \sum_{v \sim u} \overline{\omega((u, v))}F(v). \end{aligned} \tag{1}$$

We remark that the notation $v \sim u$ means that the vertex v is adjacent to the vertex u, and that the third equality follows by using a property of the expectation operation which allows us to compute the expectation of a certain event subject to a condition in terms of the expectations of individual events which describe the condition multiplied by their individual probabilities.

This computation is surprisingly meaningful. It suggests that the value of the function F at any vertex can be characterized by the average of the values of F at vertices adjacent to the one of interest, multiplied by the oriented angular displacement quantity ω between them! This is an example of what we will later term the *magnetic mean value property*, which the reader may recall from the study of *harmonic functions*. The reader may be surprised that the author wishes not to provide a more explicit description of our function F– rather, the author wishes to arrive at this point because it illustrates how a rather abstract property which is integral to this paper shows up in even a simple toy example concerning the angular orientation of a randomly moving molecule.

1.2. **Differential operations: continuous to discrete.** In multivariable calculus, the reader probably encountered what is usually termed the *Laplacian*, denoted by a symbol Δ. Specifically, if one has a function $u : \mathbb{R}^3 \to \mathbb{R}$ which has continuous second-order partial derivatives in the variables x, y, z, we may write

$$\Delta u = u_{xx} + u_{yy} + u_{zz}$$

where subscripts indicate derivatives taken in the obvious sense. This is considered an extremely important tool in both calculus and the study of physical systems and models; it is an example of what we call a 'differential operator,' which acts on functions u by taking derivatives and combining them in a linear fashion. The term 'operator,' which is more general, refers to linear transformations acting on vector spaces, e.g., spaces of continuously differentiable functions. The experienced reader may recall that these operators often yield what we call *partial differential equations*, which are equations relating an unknown function to one or more of its partial derivatives. In particular, the Laplacian defines, among others, two very useful partial differential equations. Staying in the three-variable setting, let us suppose we have some bounded region $\Omega \subset \mathbb{R}^3$ with a boundary denoted $\partial\Omega$. Moreover, suppose we are given continuous functions $\phi : \Omega \to \mathbb{R}$ and $\psi : \partial\Omega \to \mathbb{R}$. The *Dirichlet problem* associated to Ω with *boundary condition* ψ asks the mathematician to find an unknown function u satisfying

$$\begin{cases} \Delta u = 0 & \text{on } \Omega \\ u = \psi & \text{on } \partial\Omega \end{cases} . \tag{2}$$

The function u is called *harmonic* on Ω, since its Laplacian vanishes there. The experienced reader might recall an important characterization of harmonic functions like u above: their values at a particular point can be found by looking at the average of the values around the point. We omit a formal statement of this property, since it requires some technical jargon that would take us off point; the interested reader is referred to an introductory text concerning partial differential equations such as [13]. As mentioned in the motivating example, a discrete version of this property will arise later on.

A second problem of interest is the *Poisson problem* with boundary condition ψ and *source term* ϕ, one formulation of which asks the mathematician to identify a function u for which

$$\begin{cases} \Delta u = \phi & \text{on } \Omega \\ u = \psi & \text{on } \partial\Omega \end{cases} . \tag{3}$$

The especially informed reader may recall that both of these equations have important physical interpretations which relate to concepts such as electric and magnetic potential; the exact nature of these relationships are outside of the scope of this exposition, and the author refers the interested reader to any intermediate physics textbook for more information.

A key characteristic of these equations is the nature of the space in which they are interested; the set Ω is usually a subset of the space $\mathbb{R}^3$ containing infinitely many points. In a computational setting, it is often extremely useful to consider similar problems on spaces which are easier to perform computations in; in particular, what are often called *discrete* representations of such spaces. For example, the space $\mathbb{R}^3$, which contains all triples of real numbers, may be simplified by considering instead the space $\mathbb{Z}^3$, which contains all triples of integers. This space is still infinite, but countable. To the mathematician, this is much smaller, and functions on this space can be easier to analyze computationally. Such discretizations of large regions naturally give rise to the question of adapting differential operators to functions on these spaces, which no longer have well-defined derivatives taken in the traditional sense. These are often called *discrete differential operators*, or *finite difference operators*. For example, if one has a function

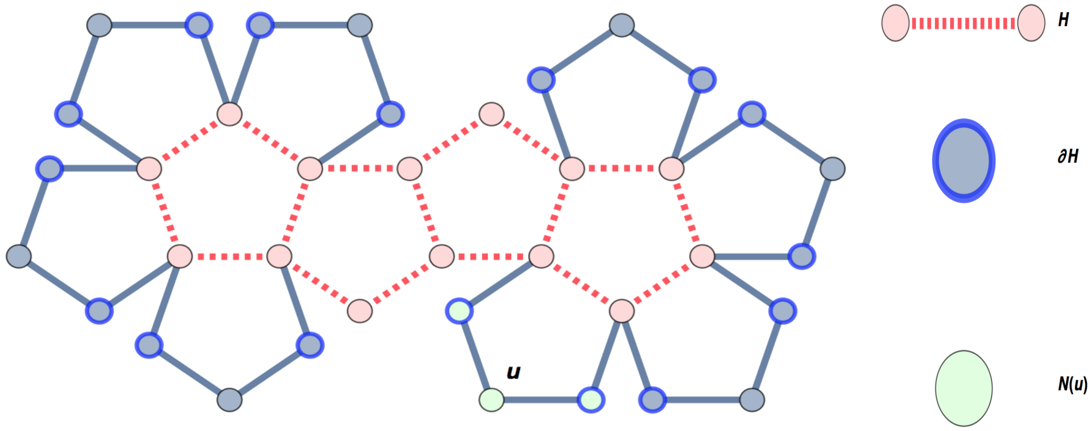

FIGURE 2. A dodecaheral platonic graph with subconnected subset H, its vertex boundary ∂H, and a particular vertex neighborhood $N(u)$.

p on the space $\mathbb{Z}^3$, that is, $p : \mathbb{Z}^3 \to \mathbb{R}$, we may define a *discrete Laplace operator* D by the following:

$$\begin{aligned}(Dp)(x_i, y_i, z_i) := {} & 2p(x_i, y_i, z_i) - p(x_{i+1}, y_i, z_i) - p(x_{i-1}, y_i, z_i) \\ & + 2p(x_i, y_i, z_i) - p(x_i, y_{i+1}, z_i) - p(x_i, y_{i-1}, z_i) \\ & + 2p(x_i, y_i, z_i) - p(x_i, y_i, z_{i+1}) - p(x_i, y_i, z_{i-1})\end{aligned}$$

which basically evaluates the differences of the function p along all of the points close to the point of interest $(x_i, y_i, z_i) \in \mathbb{Z}^3$, and adds them up, yielding a real number. Let us now consider a discrete analog of the Laplacian in a different kind of space: a graph. The reader can understand why this is useful in the following sense. In the case of $\mathbb{Z}^3$, we have a natural sense of two points being 'close;' exactly one of their coordinates being separated by a distance of 1. They are adjacent in the sense of being near one another along a particular integer axis. We can extend this to the case where our space is not $\mathbb{Z}^3$, but a combinatorial graph $G = (V, E)$ consisting of a finite vertex set and an edge set identifying which vertices are adjacent to one another. If we have a function $p : V \to \mathbb{R}$, we can define its *combinatorial discrete Laplacian*, denoted $\Delta_G p : V \to \mathbb{R}$ by

$$(\Delta_G p)(u) = \sum_{v \sim u} (p(u) - p(v))$$

which sums the differences of p along the vertices adjacent to u, similar to what we saw in the previous example D. Developed in [16] are some interesting general results related to this area, and some surprising limitations on the ability of discrete Laplace operators to simultaneously satisfy discrete analogues of those algebraic and analytic properties enjoyed by their relatives for differentiable functions on Euclidean spaces.

1.3. **Some graph theory and linear algebra.** Let $G = (V(G), E(G))$ be an undirected graph on $n < \infty$ vertices, without loops or multiple edges, and let $V(G)$ and $E(G)$ denote its vertex and edge sets, respectively. Henceforth, we will call such a graph *simple*. If $v \in V(G)$, we denote by d_v^G as the *degree* of the vertex v in the graph G; that is, the number of vertices adjacent to v. If two vertices $u, v \in V(G)$ are adjacent, we write $u \sim v$. A graph is called *connected* if each pair of vertices may be joined by a path in the graph.

If $u \in V(G)$, we define the *vertex neighborhood of* u to be the set

$$N(u) := \{v \sim u : v \in V(G)\} \cup \{u\} \subset V(G).$$

We shall term a proper subset of vertices $H \subsetneq V(G)$ a *subconnected* subset of $V(G)$ or G if it induces a connected subgraph. For example, and vertex neighborhood would be subconnected. Let us impose on a subset $H \subset V(G)$ a few useful anatomical structures. First, we define the *vertex boundary* of H to be given by

$$\partial H := \big\{u \in V(G) : \exists \{u, v\} \in E(G),\ v \in H, u \notin H\big\} \tag{4}$$

which for our purposes is a good way to define the boundary of H. The *closure* of H, denoted $\overline{H}$, will be the set $H \cup \partial H \subset V(G)$. We supply an illustration of these definitions in Figure 2.

We define the *adjacency matrix* of G to be the matrix $\mathbf{A}_G$ indexed by some enumeration of the vertex set of G, and defined by

$$\mathbf{A}_G(u,v) = \begin{cases} 1 & u \sim v, \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Let us define the *oriented edge set* of a graph G by

$$E^{\mathrm{or}}(G) := \big\{(u,v),\ (v,u) : \{u,v\} \in E(G)\big\}.$$

By a *signature* on a graph G, we mean a map

$$\sigma : E^{\mathrm{or}}(G) \to \{z \in \mathbb{C} : |z| = 1\} : (u,v) \mapsto \sigma_{uv}$$

satisfying the algebraic condition $\sigma_{vu} = \overline{\sigma_{uv}} = \sigma_{uv}^{-1}$. The reader may recall the 'angular displacement' function ω from the motivating example; a 'signature' is a formalization of this concept. The *trivial signature* is given by $\sigma \equiv 1$, and the *negative signature* is given by $\sigma \equiv -1$. By a *magnetic graph*, we mean a pair (G,σ) consisting of a simple graph G and a particular signature σ.

The following definition is a property achieved by some graph signatures, which will be useful later.

Definition 1.3.1. Let (G,σ) be a magnetic graph. We say that (G,σ) is *balanced* if for every cycle

$$C = \{u_0, u_1, ..., u_{n+1}\} \subset V(G),$$

where $u_i \sim u_{i+1}$ for $0 \leqslant i \leqslant n$, it being understood that $u_{n+1} := u_0$, one has

$$\prod_{i=0}^{n} \sigma_{u_i u_{i+1}} = 1.$$

In other words, the product of the signature along every cycle comes to 1. In any other case, we shall say (G,σ) is *unbalanced*.

For example, the cycle graph with which we worked in the motivating example, equipped with the signature structure defined by ω, is a balanced magnetic graph.

Definition 1.3.2. Suppose J, K are two simple graphs. We define their *Kronecker product graph*, denoted $J \times K$, by the vertex set $V(J) \times V(K)$ and the edge set

$$E(J \times K) := \{\{(u,v),(u',v)\} : (u,u') \in E(J)\} \cup \{\{(u,v),(u,v')\} : (v,v') \in E(K)\}.$$

In the case where we wish to form a product of magnetic graphs, we have the following construction of a 'product signature.'

Definition 1.3.3. Let $(J,\rho^J), (K,\rho^K)$ be two magnetic graphs. For two possible pairs of adjacent vertices in $V(J \times K)$ of the oriented edge form $((u,v),(u',v))$, and $((u,v),(u,v'))$, define a new signature ρ on the product graph by

$$\rho\big((u,v),(u',v)\big) = \rho^J_{uu'}$$
$$\rho\big((u,v),(u,v')\big) = \rho^K_{vv'}$$

i.e. 'recycle' the signature from the original graph from which the particular oriented edge originated.

The reader is invited to verify that this indeed forms a signature on the product graph.

We will be working in function spaces of the form

$$\ell_2\big(V(G)\big) := \big\{f : V(G) \to \mathbb{C}\big\}$$

with obvious generalizations to any subset of $V(G)$. We equip this space with standard complex inner product $\langle \cdot, \cdot \rangle_G$ given by

$$\langle f, g \rangle_G = \sum_{u \in V(G)} f(u)\overline{g(u)}$$

where the subscript on the bottom right of the bracket indicates the graph or vertex set over which the inner product is being taken, if not obvious from the context. The reader who is unfamiliar with the notions of a complex inner product is referred to any intermediate linear algebra text, such as [1]; put simply, it is a generalization of the dot product to complex vector spaces. We observe that the above function space is naturally isomorphic to the finite-dimensional complex inner product space $\mathbb{C}^n$, where n is the number of vertices in the domain of interest. In general, we identify functions in ℓ_2 with column vectors in $\mathbb{C}^n$ and speak of them equivalently. If two such functions have an inner product of 0, we say they are *orthogonal.* We define a *norm* on $\ell_2(V(G))$, or generalized length, by $||f||^2 = \langle f, f\rangle_G$ for each $f \in \ell_2(V(G))$. An *orthonormal basis* for $\ell_2(V(G))$ is a collection of mutually orthogonal functions with norm 1 which form a basis for $\ell_2(V(G))$ in the vector space sense.

We will now move on to constructing some 'discrete differential operators' that will be used to formulate the problems of interest in this paper. Let us begin by slightly reformulating the combinatorial Laplace operator mentioned in the previous subsection:

Definition 1.3.4. The *combinatorial Laplacian* associated to a simple graph G consisting of n vertices is the $n \times n$ matrix Δ_G, with rows and columns indexed by some enumeration of $V(G)$, defined by

$$\Delta_G(u,v) = \begin{cases} d_v^G & u = v, \\ -1 & u \sim v, \\ 0 & \text{otherwise} \end{cases}.$$

If $f \in \ell_2(V(G))$, we may speak of its *combinatorial Laplacian* as the matrix product $\Delta_G f$. We then have the formula

$$(\Delta_G f)(u) = \sum_{v \sim u} \big(f(u) - f(v)\big) \tag{6}$$

as desired. Using the same framework as in definition (1.3.4) and taking into account the signature, we have the following definition.

Definition 1.3.5. The *magnetic Laplacian* of a magnetic graph (G, σ), consisting of n vertices, is the $n \times n$ matrix with rows and columns indexed by some enumeration of the vertex set of G with entries given by

$$\Delta_G^\sigma(u,v) = \begin{cases} d_v^G & u = v, \\ -\sigma_{uv} & u \sim v, \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, if $f \in \ell_2(V(G))$ we define the *magnetic Laplacian of f* to be the product $\Delta_G^\sigma f$, and we have the equation

$$(\Delta_G^\sigma f)(u) = \sum_{v \sim u} \big(f(u) - \sigma_{uv} f(v)\big). \tag{7}$$

If $H \subsetneq V(G)$ is a proper subset of vertices in G, then the symbol Δ_H^σ will be used to refer to the magnetic Laplacian associated to the subgraph in G induced by H. *Warning!* To avoid burdensome notation, since the combinatorial Laplacian will not be used beyond this introduction section, going forward *we will often omit the superscript σ when using the magnetic Laplacian* when the signature is absolutely clear from the context of the exposition.

We observe that as a linear operator on $\ell_2(V(G))$, Δ_G^σ is *self-adjoint*, since its matrix representation is easily verified from the definition of σ to be a Hermitian matrix. The reader who is unfamiliar with this terminology is referred to an intermediate linear algebra text for additional information, such as the very accessible text [1], but is reminded that the technical observations above mean that for any two functions $f, g \in \ell_2(V(G))$ we have

$$\langle \Delta_G^\sigma f, g\rangle_G = \langle f, \Delta_G^\sigma g\rangle_G.$$

As a consequence, there exists an orthonormal basis $\{\phi_1, \phi_2, ..., \phi_n\}$ for $\ell_2(V(G))$, and an associated set of real eigenvalues, $\{\lambda_1, \lambda_2, ..., \lambda_n\}$ so that $\Delta_G^\sigma \phi_i = \lambda_i \phi_i$ for each $1 \leqslant i \leqslant n$. The family $\{\phi_1, \phi_2, ..., \phi_n\}$ will be called *eigenvectors* and/or *eigenfunctions* for Δ_G^σ. Sometimes we refer to these two families together as the *spectral system* associated to Δ_G^σ.

If the Laplacian of a function vanishes at a vertex v, then we say the function is *harmonic* at v. If a function is harmonic at every point in a set $H \subset V(G)$, then we say the function is harmonic on H.

Let us define two final operators, this time optimized for analysis on a subset of $V(G)$.

Definition 1.3.6. Suppose $H \subsetneq V(G)$ as above. We define the *magnetic Dirichlet Laplacian* of H to be the principal submatrix L_H of Δ_G^σ indexed by some enumeration of the set H.

L_H is self-adjoint on $\ell_2(H)$ as well, inheriting this from Δ_G^σ. The reader is invited to check this remark.

Definition 1.3.7. Let (G,σ), $H \subsetneq V(G)$ be as before. We define the *normal derivative* to be the operator $\frac{\partial}{\partial\eta}$ on $\ell_2(\overline{H})$ given by

$$\frac{\partial f}{\partial \eta}(u) = \sum_{\substack{v\sim u \\ v\in V(H)}} \big(f(u) - \sigma_{uv} f(v)\big)$$

for each $f \in \ell_2(\overline{H}), u \in \overline{H}$.

This discrete derivative operator, heuristically speaking, outputs a signed quantity measuring how much the function f 'flows inward' towards a vertex u. Let us now give a characterization of harmonic functions, which was discussed tangentially in the motivational subsections, and a maximum modulus principle which we will use later.

Theorem 1.1 (Magnetic Mean Value Property)**.** Let (G,σ) be a magnetic graph. A function $f \in \ell_2(V(G))$ is harmonic at a vertex $u \in V(G)$ if and only if the following holds:

$$f(u) = \frac{1}{d_u^G}\Bigg(\sum_{\substack{v\sim u \\ v\in G}} \sigma_{uv} f(v)\Bigg).$$

Proof. We verify the claim directly:

$$(\Delta_G f)(u) = 0 \iff \sum_{\substack{v\sim u \\ v\in G}} \big(f(u) - \sigma_{uv} f(v)\big) = 0 \iff f(u) = \frac{1}{d_u^G}\Bigg(\sum_{\substack{v\sim u \\ v\in G}} \sigma_{uv} f(v)\Bigg).$$

□

We wish to draw the reader's attention back to the equation (1) from the motivating example. If we rearrange it slightly, one observes that at each vertex u, we have

$$\sum_{v\sim u} \big(F(u) - \overline{\omega((u,v))}F(v) = 0\big).$$

The quantity on the left is, in fact, what we now call the *magnetic Laplacian* of F. With the new terminology established in this section, we now see that the function of interest F in the first example is actually harmonic, in the sense of the magnetic Laplacian (note that what we called ω assumes the role of σ in the preceding theorem, after the application of a complex conjugate on ω as a formality).

We round out this preliminary subsection with a final useful result.

Theorem 1.2 (Maximum Modulus Principle)**.** Let (G,σ) be a magnetic graph, and let $H \subset V(G)$ be a sub-connected subset of vertices in G, with vertex boundary ∂H. Suppose $f \in \ell_2(\overline{H})$ is harmonic on $\overline{H}$. Then, f satisfies

$$\max_{u\in\overline{H}} |f(u)| = \max_{u\in\partial H} |f(u)|.$$

Proof. Let us assume that for some vertex $u^* \in H$, we have

$$|f(u^*)| > \max_{u\in\partial H} |f(u)|.$$

We observe that, via the mean value principle in the preceding result,

$$|f(u^*)| = \frac{1}{d_{u^*}}\left|\sum_{v\sim u^*} \sigma_{u^*v} f(v)\right| \leqslant \frac{1}{d_{u^*}} \sum_{v\sim u^*} |f(v)| \leqslant |f(u^*)|.$$

In turn, we find that the values of f at vertices $v \sim u^*$ have the same modulus as $f(u^*)$; this argument then applies to each of the neighbors of v, their neighbors, etc.. In turn, we can see that if, as we assumed, a maximum modulus is attained strictly within H, every vertex in $\overline{H}$ must have this same modulus, including those on the boundary. Appealing to contradiction, this completes the proof. □

1.4. **Some remarks on probability.** In this paper, we will make use of a few fairly standard notions from the theory of probability, and we dedicate this subsection to a brief review. The reader who is unfamiliar with these concepts is referred to any standard probability text; for instance, [9], or [11] for a more applied approach. By $\mathbb{P}[P]$ we mean the probability that an event P occurs. By $\mathbb{P}[P : Q]$, we mean a conditional probability; that is, the probability that P occurs knowing that Q has already occurred. If we have a random variable X, i.e. a real- or complex-valued function whose output or variable may take random values, we denote by $\mathbb{E}[X]$ the expectation of X taken over all possible events, and similarly, by $\mathbb{E}[X : P]$ we denote the expectation of X subject to the condition that the event P has occurred.

On a final note, recall that in the motivating example, we utilized an important fact concerning conditional expectations. Suppose that the set of all outcomes Ω over which a random variable X is considered may be partitioned into a disjoint union of a finite family of outcomes, say P_i; that is, $\Omega = \bigcup_{i=1}^n P_i$, and $P_i \cap P_k = \varnothing$ for $i \neq k$. Then we may express the total expectation of the random variable X subordinate to this partition in the following manner:

$$\mathbb{E}[X] = \sum_{i=1}^{n} \mathbb{E}[X : P_i] \cdot \mathbb{P}[P_i]. \tag{8}$$

This fact can be found in more detail in, for example, the text [11].

2. Magnetic Dirichlet Problem via Random Walks

In this section, we will revisit in detail the concepts to which the author alluded in the motivating example from the introduction. In particular, we will clearly formulate a discrete version of the Dirichlet problem in equation (2) for magnetic graphs and solve it in two ways using the framework of random walks on a graph. The first approach will be for a general, connected magnetic graph on an appropriate subset of vertices. The second approach, which will yield a slightly simpler solution, will be suited specifically for those sufficiently connected magnetic graphs whose signatures take values in a finite subgroup of $\{z \in \mathbb{C} : |z| = 1\}$ (viewed as a group itself under multiplication). This second approach will utilize a concept known as the *magnetic lift graph*, which is associated to the magnetic graph of interest. The reader who wishes to find more information concerning how random walks can be utilized to solve discrete boundary value problems is encouraged to explore the text by Lawler [11].

2.1. **Formulation of the problem, first solution.** Let us first formulate the problem, tackle some technical remarks, and then present and prove the first approach to the solution.

Let (G, σ) be a simple, connected magnetic graph and let $H \subsetneq V(G)$ be a proper, subconnected subset of vertices in $V(G)$. Let $f \in \ell_2(\partial H)$ be a given boundary condition. We wish to find a function $\Psi \in \ell_2(\overline{H})$ for which

$$\begin{cases} (\Delta_G \Psi)(u) = 0 & u \in H \\ \Psi(u) = f(u) & u \in \partial H \end{cases}. \tag{9}$$

Heuristically speaking, the approach to this problem will be as follows. We would like to begin a random walk process somewhere in H (where the values of Ψ are undetermined), let it proceed throughout H, and then record the value of the boundary condition at the point where the walk exits the set H and touches the boundary ∂H, multiplied by the product of the values of the signature along the path determined by the random walk process. The main concern in this approach is the need for probabilistic certainty that the random walk will eventually encounter the boundary, regardless of where it begins in H.

The resolution of this important detail comes from viewing the random walk on our graph in a slightly more technical framework. In particular, a random walk process on a graph is often viewed as a *discrete time Markov chain*. This is essentially a formal framework that gives structure to the concept of a random walk process, as a special kind of random variable which evolves through time. In our case, the vertices in H would be called our 'transient' states of the process, and the boundary vertices in ∂H would be called 'absorbing' or 'stopping' states of the process, since in our preceding heuristic explanation of the random walk of interest, the walker will 'stop' once reaching the boundary set. In the Markov Chain text [14, ch. 1], the author sets down a proof that as long as the Markov chain is *irreducible*, the probability that the process is eventually absorbed by one of the stopping states is in fact 1. However, this useful fact need be translated back into our language of graphs. In [7], Chung states a well-known property of graphs which characterizes the irreducibility of the random walk process, which we will recall below.

Lemma 2.1.1. Let G be a simple graph, and consider the random walk process (S_t) originating at any vertex in G. Then, the process (S_t) is irreducible, i.e., for each $u, v \in V(G)$,

$$\mathbb{P}\left[\min\{t : S_t = v\} < \infty : S_0 = u\right] > 0,$$

if and only if G is connected.

This is all to say that as long as our original graph G is connected, and the proper vertex subset H is subconnected, then we can be certain (with probability 1) that any random walk originating in H will in fact eventually reach the boundary ∂H. We now present the first solution to the problem in (9), the framework for which was inspired by the book [11], wherein a similar solution is given for the combinatorial Laplace operator.

Theorem 2.1 (Dirichlet Solution 1)**.** Let G be a connected magnetic graph, and $H \subsetneq V(G)$ a proper, subconnected subset of vertices in G. Let f be a given boundary condition. Let $(S_t) = (S_0, S_1, ..., S_t)$ be a random walk originating at $S_0 \in H$ which moves between adjacent vertices with uniform probability of transitioning from any vertex to one of its neighbors, represented as an ordered sequence of vertices. Set $T = \min\{t : S_t \in \partial H\}$, and let $\widetilde{S}_t = S_{\min\{t,T\}}$ be the modified random walk which 'stops' upon reaching ∂H. Then the unique solution Ψ to the Dirichlet problem

$$\begin{cases} (\Delta_G \Psi)(u) = 0 & u \in H \\ \Psi(u) = f(u) & u \in \partial H \end{cases}$$

may be given by

$$\Psi(u) = \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : S_0 = u], \quad u \in \overline{H}. \tag{10}$$

Proof. First, note that uniqueness follows from applying the maximum modulus principle in Theorem 1.2 to the difference of two distinct solutions $\Psi_1 - \Psi_2$, whose values on ∂H become 0. We now simply check that the solution as stated in equation (10) indeed solves the problem (9). Let Ψ be given by equation (10). If $u \in \partial H$, we check

$$\Psi(u) = \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : S_0 = u] = \mathbb{E}[f(u) : S_0 = u] = f(u).$$

Now if $u \in H$, we verify

$$\begin{aligned} \Psi(u) &= \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : S_0 = u] \\ &= \sum_{v \sim u} \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : S_0 = u, S_1 = v] \mathbb{P}[S_1 = v : S_0 = u] \\ &= \sum_{v \sim u} \frac{1}{d_u^G} \mathbb{E}[f(\widetilde{S_T}) \sigma_{uv} \prod_{i=2}^{T} \sigma_{S_{i-1}S_i} : S_0 = u, S_1 = v] \\ &= \sum_{v \sim u} \frac{1}{d_u^G} \sigma_{uv} \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : S_0 = v] = \frac{1}{d_u^G}\left(\sum_{v \sim u} \sigma_{uv} \Psi(v)\right). \end{aligned}$$

We appeal to the mean value characterization of harmonic functions in Theorem 1.1 to see that Ψ is indeed harmonic on H. This completes the proof. □

2.2. **Magnetic lifts, second solution.** The main downside to the previous solution is the product of the signatures along the path, in the sense that it serves as an additional quantity which need be computed alongside the sequence of vertices encountered by the random walk. To somewhat resolve this disadvantage and produce a second formulation of the solution, we introduce the notion of a magnetic lift graph. This construction seems to have originated as a discrete interpretation of a topological covering space, which was then reformulated and adapted to the setting of a magnetic graph. Some interesting exposition can be found in Biggs, [5, ch. 19]. At the present time, this construction is limited to the case where a magnetic graph is paired with a signature taking values in a finite subgroup of $S^1 \subset \mathbb{C} := \{z \in \mathbb{C} : |z| = 1\}$.

Definition 2.2.1. Let (G, σ) be a magnetic graph. Further assume that σ takes values strictly in a subgroup of the complex unit circle consisting of the pth primitive roots of unity, denoted $\mathbf{S}_p^1$ for some integer $p \geqslant 2$. Write

$\mathbf{S}_p^1 = \{\omega_i\}_{i=0}^{p-1} = \{e^{2\pi ji}\}_{i=0}^{p-1}$. We define the *lift* of G to be the non-magnetic graph $\widehat{G}$ consisting of vertex set $G \times \mathbf{S}_p^1$ and edges defined by

$$(u, \omega_i) \sim (v, \omega_k) \text{ in } \widehat{G} \iff u \sim v \text{ in } G \text{ and } \omega_k = \omega_i \sigma_{uv}.$$

The subsets $G \times \{\omega_i\} \subsetneq V(\widehat{G})$ for each fixed $\omega_i \in \mathbf{S}_p^1$ are called the *levels* of the magnetic graph.

As the reader will see, magnetic lifts are an appropriate setting in which to start a random walk. However, before attempting to do so, we must resolve some of the same issues that we encountered when extending Green's functions to products. Namely, knowing only that G is connected, we do not necessarily know that its lift $\widehat{G}$ satisfies the same property, and in turn we may not be able to apply the result in Lemma 2.1.1 to a random walk process on $\widehat{G}$ to obtain a solution as before. We present a strong implication of the connectedness of $\widehat{G}$, and give a partial converse.

Theorem 2.2. Let (G, σ) be a connected magnetic graph, and assume σ takes values in $\mathbf{S}_p^1$ for some $p \geqslant 2$. Then if the magnetic lift $\widehat{G}$ is connected, then σ is unbalanced. Moreover, if $p = 2$, then the converse holds.

Proof. Assume $\widehat{G}$ is connected and $p \geqslant 2$. Fix any $u \in V(G)$ and look at a path in $\widehat{G}$ starting at $(u, 1) \in V(\widehat{G})$ and terminating at (u, ω) for some $\omega \in \mathbf{S}_p^1 \backslash \{1\}$. By projecting this path onto the original graph G; that is, viewing the first coordinates of the path in $\widehat{G}$ as a path in G, we find that it in fact is a cycle. Moreover, since this path began on one level in $\widehat{G}$ and ended on another level in the lift graph, the definition of the edge set of the magnetic lift precisely implies that the product of the signatures along the associated cycle in G cannot be equal to 1 since $\omega \neq 1$ by assumption. In other words, σ must be unbalanced. For the partial converse, let us now assume that σ is unbalanced and $p = 2$. Let $(u, s_1), (v, s_2) \in V(\widehat{G})$ be fixed. Since G is connected, we may find a path $R := \{u, ..., v\} \subset V(G)$ connecting u and v. Also, since σ is unbalanced, there exists some cycle $C' := \{u_0, u_1, ..., u_n, u_{n+1}\}$ in G for which

$$\prod_{i=0}^{n} \sigma_{u_i, u_{i+1}} = -1$$

where $u_{n+1} \equiv u_0$. Now by viewing the path R on the lift graph, we may obtain a new path beginning at $(u, s_1) \in V(\widehat{G})$, concatenated with the vertices in $\widehat{G}$ whose first coordinates are the vertices in the original path R, and which terminates at (v, s) for some $s = \pm 1$. If $s = s_2$ then we have found the desired path connecting the two vertices in the lift identified at the beginning. If $s \neq s_2$, then proceed by looking at the cycle in G obtained by concatenating a fixed path connecting v and u_0 with the cycle C', and then with the reverse of path connecting v to u_0. Because the cycle contains the one identified as having a signature product of -1, we may view it as a path in the lift originating at (v, s), and since $s \neq s_2$ and $p = 2$, it terminates at (v, s_2). By concatenating $\widehat{R}$ with this new path in the lift, we have obtained a path originating at (u, s_1), and terminating at (v, s_2). This completes the proof. ☐

We round out this subsection by presenting our second formulation of the solution to the Dirichlet problem, now utilizing the magnetic lift structure.

Theorem 2.3. Let G, H, f, Ψ be as in Theorem 2.1. Assume further that σ takes values in some $\mathbf{S}_p^1 = \{\omega_i\}_{i=0}^{p-1}$, ordered as in Definition 2.2.1, where $p \geqslant 2$, and that the lift $\widehat{G}$ is connected. Let $(\widehat{S}_t) = ((S_0, \sigma_0), (S_1, \sigma_1), ..., (S_t, \sigma_t))$ be a random walk on $\widehat{G}$, which originates at $(S_0, \sigma_0) \in H \times \mathbf{S}_p^1$, and is represented as an ordered sequence of vertices. Once again, set $T = \min\{t : (S_t, \sigma_t) \in \partial H \times \mathbf{S}_p^1\}$, and let

$$\widetilde{\widehat{S}}_t = ((\widetilde{S_0}, \widetilde{\sigma_0}), (\widetilde{S_1}, \widetilde{\sigma_1}), ..., (\tilde{S}_t, \tilde{\sigma}_t)) = \widehat{S_{\min\{t,T\}}}$$

be the modified random walk which 'stops' upon reaching $\partial H \times \mathbf{S}_p^1$. Then the unique solution to (9) may be given by

$$\Psi(u) = \mathbb{E}[f(\widetilde{S_T})\widetilde{\sigma_T} : S_0 = (u, 1)], \quad u \in \overline{H}. \tag{11}$$

Proof. This is just a special case of the previous solution derivation, which we sketch. All that need be checked is (i) that uniqueness holds, via the maximum modulus principle in Theorem 1.2 as before; (ii) that $\widetilde{\sigma(T)}$ is equal to the signature product in (2.1), which one verifies from the definition of the edge set of $\widehat{G}$ in Definition 2.2.1; and (iii) that $f(\widetilde{S_T})$ is a well-defined random variable when the walk is on $\widehat{G}$ and not G, which follows from Lemma 2.1.1. ☐

3. Magnetic Poisson Problem via Spectral Theory

In this section, we will state and prove a useful Green's identity, and then formulate and solve the Poisson problem associated to the magnetic Laplacian. Finally, we will focus on what will be called a 'discrete Green's function,' and extend its formulation to the case of product graphs.

3.1. Magnetic Green's identity and Green's function.

This part will concern the aforementioned Green's identity, the continuous version of which the reader may recall from multivariable calculus. Generally speaking, Green's identities (of which there are several formulations) are useful tools in topics like partial differential equations and multivariable analysis; see [13]. In this subsection, we will formulate a magnetic Green's identity, and then write up a useful technical lemma that will be used later. This was originally inspired by the identities developed in [3] for the combinatorial Laplace operator. At the end, we give some exposition concerning a discrete analog of what is known as a Green's function.

Theorem 3.1 (Magnetic Green's Identity)**.** Let (G,σ) be a magnetic graph, and $H \subsetneq V(G)$. Let $f, g \in \ell_2(V(\overline{H}))$. Then the following holds:

$$\sum_{u\in H}\left[(\Delta_{\overline{H}}f)(u)\overline{g(u)} - f(u)\overline{(\Delta_{\overline{H}}g)(u)}\right] = \sum_{u\in\partial H}\left[f(u)\overline{\frac{\partial g}{\partial\eta}(u)} - \frac{\partial f}{\partial\eta}(u)\overline{g(u)}\right].$$

Proof. We prove the identity by a direct computational argument. First, notice that

$$\begin{aligned}
&\sum_{u\in H}\left(\Delta_{\overline{H}}f(u)\overline{g(u)} - f(u)\overline{\Delta_{\overline{H}}g(u)}\right)\\
&= \sum_{u\in H}\overline{g(u)}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(f(u)-\sigma_{uv}f(v)\right) - \sum_{u\in H}f(u)\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\overline{g(u)-\sigma_{uv}g(v)}\right)\\
&= \sum_{u\in H}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\overline{g(u)}f(u) - \sigma_{uv}\overline{g(u)}f(v)\right) - \left(f(u)\overline{g(u)} - \sigma_{vu}f(u)\overline{g(v)}\right)
\end{aligned}$$

which yields the following:

$$\sum_{u\in H}\left(\Delta_{\overline{H}}f(u)\overline{g(u)} - \overline{\Delta_{\overline{H}}g(u)}f(u)\right) = \sum_{u\in H}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\sigma_{vu}f(u)\overline{g(v)} - \sigma_{uv}\overline{g(u)}f(v)\right). \tag{12}$$

The reader may check that the summand on the R.H.S. is anti-symmetric in the following sense: For any pair $u\sim v$ with $u, v\in H$, the two terms in the sum evaluated at these vertices in different order will be negatives of each other, and cancel. Hence, all terms in the sum that were evaluated over edges strictly inside of H will vanish. The only terms that will not completely cancel are those from evaluation on vertices inside of H with neighbors in the vertex boundary ∂H. As a formality, we switch the role of u and v, negate the summand appropriately, and obtain from (12) the following:

$$\sum_{u\in H}\left(\Delta_{\overline{H}}f(u)\overline{g(u)} - \overline{\Delta_{\overline{H}}g(u)}f(u)\right) = \sum_{u\in\partial H}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\sigma_{uv}\overline{g(u)}f(v) - \sigma_{vu}f(u)\overline{g(v)}\right).$$

This will yield the identity as follows:

$$\begin{aligned}
&\sum_{u\in\partial H}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\sigma_{uv}\overline{g(u)}f(v) - \sigma_{vu}f(u)\overline{g(v)}\right)\\
&= \sum_{u\in\partial H}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(f(u)\overline{g(u)} - f(u)\overline{\sigma_{uv}g(v)}\right) - \left(f(u)\overline{g(u)} - \sigma_{uv}\overline{g(u)}f(v)\right)\\
&= \sum_{u\in\partial H}\left[f(u)\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(\overline{g(u)-\sigma_{uv}g(v)}\right) - \overline{g(u)}\sum_{\substack{v\sim u\\ v\in\overline{H}}}\left(f(u)-\sigma_{uv}f(v)\right)\right]\\
&= \sum_{u\in\partial H}\left[f(u)\overline{\frac{\partial g}{\partial\eta}(u)} - \frac{\partial f}{\partial\eta}(u)\overline{g(u)}\right].
\end{aligned}$$

∎

Let us now move on to a useful technical lemma.

Lemma 3.1.1. Let (G, σ) be a connected magnetic graph, and $H \subsetneq V(G)$ a subconnected subset of vertices. Then L_H is an invertible matrix.

Proof. Assume per contradiction that there exists a nonzero solution $h \in \ell_2(H)$ to the homogeneous linear equation

$$L_H h \equiv 0.$$

Put $|h(u^*)| = \max_{u \in H} |h(u)| > 0$. Then from the definition of L_H, we have

$$|h(u^*)| = \frac{1}{d^G_{u^*}} \left| \sum_{\substack{v \sim u^* \\ v \in H}} \sigma_{u^* v} h(v) \right| \leqslant \frac{1}{d^G_{u^*}} \sum_{\substack{v \sim u^* \\ v \in H}} |h(v)| \leqslant \frac{1}{d^H_{u^*}} \sum_{\substack{v \sim u^* \\ v \in H}} |h(u^*)| = |h(u^*)|$$

where $d^H_{u^*}$ is the degree of the vertex u in the subgraph induced by H. From this we have forced two conclusions: first, that the degree of u^* in G is the same as in the subgraph induced by H; and second, that $|h(v)| = |h(u^*)|$ for each v adjacent to u^* in H. Hence we may do the same analysis on any vertex adjacent to u^* in H; in turn, the conclusions we made apply to all of these vertices as well, and their neighbors in H, and so on. Since H is connected when viewed as an induced subgraph of G, after finitely many iterations of this process we have the conclusion that the degree of each vertex $u \in H$ taken in H agrees with the degree of said vertex taken in G. This cannot be the case since we assumed that G is connected, and that H induces a *proper* subgraph of G. The claim follows. ☐

Some remarks concerning this lemma are in order. The matrix L_H^{-1} we have now encountered is very interesting. As the reader will shortly see, it is an important part of the solution to the magnetic Poisson problem which will soon be formulated. Generally speaking, in the continuous case, both the Poisson problem as formulated in the introduction, and some very closely related partial differential equations like the heat equation, utilize in their solutions what is known as a Green's function. These functions usually depend on several factors, e.g. the domain of interest, the type of equation, and in particular, the source term of the equation. If one is lucky enough, oftentimes the solution to the equation has a simple integral representation involving the Green's function. As the reader will see explicitly in the sequel, this inverse matrix L_H^{-1} serves precisely this role in a discrete sense; its interpretation as a 'discrete Green's function' is founded in this fact.

3.2. **Magnetic Poisson problem.** The reader is invited to refer once again to the equation (3) in the second motivational section. With our discrete magnetic Laplace operator on hand, we are ready to reformulate it in the setting of a magnetic graph. We will phrase the new formulation and its solution in the form of a theorem, and dedicate this section to proving it by obtaining the solution from two associated problems. The proof utilizes techniques seen in [6], which have been adapted to the setting of the magnetic Laplace operator.

Theorem 3.2 (Magnetic Poisson problem)**.** Let (G, σ) be a magnetic graph, and let $H \subsetneq V(G)$ be a proper subconnected subset of $m \geqslant 1$ vertices in G. Additionally, let $f \in \ell_2(H)$ and $g \in \ell_2(\partial H)$ be given functions, called the *source* and *boundary* conditions, respectively. The unique solution $\Psi \in \ell_2(\overline{H})$ to the equation

$$\left\{ \begin{array}{cc} (\Delta_G \Psi)(w) = f(w) & w \in H \\ \Psi(w) = g(w) & w \in \partial H \end{array} \right. \tag{13}$$

is given by

$$\Psi(w) = \left\{ \begin{array}{cc} (L_H^{-1} f)(w) - \sum_{i=1}^m \frac{e_i(w)}{\lambda_i} \left[\sum_{u \in \partial H} \overline{\frac{\partial \widetilde{e_i}}{\partial \eta}(u)} g(u) \right] & w \in H \\ g(w) & w \in \partial H \end{array} \right. \tag{14}$$

where $\{e_1, e_2, ..., e_m\} \subset \ell_2(H)$ and $\{\lambda_1, \lambda_2, ..., \lambda_m\} \subset \mathbb{R}$ is an orthonormal basis of $\ell_2(H)$, which are eigenfunctions for L_H, and their associated eigenvalues resp.; and $\{\widetilde{e_1}, \widetilde{e_2}, ..., \widetilde{e_m}\} \subset \ell_2(\overline{H})$ are their extensions to the closure of H, uniformly taking the value 0 on the vertices ∂H and agreeing with the original eigenfunctions on H.

Before proving this claim, we make a quick remark on the conditions we asked of H. In particular, we required that it be a subconnected subset of $V(G)$. The reader will see shortly that this is to ensure L_H is invertible. In the case where the mathematician wishes to apply this result to a subset H which induces a disconnected subgraph, she would simply apply this result to the problems obtained by looking at each of the subsets of H which induce separate connected components individually, then defining the full solution on the whole set by adding together the solutions on each of the subconnected subsets of H, extended appropriately.

Proof. This proof follows the general strategy seen in [6], adapted to the magnetic Laplace operator. The especially informed reader who has encountered the differential equation (3) in class may recall that it can be solved by looking at two associated problems individually. To this extent, let us first examine the following problem wherein we have ignored the source condition f. Let $\psi \in \ell_2(\overline{H})$ solve

$$\begin{cases} (\Delta_G \psi)(w) = 0 & w \in H \\ \psi(w) = g(w) & w \in \partial H \end{cases} \tag{15}$$

Let $\{e_i\}_{1 \leqslant i \leqslant m}$ be an orthonormal basis of $\ell_2(H)$ of eigenvectors for L_H, associated to real eigenvalues $\{\lambda_i\}_{1\leqslant i\leqslant m}$, counted with multiplicity. Extend this family of functions on H to a family $\{\widetilde{e_i}\}$ on $\overline{H}$ by setting $\widetilde{e_i} \equiv 0$ on ∂H. We know the values of ψ in ∂H, so we solve for the values of ψ in H. To this end, for $w \in H$ we have a unique expression of ψ as a linear combination of the e_i's:

$$\psi(w) = \sum_{i=1}^{m} c_i e_i(w), \qquad w \in H. \tag{16}$$

Let us solve for the currently undetermined constants c_i. First,

$$\begin{aligned} c_i &= \langle \psi, e_i \rangle_H \\ \lambda_i c_i &= \lambda_i \langle \psi, e_i \rangle_H \\ &= \langle \psi, L_H e_i \rangle_H . \end{aligned} \tag{17}$$

Next, let an extension $g_0 : \overline{H} \to \mathbb{C}$ of g be given by

$$g_0(w) = \begin{cases} 0 & w \in H \\ g(w) & w \in \partial H \end{cases}.$$

Then (17) becomes

$$\begin{aligned} \lambda_i c_i &= \langle \psi - g_0, L_H e_i \rangle_H \\ &= \langle L_H(\psi - g_0), e_i \rangle_H \\ &= \langle \Delta_{\overline{H}}(\psi - g_0), \widetilde{e_i} \rangle_{\overline{H}} \\ &= \langle -\Delta_{\overline{H}} g_0, \widetilde{e_i} \rangle_{\overline{H}} \\ &= \sum_{u \in \overline{H}} -\Delta_{\overline{H}} g_0(u) \overline{\widetilde{e_i}(u)} \\ &= \sum_{u \in H} \left[g_0(u) \overline{\Delta_{\overline{H}} \widetilde{e_i}(u)} - \Delta_{\overline{H}} g_0(u) \overline{\widetilde{e_i}(u)} \right] \end{aligned}$$

where $\Delta_{\overline{H}}$ is the magnetic Laplacian associated to the connected (magnetic) subgraph in G induced by $\overline{H}$. Moreover, the last equality follows by noting that $\widetilde{e_i} \equiv 0$ on ∂H, and $g_0 \equiv 0$ on H. By complicating the sum a bit, we have clear access to the Green's identity from Theorem 3.1, though the reader should note that a complex conjugation was applied. The computation is almost complete:

$$\begin{aligned} \lambda_i c_i &= \sum_{u \in \partial H} \left[\overline{\widetilde{e_i}(u)} \frac{\partial g_0}{\partial \eta}(u) - \overline{\frac{\partial \widetilde{e_i}}{\partial \eta}(u)} g_0(u) \right] \\ &= - \sum_{u \in \partial H} \overline{\frac{\partial \widetilde{e_i}}{\partial \eta}(u)} g(u) \end{aligned}$$

whence, recalling equation (16), the solution ψ to equation (15) may be expressed

$$\psi(w) = \begin{cases} -\sum_{i=1}^{m} \frac{e_i(w)}{\lambda_i} \left[\sum_{u \in \partial H} \overline{\frac{\partial \widetilde{e_i}}{\partial \eta}(u)} g(u) \right] & w \in H \\ g(w) & w \in \partial H \end{cases}.$$

With ψ in hand, we continue by considering a second problem wherein we have now ignored the boundary condition. Let $\phi \in \ell_2(\overline{H})$ solve

$$\begin{cases} (\Delta_G \phi)(w) = f(w) & w \in H \\ \phi(w) = 0 & w \in \partial H \end{cases}. \tag{18}$$

To solve this problem, we simply apply some linear algebra and make use of Lemma 3.1.1. First, since ϕ is assumed to take the value 0 on ∂H, one verifies that on $\overline{H}$, it holds that

$$\Delta_G \phi \equiv \Delta_{\overline{H}} \phi \equiv L_H \phi,$$

whence (18) is equivalently stated

$$\begin{cases} (L_H\phi)(w) = f(w) & w \in H \\ \phi(w) = 0 & w \in \partial H \end{cases}.$$

In turn, the unique solution ϕ to (18) may be written

$$\phi(w) = \begin{cases} (L_H^{-1} f)(w) & w \in H \\ 0 & w \in \partial H \end{cases}. \tag{19}$$

Returning to the original claim of the section, the reader is invited to check that the sum $\phi + \psi$, based not on their explicit solutions but rather on the problems which they were chosen to solve, in fact, solves the original problem in equation (13). To be thorough, we conclude the claim:

$$\Psi(w) = \phi(w) + \psi(w) = \begin{cases} (L_H^{-1} f)(w) - \sum_{i=1}^m \frac{e_i(w)}{\lambda_i}\left[\sum_{u\in\partial H} \overline{\frac{\partial \tilde{e_i}}{\partial \eta}(u)} g(u)\right] & w \in H \\ g(w) & w \in \partial H \end{cases}.$$

This completes our proof. ☐

3.3. **Green's functions and product graphs.** Let us now take a slight detour. The reader may recall some exposition in subsection 3.1 concerning the description of the matrix L_H^{-1} as a discrete Green's function. In our final remarks for this part of the paper, we wish to actually construct this matrix from the eigenfunctions and eigenvalues of the magnetic Laplacian, and show how we may be construct a Green's function for the product of two magnetic graphs, when their respective eigenfunctions and eigenvalues are identified. First, a lemma.

Lemma 3.3.1. Let (G, σ) be a magnetic graph, and let $H \subsetneq V(G)$ be a proper subconnected subset consisting of m vertices. Let $\{e_i\}_{i=1}^m$, and $\{\lambda_i\}_{i=1}^m$ be the orthonormal system associated to L_H as in the statement of the solution in the previous subsection, *cf* equation (14). If we interpret L_H^{-1} as a function on $H \times H$, we have the following equation

$$L_H^{-1}(p,q) = \sum_{i=1}^m \frac{1}{\lambda_i} e_i(p)\overline{e_i(q)}$$

where $(p,q) \in H \times H$.

Proof. Since L_H is a Hermitian matrix, it admits a matrix factorization of the form

$$L_H = \mathbf{U} D \mathbf{U}^*$$

where $D = \text{diag}(\lambda_1, \lambda_2, ..., \lambda_m)$ is a diagonal matrix of eigenvalues, $\mathbf{U} = [e_1 \;\; e_2 \;\; ... \;\; e_m]$ is the matrix of eigenvectors, and $\mathbf{U}^* = \overline{\mathbf{U}^T}$ is its complex conjugate transpose matrix. After carrying out a pointwise computation for the entries in the inverse matrix, $L_H^{-1} = \mathbf{U} D^{-1} \mathbf{U}^*$, the claim follows. ☐

The preceding lemma is particularly useful in that an explicit construction of the Green's function for H can be found with a determined spectral system associated to H. Though this can be a difficult system to find in practice, obtaining it using a computational software for a particular graph is usually a tractable task. The identification of these systems for general families of graphs remains an interesting, and quite open, research question; especially in the magnetic case.

The extension of the previous theorem to a product graph is not very difficult. Indeed, it requires only that we identify with some care the spectral system associated to the product of two proper subsets. However, a technicality stands in our way of this identification. Recall that whenever graphs G, H are not necessarily connected, we cannot always conclude that L_H is invertible. This becomes a problem because even if two graphs are connected, we have no reason to believe that their product is itself connected. As such, we must recall a result proved in [17] which clarifies the conditions required for a product to be connected. For some additional information about Kronecker product graphs, see [4].

Theorem 3.3 (Weichsel)**.** Let G_1, G_2 be connected graphs. Then the following are equivalent:

(a) The Kronecker product $G_1 \times G_2$ is connected.

(b) At most one of G_1 or G_2 is bipartite.
(c) There is at least one cycle in either G_1 or G_2 of odd length.

Theorem 3.4. Let $(J, \rho^J), (K, \rho^K)$ be two signed, connected graphs and let $M \subsetneq V(J)$, $N \subsetneq V(K)$ be two proper subconnected subsets consisting of m, n vertices, respectively, and let ρ be the product signature as in Definition 1.3.3. Assume that $J \times K$ is connected (i.e. the pair satisfies some condition in Theorem 3.3). Finally, let $\{x_i\}_{i=1}^m$ and $\{y_k\}_{k=1}^n$ be orthonormal bases for $\ell_2(M), \ell_2(N)$ respectively, associated to eigenvalues $\{\mu_i\}, \{\nu_k\}$ counted with multiplicity. Then, the eigenvectors for the operator $L_{M\times N}$ on $\ell_2(M \times N)$ may be identified as $\{x_i y_k\}_{i,k}$, where $x_i y_k$ is defined pointwise. The corresponding eigenvalues are $\{\mu_i + \nu_k\}_{i,k}$.

Proof. Let us fix some $(p, q) \in M \times N$ and $1 \leqslant i, k \leqslant m, n$ (resp.) and compute

$$\begin{aligned}
\big(L_{M\times N} x_i y_k\big)(p, q) &= \sum_{\substack{(p',q')\sim(p,q)\\(p',q')\in M\times N}} x_i(p)y_k(q) - \rho((p, q), (p', q'))x_i(p')y_k(q') \\
&= \sum_{\substack{p'\sim p\\p'\in M}} x_i(p)y_k(q) - \rho^J_{pp'} x_i(p')y_k(q) \\
&\qquad + \sum_{\substack{q'\sim q\\q'\in N}} x_i(p)y_k(q) - \rho^K_{qq'} x_i(p)y_k(q') \\
&= y_k(q)\big(L_M x_i\big)(p) + x_i(p)\big(L_N y_k\big)(q) \\
&= (\mu_i + \nu_k)(x_i(p)y_k(q)).
\end{aligned}$$

This shows $\{x_i y_k\}_{i,k}$ are all eigenvectors with eigenvalues $\{\mu_i + \nu_k\}_{i,k}$. One readily checks that this family of eigenvectors is indeed linearly independent; and since

$$\dim\left(\ell_2(M \times N)\right) = \dim \ell_2(M) \cdot \dim \ell_2(N),$$

these account for all of the eigenvectors and, with multiplicity, the eigenvalues associated to $L_{M\times N}$. ☐

We will now draw this subsection to a close by giving a formula for the Green's function on a product (Note that its proof is implicit in its statement).

Theorem 3.5. Let $(J, \rho^J), (K, \rho^K)$, M, N, and $\{x_i y_k\}_{i,k=1}^{m,n}$, $\{\mu_i + \nu_k\}_{i,k}$ be as in Theorem 3.4. Recalling Lemma 3.3.1, we have the following expression for the Green's function $L^{-1}_{M\times N}$:

$$L^{-1}_{M\times N}\big((p, q), (p', q')\big) = \sum_{i=1}^{m} \sum_{k=1}^{n} \frac{x_i(p)y_k(q)\overline{x_i(p')y_k(q')}}{\mu_i + \nu_k}$$

where $\big((p, q), (p', q')\big) \subset M \times N$.

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