DISCRETE TRACE THEOREMS AND ENERGY MINIMIZING SPRING EMBEDDINGS OF PLANAR GRAPHS

JOHN C. URSCHEL AND LUDMIL T. ZIKATANOV

Abstract. Tutte’s spring embedding theorem states that, for a three-connected planar graph, if the outer face of the graph is fixed as the complement of some convex region in the plane, and all other vertices are placed at the mass center of their neighbors, then this results in a unique embedding, and this embedding is planar. It also follows fairly quickly that this embedding minimizes the sum of squared edge lengths, conditional on the embedding of the outer face. However, it is not at all clear how to embed this outer face. We consider the minimization problem of embedding this outer face, up to some normalization, so that the sum of squared edge lengths is minimized. In this work, we show the connection between this optimization problem and the Schur complement of the graph Laplacian with respect to the interior vertices. We prove a number of discrete trace theorems, and, using these new results, show the spectral equivalence of this Schur complement with the boundary Laplacian to the one-half power for a large class of graphs. Using this result, we give theoretical guarantees for this optimization problem, which motivates an algorithm to embed the outer face of a spring embedding.

1. Introduction

Graph drawing is an area at the intersection of mathematics, computer science, and more qualitative fields. Despite the extensive literature in the field, in many ways the concept of what constitutes the optimal drawing of a graph is heuristic at best, and subjective at worst. For a general review of the major areas of research in graph drawing, we refer the reader to [1, 10]. When energy minimization is desired (i.e. Hall’s energy, the sum of squared distances between adjacent vertices), the optimal embedding in the plane is given by the two-dimensional diffusion map induced by the eigenvectors of the two smallest non-zero eigenvalues of the graph Laplacian [12, 13, 14]. This general class of graph drawing techniques is referred to as spectral layouts. However, in the case of a planar graph, this drawing is not guaranteed to produce a planar layout. When looking at triangulations of a given domain, it is commonplace for the near-boundary points of the spectral layout to “grow” out of the boundary, or lack any resemblance to a planar embedding. For instance, see the spectral layout of a random triangulation of a disk and rectangle in Figure 1.

In his 1962 work titled “How to Draw a Graph,” Tutte found an elegant technique to produce planar embeddings of planar graphs that also minimize “energy” in some sense [19]. In particular, for a three-connected planar graph, he showed that if the outer face of the graph is fixed as the complement of some convex region in the plane, and every other point is located at the mass center of its neighbors, then the resulting embedding is planar. This embedding minimizes Hall’s energy, conditional on the embedding of the boundary face. This result is now known as Tutte’s spring embedding theorem, and this general class of graph drawing techniques is known as force-based layouts. While this result is well known (see [11], for example), it is not so obvious how to embed the outer face. This, of course, should vary from case to case, depending on the dynamics of the interior.

In this work, we examine how to embed the boundary face such that the embedding is convex and minimizes Hall’s energy over all such convex embeddings with some given normalization. While
it is not clear how to exactly minimize energy over all convex embeddings in polynomial time, it also is not clear that this is a NP-hard optimization problem. Proving that this optimization problem is NP-hard appears to be extremely difficult, as the problem itself seems to lack any natural relation to a known NP-complete problem. In what follows, we analyze this problem and give theoretical guarantees for a large class of three-connected planar graphs through trace theorems. Trace theorems are a class of results in theory of partial differential equations relating norms on the domain to norms on the boundary, which are used to provide a priori estimates on the Dirichlet integral of functions with given data on the boundary. We construct a discrete version of a trace theorem in the plane, and even use this construction to imply a continuous energy-only trace theorem for $H^1(\Omega)$ and $H^{1/2}(\Gamma)$, $\Omega \subset \mathbb{R}^2$. In what follows, we show that the Schur complement of the graph Laplacian with respect to the interior vertices is the correct matrix to consider when choosing an optimal embedding of boundary vertices. See Figure 2 for a visual example of a spring embedding using the two minimal non-trivial eigenvectors of the Schur complement. Using discrete trace theorems, we can quantify the behavior of this Schur complement. In particular, using these trace theorems, we show that this Schur complement is spectrally equivalent to the boundary Laplacian to the one half power. This spectral equivalence result produces theoretical guarantees for the energy minimizing spring embedding problem, but is also of independent interest and applicability in the study of spectral properties of planar graphs. These theoretical guarantees give rise to a natural algorithm with provable guarantees. The performance of this algorithm is also illustrated through numerical experiments.

The remainder of the paper is as follows. In Section 2, we formally introduce Tutte’s spring embedding theorem and characterize the optimization problem under consideration. In Section 3, we consider trace theorems for Lipschitz domains from the theory of elliptic partial differential equations, prove discrete energy-only variants of these results for the plane, and show that the Schur complement with respect to the interior is spectrally equivalent to the boundary Laplacian to the one half power. In Section 4, we use the results from the previous section to give theoretical guarantees regarding approximate solutions to the original optimization problem, and use these theoretical results to motivate an algorithm to embed the outer face of a spring embedding. We present numerical results to illustrate both the behavior of Schur complement-based embeddings compared to variations of natural spectral embeddings, and the practical performance of the algorithm introduced.

2. Spring Embeddings and the Schur Complement

In this section, we introduce the main definitions and notation of the paper, formally define the optimization problem under consideration, and show how the Schur complement is closely related to this optimization problem.

2.1. Definitions and Notation. Let $G = (V, E)$, $V = \{1, \ldots, n\}, E \subset \{e \subset V \mid |e| = 2\}$, be a simple, connected, undirected graph. $G$ is $k$-connected if it remains connected upon the removal of any $k - 1$ vertices, and is planar if it can be drawn in the plane such that no edges intersect (save for adjacent edges at their mutual endpoint). Let $G_n$ be the set of all ordered pairs $(G, \Gamma)$, where $G$ is a simple, undirected, planar, three-connected graph of order $n > 3$, and $\Gamma \subset V$, $n\Gamma := |\Gamma|$, defines a face of $G$. Let $N(i)$ and $d(i)$ be the neighborhood and degree of vertex $i$, and $d_G(i, j)$ be the distance between vertices $i$ and $j$. Let $G[S]$ be the graph induced by the vertices $S$, and $d_S(i, j)$ be the distance between vertices $i$ and $j$ in $G[S]$. The graph Laplacian $L_G \in \mathbb{R}^{n \times n}$ of $G$ is the symmetric matrix defined by

$$\langle L_Gx, x \rangle = \sum_{\{i, j\} \in E} (x_i - x_j)^2,$$
and, in general, a matrix is the graph Laplacian of some weighted graph if it is symmetric diagonally dominant, has non-positive off-diagonal entries, and the vector $\mathbf{1} := (1, \ldots, 1)^T$ lies in its nullspace. The convex hull of a finite set of points $X$ is denoted by $\text{conv}(X)$, and a point $x \in X$ is a vertex of $\text{conv}(X)$ if $x \not\in \text{conv}(X \setminus x)$. Given a matrix $A$, we denote the $i^{th}$ row by $A_{i,\cdot}$, the $j^{th}$ column by $A_{\cdot,j}$, and the entry in the $i^{th}$ row and $j^{th}$ column by $A_{i,j}$.

2.2. Spring Embeddings. Here and in what follows, we refer to $\Gamma$ as the “boundary” of the graph $G$, $V \setminus \Gamma$ as the “interior,” and generally assume $n_\Gamma := |\Gamma|$ to be relatively large (typically

Figure 1. Delaunay triangulations of 1250 points randomly generated on the disk (A) and rectangle (B), their non-planar spectral layouts (C) and (D), and planar layouts using a spring embedding of the Schur complement of the graph Laplacian with respect to the interior vertices (E) and (F).
Figure 2. A visual example of embeddings of the 2D finite element discretization graph 3elt, taken from the SuiteSparse Matrix Collection [5]. Figure (A) is the non-planar spectral layout of this 2D mesh, and Figure (B) is a planar spring embedding of the mesh, using the minimal non-trivial eigenvectors of the Schur complement to embed the boundary.

Figure 2. A visual example of embeddings of the 2D finite element discretization graph 3elt, taken from the SuiteSparse Matrix Collection [5]. Figure (A) is the non-planar spectral layout of this 2D mesh, and Figure (B) is a planar spring embedding of the mesh, using the minimal non-trivial eigenvectors of the Schur complement to embed the boundary.

By embedding $G$ in the plane and traversing the embedding, one can easily find all the induced cycles of $G$ in linear time and space [3]. However, depending on the application from which the graph originated, the boundary face is often already designated. Without loss of generality, suppose that $\Gamma = \{n - n_\Gamma + 1, \ldots, n\}$. A matrix $X \in \mathbb{R}^{n \times 2}$ is said to be a planar embedding of $G$ if the drawing of $G$ using straight lines and with vertex $i$ located at coordinates $X_i, \cdot$ for all $i$ is a planar drawing. A matrix $X_\Gamma \in \mathbb{R}^{n_\Gamma \times 2}$ is said to be a convex embedding of $\Gamma$ if the embedding is planar and every point is a vertex of the convex hull $\text{conv}\{[X_\Gamma]_i, i = 1, \ldots, n\}$. Tutte’s spring embedding theorem states that if $X_\Gamma$ is a convex embedding of $\Gamma$, then the system of equations

$$X_{i, \cdot} = \begin{cases} \frac{1}{d(i)} \sum_{j \in N(i)} X_{j, \cdot} & i = 1, \ldots, n - n_\Gamma \\ [X_\Gamma]_{i - (n - n_\Gamma)}, & i = n - n_\Gamma + 1, \ldots, n \end{cases}$$

has a unique solution $X$, and this solution is a planar embedding of $G$ [19].

We can write both the Laplacian and embedding of $G$ in block-notation, differentiating between interior and boundary vertices as follows:

$$L_G = \begin{pmatrix} L_0 + D_o & -A_{o, \Gamma} \\ -A_{o, \Gamma}^T & L_\Gamma + D_\Gamma \end{pmatrix} \in \mathbb{R}^{n \times n}, \quad X = \begin{pmatrix} X_o \\ X_\Gamma \end{pmatrix} \in \mathbb{R}^{n \times 2},$$

where $L_o, D_o \in \mathbb{R}^{(n - n_\Gamma) \times (n - n_\Gamma)}$, $L_\Gamma, D_\Gamma \in \mathbb{R}^{n_\Gamma \times n_\Gamma}$, $A_{o, \Gamma} \in \mathbb{R}^{(n - n_\Gamma) \times n_\Gamma}$, $X_o \in \mathbb{R}^{(n - n_\Gamma) \times 2}$, $X_\Gamma \in \mathbb{R}^{n_\Gamma \times 2}$, and $L_o$ and $L_\Gamma$ are the Laplacians of $G[V \setminus \Gamma]$ and $G[\Gamma]$, respectively. Using block notation, the system of equations for the Tutte spring embedding of some convex embedding $X_\Gamma$ is given by

$$X_o = (D_o + D[L_o])^{-1}[(D[L_o] - L_o)X_o + A_{o, \Gamma}X_\Gamma],$$

where $D[A]$ is the diagonal matrix with diagonal entries given by the diagonal of $A$. Therefore, the unique solution to this system is

$$X_o = (L_o + D_o)^{-1}A_{o, \Gamma}X_\Gamma.$$
We note that this choice of \( X_o \) not only guarantees a planar embedding of \( G \), but one can also easily verify that this also minimizes Hall’s energy, namely,

\[
\arg\min_{X_o} h(X) = (L_o + D_o)^{-1}A_o,\Gamma X_\Gamma,
\]

where \( h(X) := \text{Tr}(X^T L X) \) (see [14] for more on Hall’s energy).

While Tutte’s theorem is a very powerful result, guaranteeing that, given a convex embedding of any face, the energy-minimizing embedding of the remaining vertices results in a planar embedding, it gives no direction as to how this outer face should be embedded. In this work, we consider the problem of producing a planar embedding which is energy-minimizing, subject to some normalization. In this work, we consider embeddings which satisfy \( X_\Gamma^T X_\Gamma = I \) and \( X_\Gamma^T 1 = 0 \), though other normalizations, such as \( X^T X = I \) and \( X^T 1 = 0 \), would be equally appropriate. The analysis that follows in this paper can be readily applied to this alternate normalization, but does require the additional step of verifying a norm equivalence between \( V \) and \( \Gamma \) for the harmonic extension of low energy vectors, which can be produced relatively easily for the class of graphs considered in Section 3. Let \( \mathcal{X} \) be the set of all convex, planar embeddings \( X_\Gamma \) which satisfy \( X_\Gamma^T X_\Gamma = I \) and \( X_\Gamma^T 1 = 0 \). The main optimization problem under consideration is

\[
(2.1) \quad \min h(X) \quad s.t. \quad X_\Gamma \in \text{cl}(\mathcal{X}),
\]

where \( \text{cl}(\cdot) \) is the closure of a set. The normalizations \( X_\Gamma^T 1 = 0 \) and \( X_\Gamma^T X_\Gamma = I \) ensure that the solution does not degenerate into a single point or line. In what follows we are primarily concerned with approximately solving this optimization problem. However, we do not determine whether the class of optimization problems of the form \( (2.1) \) is NP-hard. If \( (2.1) \) is NP-hard, it seems extremely difficult to verify that this is indeed the case.

2.3. Schur Complement of \( V \setminus \Gamma \). Given some choice of \( X_\Gamma \), by Tutte’s theorem the minimum value of \( h(X) \) is attained when \( X_o = (L_o + D_o)^{-1}A_o,\Gamma X_\Gamma \), and given by

\[
h(X) = \text{Tr} \left[ \left((L_o + D_o)^{-1}A_o,\Gamma X_\Gamma \right)^T \left[ X_\Gamma^T \begin{pmatrix} L_o + D_o & -A_o,\Gamma \\ -A_o,\Gamma & L_\Gamma + D_\Gamma \end{pmatrix} \left( (L_o + D_o)^{-1}A_o,\Gamma X_\Gamma \right) \right] \right]
\]

\[
= \text{Tr} \left( X_\Gamma^T \left[ L_\Gamma + D_\Gamma - A_o,\Gamma (L_o + D_o)^{-1}A_o,\Gamma \right] X_\Gamma \right) = \text{Tr} \left( X_\Gamma^T S_\Gamma X_\Gamma \right),
\]

where \( S_\Gamma \) is the Schur complement of \( L_\Gamma \) with respect to \( V \setminus \Gamma \),

\[
S_\Gamma = L_\Gamma + D_\Gamma - A_o,\Gamma (L_o + D_o)^{-1}A_o,\Gamma.
\]

For this reason, we can treat \( X_o \) as a function of \( X_\Gamma \) and instead consider the optimization problem

\[
(2.2) \quad \min h_\Gamma(X_\Gamma) \quad s.t. \quad X_\Gamma \in \text{cl}(\mathcal{X}),
\]

where

\[
h_\Gamma(X_\Gamma) := \text{Tr}(X_\Gamma^T S_\Gamma X_\Gamma).
\]

In the following proposition, we present a number of basic properties of the Schur complement of a graph Laplacian. For more information on the Schur complement, we refer the reader to [2, 6, 21].

Proposition 2.1. Let \( G = (V, E) \), \( n = |V| \), be a graph, \( L_G \in \mathbb{R}^{n \times n} \) the associated graph Laplacian, and \( L_G \) and vectors \( v \in \mathbb{R}^n \) be written in block form

\[
L(G) = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}, \quad v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},
\]

where \( L_{22} \in \mathbb{R}^{m \times m}, \ v_2 \in \mathbb{R}^m, \) and \( L_{12} \neq 0 \). Then

(1) \( S = L_{22} - L_{21}L_{11}^{-1}L_{12} \) is a graph Laplacian,
(2) \[ \sum_{i=1}^{m} (e_i^T L_{22} 1_m)e_i e_i^T - L_{21} L_{11}^{-1} L_{12} \] is a graph Laplacian,

(3) \[ \langle Sw, w \rangle = \inf \{ \langle Lv, v \rangle | v_2 = w \} \]

Proof. Let \( P = \begin{pmatrix} -L_{11}^{-1} L_{12} \\ I \end{pmatrix} \) \( \in \mathbb{R}^{n \times m} \). Then

\[ P^T LP = (-L_{21} L_{11}^{-1} I) \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} -L_{11}^{-1} L_{12} \\ I \end{pmatrix} = L_{22} - L_{21} L_{11}^{-1} L_{12} = S. \]

Because \( L_{11} 1_{n-m} + L_{12} 1_m = 0 \), we have \( 1_{n-m} = -L_{11}^{-1} L_{12} 1_m \). Therefore \( P 1_m = 1_n \), and, as a result,

\[ S 1_m = P^T L P 1_m = P^T L 1_n = P^T 0 = 0. \]

In addition,

\[ \begin{bmatrix} \sum_{i=1}^{m} (e_i^T L_{22} 1_m)e_i e_i^T - L_{21} L_{11}^{-1} L_{12} \end{bmatrix} 1_m = \begin{bmatrix} \sum_{i=1}^{m} (e_i^T L_{22} 1_m)e_i e_i^T - L_{22} \end{bmatrix} 1_m + S 1_m \]

\[ = \sum_{i=1}^{m} (e_i^T L_{22} 1_m)e_i - L_{22} 1_m \]

\[ = \begin{bmatrix} \sum_{i=1}^{m} e_i e_i^T - 1_m \end{bmatrix} L_{22} 1_m = 0. \]

\( L_{11} \) is an M-matrix, so \( L_{11}^{-1} \) is a non-negative matrix. \( L_{21} L_{11}^{-1} L_{12} \) is the product of three non-negative matrices, and so must also be non-negative. Therefore, the off-diagonal entries of \( S \) and \( \sum_{i=1}^{m} (e_i^T L_{22} 1_m)e_i e_i^T - L_{21} L_{11}^{-1} L_{12} \) are non-positive, and so both are graph Laplacians.

Consider

\[ \langle Lv, v \rangle = \langle L_{11} v_1, v_1 \rangle + 2 \langle L_{12} v_2, v_1 \rangle + \langle L_{22} v_2, v_2 \rangle, \]

with \( v_2 \) fixed. Because \( L_{11} \) is symmetric positive definite, the minimum occurs when

\[ \frac{\partial}{\partial v_1} \langle Lv, v \rangle = 2 L_{11} v_1 + 2 L_{12} v_2 = 0. \]

Setting \( v_1 = -L_{11}^{-1} L_{12} v_2 \), the desired result follows. \( \square \)

The Schur complement Laplacian \( S_\Gamma \) is the sum of two Laplacians \( L_\Gamma \) and \( D_\Gamma - A_{\alpha,\Gamma}^T (L_\alpha + D_\alpha)^{-1} A_{\alpha,\Gamma} \), where the first is the Laplacian of \( G[\Gamma] \), and the second is a Laplacian representing the dynamics of the interior. One can think of the second Laplacian as a perturbation of sorts to the standard cycle.

Now that we have properly introduced the optimization problem under consideration, in the next section we prove the spectral equivalence of \( S_\Gamma \) and \( L_\Gamma^{1/2} \) for a large class of \( G_n \) by first proving discrete energy-only trace theorems. Then, in Section 4, we use this spectral equivalence to prove theoretical properties of (2.2) and motivate an algorithm to approximately solve this optimization problem.

3. Trace Theorems for Planar Graphs

The main result of this section takes classical trace theorems from the theory of partial differential equations and extends them to a class of planar graphs. However, for our purposes, we require a stronger form of trace theorem, one between energy semi-norms (i.e., no \( l^2 \) term), which we refer to as “energy-only” trace theorems. These energy-only trace theorems imply their classical variants.
with \(l^2\) terms almost immediately. We then use these new results to prove the spectral equivalence of \(S_G\) and \(L_{1/2}^G\) for the class of graphs under consideration. This class of graphs is rigorously defined below, but includes planar three-connected graphs which have some regular structure (such as graphs of finite element discretizations). In what follows, we prove spectral equivalence with explicit constants. While this does make the analysis slightly messier, it has the benefit of showing that equivalence holds for constants that are not too large, thereby verifying that the equivalence is a practical result which can be used in the analysis of algorithms. We begin by formally describing the classical trace theorem.

Let \(\Omega \subset \mathbb{R}^d\) be a domain with boundary \(\Gamma = \partial \Omega\) which, locally, is a graph of a Lipschitz function. \(H^1(\Omega)\) is the Sobolev space of square integrable functions with square integrable gradient, with norm

\[
\|u\|_{H^1(\Omega)}^2 = \|\nabla u\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\Omega)}^2, \quad \text{where} \quad \|u\|_{L^2(\Omega)}^2 = \int_{\Omega} u^2 \, dx.
\]

Let

\[
\|\varphi\|_{H^{1/2}(\Gamma)}^2 = \|\varphi\|_{L^2(\Gamma)}^2 + \iint_{\Gamma \times \Gamma} \frac{(\varphi(x) - \varphi(y))^2}{|x - y|^d} \, dx \, dy
\]

for functions defined on \(\Gamma\), and denote by \(H^{1/2}(\Gamma)\) the Sobolev space of functions defined on the boundary \(\Gamma\) for which \(\|\cdot\|_{1/2,\Gamma}\) is finite. The trace theorem for functions in \(H^1(\Omega)\) is one of the most popular and used trace theorems in the theory of partial differential equations. More general results for traces on boundaries of Lipschitz domains, which involve \(L^p\) norms and fractional derivatives, are due E. Gagliardo [7] (see also [4]). Gagliardo’s theorem, when applied to the case of \(H^1(\Omega)\) and \(H^{1/2}(\Gamma)\), states that if \(\Omega \subset \mathbb{R}^d\) is a Lipschitz domain, then the norm equivalence

\[
\|\varphi\|_{1/2,\Omega} \simeq \inf\{\|u\|_{1,\Omega} \mid u|\Gamma = \varphi\}
\]

holds. These results are key tools in proving a priori estimates on the Dirichlet integral of functions with given data on the boundary of a domain \(\Omega\). Roughly speaking, a trace theorem gives a bound on the energy of a harmonic function via norm of the trace of the function on \(\Gamma = \partial \Omega\). In addition to the classical references given above, further details on trace theorems and their role in the analysis of PDEs (including the case of Lipschitz domains) are found in the monograph by Lions and Magenes [15] and Nečas [17]. There are several analogues of this theorem for finite element discretizations (finite dimensional subspaces of \(H^1(\Omega)\)), for instance, in [16] it is shown that the finite element discretization of the Laplace-Beltrami operator on the boundary to power one-half provides a norm which is equivalent to the \(H^{1/2}(\Gamma)\)-norm. Here we prove energy-only analogues of the classical trace theorem for graphs \((G,\Gamma) \in \mathcal{G}_n\), using energy semi-norms

\[
|u|_G^2 = \langle L_G u, u \rangle \quad \text{and} \quad |\varphi|_G^2 = \sum_{p<q} \frac{(\varphi(p) - \varphi(q))^2}{d_G^2(p,q)}.
\]

The energy semi-norm \(|\cdot|_G\) is a discrete analogue of \(\|\nabla u\|_{L^2(\Omega)}\), and the boundary semi-norm \(|\cdot|_\Gamma\) is a discrete analogue of the quantity \(\iint_{\Gamma \times \Gamma} \frac{(\varphi(x) - \varphi(y))^2}{|x - y|^2} \, dx \, dy\). In addition, by connectivity, \(|\cdot|_G\) and \(|\cdot|_\Gamma\) are norms on the quotient space orthogonal to \(1\). We aim to prove that for any \(\varphi \in \mathbb{R}^{n_G}\),

\[
\frac{1}{c_1} |\varphi|_\Gamma \leq \min_{u|\Gamma = \varphi} |u|_G \leq c_2 |\varphi|_\Gamma
\]

for some constants \(c_1, c_2\) which do not depend on \(n_G, n\). We begin by proving these results for a simple class of graphs, and then extend our analysis to more general graphs.
3.1. Trace Theorems for a Simple Class of Graphs. Let $G_{k,\ell} = C_k \square P_\ell$ be the Cartesian product of the $k$ vertex cycle $C_k$ and the $\ell$ vertex path $P_\ell$, where $4 \ell < k < 2c\ell$ for some constant $c \in \mathbb{N}$. Vertex $(i,j)$ in $G_{k,\ell}$ corresponds to the product of $i \in C_k$ and $j \in P_\ell$, $i = 1, \ldots, k; j = 1, \ldots, \ell$.

The boundary of $G_{k,\ell}$ is defined to be $\Gamma = \{(i,1)\}_{i=1}^k$. Let $u \in \mathbb{R}^{k \times \ell}$ and $\varphi \in \mathbb{R}^k$ be functions on $G_{k,\ell}$ and $\Gamma$, respectively, with $u[(i,j)]$ denoted by $u(i,j)$ and $\varphi[(i,1)]$ denoted by $\varphi(i)$. For the remainder of the section, we consider the natural periodic extension of $u(i,j)$ and $\varphi(i)$ to the indices $i \in \mathbb{Z}$. In particular, if $i \not\in \{1, \ldots, k\}$, then $\varphi(i) = \varphi(i^*)$ and $u(i,j) = u(i^*,j)$, where $i^* \in \{1, \ldots, k\}$ and $i^* = i \bmod k$.

We have broken the proof of the trace theorem into two lemmas. Lemma 3.1 shows that the discrete trace operator is bounded, and Lemma 3.2 shows that it has a continuous right inverse. Taken together, these lemmas imply our desired result.

**Lemma 3.1.** Let $G_{k,\ell} = C_k \square P_\ell$, $4 \ell < k < 2c\ell$, $c \in \mathbb{N}$, with boundary $\Gamma = \{(i,1)\}_{i=1}^k$. For any $u \in \mathbb{R}^{k \times \ell}$, the vector $\varphi = u|_\Gamma$ satisfies

$$|\varphi|_\Gamma \leq \max\{\sqrt{3c}, 2\pi\} |u|_G.$$

**Proof.** We can decompose $\varphi(p+h) - \varphi(h)$ into a sum of differences, given by

$$\varphi(p+h) - \varphi(p) = \sum_{i=1}^{s-1} u(p+h,i) - u(p+h,i+1)$$

$$+ \sum_{i=1}^{h} u(p+i,s) - u(p+i-1,s)$$

$$+ \sum_{i=1}^{s-1} u(p,s-i+1) - u(p,s-i),$$

where $s = \left\lceil \frac{h}{c} \right\rceil$. By Cauchy-Schwarz,

$$\sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left( \frac{\varphi(p+h) - \varphi(p)}{h} \right)^2 \leq 3 \sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left( \frac{1}{h} \sum_{i=1}^{s-1} u(p+h,i) - u(p+h,i+1) \right)^2$$

$$+ 3 \sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left( \frac{1}{h} \sum_{i=1}^{h} u(p+i,s) - u(p+i-1,s) \right)^2$$

$$+ 3 \sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left( \frac{1}{h} \sum_{i=1}^{s-1} u(p,s-i+1) - u(p,s-i) \right)^2.$$
We bound the first and the second term separately. The third term is identical to the first. Using Hardy’s inequality [8, Theorem 326], we can bound the first term by
\[
\left(\sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left(\frac{1}{h} \sum_{i=1}^{s-1} u(p, i) - u(p, i + 1)\right)^2 \right) \leq \frac{\pi^2}{6} \sum_{p=1}^{k} \sum_{h=1}^{\ell} \left(\frac{1}{h} \sum_{i=1}^{s-1} u(p, i) - u(p, i + 1)\right)^2.
\]

For the second term, we have
\[
\left(\sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \left(\frac{1}{h} \sum_{i=1}^{s-1} u(p, i, s) - u(p + i - 1, s)\right)^2 \right) \leq \sum_{p=1}^{k} \sum_{h=1}^{\lfloor k/2 \rfloor} \frac{1}{h} \sum_{i=1}^{s-1} (u(p, i) - u(p, i + 1))^2.
\]

Combining these bounds produces the desired result
\[
|\varphi|_\Gamma \leq \max\{\sqrt{3c}, 2\pi\} |u|_G.
\]

In order to show that the discrete trace operator has a continuous right inverse, we need to produce a provably low-energy extension of an arbitrary function on \(\Gamma\). Let
\[
a = \frac{1}{k} \sum_{p=1}^{k} \varphi(p) \quad \text{and} \quad a(i, j) = \frac{1}{2j-1} \sum_{h=1-j}^{j-1} \varphi(i + h).
\]

We consider the natural extension
\[
(3.1) \quad u(i, j) = \frac{j-1}{\ell-1} a + \left(1 - \frac{j-1}{\ell-1}\right) a(i, j),
\]
and prove the following inverse result for the discrete trace operator.

**Lemma 3.2.** Let \(G_{k,\ell} = C_k \square P_\ell\), \(4 \ell < k < 2c\ell\), \(c \in \mathbb{N}\), with boundary \(\Gamma = \{(i, 1)\}_{i=1}^{k}\). For any \(\varphi \in \mathbb{R}^k\), the vector \(u\) defined by (3.1) satisfies
\[
|u|_G \leq \sqrt{\frac{c + 121}{9}} |\varphi|_\Gamma.
\]

**Proof.** We can decompose \(|u|_G^2\) into two parts, namely,
\[
|u|_G^2 = \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(i, j) - u(i, j))^2 + \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} (u(i, j + 1) - u(i, j))^2.
\]

We bound each sum separately, beginning with the first. We have
\[
u(i + 1, j) - u(i, j) = \left(1 - \frac{j-1}{\ell-1}\right) (a(i + 1, j) - a(i, j)) = \left(1 - \frac{j-1}{\ell-1}\right) \frac{\varphi(i + j) - \varphi(i + 1 - j)}{2j-1}.
\]
We now consider the second sum. Each term can be decomposed as

\[ (u(i+1, j) - u(i, j))^2 \leq \sum_{i=1}^{k} \sum_{j=1}^{\ell} \left[ \frac{\varphi(i+j) - \varphi(i+1-j)}{2j-1} \right]^2 \]

Squaring both sides and noting that \( 4\ell < k \), we have

\[ \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(i+1, j) - u(i, j))^2 \leq \sum_{i=1}^{k} \sum_{j=1}^{\ell} \left[ \frac{\varphi(i+j) - \varphi(i+1-j)}{2j-1} \right]^2 \]

\[ \leq \sum_{i=1}^{k} \sum_{j=1}^{2\ell-1} \left[ \frac{\varphi(p+h) - \varphi(p)}{h} \right]^2 \leq |\varphi|^2_{1}. \]

We now consider the second sum. Each term can be decomposed as

\[ u(i, j+1) - u(i, j) = \frac{a - a(i, j)}{\ell - 1} + \left( 1 - \frac{j}{\ell - 1} \right) [a(i, j+1) - a(i, j)], \]

which leads to the upper bound

\[ \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} (u(i, j+1) - u(i, j))^2 \leq 2 \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} \left[ \frac{a - a(i, j)}{\ell - 1} \right]^2 + 2 \sum_{i=1}^{k} \sum_{j=1}^{\ell-2} (a(i, j+1) - a(i, j))^2. \]

We estimate these two terms in the previous equation separately, beginning with the first. The difference \( a - a(i, j) \) can be written as

\[ a - a(i, j) = \frac{1}{k} \sum_{p=1}^{k} \varphi(p) - \frac{1}{2j-1} \sum_{h=1-j}^{j-1} \varphi(i + h) \]

\[ = \frac{1}{k(2j-1)} \sum_{p=1}^{k} \sum_{h=1-j}^{j-1} \varphi(p) - \varphi(i + h). \]

Squaring both sides,

\[ (a - a(i, j))^2 = \frac{1}{k^2(2j-1)^2} \left( \sum_{p=1}^{k} \sum_{h=1-j}^{j-1} \varphi(p) - \varphi(i + h) \right)^2 \]

\[ \leq \frac{1}{k(2j-1)} \sum_{p=1}^{k} \sum_{h=1-j}^{j-1} (\varphi(p) - \varphi(i + h))^2. \]

Summing over all \( i \) and \( j \) gives

\[ \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} \left( \frac{(a - a(i, j))}{\ell - 1} \right)^2 \leq \frac{1}{(\ell - 1)^2} \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} \frac{1}{k(2j-1)} \sum_{p=1}^{k} \sum_{h=1-j}^{j-1} (\varphi(p) - \varphi(i + h))^2 \]

\[ = \frac{k}{4(\ell - 1)^2} \sum_{j=1}^{\ell-1} \frac{1}{2j-1} \sum_{h=1-j}^{j-1} \sum_{i,p=1}^{k} (\varphi(p) - \varphi(i + h))^2 \]

\[ \leq \frac{k^2}{4(\ell - 1)} |\varphi|^2_{1} \leq c|\varphi|^2_{1}. \]

This completes the analysis of the first term. For the second term, we have

\[ a(i, j+1) - a(i, j) = \frac{1}{2j+1} \left[ \varphi(i+j) + \varphi(i-j) - \frac{2}{2j-1} \sum_{h=1-j}^{j-1} \varphi(i+h) \right]. \]
Next, we note that

\[ \left| \varphi(i + j) - \frac{1}{2j - 1} \varphi(i) - \frac{2}{2j - 1} \sum_{h=1}^{j-1} \varphi(i + h) \right| = \left| \frac{\varphi(i + j) - \varphi(i)}{2j - 1} + 2 \sum_{h=1}^{j-1} \frac{\varphi(i + j) - \varphi(i + h)}{2j - 1} \right| \leq 2 \sum_{h=0}^{j-1} \frac{|\varphi(i + j) - \varphi(i + h)|}{2j - 1}, \]

and, similarly,

\[ \left| \varphi(i - j) - \frac{1}{2j - 1} \varphi(i) - \frac{2}{2j - 1} \sum_{h=1}^{j-1} \varphi(i - h) \right| = \left| \frac{\varphi(i - j) - \varphi(i)}{2j - 1} + 2 \sum_{h=1}^{j-1} \frac{\varphi(i - j) - \varphi(i - h)}{2j - 1} \right| \leq 2 \sum_{h=0}^{j-1} \frac{|\varphi(i - j) - \varphi(i - h)|}{2j - 1}. \]

Hence,

\[
\sum_{j=1}^{l-1} (a(i,j+1) - a(i,j))^2 \leq \sum_{j=1}^{l-1} \frac{8}{(2j + 1)^2} \left[ \left( \sum_{h=0}^{j-1} \frac{|\varphi(i + j) - \varphi(i + h)|}{2j - 1} \right)^2 + \left( \sum_{h=0}^{j-1} \frac{|\varphi(i - j) - \varphi(i - h)|}{2j - 1} \right)^2 \right].
\]

Once we sum over all \( i \), the sum of the first and second term are identical, and therefore

\[
\sum_{i=1}^{k} \sum_{j=1}^{l-1} (a(i,j+1) - a(i,j))^2 \leq 16 \sum_{i=1}^{k} \sum_{j=1}^{l-1} \left( \sum_{h=0}^{j-1} \frac{|\varphi(i + j) - \varphi(i + h)|}{(2j - 1)(2j + 1)} \right)^2.
\]

We have

\[
\sum_{h=0}^{j-1} \frac{|\varphi(i + j) - \varphi(i + h)|}{(2j - 1)(2j + 1)} \leq \frac{1}{3j} \sum_{p=i}^{i+j-1} \frac{|\varphi(i + j) - \varphi(p)|}{j} \leq \frac{1}{3j} \sum_{p=i}^{i+j-1} \frac{|\varphi(i + j) - \varphi(p)|}{i + j - p},
\]

which implies that

\[
16 \sum_{i=1}^{k} \sum_{j=1}^{l-1} \left( \sum_{h=0}^{j-1} \frac{|\varphi(i + j) - \varphi(i + h)|}{(2j - 1)(2j + 1)} \right)^2 \leq 16 \left( \sum_{i=1}^{k} \sum_{j=1}^{l-1} \left( \frac{1}{j} \sum_{p=i}^{i+j-1} \frac{|\varphi(i + j) - \varphi(p)|}{i + j - p} \right)^2 \right) \leq 16 \left( \sum_{q=1}^{k} \sum_{m=1}^{l-1} \left( \frac{1}{q - m} \sum_{p=m}^{q-1} \frac{|\varphi(q) - \varphi(p)|}{q - p} \right)^2 \right).
\]
Letting \( r = q - m, s = q - p \), and using Hardy’s inequality [8, Theorem 326], we obtain

\[
\frac{16}{9} \sum_{q=1}^{k-\ell-1} \sum_{m=1}^{q-1} \left( \frac{1}{q-m} \sum_{p=m}^{q-1} \left| \varphi(q) - \varphi(p) \right| \right)^2 = \frac{16}{9} \sum_{q=1}^{k-\ell-1} \sum_{r=1}^{q-1} \left( \frac{1}{r} \sum_{s=1}^{r} \left| \varphi(q) - \varphi(q-s) \right| \right)^2 \\
\leq \frac{64}{9} \sum_{q=1}^{k-\ell-1} \sum_{r=1}^{q-1} \left[ \frac{\varphi(q) - \varphi(q-r)}{r} \right]^2 \\
= \frac{32}{9} \sum_{q_1,q_2=1}^{k-\ell-1} \left[ \frac{\varphi(q_1) - \varphi(q_2)}{q_1 - q_2} \right]^2 \\
\leq \frac{32}{9} \sum_{q_1,q_2=1}^{k-\ell-1} \left[ \frac{\varphi(q_1) - \varphi(q_2)}{d_G((q_1,1),(q_2,1))} \right]^2,
\]

where, if \( q > k \), we associate \((q,1)\) with \((q^*,1)\), where \( q^* = q \mod k \) and \( 1 \leq q^* \leq k \). The previous sum consists of some amount of over-counting, with some terms \((\varphi(q_1) - \varphi(q_2))^2\) appearing eight times. However, the chosen indexing of the cycle \( C_k \) is arbitrary. Therefore, we can average over all \( k \) different choices of ordering that preserve direction. In particular,

\[
\sum_{i=1}^{k-1} \sum_{j=1}^{l-1} (a(i, j+1) - a(i, j))^2 \leq \frac{32}{9k} \sum_{t=0}^{k-\ell-1} \sum_{q_1,q_2=1}^{k-\ell-1} \left[ \frac{\varphi(q_1+t) - \varphi(q_2+t)}{d_G((q_1,1),(q_2,1))} \right]^2.
\]

For each choice of \( t \), there are \( \ell - 1 \) indices which are over-counted by both summations. Let us consider a specific term corresponding to the indices \( q_1 \) and \( q_2 \). If neither of these are over-counted indices, the term will appear twice. If exactly one is an over-counted index, the term will appear four times. Finally, if both are over-counted indices, the term will appear eight times. Summing over all choices of \( t \) any term appears at most \( 2(k-\ell) + 8\ell \) times, which leads to the upper bound

\[
\sum_{i=1}^{k-1} \sum_{j=1}^{l-1} (a(i, j+1) - a(i, j))^2 \leq \frac{32}{9} \frac{2(k-\ell) + 8\ell}{k} |\varphi|^2 < \frac{112}{9} |\varphi|^2.
\]

Combining all our estimates, we obtain the desired result

\[
|u|_G \leq \sqrt{c + \frac{121}{9} |\varphi|_\Gamma}.
\]

\( \square \)

Combining Lemmas 3.1 and 3.2, we obtain our desired trace theorem.

**Theorem 3.3.** Let \( G_{k,\ell} = C_k \square P_\ell, 4\ell < k < 2c\ell, c \in \mathbb{N} \), with boundary \( \Gamma = \{ (i,1) \}_{i=1}^{k} \). For any \( \varphi \in \mathbb{H}_k \),

\[
\frac{1}{\max \{ \sqrt{3c}, 2\pi \}} |\varphi|_\Gamma \leq \min_{u \mid \gamma = \varphi} |u|_G \leq \sqrt{c + \frac{121}{9} |\varphi|_\Gamma}.
\]

With a little more work, we can prove a similar result for a slightly more general class of graphs. In particular, let \( G_{k,\ell}^* \) be the graph resulting from adding to \( G_{k,\ell} \) all edges of the form \( \{(i,j), (i-1,j+1)\} \) and \( \{(i,j), (i+1,j+1)\}, i = 1, \ldots, k, j = 1, \ldots, \ell - 1 \). Using Theorem 3.3, we can almost immediately prove a trace theorem for any graph \( H \) satisfying \( G_{k,\ell} \subset H \subset G_{k,\ell}^* \). In fact, Lemma
3.1 carries over immediately. In order to prove a new version of Lemma 3.2, it suffices to bound the energy of \( u \) on the edges in \( G_{k,ℓ}^* \) not contained in \( G_{k,ℓ} \). By Cauchy-Schwarz,

\[
|u|_{G^*}^2 = |u|_G^2 + \sum_{i=1}^k \sum_{j=1}^\ell (u(i, j + 1) - u(i - 1, j))^2 + (u(i, j + 1) - u(i + 1, j))^2
\]

\[
\leq 3 \sum_{i=1}^k \sum_{j=1}^\ell (u(i + 1, j) - u(i, j))^2 + 2 \sum_{i=1}^k \sum_{j=1}^\ell (u(i, j + 1) - u(i, j))^2,
\]

and therefore Corollary 3.4 follows immediately from the proofs of Lemmas 3.1 and 3.2.

**Corollary 3.4.** Let \( H \) satisfy \( G_{k,ℓ} \subset H \subset G_{k,ℓ}^* \), \( 4ℓ < k < 2cℓ \), \( c \in \mathbb{N} \), with boundary \( Γ = \{(i, 1)\}_{i=1}^k \). For any \( φ \in \mathbb{R}^k \),

\[
\frac{1}{\max\{\sqrt{3c}, 2π\}} |φ|_Γ \leq \min_{u|_Γ = φ} |u|_H \leq \sqrt{3c + 28} |φ|_Γ.
\]

### 3.2. Trace Theorems for General Graphs

In order to extend Corollary 3.4 to more general graphs, we introduce a graph operation which can be roughly thought of as an aggregation (a partition of \( V \) into connected subsets) in which the size of aggregates are bounded. In particular, we give the following definition.

**Definition 3.5.** The graph \( H, G_{k,ℓ} \subset H \subset G_{k,ℓ}^* \), is said to be an \( M \)-aggregation of \((G, Γ) ∈ \mathcal{G}_n \) if there exists an aggregation \( A = a_* \cup \{a_{i,j}\}_{i=1}^k \) of \((G, Γ)\) satisfying

1. \( G[a_{i,j}] \) is connected and \( |a_{i,j}| \leq M \) for all \( i = 1, ..., k, j = 1, ..., ℓ \),

2. \( Γ \subset \bigcup_{i=1}^k a_{i,1} \), and \( Γ \cap a_{i,1} \neq ∅ \) for all \( i = 1, ..., k \),

3. \( N_G(a_*) \subset a_* \cup \bigcup_{i=1}^k a_{i,ℓ} \),

4. the aggregation graph of \( A \backslash a_* \), given by \( ( A \backslash a_*, \{(a_{i,j_1}, a_{i,j_2}) \mid N_G(a_{i,j_1}) \cap a_{i,j_2} \neq ∅ \} ) \), is isomorphic to \( H \).

This definition allows us to prove trace theorems for a much larger class of graphs than just graphs \( H \) of the form \( G_{k,ℓ} \subset H \subset G_{k,ℓ}^* \). However, this is the not only operation for which we can control the behavior of the energy and boundary semi-norms. For instance, the behavior of our semi-norms under the deletion of some number of edges can be bounded easily if there exists a set of paths of constant length, with one path between each pair of vertices which are no longer adjacent, such that no edge is in more than a constant number of these paths. In addition, the behavior of these semi-norms under the disaggregation of large degree vertices is relatively well-behaved, see [9] for details. We give the following main result regarding graphs \((G, Γ)\) for which some \( H, G_{k,ℓ} \subset H \subset G_{k,ℓ}^* \), is an \( M \)-aggregation of \((G, Γ)\), but note that a large number of minor refinements are possible, such as the two briefly mentioned in this paragraph.

**Theorem 3.6.** If \( H, G_{k,ℓ} \subset H \subset G_{k,ℓ}^* \), \( 4ℓ < k < 2cℓ \), \( c \in \mathbb{N} \), is an \( M \)-aggregation of \((G, Γ) ∈ \mathcal{G}_n \), then for any \( φ \in \mathbb{R}^{nΓ} \),

\[
\frac{1}{6M \sqrt{M + 3} \max\{\sqrt{3c}, 2π\}} |φ|_Γ \leq \min_{u|_Γ = φ} |u|_G \leq 2M^2 \sqrt{146(3c + 14)} |φ|_Γ.
\]
Proof. We first prove that there is an extension $u$ of $\varphi$ which satisfies $|u|_G \leq c_1|\varphi|_\Gamma$ for some $c_1$. To do so, we define auxiliary functions $\hat{u}$ and $\hat{\varphi}$ on $(G_{2k,\ell}^*, \Gamma_{2k,\ell})$. Let

$$\hat{\varphi}(p) = \begin{cases} 
\max_{q \in \Gamma \cap a(p+1)/2} \varphi(q) & \text{if } p \text{ is odd}, \\
\min_{q \in \Gamma \cap a(p)/2} \varphi(q) & \text{if } p \text{ is even},
\end{cases}$$

and $\hat{u}$ be extension (3.1) of $\hat{\varphi}$. The idea is to upper bound the semi-norm for $u$ by $\hat{u}$, for $\hat{u}$ by $\hat{\varphi}$ (using Corollary 3.4), and for $\hat{\varphi}$ by $\varphi$. On each aggregate $a_{i,j}$, let $u$ take values between $\hat{u}(2i - 1, j)$ and $\hat{u}(2i, j)$, and let $\hat{u}$ equal $a$ on $a_*$. We can decompose $|u|^2_G$ into

$$|u|^2_G = \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(p) - u(q))^2 + \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(p) - u(q))^2 + \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(p) - u(q))^2 + \sum_{i=1}^{k} \sum_{j=1}^{\ell} (u(p) - u(q))^2,$$

and bound each term of $|u|^2_G$ separately, beginning with the first. The maximum energy semi-norm of an $m$ vertex graph that takes values in the range $[a, b]$ is bounded above by $(m/2)^2(b - a)^2$. Therefore,

$$\sum_{p, q \in \Gamma \cap a_{i,j}, \ p \sim q} (u(p) - u(q))^2 \leq \frac{M^2}{4} (\hat{u}(2i - 1, j) - \hat{u}(2i, j))^2.$$

For the second term,

$$\sum_{p \in \Gamma \cap a_{i,j}, \ q \in \Gamma \cap a_{i-1,j+1}, \ p \sim q} (u(p) - u(q))^2 \leq M^2 \max_{i_1 \in \{2i-1, 2i\}, \ i_2 \in \{2i+1, 2i+2\}} (\hat{u}(i_1, j) - \hat{u}(i_2, j))^2 \leq 3M^2 [(\hat{u}(2i - 1, j) - \hat{u}(2i, j))^2 + (\hat{u}(2i, j) - \hat{u}(2i + 1, j))^2 + (\hat{u}(2i + 1, j) - \hat{u}(2i + 2, j))^2].$$

The exact same type of bound holds for the third and fourth terms. For the fifth term,

$$\sum_{p \in \Gamma \cap a_{i,j}, \ q \in \Gamma \cap a_{i+1,j}, \ p \sim q} (u(p) - u(q))^2 \leq M^2 \max_{i_1 \in \{2i-1, 2i\}, \ i_2 \in \{2i-1, 2i\}} (\hat{u}(i_1, j) - \hat{u}(i_2, j + 1))^2,$$

and, unlike terms two, three, and four, this maximum appears in $|\hat{u}|^2_{G_{2k,\ell}^*}$. Combining these three bounds, we obtain

$$|u|_G \leq \frac{\sqrt{73}M}{2} |\hat{u}|_{G_{2k,\ell}^*}.$$

Next, we lower bound $|\varphi|_\Gamma$ by a constant times $|\hat{\varphi}|_{\Gamma_{2k,\ell}}$. By definition, in $\Gamma \cap a_{i,1}$ there is a vertex which takes value $\hat{\varphi}(2i - 1)$ and a vertex which takes value $\hat{\varphi}(2i)$. This implies that every term in $|\hat{\varphi}|_{\Gamma_{2k,\ell}}$ is a term in $|\varphi|_\Gamma$, with possibly different denominator. Distances between vertices on $\Gamma$ can be decreased by at most a factor of $2M$ on $\Gamma_{2k,\ell}$. In addition, it may be the case that an aggregate
contains only one vertex of $\Gamma$, which results in $\bar{c}(2i - 1) = \bar{c}(2i)$. Therefore, a given term in $|\varphi|^2$ could appear four times in $|\bar{c}|^2_{G_{2k,\ell}}$. Combining these two facts, we immediately obtain the bound

$$|\bar{c}|_{G_{2k,\ell}} \leq 4M|\varphi|,$$

which gives the estimate

$$|u|_G \leq \frac{\sqrt{73}M}{2}|u|_{G_{2k,\ell}} \leq \frac{\sqrt{73}M}{2}\sqrt{6c + 28}|\bar{c}|_{G_{2k,\ell}} \leq 2M^2 \sqrt{146(3c + 14)} |\varphi|,$$

and completes the first half of the proof.

All that remains is to show that for any $u$, $|\varphi| \leq c_2|u|$ for some $c_2$. To do so, we define auxiliary functions $\tilde{u}$ and $\tilde{c}$ on $(G_{2k,2\ell}, \Gamma_{2k,2\ell})$. Let

$$\tilde{u}(i, j) = \begin{cases} 
\max_{p \in a_{i/2}, j/2} u(p) & \text{if } i = j \mod 2, \\
\min_{p \in a_{i/2}, j/2} u(p) & \text{if } i \neq j \mod 2.
\end{cases}$$

Here, the idea is to lower bound the semi-norm for $u$ by $\tilde{u}$, for $\tilde{u}$ by $\tilde{c}$ (using Corollary 3.4), and for $\tilde{c}$ by $\varphi$. We can decompose $|\tilde{u}|^2_{G_{2k,2\ell}}$ into

$$|\tilde{u}|^2_{G_{2k,2\ell}} = 4 \sum_{i=1}^{k} \sum_{j=1}^{\ell} (\tilde{u}(2i - 1, 2j - 1) - \tilde{u}(2i, 2j - 1))^2$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{\ell} (\tilde{u}(2i, 2j - 1) - \tilde{u}(2i + 1, 2j - 1))^2 + (\tilde{u}(2i, 2j) - \tilde{u}(2i + 1, 2j))^2$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{\ell-1} (\tilde{u}(2i - 1, 2j) - \tilde{u}(2i - 1, 2j + 1))^2 + (\tilde{u}(2i, 2j) - \tilde{u}(2i, 2j + 1))^2,$$

and bound each term separately, beginning with the first. The minimum squared energy semi-norm of an $m$ vertex graph that takes value $a$ at some vertex and value $b$ at some vertex is bounded below by $(b - a)^2/m$. Therefore,

$$(\tilde{u}(2i - 1, 2j - 1) - \tilde{u}(2i, 2j - 1))^2 \leq M \sum_{p,q \in a_{i,j}, p \sim q} (u(p) - u(q))^2.$$

For the second term, we first note that

$$\min_{i_1 \in \{2i-1,2i\}, i_2 \in \{2i+1,2i+2\}} (\tilde{u}(i_1, 2j) - \tilde{u}(i_2, 2j))^2 \leq \sum_{p,q \in a_{i,j}, q \sim p} (u(p) - u(q))^2.$$

One can quickly verify by application of Cauchy-Schwarz that

$$(\tilde{u}(2i - 1, 2j) - \tilde{u}(2i + 2, 2j))^2 + (\tilde{u}(2i, 2j) - \tilde{u}(2i + 1, 2j))^2$$

is bounded above by

$$3(\tilde{u}(2i - 1, 2j) - \tilde{u}(2i, 2j))^2 + 3(\tilde{u}(2i + 1, 2j) - \tilde{u}(2i + 2, 2j))^2 + 4 \min_{i_1 \in \{2i-1,2i\}, i_2 \in \{2i+1,2i+2\}} (\tilde{u}(i_1, 2j) - \tilde{u}(i_2, 2j))^2.$$

The technique for the third term is identical to that of the second term. Therefore,

$$|\tilde{u}|_{G_{2k,2\ell}} \leq 2\sqrt{M} + 3|u|_G.$$
Next, we upper bound $|\varphi|_r$ by a constant multiple of $|\tilde{\varphi}|_{\Gamma_{2k,2\ell}}$. We can write $|\varphi|^2_\Gamma$ as

$$|\varphi|^2_\Gamma = \sum_{i=1}^{k} \sum_{p,q \in \Gamma \cap a_{i,1}} \frac{(\varphi(p) - \varphi(q))^2}{d^2_G(p,q)} + \sum_{i=1}^{k-1} \sum_{p \in \Gamma \cap a_{i,1}, q \in \Gamma \cap a_{i+1,1}} \frac{(\varphi(p) - \varphi(q))^2}{d^2_G(p,q)},$$

and bound each term separately. The first term is bounded by

$$\sum_{p,q \in \Gamma \cap a_{i,1}} \frac{(\varphi(p) - \varphi(q))^2}{d^2_G(p,q)} \leq \frac{M^2}{4} (\tilde{\varphi}(2i - 1) - \tilde{\varphi}(2i))^2.$$ 

For the second term, we first note that $d_G(p,q) \geq 3d_{\Gamma_{2k,2\ell}}((m_1,1),(m_2,1))$ for $p \in \Gamma \cap a_{i,1}$, $q \in \Gamma \cap a_{i+1,1}$, $m_1 \in \{2i_1 - 1, 2i_1\}$, $m_2 \in \{2i_2 - 1, 2i_2\}$, which allows us to bound the second term by

$$\sum_{p \in \Gamma \cap a_{i,1}, q \in \Gamma \cap a_{i+1,1}} \frac{(\varphi(p) - \varphi(q))^2}{d^2_G(p,q)} \leq 9M^2 \max_{m_1 \in \{2i_1 - 1, 2i_1\}} \max_{m_2 \in \{2i_2 - 1, 2i_2\}} \frac{(\tilde{\varphi}(m_1) - \tilde{\varphi}(m_2))^2}{d^2_{\Gamma_{2k,2\ell}}(m_1, m_2)}.$$ 

This immediately implies that

$$|\varphi|_r \leq 3M|\tilde{\varphi}|_{\Gamma_{2k,2\ell}},$$

and, therefore,

$$|\varphi|_r \leq 3M|\tilde{\varphi}|_{\Gamma_{2k,2\ell}} \leq 3M \max\{\sqrt{3c}, 2\pi\} |\tilde{u}|_{G_{2k,2\ell}} \leq 6M \sqrt{M + 3 \max\{ \sqrt{3c}, 2\pi \}} |u|_G.$$ 

This completes the proof. \qed

The above proof also immediately implies a similar result. Let $\tilde{L} \in \mathbb{R}^{n_r \times n_r}$ be the Laplacian of the complete graph on $\Gamma$ with weights $\bar{w}(i,j) = d^2_\Gamma(i,j)$. The same proof implies the following.

**Corollary 3.7.** If $H, G_{k,\ell} \subset H \subset G^*_d, 4\ell < k < 2c\ell$, $c \in \mathbb{N}$, is an $M$-aggregation of $(G,\Gamma) \in \mathcal{G}_n$, then for any $\varphi \in \mathbb{R}^{n_r}$,

$$\frac{1}{6 M \sqrt{M + 3 \max\{ \sqrt{3c}, 2\pi \}}} (\tilde{L}\varphi, \varphi)^{1/2} \leq \min_{u \parallel \varphi_0} |u|_G \leq 2M^2 \sqrt{146(3c + 14)} (\tilde{L}\varphi, \varphi)^{1/2}.$$ 

### 3.3. Spectral Equivalence of $S_\Gamma$ and $L_\Gamma^{1/2}$. By Corollary 3.7, in order to prove spectral equivalence between $S_\Gamma$ and $L_\Gamma^{1/2}$, it suffices to show that $L_\Gamma^{1/2}$ and $\tilde{L}$ are spectrally equivalent. This can be done relatively easily, and leads to a proof of the main result of the section.

**Theorem 3.8.** If $H, G_{k,\ell} \subset H \subset G^*_d, 4\ell < k < 2c\ell$, $c \in \mathbb{N}$, is an $M$-aggregation of $(G,\Gamma) \in \mathcal{G}_n$, then for any $\varphi \in \mathbb{R}^{n_r}$,

$$\frac{1}{36M^2(M + 3 \max\{3c, 4\pi^2\}) \left(2\frac{2}{\pi^2} + \frac{\sqrt{2}}{2\pi}\right)} (L_{\Gamma}^{1/2}\varphi, \varphi) \leq (S_\Gamma \varphi, \varphi) \leq \frac{584M^4(3c + 14)}{(\frac{1}{2\pi} - \frac{\sqrt{2}}{12})} (L_{\Gamma}^{1/2}\varphi, \varphi).$$

Proof. Let $\phi(i,j) = \min \{i - j \mod n_r, j - i \mod n_r\}$. $G[\Gamma]$ is a cycle, so $\tilde{L}(i,j) = -\phi(i,j)^2$ for $i \neq j$. The spectral decomposition of $L_\Gamma$ is well known, namely,

$$L_\Gamma = \sum_{k=1}^{n_r/2} \lambda_k(L_\Gamma) \left[ \frac{x_k x_k^T}{\|x_k\|^2} + \frac{y_k y_k^T}{\|y_k\|^2} \right],$$

where $\lambda_k(L_\Gamma) = 2 - 2\cos \frac{2\pi k}{n_r}$ and $x_k(j) = \sin \frac{2\pi kj}{n_r}$, $y_k(j) = \cos \frac{2\pi kj}{n_r}, j = 1, ..., n_r$. If $n_r$ is odd, then $\lambda_{(n_r-1)/2}$ has multiplicity two, but if $n_r$ is even, then $\lambda_{n_r/2}$ has only multiplicity one, as $x_{n_r/2} = 0.$
If \( k \neq n_\Gamma / 2 \), we have
\[
\|x_k\|^2 = \sum_{j=1}^{n_\Gamma} \sin^2 \left( \frac{2\pi k j}{n_\Gamma} \right) = \frac{n_\Gamma}{2} - \frac{1}{2} \sum_{j=1}^{n_\Gamma} \cos \left( \frac{4\pi k j}{n_\Gamma} \right) = \frac{n_\Gamma}{2} - \frac{1}{4} \left[ \sin(2\pi k (2 + \frac{1}{n_\Gamma})) - 1 \right] = \frac{n_\Gamma}{2},
\]
and so \( \|y_k\|^2 = \frac{n_\Gamma}{2} \) as well. If \( k = n_\Gamma / 2 \), then \( \|y_k\|^2 = n_\Gamma \). If \( n_\Gamma \) is odd,
\[
L_{1/2}(i, j) = \frac{2\sqrt{2}}{n_\Gamma} \sum_{k=1}^{n_\Gamma / 2} \left[ 1 - \cos \left( \frac{2k\pi}{n_\Gamma} \right) \right]^{1/2} \left[ \sin \left( \frac{2\pi k i}{n_\Gamma} \right) \sin \left( \frac{2\pi k j}{n_\Gamma} \right) - \cos \left( \frac{2\pi k i}{n_\Gamma} \right) \cos \left( \frac{2\pi k j}{n_\Gamma} \right) \right]^{1/2}
\]
and if \( n_\Gamma \) is even,
\[
L_{1/2}(i, j) = \frac{2}{n_\Gamma} (-1)^{i+j} + \frac{4}{n_\Gamma} \sum_{k=1}^{n_\Gamma / 2 - 1} \sin \left( \frac{\pi 2k}{n_\Gamma} \right) \cos \left( \phi(i, j) \frac{2k}{n_\Gamma} \right)
\]
\[= \frac{2}{n_\Gamma} \sum_{k=0}^{n_\Gamma / 2 - 1} \sin \left( \frac{\pi 2k}{n_\Gamma} \right) \cos \left( \phi(i, j) \frac{2k}{n_\Gamma} \right).
\]
\( L_{1/2}(i, j) \) is simply the trapezoid rule applied to the integral of \( \sin(\frac{\pi x}{2}) \cos(\phi(i, j)\pi x) \) on the interval \([0, 2]\). Therefore,
\[
\left| L_{1/2}(i, j) + \frac{2}{\pi(4\phi(i, j)^2 - 1)} \right| = \left| L_{1/2}^\Gamma(i, j) - \int_0^2 \sin \left( \frac{\pi x}{2} \right) \cos(\phi(i, j)\pi x) \, dx \right| \leq \frac{2}{3n_\Gamma},
\]
where we have used the fact that if \( f \in C^2([a, b]) \), then
\[
\left| \int_a^b f(x) \, dx - \frac{f(a) + f(b)}{2} (b - a) \right| \leq \frac{(b - a)^3}{12} \max_{\xi \in [a, b]} |f''(\xi)|.
\]
Noting that \( n_\Gamma \geq 3 \), it quickly follows that
\[
\left( \frac{1}{2\pi} - \frac{\sqrt{2}}{12} \right) \langle L_{1/2}^\Gamma \varphi, \varphi \rangle \leq \langle L_{1/2}^\Gamma \varphi, \varphi \rangle \leq \left( \frac{2}{3\pi} + \frac{\sqrt{2}}{27} \right) \langle L_{1/2}^\Gamma \varphi, \varphi \rangle.
\]
Combining this result with Corollary 3.7, and noting that \( \langle \varphi, S_{\Gamma} \varphi \rangle = |\hat{u}|^2_{L^2} \), where \( \hat{u} \) is the harmonic extension of \( \varphi \), we obtain the desired result
\[
\frac{1}{36M^2(M + 3) \max \{ 3c, 4\pi^2 \} \left( \frac{2}{3\pi} + \frac{\sqrt{2}}{27} \right)} \langle L_{1/2}^\Gamma \varphi, \varphi \rangle \leq \langle S_{\Gamma} \varphi, \varphi \rangle \leq \frac{584M^4(3c + 14)}{\left( \frac{1}{2\pi} - \frac{\sqrt{2}}{12} \right)} \langle L_{1/2}^\Gamma \varphi, \varphi \rangle.
\]
\[
\square
\]
3.4. An Illustrative Example. While the concept of a graph \((G, \Gamma)\) having some \( H, G_{k, \ell} \subset H \subset G_{k, \ell} \), as an \( M \)-aggregation seems somewhat abstract, this simple formulation in itself is quite powerful. As an example, we illustrate that this implies a trace theorem (and, therefore, spectral equivalence) for all three-connected planar graphs with bounded face degree and for which there exists a planar spring embedding with a convex hull that is not too thin (a bounded distance to Hausdorff distance ratio for the boundary with respect to some point in the convex hull) and satisfies bounded edge length and small angle conditions. Let \( G_{n}^{f \leq c} \) be the elements of \((G, \Gamma) \in \mathcal{G}_{n} \) for which every face other than the outer face \( \Gamma \) has at most \( c \) edges. We have the following theorem.

**Theorem 3.9.** If there exists a planar spring embedding \( X \) of \((G, \Gamma) \in \mathcal{G}_{n}^{f \leq c} \) for which
(1) $K = \text{conv}([(X_j^i),_{i=1}^n])$ satisfies

$$\sup_{u \in K} \inf_{v \in \delta K} \sup_{w \in \delta K} \|u - v\| \geq c_2,$$

(2) $X$ satisfies

$$\max_{\{i_1, i_2\} \in E} \|X_{i_1, i} - X_{i_2, i}\| \leq c_3 \text{ and } \min_{\{j_1, j_2\} \in E} \angle (X_{j_1, i}, X_{i_1, i}, X_{j_2, i}) \geq \theta,$$

then there exists an $H, G_{k, \ell} \subset H \subset G^*_{k, \ell}$, $4\ell < k < 2\ell$, $c \in \mathbb{N}$, such that $H$ is an $M$-aggregation of $(G, \Gamma)$ where $c$ and $M$ are constants that depend on $c_1, c_2, c_3$, and $\theta$.

**Proof.** The general plan of the proof is to construct sub-regions of $K$, and argue the existence of an $M$-aggregation of $(G, \Gamma)$ by using the vertices contained in each sub-region to construct an aggregation. The properties which must be verified are that each aggregate is indeed connected, the necessary adjacent aggregates are connected, and no non-adjacent aggregates are connected.

We begin by proving a number of properties regarding the interior faces of the embedding $X$. The conditions of the theorem do not depend on the scale or relative location of $X$, so we may suppose that the maximizing choice of $u$ is the origin and the minimum edge length

$$\min_{\{i_1, i_2\} \in E} \|X_{i_1, i} - X_{i_2, i}\| = 1.$$

From here, we can make a number of estimates regarding the embedding $X$. These estimates are not tight in general, and here simplicity is preferred over optimal constants. The maximum edge length is at most $c_3$ and the diameter of every interior face is at most $\frac{1}{2}c_1c_3$. The area of each interior face is bounded below by $a_1 := \frac{1}{2} \sin \theta$, the area of a triangle with two sides of length one and internal angle $\theta$, and above by $a_2 := \frac{1}{4}c_1c_3^2 \cot \frac{\pi}{c_3}$, the area of a regular $c_1$-gon with side lengths $c_3$. By Euler’s formula and the property of three-connectedness, we can quickly conclude that $G$ has at least $\frac{2a_2}{c_1}n$ faces, and at most $2an$ faces, which implies that the area of $K$ is at least $\frac{2a_1}{c_1}n$ and at most $2a_2n$. Therefore, we can upper bound the distance and lower bound the Hausdorff distance (denoted by $d_H(\cdot, \cdot)$) between $o$ and $\delta K$ by

$$d(o, \delta K) \leq \frac{2a_2n}{\pi} \text{ and } d_H(o, \delta K) \geq \frac{2a_1n}{\pi c_1}.$$

Combining this estimate with condition (1) of the theorem, we obtain the following lower and upper estimates on $d(o, \delta K)$, $d_H(o, \delta K)$, and the length of $\delta K$ (denoted $L(\delta K)$):

$$c_2 \frac{2a_1n}{\pi c_1} \leq d(o, \delta K) \leq \frac{2a_2n}{\pi},$$

$$\sqrt{\frac{2a_1n}{\pi c_1}} \leq d_H(o, \delta K) \leq \frac{1}{c_2} \sqrt{\frac{2a_2n}{\pi}},$$

$$2 \sqrt{\frac{2\pi a_1n}{c_1}} \leq L(\delta K) \leq \frac{2}{c_2} \sqrt{2\pi a_2n}.$$

The curvature of $\delta K$ is bounded by a function of the constants $c_1$, $c_2$, $c_3$, $\theta$, and, therefore, there exists a constant $c_4$ such that

$$\min_{v, w \in \delta K} \frac{\|v - w\|}{d_{\delta K}(v, w)} \geq c_4,$$

where $d_{\delta K}(v, w)$ is the minimum length curve between $v$ and $w$ contained completely in $\delta K$. 


We are now prepared to define our aggregation. Let us break \( \delta K \) into curves \( dK_1, \ldots, dK_k \), with each of equal length \( L/k \), where \( k \) is chosen to be the maximal integer satisfying \( L/k \geq 16c_1c_3c_4^{-1} \). In addition, let \( \ell \) be the largest integer satisfying
\[
\frac{c_2\sqrt{\frac{2a_{1,n}}{\pi c_1}}}{2\ell} \geq 8c_1c_3.
\]
Let \( \hat{dK}_i \) be the line segment connecting the two endpoints of the curve \( dK_i \), \( i = 1, \ldots, k \). We partition \( K \) into subregions in the following manner:

\[
K_{i,1} = \text{conv} \left( dK_i, \left[ 1 - \frac{1}{2\ell} \right] \hat{dK}_i \right), \quad i = 1, \ldots, k
\]

\[
K_{i,j} = \text{conv} \left( \left[ 1 - \frac{j-1}{2\ell} \right] \hat{dK}_i, \left[ 1 - \frac{j}{2\ell} \right] \hat{dK}_i \right), \quad i = 1, \ldots, k, \ j = 2, \ldots, \ell,
\]

\[
K_a = \text{conv} \left( \frac{1}{2} \bigcup_{i=1}^{k} \hat{dK}_i \right).
\]

Each \( K_{i,j}, \ j \neq 1 \), is a quadrilateral with each side of length at least \( 4c_1c_3 \) (the side lengths can also be bounded by using the upper bounds for \( d_H(o, \delta K) \) and \( L(\delta K) \)). This, paired with the lower bound for the area and the upper bound for the diameter of an interior face, implies that the number of vertices in a given \( K_{i,j} \) is a function of the constants defined above.

We have already shown \( c \) to be a constant by our definitions of \( k \) and \( \ell \). What remains is to define our aggregation, verify that \( M \) is a constant, \( G[a_{i,j}] \) is connected, adjacent aggregates are connected (with respect to \( G_k, \ell \)), and non-adjacent aggregates are not connected (with respect to \( G^k, \ell \)). Let us add to each aggregate \( a_{i,j} \) all vertices which are contained in \( K_{i,j} \), and are at distance at least \( 2c_1c_3 \) from \( K \setminus K_{i,j} \). In addition, let \( a_{i,j} \) always be a subset of the vertices which are within distance \( 2c_1c_3 \) of \( K_{i,j} \). In particular,

\[
\{ u \in V(G) \mid X_{u,i} \in K_{i,j}, d(X_{u,i}, K \setminus K_{i,j}) \geq 2c_1c_3 \} \subset a_{i,j} \subset \{ u \in V(G) \mid d(X_{u,i}, K_{i,j}) \leq 2c_1c_3 \}.
\]

By the last condition, we can already guarantee that \( M \) is a constant and \( a_{i,j} \) is not connected to any non-adjacent aggregate. However, each \( a_{i,j} \) may not be connected. We extend each \( a_{i,j} \) (currently consisting of all vertices contained in \( K_{i,j} \) and distance at least \( 2c_1c_3 \) from \( K \setminus K_{i,j} \)) to the connected graph which consists of vertices which are at maximum distance from \( K \setminus K_{i,j} \). Now, each \( a_{i,j} \) is connected and this extension decreases the distance to the boundary by at most \( 1/2c_1c_3 \) (the maximum diameter of an interior face). For each pair of aggregates \( a_{i,j} \) and \( a_{i,j+1} \) (and similarly for \( a_{i,j} \) and \( a_{i+1,j} \)), we choose the shortest path from a vertex in \( a_{i,j} \) to a vertex in \( a_{i,j+1} \) consisting of vertices exclusively contained in \( K_{i,j} \cup K_{i,j+1} \). We add the portion of the path contained in \( K_{i,j} \) to \( a_{i,j} \) and the portion contained in \( K_{i,j+1} \) to \( a_{i,j+1} \). After this procedure is complete, we now have that adjacent aggregates are connected. All that remains is to perform a simultaneous breadth first search from all aggregates until every vertex in each \( K_{i,j} \) belongs to an aggregate, and the aggregation is complete. \( \Box \)

We also note that the results of this section implies an energy-only trace theorem for \( H^1(\Omega) \) functions with traces on \( \Gamma = \partial \Omega \). Let \( B^2 \) and \( S^1 \) be the unit disk and circle in \( \mathbb{R}^2 \), respectively. We have the following corollary.

**Corollary 3.10.** Let \( \Omega \subset \mathbb{R}^2 \) be a connected polygonal domain with boundary \( \Gamma = \partial \Omega \). If there exists a bi-Lipschitz bijection \( f : \Omega \to B^2 \) such that \( f(\Gamma) = S^1 \), then there exists constants \( c, C \) depending only on \( \Omega \) such that, for all \( \varphi \in H^{1/2}(\Gamma) \),

\[
c|\varphi|_{H^{1/2}(\Gamma)} \leq \inf_{u \in H^{1}(\Omega)} \| \nabla u \|_{L^2(\Omega)} \leq C|\varphi|_{H^{1/2}(\Gamma)}.
\]
Proof. It is well known that for piece-wise linear continuous functions on any triangulation of $\Omega$, the seminorm on $|\cdot|_\Gamma$ is equivalent to the $|\cdot|_{H^{1/2}(\Gamma)}$ (see [16]). Because the constants in the trace inequalities in Corollary 3.4 are independent of the number of vertices in the graph, and the piece-wise linear continuous functions are dense in $H^1(\Omega)$ when the triangulations are refined, the result immediately follows.

\[\Box\]

4. Approximately Energy Minimizing Embeddings

In this section, we make use of the analysis of Section 3 to give theoretical guarantees regarding approximate solutions to (2.2), which inspires the construction of a natural algorithm to approximately solve this optimization problem. In addition, we give numerical results for our algorithm applied to a wide range of graphs. Though in the previous section we took great care to produce results with explicit constants for the purpose of illustrating practical usefulness, in what follows we simply suppose that we have the spectral equivalence

\[\frac{1}{c_1} \langle L^{1/2}_\Gamma x, x \rangle \leq \langle S_\Gamma x, x \rangle \leq c_2 \langle L^{1/2}_\Gamma x, x \rangle,\]

for all $x \in \mathbb{R}^{n_\Gamma}$ and some constants $c_1$ and $c_2$ which are not too large and can be explicitly chosen based on the results of Section 3.

4.1. Theoretical Guarantees. Again, we note that if the minimal two non-trivial eigenvectors of $S_\Gamma$ produce a convex embedding, then this is the exact solution of (2.2). However, if this is not the case, then, by spectral equivalence, we can still make a number of statements.

The convex embedding $X_C$ given by

\[[X_C]_j. = \frac{2}{n_\Gamma} \left( \cos \frac{2\pi j}{n_\Gamma}, \sin \frac{2\pi j}{n_\Gamma} \right), \quad j = 1, \ldots, n_\Gamma,\]

is the embedding of the two minimal non-trivial eigenvectors of $L^{1/2}_\Gamma$, and therefore,

\[h_\Gamma(X_C) \leq 4c_2 \sin \frac{\pi}{n_\Gamma} \leq c_1 c_2 \min_{X_\Gamma \in \mathcal{X}} h_\Gamma(X_\Gamma),\]

thereby producing a $c_1 c_2$ approximation guarantee for (2.2).

In addition, we can guarantee that the optimal embedding is largely contained in the subspace corresponding to the minimal $k$ minimal eigenvalues of $L^{1/2}_\Gamma$ when $k$ is a reasonably large constant. In particular, if $X^*_\Gamma$ minimizes (2.2), and $\Pi_i$ is the $\ell^2$-orthogonal projection onto the direct sum of the eigenvectors corresponding to the $i$ minimal non-trivial eigenvalues (counted with multiplicity) of $L^{1/2}_\Gamma$, then

\[h_\Gamma(X^*_\Gamma) \geq \text{Tr}(\langle (I - \Pi_{2i})X^*_\Gamma^T S_\Gamma(I - \Pi_{2i})X^*_\Gamma \rangle) \geq \frac{1}{c_1} \text{Tr}(\langle (I - \Pi_{2i})X^*_\Gamma^T L^{1/2}_\Gamma(I - \Pi_{2i})X^*_\Gamma \rangle) \geq \frac{2}{c_1} \sin \left( \frac{\pi(i + 1)}{n_\Gamma} \right) \text{Tr}(\langle (I - \Pi_{2i})X^*_\Gamma^T(I - \Pi_{2i})X^*_\Gamma \rangle),\]

and $h_\Gamma(X^*_\Gamma) \leq h_\Gamma(X_C)$, which, by using the property $\frac{2x}{\pi} \leq \sin x \leq x$ for all $x \in \left[0, \frac{\pi}{2}\right]$, implies that

\[\text{Tr}(\langle (I - \Pi_{2i})X^*_\Gamma^T(I - \Pi_{2i})X^*_\Gamma \rangle) \leq \frac{2c_1 c_2 \sin (\pi/n_\Gamma)}{\sin (\pi(i + 1)/n_\Gamma)} \leq \frac{\pi c_1 c_2}{i + 1}.\]
4.2. Algorithmic Considerations. The theoretical analysis of this section gives rise to a number of natural techniques to approximately solve (2.2), such as exhaustively searching the direct sum of some constant number of low energy eigenspaces. However, numerically, it appears that when the pair \((G, \Gamma)\) satisfies certain conditions, such as the conditions of Theorem 3.9, the minimal non-trivial eigenvector pair often produces a convex embedding, and when it does not, the removal of some small number of boundary vertices produces a convex embedding. If the embedding is almost convex (i.e., convex after the removal of some small number of vertices), a convex embedding can be produced by simply moving these vertices so that they are on the boundary and between their convex (i.e., convex after the removal of some small number of vertices), a convex embedding can be produced by simply moving these vertices so that they are on the boundary and between their two neighbors. Given an approximate solution to (2.2), one natural approach simply consists of iteratively applying a smoothing matrix, such as \(dI - S_{\Gamma}\), or the inverse \(S_{\Gamma}^{-1}\) defined on the subspace \(\{x \mid \langle x, 1 \rangle = 0\}\), until the matrix \(X_{\Gamma}\) is no longer a convex embedding. In fact, applying this procedure to \(X_C\) immediately produces a technique that approximates the optimal solution within a factor of at least \(c_1c_2\), and possibly better given smoothing. In order to have the theoretical guarantees that result from using \(X_C\), and benefit from the possibly nearly-convex Schur complement low energy embedding, we introduce Algorithm 1.

Algorithm 1 takes a graph \((G, \Gamma) \in \mathcal{G}_n\) as input, and first computes the minimal two non-trivial eigenvectors of the Schur complement, denoted by \(X\). If \(X\) is planar and convex, the algorithm terminates and outputs \(X\), as it has found the exact solution to (2.2). If \(X\) is non-planar, then this embedding is replaced by \(X_C\), the minimal two non-trivial eigenvectors of the boundary Laplacian to the one half power. If \(X\) is planar, but non-convex, then some procedure is applied to transform \(X\) into a convex embedding. The embedding is then shifted so that the origin is the center of mass, and a change of basis is applied so that \(X^TX = I\). However, if \(h_\Gamma(X) > h_\Gamma(X_C)\), then clearly \(X_C\) is a better initial approximation, and we still replace \(X\) by \(X_C\). We then perform some type of smoothing to our embedding \(X\), resulting in a new embedding \(\hat{X}\). If \(\hat{X}\) is non-planar, the algorithm terminates and outputs \(X\). If \(\hat{X}\) is planar, we again apply some procedure to transform \(\hat{X}\) into a convex embedding, if it is not already convex. Now that we have a convex embedding \(\hat{X}\), we shift \(\hat{X}\) and apply a change of basis, so that \(\hat{X}^T1 = 0\) and \(\hat{X}^T\hat{X} = I\). If \(h_\Gamma(\hat{X}) < h_\Gamma(X)\), then we replace \(X\) by \(\hat{X}\) and repeat this smoothing procedure, producing a new \(\hat{X}\), until the algorithm terminates. If \(h_\Gamma(\hat{X}) \geq h_\Gamma(X)\), then we terminate the algorithm and output \(X\).

It is immediately clear from the statement of the algorithm that the following holds.

**Proposition 4.1.** The embedding \(X_\Gamma\) of Algorithm 1 satisfies \(h_\Gamma(X_\Gamma) \leq c_1c_2 \min_{X_\Gamma \in \mathcal{X}} h_\Gamma(X_\Gamma)\).

We now discuss some of the finer details of Algorithm 1. Determining whether an embedding is planar can be done in near-linear time using the sweep line algorithm [18]. If the embedding is planar, testing if it is also convex can be done in linear time. One such procedure consists of shifting the embedding so the origin is the mass center, checking if the angles each vertex makes with the x-axis are properly ordered, and then verifying that each vertex \(x_i\) is not in \(\text{conv}\{o, x_{i-1}, x_{i+1}\}\). Also, in practice, it is advisable to replace conditions of the form \(h_\Gamma(X) - h_\Gamma(\hat{X}) > 0\) in Algorithm 1 by the condition \(h_\Gamma(X) - h_\Gamma(\hat{X}) > \text{tol}\) for some small value of \(\text{tol}\), in order to ensure that the algorithm terminates after some finite number of steps.

There are a number of different choices for smoothing procedures and techniques to make a planar embedding convex. For the numerical experiments that follow, we simply consider the smoothing operation \(X \leftarrow S_{\Gamma}^{-1}X\), and make a planar embedding convex by replacing the embedding by its convex hull, and place vertices equally spaced along each line. For example, if \(x_1\) and \(x_2\) are vertices of the convex hull, but \(x_2, x_3, x_4\) are not, then we set \(x_2 = 3/4x_1 + 1/4x_5\), \(x_3 = 1/2x_1 + 1/2x_5\), and \(x_4 = 1/4x_1 + 3/4x_5\). Given the choices of smoothing and making an embedding convex that we have outlined, the version of Algorithm 1 that we are testing has complexity near-linear in \(n\). The main cost of this procedure is in fact computations which involve \(S_{\Gamma}\).
Algorithm 1 Embed the Boundary $\Gamma$

\[ X = \text{minimaleigenvectors}(G, \Gamma) \]

If isplanar($X$) = 0,

\[ X \leftarrow \left\{ \frac{2}{n_\Gamma} \left( \cos \frac{2\pi j}{n_\Gamma}, \sin \frac{2\pi j}{n_\Gamma} \right) \right\}_{i=1}^{n_\Gamma} \]

Else

If isconvex($X$) = 1,

\[ X_{\text{alg}} = X \]

end Algorithm

Else

\[ X \leftarrow \text{makeconvex}(X) \]

\[ X \leftarrow X - \frac{1_{n_\Gamma}^T 1_{n_\Gamma}}{n_\Gamma} X \]

solve $[X^T X]Q = QA, Q$ orthogonal, $A$ diagonal

\[ X \leftarrow XQA^{-1/2} \]

If $h_{\Gamma}(X) > h_{\Gamma}\left( \left\{ \frac{2}{n_\Gamma} \left( \cos \frac{2\pi j}{n_\Gamma}, \sin \frac{2\pi j}{n_\Gamma} \right) \right\}_{i=1}^{n_\Gamma} \right)$,

\[ X \leftarrow \left\{ \frac{2}{n_\Gamma} \left( \cos \frac{2\pi j}{n_\Gamma}, \sin \frac{2\pi j}{n_\Gamma} \right) \right\}_{i=1}^{n_\Gamma} \]


All variants of Algorithm 1 require the repeated application of $S$ or $S^{-1}$ to a vector in order to compute the minimal eigenvectors of $S$ (possibly also to perform smoothing). The Schur complement $S$ is a dense matrix and requires the inversion of an $n \times n$ matrix, but can be represented as the composition of functions of sparse matrices. In practice, $S$ should never be formed explicitly. Rather, the operation of applying $S$ to a vector $x$ should occur in two steps. First, the sparse Laplacian system $(L_o + D_o)y = A_{o,\Gamma}x$ should be solved for $y$, and then the product $Sx$ is given by $Sx = (L_\Gamma + D_\Gamma)x - A_{\Gamma,\Gamma}^T y$. Each application of $S$ is therefore an $O(n \log n)$ procedure (using an $O(n \log n)$ Laplacian solver). The application of the inverse $S^{-1}$ defined on the subspace $\{x | \langle x, 1 \rangle = 0\}$ also requires the solution of a Laplacian system. As noted in [20], the action of $S^{-1}$
Table 1. Numerical results for experiments on Delaunay triangulations of \( n \) points randomly generated in a disk or rectangle. One hundred experiments were performed for each convex body and choice of \( n \). The row “% planar” gives the percent of the samples for which the boundary embedding was planar. The row “crossings per edge” reports the average number of edge crossings per edge, where the average is taken over all non-planar embeddings. In some cases all one hundred experiments result in planar embeddings, in which case this entry does not contain a value. The row “# not convex” reports the average fraction of vertices which are not also vertices of the resulting convex hull. This average is taken over all planar embeddings. The row “energy ratio” reports the average ratio between the value of the objective function \( h_{\Gamma}(\cdot) \) for the embedding under consideration and \( h_{\Gamma}(X_s) \). This, again, is an average over all planar embeddings.

4.3. Numerical Results. We perform a number of simple experiments, which illustrate the benefits of using the Schur complement to produce an embedding. In particular, we consider the same two types of triangulations as in Figure 1, random triangulations of the unit disk and the 3-by-1 rectangle. For each of these two convex bodies, we sample \( n \) points uniformly at random and compute a Delaunay triangulation. For each triangulation, we compute the minimal two non-trivial eigenvectors of the graph Laplacian \( L_G \), and the minimal two non-trivial eigenvectors of the...
Schur complement $S_\Gamma$ of the Laplacian $L_G$ with respect to the interior vertices $V \setminus \Gamma$. The properly normalized and shifted versions of the Laplacian and Schur complement embeddings are denoted by $X_l$ and $X_s$, respectively. We then check whether each of these embeddings of the boundary is planar. If the embedding is not planar, we note how many edge crossings the embedding has. If the embedding is planar, we also determine if it is convex, and compute the number of boundary vertices which are not vertices of the convex hull. If the embedding is planar, but not convex, then we simply replace the embedding by the natural embedding corresponding to the convex hull of the original layout. This convex-adjusted layout of the Laplacian and Schur complement embedding (shifted and properly scaled) is denoted by $X_{lc}$ and $X_{sc}$, respectively. The embedding defined by minimal two non-trivial eigenvectors of the boundary Laplacian $L_\Gamma$, denoted by $X_C$, is the typical circular embedding of a cycle, and formally defined in the previous subsection. Of course the value $h_\Gamma(X_s)$ is a lower bound for the minimum of (2.2), and this estimate is exact if $X_s$ is a planar and convex embedding. The embedding resulting from Algorithm 1 is denoted by $X_{alg}$. For each triangulation, we compute the ratio of $h_\Gamma(X_s)$ to $h_\Gamma(X_l)$, $h_\Gamma(X_{sc})$, $h_\Gamma(X_{alg})$, $h_\Gamma(X_{lc})$, and $h_\Gamma(X_C)$, conditional on each of these layouts being planar. We perform this procedure one hundred times each for both convex bodies and a range of values of $n$. We report the results in Table 4.3.

These numerical results illustrate a number of phenomena. For instance, when considering the disk both the Laplacian embedding and Schur complement are always planar, usually close to convex, and both perform reasonably well compared to the lower bound $h_\Gamma(X_s)$ for Problem (2.2). The embedding $X_{alg}$ from Algorithm 1 produced small improvements over the results of the Schur complement, but this improvement was negligible when average ratio was rounded to the thousands place. As expected, the $L_\Gamma$-based embedding $X_C$ performs well in this instance, as the original embedding of the boundary in the triangulation is already a circle. Most likely, any graph which possesses a high level of macroscopic symmetry shares similar characteristics. However, when we consider the rectangle, the convex version of the Schur complement embedding has a significantly better performance than the Laplacian-based embedding. In fact, for a large percentage of the simulations the Laplacian based-embedding was non-planar, and possessed a relatively large number of average crossings per edge. We give a visual representation of the typical difference in the Laplacian vs Schur complement embeddings of the boundary in Figure 3. In addition, in this instance, the smoothing procedure of Algorithm 1 leads to small, but noticeable improvements. Of course, the generic embedding $X_C$ performs poorly in this case, as the embedding does not take into account any of the dynamics of the interior.

The Schur complement embedding clearly outperforms the Laplacian embedding, especially for triangulations of the rectangle. From this, we can safely conclude that Laplacian embedding is...
not a reliable method to embed graphs, and note that, while spectral equivalence does not imply that the minimal two non-trivial eigenvectors produce a planar, near-convex embedding, practice illustrates that for well-behaved graphs with some level of structure, this is a likely result.

Acknowledgements

The work of L. Zikatanov was supported in part by NSF grants DMS-1720114 and DMS-1819157. The work of J. Urschel was supported in part by ONR Research Contract N00014-17-1-2177. The authors are grateful to Louisa Thomas for greatly improving the style of presentation.

References

Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA, USA.
E-mail address: urschel@mit.edu, Corresponding author.

Department of Mathematics, The Pennsylvania State University, University Park, Pennsylvania, 16802, USA; Institute for Mathematics and Informatics, Bulgarian Academy of Sciences, Sofia, Bulgaria.
E-mail address: ludmil@psu.edu