Diffuse scattering on graphs

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Abstract

We formulate and analyze difference equations on graphs analogous to time-independent diffusion equations arising in the study of diffuse scattering in continuous media. Moreover, we show how to construct solutions in the presence of weak scatterers from the solution to the homogeneous (background problem) using Born series, providing necessary conditions for convergence and demonstrating the process through numerous examples. In addition, we outline a method for finding Green’s functions for Cayley graphs for both abelian and non-abelian groups. Finally, we conclude with a discussion of the effects of sparsity on our method and results, outlining the simplifications that can be made provided that the scatterers are weak and well-separated.

1 Introduction

Spectral graph theory is a rich and well-developed theory for both the combinatorial and analytic properties of graphs. The following set-up is generally considered. Let $G = (V, E)$ be a graph with vertex set $V$ and edge set $E$, and $L$ be the combinatorial Laplacian $L$, or some suitably rescaled variant [7]. We can then formulate a graph analog of Poisson’s equation

\[
\begin{cases}
(Lu)(x) = f(x), & x \in V \\
u(x) = g(x), & x \in \delta V
\end{cases}
\]  

(1)

where $\delta V$ is the set of boundary vertices, which will be discussed in more detail later, and the functions $f$ and $g$ represent internal and boundary sources, respectively. Equation (1) have been studied both when the edges are equally-weighted and when the edge weighting varies throughout the graph [7, 8, 5]. In this work, as in [4], we consider the effect of introducing inhomogeneities on the vertices rather than on the edges, as represented by the addition of a (vertex) potential term to equation (1). We call this problem the problem of diffuse scattering on graphs because of its analogy to related problem in the continuous setting, where the vertex potential is often called the absorption. In order to develop the

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necessary foundations to formulate corresponding inverse problems, which will be analyzed in subsequent works, we also study the role of boundary conditions on the solutions. In particular, we consider Dirichlet and Neumann boundary conditions, and formulate a suitable graph analog of Robin, or mixed, boundary conditions, which are often employed in the continuous setting.

Green’s functions for graphs were introduced in 2000 by Yau and Chung, who examined a graph-theoretic analog of Poisson’s equation [8]. Since then, Green’s function methods have proved useful in many fields, yielding interesting results in many areas including the properties of random walks [8, 16], chip-firing games [14], analysis of online communities [19], machine learning algorithms [31, 23] and load balancing in networks [6].

The graph analog of Poisson’s equation is related to the classical problem of resistor networks first studied by Kirchhoff in 1847 [17]. In that setting, one is given a collection of interconnected resistors to which a voltage source is attached at various points [10]. The resulting system can be thought of as a weighted graph, with each edge corresponding to a particular resistor and the vertices representing the connections between them [10]. In the event that all the resistors are identical, the voltage at each point satisfies Poisson’s equation on the associated graph [9]. In this setting, one seeks either to map the network, finding its corresponding graph [10], solely by measuring the current or potential at various points in the network. This physical analogy is also employed for graph sparsification [26], as well as in near linear-time solvers for symmetric, diagonally dominant linear systems [18, 30, 11].

Discrete analogs of PDEs on graphs are not limited to Poisson-type problems and are used extensively in lattice dynamics where we consider the graph analog of the Helmholtz equation [20, 29], which arises when considering the Fourier transform of the wave equation. In lattice theory, one problem of particular importance is to examine the propagation of phonons through a crystal in order to determine the size and location of imperfections [20, 29].

In this paper we consider the problem of diffuse scattering on graphs. As in the analogous continuous problem, we are particularly interested in systems with nearly uniform absorption. By this we mean that the variations in the absorption are small relative to the mean and are typically limited to a small subset of vertices. By defining and applying a discrete version of the Born series we obtain, under suitable conditions, a series solution to the forward problem for a heterogeneous medium, given in terms of the Green’s function for the diffusion equation on the same graph but with uniform absorption, called the background Green’s function. We then provide necessary conditions on the inhomogeneities for the series solution to converge to the correct solution and provide estimates for the rate of convergence.

Although there are many similarities between the equations considered here and those previously mentioned, changing the underlying differential operator gives rise to significant differences in the qualitative behaviour of the solutions. In Section 2 we illustrate these differences through various examples and connect the results with their continuous coun-
terparts when such analogues exist. We also consider the important special case of graphs with boundaries, since in applications measurements are carried out on the boundary. In cataloguing the possible boundary conditions, we discuss the well-known Dirichlet and Neumann boundary conditions before formulating a graph equivalent of Robin boundary conditions, similar to those considered in [3]. The introduction of the added parameter representing the mixture of Dirichlet and Neumann boundary conditions will be useful in subsequent work when we consider the inverse problem.

In Section 3 we develop the necessary tools to construct the Born series from the background Green’s function. In particular, we prove necessary conditions for the convergence of the series, and discuss the dependence of the rate of convergence on the structure of the graph.

The above results are then applied in Section 4 to various families of graphs. Many of these computations depend upon the use of symmetries to simplify the calculations. In Section 5 we discuss the connection between the symmetries of vertex-transitive graphs and group representation theory, showing how to use knowledge of the symmetry group of a graph to obtain an expression for the corresponding background Green’s function.

In Section 6, we consider the discrete analogue of a classical problem in scattering theory; the scattering due to a small collection of point absorbers. In the case where there are only one or two point absorbers present, we explicitly sum the Born series and give exact formulae for the scattered fields provided the Green’s function for the homogeneous medium is known. Finally, we compare the scattering of light from point absorbers on infinite one-dimensional and two-dimensional lattice graphs with the well-known formulae for the continuous problem of the same dimensions.

2 Preliminaries

2.1 Time-independent diffusion equations on graphs

Let $\Gamma = (E', V')$ be the graph with edge set $E'$ and vertex set $V'$. Given a subgraph $\Sigma = (E, V)$ of $\Gamma$, we define the vertex boundary of $\Sigma$, $\delta V$, by [7]

$$\delta V = \{ y \in V' \setminus V \mid \exists x \in \Sigma \text{ such that } \{ x, y \} \in E' \}. \quad (2)$$

As in [7] we consider the (vertex) Laplacian $L : V \times (V \cup \Sigma) \to \mathbb{R}$ defined by

$$L(x, y) = \begin{cases} 
    d_x & \text{if } y = x \\
    -1 & \text{if } y \sim x \\
    0 & \text{otherwise,}
\end{cases} \quad (3)$$

where \(d_x\) is the degree of the vertex \(x\) and \(x \sim y\) if \(x\) is adjacent to the vertex \(y\). Often it is more convenient to work with the normalized Laplacian matrix \([7]\)

\[
L(x, y) = \begin{cases} 
1 & \text{if } x = y \\
\frac{-1}{\sqrt{d_x d_y}} & \text{if } x \sim y \\
0 & \text{otherwise},
\end{cases}
\] (4)

which can be obtained from \(L\) via the identity

\[
L = T^{-\frac{1}{2}}LT^{-\frac{1}{2}},
\]

where \(T(x, y) = \delta_{x,y} d_y\) and \(T^{-1}(x, x) = 0\) for \(d_x = 0\).

To develop the time-independent diffusion equation on graphs we require suitable boundary conditions analogous to those arising in partial differential equations (PDEs). We say a function \(u : V' \rightarrow \mathbb{R}\) satisfies a homogeneous Dirichlet boundary condition if its restriction to \(\delta V\) is identically zero \([7]\). To obtain appropriate derivative-type boundary conditions we assume \(\Gamma\) is of bounded degree and define the discrete analog of the normal derivative \(\partial : \ell^2(V \cup \delta V) \rightarrow \ell^2(\delta V)\) by

\[
\partial u(y) = \sum_{x \in V, x \sim y} [u(y) - u(x)].
\] (5)

A function \(u : (V \cup \delta V) \rightarrow \mathbb{R}\) satisfies a homogeneous Neumann boundary condition \([7]\) if \(\partial u(x) = 0\) for all \(x \in \delta V\) and satisfies a Robin boundary condition if there exists a constant \(t\) such that

\[
t u(x) + \partial u(x) = 0
\] (6)

for all \(x \in \delta V\). Note that choosing \(t = 0\) yields Neumann boundary conditions while letting \(t \rightarrow \infty\) produces Dirichlet boundary conditions. Given a function \(g : \delta V \rightarrow \mathbb{R}\) we can also define corresponding inhomogeneous boundary conditions

\[
t u(x) + \partial u(x) = g(x), \quad x \in \delta V
\] (7)

which arise when sources or sinks are located on the boundary. For a given interior source \(f\) and boundary source \(g\) we define the constant absorption, or uniform, diffusion equation

\[
\begin{cases} 
\sum_{y \in V, L(x, y) u(x) + \alpha_0 u(x) = f(x), \quad x \in V \\
t u(x) + \partial u(x) = g(x), \quad x \in \delta V.
\end{cases}
\] (8)

Here \(\alpha_0\) is a positive constant which represents the absorption of the medium. Note that \(L\) is positive semidefinite.

\[2.2\quad \text{Linear systems for finite boundary value problems}\]

In the case where \(|V|\) and \(|\delta V|\) are both finite the boundary value problem \([8]\) can be written as a linear system of equations for \(u\). We first index the vertices of \(V\) by \(1, \ldots, n = |V|\) and
those of $\delta V$ by $n + 1, \ldots, n + k$ where $k = |\delta V|$. Next we construct the $(n + k) \times (n + k)$ matrix

$$H_0 = \begin{pmatrix} L + \alpha_0 I_{n \times (n+k)} & R \\ R & D \end{pmatrix} \quad (9)$$

where $I_{n \times (n+k)}$ is the first $n$ rows of the $(n + k) \times (n + k)$ identity matrix, $R$ is the $k \times n$ matrix satisfying

$$R_{ij} = \begin{cases} -1 & \text{if } x_j \sim x_{i+n} \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

and $D$ is the $k \times k$ matrix with $i,j$th entry

$$D_{ij} = (t + |\{x_\ell \in V : x_\ell \sim x_{i+k}\}|) \delta_{ij}. \quad (11)$$

If we let $u = (u(x_1), \ldots, u(x_{n+k}))^*$ and $\tilde{f} = (f(x_1), \ldots, f(x_n), g(x_{n+1}), \ldots, g(x_{n+k}))^*$, where $w^*$ denotes the conjugate transpose of $w$, then we can rewrite the diffusion equation (8) as

$$H_0 u = \tilde{f}. \quad (12)$$

Similarly, we obtain Dirichlet boundary conditions by replacing the matrix operator $H_0$ in (9) by the matrix

$$H_0^D = \begin{pmatrix} L + \alpha_0 I_{n \times (n+k)} & 0 \\ 0 & I_{k \times k} \end{pmatrix} \quad (13)$$

where $0$ is the $n \times (n+k)$ matrix all of whose entries are zero. We say the vector $u$ satisfies the diffusion equation with Dirichlet boundary conditions if

$$H_0^D u = \tilde{f}. \quad (14)$$

Alternatively, one can obtain $u$ by noting that

$$u = \lim_{t \to \infty} u_t \quad (15)$$

where $u_t$ satisfies the equation

$$H_0 u_t = \begin{pmatrix} f \\ t g \end{pmatrix} \quad (16)$$

and $H_0$ is the matrix operator corresponding to Robin boundary conditions depending on the parameter $t$ as in (7).

It is clear by construction that $H_0$ is symmetric. As shown in the following proposition, under certain restrictions, the matrix $H_0$ is also positive definite and hence has a well-defined inverse. This is equivalent to the existence of a unique solution to the diffusion equation (8).
Proposition 1. For all $t$ such that $0 \leq t < \infty$ the smallest eigenvalue $\lambda_m$ of $H_0$ satisfies
\[ \lambda_m \geq \min\{t, \alpha_0\}. \tag{17} \]
It follows that if $t = 0$ the matrix $H_0$ is positive semidefinite and if $t > 0$ then $H_0$ is positive definite.

**Proof.** For convenience we drop the subscript 0 from $H_0$ and let $H_{i,j}$ be its $i,j$th element. From the construction of $H_0$ we know that for all $i$
\[ \sum_{j \neq i} H_{i,j} = -d_{x_i} \tag{18} \]
where, as above, $d_{x_i}$ is the degree of the vertex $x_i$. If $1 \leq i \leq n$ then
\[ H_{i,i} = d_{x_i} + \alpha_0, \tag{19} \]
while if $n + 1 \leq i \leq n + k$ then
\[ H_{i,i} = d_{x_i} + t. \tag{20} \]
From the Gerschgorin circle theorem we know that all eigenvalues of $H_0$ must lie in at least one of the circles $C_i$ where
\[ C_i = \left\{ x \in \mathbb{C} : |x - H_{i,i}| \leq \left| \sum_{j \neq i} H_{i,j} \right| \right\} \tag{21} \]
from which the result follows immediately noting that since $H_0$ is a symmetric real matrix all of its eigenvalues must lie on the real line.

Proposition 2. Consider the diffusion equation (8) on a connected graph $\Sigma$ with Neumann boundary conditions corresponding to $t = 0$. The associated matrix operator $H_0$ is positive definite for all $\alpha_0 > 0$ and moreover
\[ \lambda_m = \frac{|V|}{|V| + |\delta V|} \alpha_0 + O(\alpha_0^2) \tag{22} \]
as $\alpha_0 \to 0^+$. 

**Proof.** The proof is by contradiction. Suppose $v$ is an eigenvector of $H_0$ with eigenvalue 0. Let $A$ be the matrix
\[ A = \begin{pmatrix} L & R \\ R & D \end{pmatrix} \tag{23} \]
and $B$ the matrix defined by
\[ B_{i,j} = \begin{cases} 1, & i = j, 1 \leq i \leq n, \\ 0, & \text{otherwise}, \end{cases} \tag{24} \]
where $R$ and $D$ are defined in equations (10) and (11), respectively. By construction it is clear that

$$H_0 = A + \alpha_0 B$$

(25)

and, from the proof of the previous proposition, that both $A$ and $B$ are positive semidefinite. Note that

$$0 = v^* H_0 v = v^* A v + \alpha_0 v^* B v.$$

(26)

Since $A$ and $B$ are positive semidefinite and $B$ is diagonal it is clear that $v$ is both in the kernel of $B$ and is an eigenvector of $A$ with eigenvalue 0. Since $v \in \ker B$ it follows that its first $n$ entries must be identically zero. If $w$ denotes the last $k$ components of $v$ then we obtain

$$0 = H_0 v = A v = \begin{pmatrix} R^* w \\ D w \end{pmatrix}.$$

(27)

Note however that $D$ is a diagonal matrix whose diagonal entries are strictly positive and so $D w$ is zero if and only if $w$ is the zero vector. This implies that $v$ is a zero vector and hence cannot be an eigenvector of $H_0$ which completes the proof.

From [7] we observe that since $\Sigma$ is connected the eigenvalue 0 of $A$ has multiplicity one corresponding to the eigenvector $v = (1, \ldots, 1)^*$. It follows immediately from the theory of asymptotic analysis of linear systems, see [22] for example, that the smallest eigenvalue of $A + \alpha_0 B$ is

$$\lambda_m = \alpha_0 \frac{v^* B v}{v^* v} + O(\alpha_0^2),$$

(28)

from which the required result follows immediately.

Plots of the minimum eigenvalue of $H_0$ as a function of $\alpha_0$ are shown for a path in Figure 1a and for a complete graph in Figure 1b. As we can see, for small $\alpha_0$ the curve approaches the bound given in (28), which is shown in both plots for reference.

2.3 Spatially varying absorption

When discussing diffusion problems in the continuous setting we often wish to consider media with spatially varying properties. A similar idea can be applied to graphs through a suitable modification of the graph diffusion problem (8). Suppose the absorption at each vertex in $V$ is given by a function $\eta : V \to \mathbb{R}$. The resulting heterogeneous, or perturbed, diffusion equation is

$$\left\{ \begin{array}{ll}
\sum_{y \in V} L(x, y) u(x) + \alpha_0 [1 + \eta(x)] u(x) = f(x), & x \in V, \\
t u(x) + \partial u(x) = g(x), & x \in \delta V.
\end{array} \right.$$
Figure 1: The minimum eigenvalue of the operator $H_0$ as a function of the absorption $\alpha_0$ for: (a) a path of length 64 with Neumann boundary conditions, and (b) a complete graph on 64 vertices and Neumann boundary conditions. For both plots the line corresponds to the bound in equation (28).

To write this as a linear system we let $\tilde{\eta}$ be the $(n+k) \times (n+k)$ matrix with entries

$$
\tilde{\eta}_{ij} = \begin{cases} 
\eta(x_i), & i = j \leq n, \\
0, & \text{otherwise}.
\end{cases}
$$

(30)

It follows that $u$ solves the boundary value problem (29) if and only if it satisfies

$$
[H_0 + \alpha_0 \tilde{\eta}]u = \tilde{f}.
$$

(31)

For convenience we define $H = H_0 + \alpha_0 \tilde{\eta}$ to be the matrix operator corresponding to the more general diffusion equation.

2.4 Green’s functions for graphs

Green’s functions are a powerful tool for obtaining and analyzing solutions to PDEs such as the diffusion equation. When discussing similar equations on graphs, the analogous operator $G(x, y)$ is the inverse of $H$ [7]. Suppose the number of interior vertices of $\Sigma$ and the number of boundary vertices of $\Sigma$ are both finite. If we define $g_y = (G(x_1, y), G(x_2, y), \ldots, G(x_{n+k}, y))^*$ and let $H^*$ denotes the adjoint of the operator $H$, then $g_y$ satisfies the linear system

$$
H^* g_y = \delta_y
$$

(32)
where \( \delta_y \) is the vector whose components are all zero except for the one corresponding to \( y \) which is one. Hence we see that if \( u \) is a solution of (29) then

\[
(33)
\]

\[
g_y^* \tilde{f} = g_y^* Hu = (H^* g_y)^* u = \delta_y^* u = u(y).
\]

Though some care must be taken when \(|V| + |\delta V|\) is infinite one can define the Green’s function for such graphs in a similar way.

3 Born series

We next discuss a useful perturbative method, called Born series, for constructing series solutions to (29) using the homogeneous Green’s function.

3.1 Construction

Consider the matrix operator \( H_0 \) for the unperturbed diffusion equation (8) and let \( G_0 \) be the matrix such that \( G_0 H_0 = I \). In particular we require the columns of \( H_0 \) to be linearly independent so that \( H_0 \) has a well-defined inverse. As in the previous section, we define the matrix operator \( H \) for the perturbed problem (29) by

\[
H = H_0 + \alpha_0 \tilde{\eta},
\]

(34)

where \( \tilde{\eta} \) is once again the matrix defined in (29). If \( H^{-1} \) exists it satisfies

\[
H^{-1} = (I + \alpha_0 G_0 \tilde{\eta})^{-1} G_0
\]

(35)

and we can write a corresponding Neumann series

\[
B = \left[ \sum_{n=0}^{\infty} (-1)^n (G_0 \tilde{\eta})^n \right] G_0,
\]

(36)

which, under suitable conditions on \( G_0 \) and \( \tilde{\eta} \), is equal to the inverse of \( H \). In the context of scattering theory such an expansion is often called a Born series. Assuming the series in (36) converges to \( H^{-1} \) it follows immediately that for any source vector \( \tilde{f} \) the corresponding solution \( u \) of the time-independent diffusion equation (29) is given by

\[
u = \left[ \sum_{n=0}^{\infty} (-1)^n (G_0 \tilde{\eta})^n \right] G_0 \tilde{f}.
\]

(37)
3.2 Convergence

To show convergence of the Born series (36) with respect to a norm \(\|\cdot\|\) it is sufficient to show that the induced operator norm of \(B\), denoted by \(\|B\|\), is bounded, as shown in the following proposition.

**Proposition 3.** The series

\[
B = \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n G_0
\]

(38)

converges to the Green’s function of the perturbed problem (29) if \(\alpha_0 \|G_0\| \cdot \|\tilde{\eta}\| < 1\).

**Proof.** If \(\alpha_0 \|G_0\| \cdot \|\tilde{\eta}\| < 1\) we obtain

\[
\|B\| = \left\| \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n G_0 \right\|
\]

\[
\leq \|G_0\| \sum_{n=0}^{\infty} \alpha_0^n \|G_0\|^n \|\tilde{\eta}\|^n
\]

(39)

\[
= \frac{\|G_0\|}{1 - \alpha_0 \|G_0\| \cdot \|\tilde{\eta}\|}
\]

\[
< \infty.
\]

Since \(\|B\|\) and \(\|H\|\), defined by (36) and (34), respectively, are bounded we see that

\[
BH = \left[ \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n \right] G_0 [H_0 + \alpha_0 \tilde{\eta}]
\]

\[
= \left[ \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n \right] [I + \alpha_0 G_0 \tilde{\eta}]
\]

(40)

\[
= \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n - \sum_{n=1}^{\infty} (-1)^n \alpha_0^n (G_0 \tilde{\eta})^n
\]

\[
= I
\]

as required.

In particular we see from the previous proposition that approximating the Green’s function by a truncated Born series is more accurate when \(\|\tilde{\eta}\| \|G_0\|^{-1} \alpha_0^{-1}\) are small, sometimes called the *weak scattering limit*. We can also obtain tighter bounds if additional information about the structure of the absorption matrix \(\tilde{\eta}\) is used. In particular it is natural to assume that the matrix \(\tilde{\eta}\) has few non-zero diagonal entries. This is analogous to the physical situation where the spatial support of the scatterers is much smaller than the total volume.
Proposition 4. Suppose $\eta$ has support $\Lambda \subseteq V$ and let $I_\Lambda$ be the restriction of the identity matrix to the support of $\eta$. Further define $G_{0,\Lambda} = I_\Lambda G_0 I_\Lambda$ and let $\eta_{\max} = \sup_{x \in \Lambda} \eta(x)$. The series

$$B = \left[ \sum_{n=0}^{\infty} (-1)^n \alpha_0^n (G_0\tilde{\eta})^n \right] G_0$$

(41)

converges to the Green's function of the perturbed problem (29) if $\eta_{\max} \alpha_0 \|G_{0,\Lambda}\| < 1$. Moreover, the truncation error associated with

$$B_N = \left[ \sum_{n=0}^{N} (-1)^n \alpha_0^n (G_0\tilde{\eta})^n \right] G_0$$

(42)

is $O \left( \alpha_0^N \|G_{0,\Lambda}\|^N \cdot \eta_{\max}^N \right)$ as $N \to \infty$.

Proof. Since $\tilde{\eta}$ is a diagonal matrix it follows that $\|\tilde{\eta}\| = \eta_{\max} = \sup_{x \in V} |\eta(x)|$. Let $\Lambda$ be the support of $\eta$ and let $I_\Lambda$ be the restriction of the identity matrix to the support of $\eta$. In particular, $I_\Lambda$ is the diagonal matrix $I_\Lambda(x,y) = \delta_{x,y} \chi_{\{x \in \Lambda\}}$, where $\chi_\Lambda$ denotes the characteristic function of the set $\Lambda$. Note that $\tilde{\eta} = I_\Lambda \tilde{\eta} = \tilde{\eta} I_\Lambda$ and thus if we define $G_{0,\Lambda} = I_\Lambda G_0 I_\Lambda$ and let $n > 1$, then $(G_0\tilde{\eta})^n = G_0\tilde{\eta}(I_\Lambda G_0 I_\Lambda \tilde{\eta})^{n-1} = G_0\tilde{\eta}(G_{0,\Lambda} \tilde{\eta})^{n-1}$. Consider the truncated operator $B_N = \sum_{n=0}^{N-1} (-1)^k \alpha_0^n (G_0\tilde{\eta})^n G_0$. Clearly $B_N$ satisfies

$$\|B - B_N\| = \left\| \sum_{n=N}^{\infty} (-1)^n \alpha_0^n (G_0\tilde{\eta})^n G_0 \right\|

= \left\| G_0\tilde{\eta} \sum_{n=N-1}^{\infty} (-1)^{n+1} \alpha_0^{n+1} (G_{0,\Lambda} \tilde{\eta})^n G_0 \right\|

\leq \alpha_0^N \|G_0\|^2 \|\tilde{\eta}\| \|G_{0,\Lambda} \tilde{\eta}\|^{N-1} \sum_{n=0}^{\infty} \alpha_0^n \|G_{0,\Lambda} \tilde{\eta}\|^n

\leq \|G_0\|^2 \alpha_0^N \|G_{0,\Lambda}\|^N \eta_{\max}^N

\frac{1}{1 - \alpha_0 \|G_{0,\Lambda}\| \eta_{\max}}$$

(43)

and hence the truncation error associated with $B_N$ is $O \left( \eta_{\max}^N \alpha_0^N \|G_{0,\Lambda}\|^N \right)$ as $N \to \infty$. It follows that $B$ is bounded if $\alpha_0 \eta_{\max} \|G_{0,\Lambda}\| < 1$. \qed

4 Examples

Having developed the theory of Born series in the previous section, we now apply this method to approximate the Green’s functions for specific families of graphs, including the path, the loop, the Möbius ladder, the complete graph, the Bethe lattice, and the two-dimensional lattice.
4.1 Analysis of a path

Consider the finite path of length $n$ embedded in a path of infinite length as in Figure 2. In particular we can identify vertices with the integers $0, 1, \ldots, n, n+1$, where $0$ and $n+1$ are the boundary of the graph.

Figure 2: A diagram representing the finite path of length $n$ with boundary points 0 and $n+1$ coloured red.

Following [8] we proceed by obtaining a recursive equation for the elements of the Green’s function matrix $G$ for the time-independent homogeneous diffusion equation [8], though in our case we consider the more general Robin boundary conditions rather than the Dirichlet boundary conditions studied in [8]. We first consider the entries of $G$ for $1 \leq i \leq n+2$ and $1 \leq j \leq n$ and find the entries of $G$ for $i \leq j$. Symmetry is then used to determine the entries for $i > j$. The remaining elements of $G$ are found using a similar approach. In our discussion we consider the case of Robin boundary conditions as outlined in Section 1.2. The boundary conditions

$$ tu(0) + \partial u(0) = 0, \quad \text{and} \quad tu(n+1) + \partial u(n+1) = 0 \quad (44) $$

are enforced by adding a row to the top and bottom of the operator $(L + \alpha_0 I_{n \times (n+2)})$ yielding a matrix of the form

$$\begin{bmatrix}
1 + t & -1 & 0 & \ldots & 0 \\
-1 & 2 + \alpha_0 & -1 & \ldots & 0 \\
-1 & 2 + \alpha_0 & -1 & \ldots & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & \ldots & 0 & 1 + t
\end{bmatrix}. \quad (45)$$

Notice that unlike previous sections the boundary vertices now correspond to the first and last rows and columns of the matrix. Using the method outlined above, we obtain the following result.

**Proposition 5.** Let $\Sigma$ be a path of length $n$ such that the union of $\Sigma$ and $\delta V$ is the path of length $n+2$. The associated Green’s function for the constant absorption diffusion problem with Robin boundary conditions is

$$ G_{i+1, j+1} = \frac{(ar^i - a^{-1}r^{-i})(ar^{n+1-j} - a^{-1}r^{-(n+1-j)})}{(r - \frac{1}{r}) (a^2 r^{n+1} - a^{-2} r^{-(n+1)})}, \quad 0 \leq i \leq j \leq n + 1. \quad (46) $$
The parameter $r \geq 1$ is defined implicitly by the equation $r + 1/r = 2 + \alpha_0$ and the constant

$$a = \left[ 1 + \frac{(r^2 - 1)}{r[1 + t - r]} \right]^{1/2}$$

(47)

depends on the parameter $t$ with $t = 0$ corresponding to Neumann boundary conditions and $t \to \infty$ yielding Dirichlet boundary conditions. The remaining entries are obtained via the identity

$$G_{i,j} = G_{j,i}$$

(48)

which holds for all $1 \leq i, j \leq n + 2$.

**Proof.** For ease of notation let $G(i, j) = G_{i+1,j+1}$. If $0 < i < j$ then

$$0 = (L + \alpha_0)G(i, j) = \left[(2 + \alpha_0)G(i, j) - G(i + 1, j) - G(i - 1, j)\right].$$

(49)

Define $r$ implicitly by $r + \frac{1}{r} = 2 + \alpha_0$ in which case

$$0 = \left[-(G(i + 1, j) - rG(i, j)) + \frac{1}{r} (G(i, j) - rG(i - 1, j))\right]$$

(50)

and therefore

$$G(i + 1, y) - rG(i, j) = \frac{1}{r} [G(i, j) - rG(i - 1, j)]$$

$$= \frac{1}{r^2} [G(i - 1, j) - rG(i - 2, j)]$$

$$= \ldots$$

$$= \frac{1}{r^i} [G(1, j) - rG(0, j)].$$

(51)

If we require $G(i, j)$ to satisfy Robin boundary conditions [6], we obtain

$$t G(0, j) + [G(0, j) - G(1, j)] = 0$$

(52)

and hence $G(0, j) = G(1, j)/(1 + t)$. Letting $\gamma = 1/(1 + t)$ we obtain

$$G(i + 1, j) - rG(i, j) = \frac{1}{r^i} G(1, j)[1 - r\gamma] = \frac{c_j}{r^i},$$

(53)

from which it follows that $G(i, j) = \frac{c_j}{r^{i-1}} + rG(i - 1, j)$ and thus

$$G(i, j) = \frac{c_j}{r^{i-1}} + rG(i - 1, j)$$

$$= \frac{c_j}{r^{i-1}} + \frac{c_j}{r^{i-3}} + r^2G(i - 2, j)$$

$$= \ldots$$

$$= \frac{c_j}{r^{i-1}} \left[1 + r^2 + \cdots + r^{2(i-1)}\right] + r^iG(0, j).$$

(54)
Using the fact that $1 + r^2 + \cdots + r^{2(i-1)} = \frac{r^{2i} - 1}{r^2 - 1}$ we find that

$$G(i, j) = \frac{c_j}{r^{i-1}} \frac{r^{2i} - 1}{r^2 - 1} + r^i G(0, j)$$

$$= \frac{c_j}{r^{i-1}} \frac{r^{2i} - 1}{r^2 - 1} + r^i \gamma G(1, j)$$

$$= \frac{c_j}{r^{i-1}} \left[ r^{2i} - 1 + r^{2i} \gamma (r^2 - 1) \right].$$

Let $a = \left(1 + \frac{\gamma (r^2 - 1)}{r(1-r\gamma)}\right)^\frac{1}{2}$ and $c'_j = c_j ra$ in which case

$$G(i, j) = \frac{c'_j}{ar^i} \left[ a^2 r^{2i} - 1 \right]$$

$$= c'_j \left[ ar^i - a^{-1} r^{-i} \right].$$

Similarly, if $i < j$ we find

$$G(i, j) - rG(i, j - 1) = r \left[ G(i, j + 1) - rG(i, j) \right]$$

$$= r^2 \left[ G(i, j + 2) - rG(i, j + 1) \right]$$

$$= \cdots$$

$$= r^{n+1-j} \left[ G(i, n + 1) - rG(i, n) \right].$$

Enforcing the Robin boundary conditions we obtain $t G(i, n+1) + [G(i, n + 1) - G(i, n)] = 0$ and thus $G(i, n + 1) = \gamma G(i, n)$. Hence

$$G(i, j) - rG(i, j - 1) = r^{n+1-j} [\gamma - r] G(i, n) = c_i r^{n+1-j}$$

from which it follows that

$$G(i, j) = -c_i r^{n+1-j-2} + \frac{1}{r} G(i, j + 1)$$

$$= -c_i r^{n+1-j-2} - c_i r^{n+1-j-4} + \frac{1}{r^2} G(i, j + 2)$$

$$= \cdots$$

$$= -c_i r^{n+1-j-2} \left[ 1 + \left(\frac{1}{r}\right)^2 + \ldots + \left(\frac{1}{r}\right)^{2(n+1-j-1)} \right] + \frac{1}{r^{n+1-j}} G(i, n + 1)$$

$$= -c_i r^{n+1-j} \left(\frac{1}{r}\right)^{2(n+1-j)} - 1 + \frac{1}{r^{n+1-j}} \gamma c_i r.$$}

Upon simplification we obtain

$$G(i, j) = c'_i \left[ ar^{n+1-j} - a^{-1} r^{-(n+1-j)} \right].$$
where
\[
a = \left(1 + \frac{\gamma(r^2 - 1)}{r(1 - r\gamma)}\right)^{\frac{1}{2}},
\]
(61)
and \(c_j' = \frac{c_j}{a(1 - r^x)}\). It follows from equations (56) and (60) that
\[
G(i, j) = C \left( a^r - a^{-1}r^{-i} \right) \left( a^{n+1} - a^{-1}r^{-(n+1)-j} \right).
\]
(62)
To find the constant \(C\) we use the fact that \(1 = (L + \alpha_0)G(i, i)\) for all \(0 < i < n + 1\). In particular we obtain
\[
1 = C \left[ \left( r + \frac{1}{r} \right) (a^r - a^{-1}r^{-i}) \left( a^{n+1} - a^{-1}r^{-(n+1)-i} \right) 
- (ar^x - a^{-1}r^{-x}) \left( a^{n} - a^{-1}r^{-(n)} \right) 
- (a^{i-1} - a^{-1}r^{-(i+1)}) \left( a^{n+1} - a^{-1}r^{-(n+1)-i} \right) \right]
\]
(63)
and thus
\[
G(i, j) = \frac{(a^r - a^{-1}r^{-i})(a^{n+1} - a^{-1}r^{-(n+1)-j})}{(a^{n+1} - a^{-2}r^{-(n+1)})}
\]
for \(i \leq j, i \neq n + 1\) and \(j \neq 0\). To find \(G(0, 0)\) note that
\[
t G(0, 0) + G(0, 0) - G(0, 1) = 1
\]
(65)
so that
\[
G(0, 0) = \frac{1}{1 + t} + \frac{1}{1 + t} G(0, 1)
= \frac{(a^0 - a^{-1}r^{-0})(a^{n+1} - a^{-1}r^{-(n+1)-0})}{(a^{n+1} - a^{-2}r^{-(n+1)})}
\]
(66)
Clearly a similar result follows when \(i = j = n + 1\). Using the fact that \(H_0\) is symmetric it follows that \(G(i, j) = G(j, i)\) and so from the above formulae we can obtain the remaining entries in the matrix \(G\).

Notice that if we restrict our attention to Dirichlet boundary conditions we can reproduce the corresponding results in \([8]\) and extend them to the case where a source is located on the boundary.
Corollary 6. Let $\Sigma$ be a path of length $n$ such that the union of $\Sigma$ and $\delta \Sigma$ is the path of length $n + 2$. The associated Green’s function for the homogeneous time-independent diffusion problem (8) with Dirichlet boundary conditions is

$$G_{i+1,j+1} = \begin{cases} (r^{i-1}) (r^{n+1-i-j} - (n+1-j)) & 1 \leq i \leq j \leq n \\ (r^{-\frac{j}{2}}) (r^{n+1-i-j} - (n+1-i)) & 1 \leq j < i \leq n \\ r^{n+1-j-i} (r^{n+1-i-j} - (n+1)) & j = 0, n+1 \\ r^{i-j} (r^{n+1-i-j} - (n+1)) & i = 0, j \neq 0, \text{ and } i = n+1, j \neq n+1. \end{cases} \quad (67)$$

The Green’s function presented in [8] corresponds to the submatrix formed by removing the last row and column from the matrix $G$ defined above. Here the extra row and column are the result of allowing sources to be located on the boundary of the graph.

Proof. As in (15) we find the Green’s function for the Dirichlet boundary problem by considering a suitably-scaled limit of the Green’s function corresponding to Robin boundary conditions depending on the parameter $t$. In particular we see that the Dirichlet Green’s function $G_D$ is given by

$$G_D = \lim_{t \to \infty} GT \quad (68)$$

where $T$ is the diagonal matrix all of whose entries are 1 except for the first and the last which are $1/t$. If $j \neq 0, n+1$, the result follows immediately from the previous proposition, noting that $\lim_{t \to \infty} a = 1$. When $j$ corresponds to a boundary vertex the corresponding rows are scaled by the factor $1/t$. Note that

$$\lim_{t \to \infty} t (a - a^{-1}) = \lim_{t \to \infty} t \left[ \left(1 + \frac{r^2 - 1}{r(1+t-r)}\right)^{\frac{1}{2}} - \left(1 + \frac{r^2 - 1}{r(1+t-r)}\right)^{\frac{1}{2}} \right]$$

$$= \lim_{t \to \infty} t \left[ \left(1 + \frac{r^2 - 1}{2r(1+t-r)}\right) + \frac{1}{2} \frac{r^2 - 1}{rt} \right]$$

$$= \frac{r^2 - 1}{r}, \quad (69)$$

whence the result for the remaining entries follow immediately from the above computation and the fact that

$$\lim_{t \to \infty} a = 1, \quad (70)$$

where $a$ is defined by [61].

We can also compute the Green’s function for the centered path with vertices $-n, -n+1, \ldots, n-1, n$ and boundary vertices $-(n+1)$ and $n+1$. \qed
Corollary 7. The Green’s function for the centered path of length \((2n + 1)\) is

\[
G(i, j) = \frac{(ar^{i+n+1} - a^{-1}r^{-(i+n+1)})(ar^{n+1-j} - a^{-1}r^{-(n+1-j)})}{(r - \frac{1}{r}) (a^2 r^{2n+2} - a^2 r^{-2n+2})}
\]  

(71)

where \(-n \leq i \leq j \leq n\).

Proof. The proof follows directly from Proposition 5 through a change of variables. Letting \(i' = i + n + 1\) and \(j' = j + n + 1\) maps the centered path to a path of length \(2n + 1\) with the left boundary vertex at \(i' = 0\) and right boundary vertex at \(i' = 2n + 2\). The required result follows immediately. \(\square\)

Next we consider the Green’s function in the limit as \(n\) goes to infinity with \(i, j\) held fixed.

Corollary 8. In the limit as \(n \to \infty\) with \(i, j\) fixed we obtain

\[
G(i, j) = \frac{e^{-\log(r)|j-i|}}{2 \sinh \log r}
\]  

(72)

for all \(i, j \in \mathbb{Z}\).

Proof. From Corollary 7 we obtain

\[
G(i, j) = \frac{(ar^{i+n+1} - a^{-1}r^{-(i+n+1)})(ar^{n+1-j} - a^{-1}r^{-(n+1-j)})}{(r - \frac{1}{r}) (a^2 r^{2n+2} - a^2 r^{-2n+2})}.
\]  

(73)

In the limit as \(n \to \infty\) we obtain

\[
G(i, j) = \frac{a^2 r^{i-j+2(n+1)}}{(r - \frac{1}{r}) a^2 r^{2n+2}},
\]  

(74)

from which the result follows immediately. \(\square\)

The previous result matches the form of the free-space Green’s function of the differential equation

\[
\begin{cases}
-u''(x) + \alpha_0 u(x) = g(x), & x \in \mathbb{R}, \\
u(x) \to 0, & \text{as } |x| \to \infty,
\end{cases}
\]  

(75)

which is given by

\[
G(x, y) = \frac{e^{-\alpha_0^{1/2} |x-y|}}{2 \sqrt{\alpha_0}}.
\]  

(76)

We note that if \(r \geq 1\) satisfies \(r + 1/r = 2 + \alpha_0\) then

\[
r = 1 + \frac{1}{2} \left( \alpha_0 + \sqrt{\alpha_0^2 + 4\alpha_0} \right).
\]  

(77)
Hence \( \log r = \sqrt{\alpha_0} + O(\alpha_0) \) and \( \sinh(\log r) = \sqrt{\alpha_0} + O(\alpha_0) \) as \( \alpha_0 \to 0^+ \). It follows that the discrete and continuous case coincide in the low frequency limit when \( \alpha_0 << 1 \). In this limit the wavelength, \( 1/\sqrt{\alpha_0} \), is much larger than the edge length which is exactly the situation in which the continuous problem is approximated well by a uniform discretization of space.

Using the Green’s function obtained in Proposition 5 and the results of Section 2 we can solve the diffusion equation (29) for the path provided the absorption coefficients \( \eta(x) \) are sufficiently small. Let \( u_N = B_N \tilde{f} \) where \( \tilde{f} \) is the source vector and \( B_N \) is the truncated Born series matrix operator. Results for the particular \( \eta \) shown in Figure 3 with a unit source located at the left boundary vertex and \( t = 1/2 \) are given in Figure 4. As predicted the error decays exponentially as \( N \to \infty \) if \( \eta_{\text{max}} \) is less than a cut-off value, which is approximately 1.15. The comparison between the empirically determined cut-off for \( \eta_{\text{max}} \) and the upper bounds given by Section 3.2 is summarized in Table 1.

![Figure 3](image-url)

**Figure 3:** The absorption vector \( \eta \) used for the example of constructing a Green’s function for the heterogeneous diffusion equation (8) via Born series. The support of \( \eta \) is chosen to be a random subset of the interior vertices of size \( (2n + 2)/4 \).
Figure 4: Plots of the $\ell_\infty$ error of the truncated solution $u_N$. The green and red curves correspond to the bound on $\eta_{\text{max}}$ from Propositions 3 and 4, respectively. The other blue lines correspond to $\eta_{\text{max}}$ spaced 0.026 apart.

| Bound                  | Cut-off $\eta_{\text{max}}$ |
|------------------------|------------------------------|
| Numerical Experiment   | 1.15                         |
| Proposition 3          | 0.8333                       |
| Proposition 4          | 1.14655                      |

Table 1: Comparison of theoretical bounds and experimental results for the maximum possible value of $\eta_{\text{max}}$ for which the Neumann series converges.
4.2 Analysis of a loop

As in the previous example we can compute the Green’s function for the diffusion equation on a loop. For convenience we choose the loop to have $2n+2$ vertices, where $n$ is an integer. Similar results can be obtained for an odd number of vertices by a slight variation of the argument outlined in the following proposition.

Proposition 9. Let $\Sigma$ be the loop with $2n+2$ vertices $\{0, 1, \ldots, 2n+1\}$ as shown in Figure 5. The associated Green’s function for the diffusion equation (8) is

$$G(i, j) = \frac{r^{n+1-|i-j|\min} + r^{-(n+1-|i-j|\min)}}{(r - \frac{1}{r}) (r^{n+1} - r^{-(n+1)})}$$

(78)

for all $0 \leq i, j \leq 2n + 1$, where $|i - j|\min = \min\{|i - j|, 2n + 2 - |i - j|\}$.

Before proceeding to the proof we remark that the equation we are solving closely resembles that considered in [8], though both the ultimate aim of that work and the resulting Green’s function differ from ours. The proof we give here is based on the method for the path outlined in [8].

Proof. By symmetry we observe that $G(x, y)$ must depend only on the relative distance of the vertices $x_i$ and $x_j$ since the graph $\Sigma$ is invariant under cyclic permutation of vertices. Thus without loss of generality we can fix $j = 0$. Further notice that for all $0 < i < n$ $G(i, 0) = G(2n + 2 - i, 0)$ and hence it is sufficient to find $G(i, 0)$ when $0 \leq i \leq n + 1$. Finally, we observe that $G(n + 2, 0) = G(n, 0)$ and therefore, as in the previous example,
it is possible to write an expression for $G(n + 1, 0)$ in terms of $G(n, 0)$. In particular, if we define $r$ implicitly by $r + \frac{1}{r} = 2 + \alpha_0$ then the equation

$$0 = \left[(r + r^{-1})G(n + 1, 0) - G(n, 0) - G(n + 1, 0)\right]$$

(79)

yields

$$G(n + 1) = \frac{r + r^{-1}}{2}G(n, 0).$$

(80)

We can then apply a slight variation of the method used in the proof of Proposition 5 to obtain

$$G(i, 0) = \frac{r^{n+1-i} + r^{-(n+1-i)}}{(r - \frac{1}{r}) (r^{n+1} - r^{-(n+1)})}.$$  

(81)

The required result follows immediately by using the reflection and rotation symmetries

$$G(i, j) = G(i - (n + 1), j), \quad 0 \leq i, j \leq 2n + 1,$$
$$G(i, j) = G(i + k, j + k), \quad 0 \leq i, j, k \leq 2n + 1,$$

(82)

where all indices are taken modulo $2n + 1$.

**Corollary 10.** In the limit $n \to \infty$ with $i, j$ fixed we obtain

$$G(x, y) = \frac{e^{-\log(r)|j-i|}}{2\sinh \log r}$$

for all $i, j \in \mathbb{Z}$, which is the result obtained in Proposition 8.

**Proof.** The proof is an immediate consequence of Proposition 6 and the proof of Proposition 8. Notice that if $x$ and $y$ are fixed while $n \to \infty$ then $|i-j|_{\min} = |i-j|$ for all $n$ sufficiently large.

As in the case of the path we can use the Born series to construct Green’s solutions for the diffusion equation (29) provided that the absorption vector $\eta$, given in Figure 6, is sufficiently small. Again using a source located at the node $i = 0$ we use a truncated Born series to find approximations $u_N$ to the true solution obtained by directly solving the linear system (29). Results are shown in Figure 7 for various values of $\eta_{\text{max}}$. As expected, we see that if $\eta_{\text{max}}$ is sufficiently small the error decays exponentially with increasing $N$. If, however, $\eta_{\text{max}}$ exceeds some critical value the error grows exponentially as more terms are used. In this example the critical value of $\eta_{\text{max}}$ is approximately 2.0, though this is expected to depend on the support of $\eta$. 

Figure 6: A typical absorption vector $\eta$ used for the example of constructing a Green’s function for the heterogeneous diffusion equation (8) via Born series. The support of $\eta$ is chosen to be a random subset of the vertices of size $(2n + 1)/4$.

Figure 7: Plots of the $\ell_\infty$ error of the truncated solution $u_N$. The green and red curves correspond to the bound on $\eta_{\text{max}}$ from Propositions 3 and 4, respectively.
| Bound                      | Cut-off $\eta_{\text{max}}$ |
|---------------------------|-----------------------------|
| Numerical Experiment      | 2.0                         |
| Proposition 3             | 1.0                         |
| Proposition 4             | 1.95                        |

Table 2: Comparison of theoretical bounds, and empirical results, for the largest $\eta_{\text{max}}$ for which the Neumann series converges.

### 4.3 Analysis of a Möbius ladder

Another family of vertex-transitive graphs of particular interest in material science [25, 21, 27] and computer science [15] are the Möbius ladders on $2n + 2$ vertices. Using a similar approach as above we can compute the background Green’s function for the diffusion equation on this family of graphs. For convenience we assume $n$ is odd though a similar result can be obtained in the even case by a slight modification to the proof of the following proposition.

**Proposition 11.** Let $\Sigma$ be the Möbius ladder with $2n + 2$ vertices $\{0, 1, \ldots, 2n + 1\}$, $n$ odd, as shown in Figure 8. The associated Green’s function for the diffusion equation with uniform absorption (8) is

$$G(i, j) = \begin{cases} g_1(|i - j|_{\text{min}}) + g_2(|i - j|_{\text{min}}), & |i - j| \leq \frac{n + 1}{2} + 1 \\ g_1(|i - j|_{\text{min}}) - g_2(|i - j|_{\text{min}}), & |i - j| > \frac{n + 1}{2} \end{cases}$$

for all $0 \leq i, j \leq 2n + 1$, where $|i - j|_{\text{min}} = \min\{|i - j|, 2n + 2 - |i - j|, |i - j| - (n + 1)|\}$,

$$g_k(s) = \frac{(akr_k^{(n+1)/2} - a_{k-1}r_k^{-(n+1)/2})(akr_k^{(n+1)/2-s} - a_{k-1}r_k^{-(n+1)/2-s})}{(r_k - r_k^{-1})(akr_k^{2n+1} - a_{k-2}r_k^{-(n+1)})}, \quad k = 1, 2,$$

$r_k$ satisfies $r_k + 1/r_k = 2k + \alpha_0$,

$$a_1 = \left[1 + \frac{r_1^2 - 1}{r_1(1 + \frac{a_0}{2} - r_1)}\right]^{\frac{1}{2}},$$

and $a_2 = 1$.

**Proof.** The result is proved in a manner similar to the method of images used in PDEs []. We decompose the Green’s function into two functions one of which is symmetric and the other antisymmetric with respect to reflection through the origin. Unlike in the case of method of images, however, the ‘mirror charges’ are located within the domain of interest and we rely on cancellations to recover the desired solution. In considering the symmetries of the problem, it is clear that $G(i, j)$ must depend only on the number of vertices of the
our result can be obtained in the even case by a slight modification to the proof of the following equation on this family of graphs. For convenience we assume $27$ and computer science $[15]$ are the Möbius ladders on $2$ vertices.

### 4.3 Analysis of a Möbius ladder

Another family of vertex-transitive graphs of particular interest in material science ... a $2$.

Figure 8: The Möbius ladder with $2n + 2$ vertices.

loop lying between the two vertices $x_i$ and $x_j$, since the graph $Σ$ is invariant under cyclic permutations of its vertices. Thus, without loss of generality, we can fix $j = 0$. Letting $H_0$ be the operator associated with the homogeneous time-independent diffusion equation $[8]$, we now consider two related problems:

(A) find the vector $g_2 \in \mathbb{R}^{2n+2}$ such that $H_0 g = \frac{1}{2}(e_0 - e_{n+1})$, where $e_k$ is the kth canonical basis vector.

(B) find the vector $g_1 \in \mathbb{R}^{2n+2}$ such that $H_0 g = \frac{1}{2}(e_0 + e_{n+1})$.

In considering subproblem (A), we see by inspection that if $g_2$ is a solution then it must satisfy

$$g_2(i) = g_2(2n + 2 - i) = -g_2(n + 1 - i) = -g_2(n + 1 + i), \quad (87)$$

where once again for ease of notation we take all indices modulo $2n + 2$. It follows immediately that

$$g_2((n + 1)/2) = g_2(-(n + 1)/2) = 0. \quad (88)$$

Moreover, applying $H_0$ we see that

$$\frac{1}{2} \delta_{0,i} = (3 + \alpha_0)g_2(i) - g_2(i + n + 1) - g_2(i + 1) - g_2(i - 1), \quad (89)$$

for $-(n + 1)/2 < i < (n + 1)/2$. Hence $2g_2(i), -(n + 1)/2 < i < (n + 1)/2$ satisfies the same equation as the Green’s function for the centered path with source at $j = 0$, $\alpha_0$ replaced...
by $2 + \alpha_0$ and with Dirichlet boundary conditions at $i = \pm(n + 1)/2$. From Corollary 7 we obtain

$$ g_2(i) = \frac{(r(n+1)/2 - r^{-(n+1)/2}) (r^{(n+1)/2-i} - r^{-(n+1)/2+i})}{2(r-r^{-1})(r^{n+1} - r^{-(n+1)})} \quad (90) $$

where $r + r^{-1} = 4 + \alpha_0$.

To solve subproblem (B), we begin by noting that

$$ g_1(i) = g_1(2n + 2 - i) = g_1(n + 1 - i) = g_1(n + 1 + i), \quad (91) $$

for all $i = 0, \ldots, 2n + 1$ and where all indices are taken modulo $2n+2$. It follows that it is sufficient to find $g_1(i)$ for $i = -(n + 1)/2, \ldots, -2, -1, 0, 1, 2, \ldots, (n + 1)/2$. By symmetry we know that $g_1((n + 1)/2 - 1) = g_1((n + 1)/2 + 1)$ and $g_1(-(n + 1)/2) = g_1((n + 1)/2)$ so that

$$ 0 = (3 + \alpha_0)g_1((n + 1)/2) - g_1(-(n + 1)/2) - g_1((n + 1)/2 - 1) - g_1((n + 1)/2 + 1) = (2 + \alpha_0)g_1((n + 1)/2) - 2g_1((n + 1)/2 - 1). \quad (92) $$

Similar reasoning applies to $g_1(-(n + 1)/2)$ and hence

$$ (1 + \frac{\alpha_0}{2})g_1(\frac{n + 1}{2}) - g_1(\frac{n + 1}{2} - 1) = 0, \text{ and } (1 + \frac{\alpha_0}{2})g_1(- \frac{n + 1}{2}) - g_1(- \frac{n + 1}{2} + 1) = 0. \quad (93) $$

For all $i$, $-(n + 1)/2 < i < (n + 1)/2$ we find from the above symmetries that

$$ (2 + \alpha_0)g_1(i) - g_1(i - 1) - g_1(i + 1) = \frac{1}{2} \delta_i,0. \quad (94) $$

It follows immediately that the equations satisfied by $2g_1(i)$, $i = -(n + 1)/2, \ldots, (n + 1)/2$ are identical to those defining the Green’s function for the centered path with source at $j = 0$ and with Robin boundary conditions $t = \alpha_0/2$. Thus from Corollary 7 we find that if $r + 1/r = 2 + \alpha_0$, $t = \alpha_0/2$ and $a = \left[1 + \frac{r^2-1}{r(1+r-r^{-1})}\right]^{-\frac{1}{2}}$ then

$$ g_1(i) = \frac{(ar^{(n+1)/2} - a^{-1}r^{-(n+1)/2})(ar^{(n+1)/2-i} - a^{-1}r^{-(n+1)/2+j})}{2(r-r^{-1})(a^2r^{n+1} - a^{-2}r^{-(n+1)})}. \quad (95) $$

The remaining entries can then be found immediately by reflection.

\[\square\]

Using the results of Propositions 3 and 11 we can once again find the Green’s function for the diffusion equation (29) when the absorption is small but need not be constant. As example we consider the case where the source is located at $j = 0$ and \(\eta\) is identically 1 on its support, which is chosen to be a random subset of the vertices with size $(2n + 2)/4$, as in Figure 9. Plots of the $\ell_\infty$ difference between the actual solution, $u$, and the truncated series approximation, $u_N$, are given for different values of $N$ and $\eta_{\max}$ in Figure 10.
Figure 9: A typical absorption vector $\eta$ used for the example of constructing a Green’s function for the spatially-varying time-independent diffusion equation (8) via Born series. The support of $\eta$ is a randomly selected subset of the vertices with size $(2n + 2)/4$.

Figure 10: Plots of the $\ell_\infty$ error of the truncated solution $u_N$. The blue and teal curves correspond to the bound on $\eta_{\text{max}}$ from Propositions 3 and 4, respectively.
4.4 Analysis of the complete graph on $d$ vertices

We can perform a similar computation with the complete graph on $d$ vertices, an example of which is shown in Figure 11 for $d = 10$.

**Proposition 12.** Let $R$ be the complete graph on $d$ vertices $\{0, 1, \ldots, d-1\}$ with $d$ boundary vertices $\{0', 1', \ldots, (d-1)\}$. The associated Green’s function for the diffusion equation (8) with Robin boundary conditions is

$$G(x, y) = \begin{cases} 
\frac{\sigma}{(\sigma-1)(\sigma-1+d)} & \text{if } x = y \in V, \\
\frac{1}{(\sigma-1)(\sigma-1+d)} & \text{if } x \neq y, x, y \in V, \\
\frac{\gamma^2 \sigma}{(\sigma-1)(\sigma-1+d)} + \gamma & \text{if } x = y, x' \in \delta V,
\end{cases} \quad (96)$$

where $\gamma = 1/(1 + t)$ and $\sigma = 2 + \alpha_0 - \gamma$. The remaining entries can be obtained via the Robin boundary conditions and the identity

$$G(x, y) = G(y, x) \quad (97)$$

which holds for all $x, y \in V \cup \delta V$.

Figure 11: The complete graph on 10 vertices with 10 boundary vertices.
Proof. We first consider the case where the source is located at an interior vertex. By symmetry we may assume without loss of generality that \( y = 0 \). Note that upon fixing \( y = 0 \) the graph is invariant under a permutation of all remaining vertices, provided it preserves the edge between the vertex in \( R \) and the corresponding boundary point.

If \( x \neq 0 \) we observe that

\[
\left[ (d + \alpha_0)G(x, 0) - (d - 2)G(x, 0) - G(0, 0) - G(x', 0) \right] = 0. \tag{98}
\]

Using Robin boundary conditions we see that \( G(x', 0) = G(x, 0)/(1 + t) \) and hence

\[
G(0, 0) = [2 + \alpha_0 - \gamma] G(x, 0). \tag{99}
\]

Let \( g = G(x, 0) \) and \( \sigma = [2 + \alpha_0 - \gamma] \) in which case we obtain

\[
1 = [(d + \alpha_0)G(0, 0) - (d - 1)g - \gamma G(0, 0)]
= [(d + \alpha_0)\sigma g - (d - 1)g - \gamma \sigma g] \tag{100}
= g(\sigma - 1)(\sigma + d - 1)
\]

and thus

\[
g = \frac{1}{(\sigma - 1)(\sigma + d - 1)}. \tag{101}
\]

The remainder of the result follows immediately from noting that \( G(0, 0) = \sigma g \) and by using the symmetries of the complete graph described above.

Now suppose the source is located on the boundary. Again, without loss of generality, we may assume that the source is located at the vertex \( 0' \). If \( x \neq 0 \) then

\[
0 = [(d + \alpha_0) G(x, 0') - (d - 2)G(x, 0') - G(0, 0') - G(x', 0)]. \tag{102}
\]

If \( G(x, 0') = g \) then \( G(0, 0') = (2 + \alpha_0 - \gamma)g = \sigma g \). If \( x = 0 \) then

\[
0 = [(d + \alpha_0)\sigma g - (d - 1)g - G(0', 0')]. \tag{103}
\]

The Robin boundary condition \( tG(0', 0') + [G(0', 0') - G(0, 0')] = 1 \) implies that

\[
g = \frac{\gamma}{(d + \alpha_0)\sigma - (d - 1) - \sigma \gamma} = \frac{\gamma}{(\sigma - 1)(\sigma + d - 1)}. \tag{104}
\]

As an example, this result was used in conjunction with the Born series to solve the time-independent diffusion problem \([29]\) with \( \eta \) as given in Figure \([12]\). The associated errors for various values of \( \eta_{\text{max}} \) are shown in Figure \([13]\).
Figure 12: A typical absorption vector $\eta$ used for the example of constructing a Green’s function for the spatially-varying time-independent diffusion equation (8) via Born series. The support of $\eta$ is once again chosen to be a random sample of the interior vertices of size $d/4$.

Figure 13: Plots of the $\ell_\infty$ error of the truncated solution $u_N$. The green and red curves correspond to the bound on $\eta_{\text{max}}$ from Propositions 3 and 4, respectively.
4.5 Analysis of a Bethe lattice

We next consider the problem of finding the Green’s function for the homogeneous time-independent diffusion problem \((8)\) on a Bethe lattice, an example of which is shown in Figure 14 with coordination number 4.

**Proposition 13.** Let \(\Sigma\) be the Bethe lattice with coordination number \(k\) and define the parameter

\[
\lambda = \frac{k + \alpha_0}{2(k - 1) - \sqrt{(k + \alpha_0)^2 + (k - 2)^2 - k^2}}.
\]

(105)

If \(\lambda < 1\) the associated Green’s function for the homogeneous time-independent diffusion equation is given by

\[
G(x, y) = \frac{\lambda |x - y|}{k(1 - \lambda) + \alpha_0},
\]

(106)

where \(|x - y|\) is the distance between the vertices \(x\) and \(y\). If \(\lambda > 1\) the corresponding Green’s function is unbounded as \(|x - y| \to \infty\).

![Figure 14: The Bethe lattice with coordination number 4 up to depth 4.](image)

**Proof.** We proceed as before by first employing symmetry to reduce the number of calculations required. In particular, we note that the Bethe lattice is invariant under a change of root. Hence without loss of generality we choose one coordinate of our pair \((x, y)\) to be the root of the tree which we label as the 0th vertex. We observe by symmetry that the
Green’s function $G(x,0)$ must depend only on the distance between the vertex $x$ and the root 0. If we let $d(x)$ denote the depth of the vertex $x$, then there exists a function $g$ such that $G(x,0) = g(d(x))$. Hence we obtain

$$
[(k + \alpha_0)g(0) - kg(1)] = 1
$$
$$
[(k + \alpha_0)g(d) - g(d-1) - (k-1)g(d+1)] = 0,
$$
(107)

where $d \geq 1$. It follows that

$$
g(d+1) = \frac{1}{k-1} [(k + \alpha_0)g(d) - g(d-1)].
$$
(108)

For convenience we let $\alpha = (k + \alpha_0)/(k - 1)$ and $\beta = \frac{1}{k-1}$ in which case we find that

$$
g(d+1) = \alpha g(d) - \beta g(d-1).
$$
(109)

Defining $g_d = (g(d), g(d-1))^T$ for $d \geq 1$ we obtain

$$
g_{d+1} = \begin{bmatrix} \alpha & -\beta \\ 1 & 0 \end{bmatrix} g_d
$$
(110)

which has corresponding eigenvalues

$$
\lambda_\pm = \frac{\alpha}{2} \pm \frac{\sqrt{\alpha^2 - 4\beta}}{2}
$$
(111)

and eigenvectors $v_\pm = (\lambda_\pm, 1)^T$. All solutions of the matrix equation (110) are of the form $g_d = c_-\lambda_\pm^{d-1} v_- + c_+\lambda_\pm^{d-1} v_+$. Using the definition of $\alpha$ and $\beta$ we see that $\lambda_+ \geq 1$ and $0 < \lambda_- \leq (k + \alpha_0)/(2(k - 1))$ where $\lambda_+ = 1$ if and only if $\alpha_0 = 0$. Imposing the boundary condition $g(d) \to 0$ as $d \to \infty$ we see that this is only possible if $k$ and $\alpha_0$ are chosen so that $\lambda_- < 1$ and the coefficient $c_+$ of $\lambda_+^{d-1} v_+$ is identically zero. For ease of notation we drop the subscript on both $\lambda_-$, $c_-$ and $v_-$ so that $g_d = c\lambda^d v$. We substitute our solution into the equation (107) to obtain

$$
[(k + \alpha_0)c - \lambda k c] = 1
$$
(112)

implying that

$$
c = \frac{1}{k + \alpha_0 - \lambda k}
$$
(113)

and hence

$$
g(d) = \frac{1}{k + \alpha_0 - \lambda k} \lambda^d,
$$
(114)

which completes the proof. \qed
4.6 Analysis of a two-dimensional lattice

We conclude our catalogue of examples with a discussion of the Green’s function for the two-dimensional lattice \( \Sigma = \mathbb{Z} \times \mathbb{Z} \). For convenience, we index the vertices with ordered tuples \( V = \{ (m, n) \mid m, n \in \mathbb{Z} \} \) and hence if \( x = (m_1, n_1) \) and \( y = (m_2, n_2) \) are two vertices then \( x \sim y \) if and only if \(|m_2 - m_1| + |n_2 - n_1| = 1\). In the following proposition we obtain an integral representation of the Green’s function for the isotropic time-independent diffusion equation on the infinite two-dimensional lattice by means of a discrete Fourier transform.

**Proposition 14.** Let \( \Gamma \) be the graph \( \mathbb{Z} \times \mathbb{Z} \) with vertices labelled by \( \{ (m, n) \mid m, n \in \mathbb{Z} \} \). The Green’s function for the corresponding homogeneous time-independent diffusion equation (8) is

\[
G((m_1, n_1), (m_2, n_2)) = \frac{1}{2\pi} \int_0^{\pi} \frac{\cos(d_+v) (\cos(v))^{d_+}}{(a + \sqrt{a^2 - \cos(v)})^{d_+} \sqrt{a^2 - \cos(v)}} \, dv
\]

where \( a = 1 + \alpha_0/4 \), and \( d_\pm = |m_2 - m_1| \pm |n_2 - n_1| \). In particular, if \( (m_1, n_1) = (m_2, n_2) \) then

\[
G((m, n), (m, n)) = \frac{1}{\pi a} K\left(\frac{1}{a^2}\right)
\]

where \( K \) is the complete elliptic integral of the first kind defined by [1]

\[
K(m) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1 - m^2 \sin^2 \phi}} \, d\phi,
\]

for \( m^2 < 1 \).

**Proof.** The approach for finding the Green’s function is similar to that used for the Helmholtz equation on lattices [12, 20]. We begin by noting that the problem is invariant under translations and reflections, from which it follows that \( G \) must only depend on the quantities \( m = |m_2 - m_1| \) and \( n = |n_2 - n_1| \). Hence

\[
G((m_1, n_1), (m_2, n_2)) = G((m, n), (0, 0)) = g(m, n)
\]

for some function \( g(m, n) \in \ell^2(\mathbb{Z}^2) \). Applying the operator \( H_0 \) defined in [0], we see that \( g(m, n) \) satisfies the difference equation

\[
(4 + \alpha_0) g(m, n) - g(m - 1, n) - g(m + 1, n) - g(m, n - 1) - g(m, n + 1) = \delta_{m,0}\delta_{n,0}.
\]

We next consider the discrete Fourier transform of (119). On \( \mathbb{Z} \times \mathbb{Z} \) the Fourier transform \( \mathcal{F} : \ell^1(\mathbb{Z} \times \mathbb{Z}) \to L^1((-\pi, \pi]^2) \) of a function \( f \) is given by

\[
\hat{f}(\xi, \eta) = \mathcal{F}(f)(\xi, \eta) = \sum_{m,n \in \mathbb{Z}} e^{-im\xi - in\eta} f(m, n).
\]
Thus, upon taking the Fourier transform of equation (119), we obtain
\[
\left(4 + \alpha_0\right) - e^{i\xi} - e^{-i\xi} - e^{in} - e^{-in} \hat{g}(\xi, \eta) = 1,
\]
where \(\xi, \eta \in (-\pi, \pi]\). Using the identity
\[
e^{i\xi} + e^{-i\xi} + e^{in} + e^{-in} = (e^{i(\xi+\eta)/2} + e^{-i(\xi+\eta)/2})(e^{i(\xi-\eta)/2} + e^{-i(\xi-\eta)/2})
\]
yields
\[
\hat{g}(\xi, \eta) = \frac{1}{4 \left[ 1 + \alpha_0/4 - \cos \left( \frac{\xi+\eta}{2} \right) \cos \left( \frac{\xi-\eta}{2} \right) \right]}.
\]
Upon application of the inverse Fourier transform we find
\[
g(m, n) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{im\xi + in\eta} \frac{1}{4 \left[ 1 + \alpha_0/4 - \cos \left( \frac{\xi+\eta}{2} \right) \cos \left( \frac{\xi-\eta}{2} \right) \right]} \, d\xi \, d\eta.
\]
If we change variables, letting \(u = (\xi + \eta)/2\) and \(v = (\xi - \eta)/2\), we obtain
\[
g(m, n) = \frac{1}{2(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{i(m-n)u} e^{i(m+n)u} \frac{1}{1 + \alpha_0/4 - \cos u \cos v} \, du \, dv.
\]
If we let \(a = 1 + \alpha_0/4\) and choose \(z = e^{iu}\) we obtain
\[
g(m, n) = \frac{1}{2(2\pi)^2 i} \int_{-\pi}^{\pi} e^{i(m-n)u} \int_{-\pi}^{\pi} \frac{1}{az - \cos v} \, dz \, dv
\]
where \(C_1\) is the unit circle oriented counterclockwise. Integration then yields
\[
g(m, n) = \frac{1}{4\pi} \int_{-\pi}^{\pi} e^{i(m-n)v} \frac{(\cos v)^{m+n}}{(a + \sqrt{a^2 - \cos^2 v})^{m+n} \sqrt{a^2 - \cos^2 v}} \, dv.
\]
Using the fact that the above expression is the Fourier transform of an even function we can re-write it as a real integral, yielding
\[
g(m, n) = \frac{1}{2\pi} \int_{0}^{\pi} \frac{\cos[(m - n)v] (\cos v)^{m+n}}{(a + \sqrt{a^2 - \cos^2 v})^{m+n} \sqrt{a^2 - \cos^2 v}} \, dv.
\]
The expression for the Green’s function given in (115) follows by employing the translation and reflection symmetries outlined above. To obtain the expression (116) we observe that
\[(m_2, n_2) = (m_1, n_1)\] corresponds to \(m = n = 0\) and hence is given by

\[
g(0, 0) = \frac{1}{2\pi} \int_0^{\pi} \frac{1}{\sqrt{a^2 - \cos^2 v}} \, dv
\]

\[
= \frac{1}{2\pi a} \int_{-\pi/2}^{\pi/2} \frac{1}{\sqrt{1 - (1/a)^2 \cos^2 \phi}} \, d\phi
\]

\[
= \frac{1}{\pi a} \int_0^{\pi/2} \frac{1}{\sqrt{1 - (1/a)^2 \cos^2 \phi}} \, d\phi
\]

\[
= \frac{1}{\pi a} K \left( \frac{1}{a^2} \right). \tag{129}
\]

5. **Representation theory and the background Green’s function**

In the previous section we obtained the background Green’s function for a variety of examples by solving corresponding recurrence relations. In every example, excluding the finite path, clearly-visible symmetries were employed in an intuitive way to reduce the problem to a more tractable set of equations. This connection between symmetry and PDE analogues on graphs can be formalized using the language of representation theory.

### 5.1 Cayley graphs of finite abelian groups

As a particularly important special case we first consider Cayley graphs of abelian groups. In particular, let \(G\) be a finite abelian group and \(S\) be a symmetric subset of the elements of \(G\). Recall that \(S\) is a symmetric subset of a group \(G\) if \(g \in S\) implies \(g^{-1} \in S\). This condition is required to ensure that the resulting graph is undirected and the associated Laplacian operator is symmetric. We can then define the the Cayley graph \(X(G, S)\) to be the graph whose vertices are indexed by the elements of \(G\) with edge set \([28]\)

\[
E = \{(g, h) \in G \times G \mid gh^{-1} \in S\}. \tag{130}
\]

Looking at the examples considered in the previous section we note that the loop, Möbius ladder, and complete graph are all Cayley graphs with group \(G = \mathbb{Z}/n\mathbb{Z}\), for some \(n\), and \(S = \{-1, 1\}, \{-1, 1, -n/2, n/2\}\) and \(\{-n + 1, -n + 2, \ldots, -1, 1, \ldots, n - 2, n - 1\}\), respectively. The infinite path is the Cayley graph of the free group on 2 generators and the Bethe lattice with coordination number \(k\) is the Cayley graph of the free group on \(k\) generators. Finally, the two-dimensional lattice is the Cayley graph with group \(\mathbb{Z} \times \mathbb{Z}\) and generator set \(S = \{(-1, 0), (0, -1), (1, 0), (0, 1)\}\).
For Cayley graphs the combinatorial Laplacian can be compactly expressed using the convolution operator $\ast : \ell^2(G) \times \ell^2(G) \to \ell^2(G)$ defined by

$$(f \ast g)(x) = \sum_{y \in G} f(y) g(y^{-1}x).$$

(131)

It is clear that the adjacency matrix $A$ for $X(G, S)$ is given by [28]

$$A(f)(x) = (\delta_S \ast f)(x)$$

(132)

where $\delta_S$ is the characteristic function on the set $S$ and hence if $k = |S|$ then

$$L(f)(x) = (kI - A)(f)(x) = kf(x) - (\delta_S \ast f)(x).$$

(133)

In order to diagonalize this operator using Fourier analysis, we next define the dual group

$$\hat{G} = \operatorname{Hom}(G, \mathbb{T})$$

(134)

where $\mathbb{T}$ is the multiplicative group of complex numbers with modulus one. If $\chi \in \hat{G}$ then we call $\chi$ a character. If $G$ is a finite abelian group then it is self-dual [24], and hence $G$ is isomorphic to $\hat{G}$. We then have the following proposition, proved in [28].

**Proposition 15.** If $h \in \ell^2(G)$ then the eigenvectors of the corresponding convolution operator are equal to the characters of $G$. In particular, if $\chi \in \hat{G}$ then

$$(h \ast \chi)(x) = \hat{h}(\chi) \chi(x)$$

(135)

for all $x \in G$ and where $\hat{h}(\chi) = \sum_{x \in G} h(x) \overline{\chi(x)}$.

The following corollaries are immediate consequences of Proposition [15]

**Corollary 16.** The characters of $G$ are the eigenvectors of $L$ with corresponding eigenvalues

$$\lambda_\chi = k - \sum_{s \in S} \overline{\chi(s)}.$$  

(136)

**Corollary 17.** The Green’s function for the uniform diffusion equation is

$$G(f)(x) = \sum_{\chi \in G} \sum_{y \in G} \frac{1}{\lambda_\chi + \alpha_0} f(y) \overline{\chi(y)} \chi(x).$$

(137)

**Proof.** We begin by observing that since the eigenfunctions of $L$ are the characters of $G$ through an appropriate change of basis we may diagonalize $L$. If we denote the elements of $G$ by $x_1, \ldots, x_k$ and the characters of $G$ by $\chi_1, \ldots, \chi_k$ then we can form the corresponding $k \times k$ matrix defined by

$$X_{i,j} = \chi_j(x_i).$$

(138)
It follows from the above results that the matrix representation of \( L \) can be written as
\[
L = X \begin{pmatrix}
\lambda_{x_1} & & \\
 & \lambda_{x_2} & \\
& & \ddots \\
& & & \lambda_{x_{k-1}} \\
& & & & \lambda_{x_k}
\end{pmatrix} X^\dagger, \tag{139}
\]
where \( X^\dagger \) denotes the conjugate transpose of the matrix \( X \). Since \( XX^\dagger = I \), the \( k \times k \) identity matrix, it follows that
\[
H_0 = L + \alpha_0 I = X \begin{pmatrix}
\lambda_{x_1} + \alpha_0 & & \\
 & \lambda_{x_2} + \alpha_0 & \\
& & \ddots \\
& & & \lambda_{x_{k-1}} + \alpha_0 \\
& & & & \lambda_{x_k} + \alpha_0
\end{pmatrix} X^\dagger, \tag{140}
\]
from which the formula \( \Box \) follows immediately, using the fact that \( G = H_0^{-1} \).

### 5.2 Cayley graphs of finite groups

The results of the previous section can be extended to non-abelian groups in a natural way. As before, we use the fact that the operator \( H_0 \) can be written as a convolution operator on \( \ell^2(G) \) to find a spectral decomposition of its Fourier transform. Applying the inverse Fourier transform yields a complete set of eigenvectors and eigenvalues of \( H_0 \) from which it is straightforward to obtain an expression for the background Green’s function \( G_0 \) of the corresponding Cayley graph.

Before presenting the main results we first introduce some basic definitions and results associated with Fourier analysis on finite non-abelian groups (for a more complete description see \cite{knight2001}, for example). As in \cite{chung1997}, let \( \rho \) be a homomorphism from the group \( G \) to the automorphism group of \( V \), a \( k \)-dimensional vector space over \( \mathbb{C} \). Such a map \( \rho \) is called a \textit{k-dimensional representation} of \( G \) and is said to be \textit{irreducible} if the only subspaces of \( V \) which are invariant under \( \rho(g) \) for all \( g \in G \) are \( 0 \) and \( V \). We say that two representations \( \rho : G \to \text{GL}(V) \) and \( \tau : G \to \text{GL}(W) \) are \textit{equivalent} \cite{chung1997} if there exists an isomorphism \( f : V \to W \) such that \( \tau(g) = f \circ \rho(g) \circ f^{-1} \).

Given a representation \( \rho : G \to \text{GL}(V) \) of \( G \), let \( d_\rho = \text{dim}(V) \) denote its degree. If \( f \in \ell^1(G) \) then its \textit{Fourier transform} is the map \( \mathcal{F}[f] : \rho \to \mathbb{C}^{d_\rho} \times \mathbb{C}^{d_\rho} \) defined by \cite{knight2001}
\[
\mathcal{F}[f](\rho) = \sum_{g \in G} f(g)\rho(g). \tag{141}
\]
Observe that the Fourier transform of a function $f$ at a representation $\rho$ will, in general, be matrix-valued and is called the Fourier coefficient matrix of $f$ at $\rho$. If two representations $\rho_1$ and $\rho_2$ are equivalent then it is straightforward to show that the corresponding Fourier coefficient matrices are similar and hence the Fourier transform of $f$ is completely determined by its value on a maximal set of inequivalent irreducible representations, called the dual and denoted by $\hat{G}$. Note that if $G$ is abelian then its irreducible representations must be of degree one and this definition of $\hat{G}$ is equivalent to the one given in (134).

Given a function $h : \rho \in \hat{G} \rightarrow \mathbb{C}^{d_\rho} \times \mathbb{C}^{d_\rho}$ we can define its inverse Fourier transform by the following expression

$$\hat{h} = \mathcal{F}^{-1}[h](g) = \frac{1}{|G|} \sum_{\rho \in G} d_{\rho} \text{Tr} (\rho(g^{-1})h(\rho)).$$

(142)

The proof that $\mathcal{F}^{-1}\mathcal{F}$ is the identity operator on $\ell^2(G)$ and is independent of the choice of the elements in $\hat{G}$, provided they form a maximal set of irreducible inequivalent representations can be found in [28].

From the definitions given above it is straightforward to prove the following result [28] which will be useful in decomposing the operator $H_0$.

**Proposition 18.** Consider the convolution operator $\ast : \ell^1(G) \times \ell^1(G) \rightarrow \ell^1(G)$ defined by

$$f \ast h(g) = \sum_{r \in G} f(r^{-1})h(rg).$$

(143)

If $\hat{f} = \mathcal{F}[f]$ and $\hat{h} = \mathcal{F}(h)$ then

$$\mathcal{F}[f \ast h](\rho) = \hat{f}(\rho)\hat{h}(\rho).$$

(144)

We can now employ the theory developed above to analyze the spectrum of the Cayley graph $X(G,S)$ with vertices once again indexed by the elements of $G$ and edge generating set $S$. We begin by observing that the adjacency operator $A$ for $X(G,S)$ can be written as

$$A[f](g) = \chi_S \ast f(g), \quad \forall g \in G$$

(145)

where $\chi_S$ is the characteristic function of $S$. It follows immediately that if $e \in G$ is the identity element then

$$H_0[f](g) = ((|S| + \alpha_0)\chi_e - \chi_S) \ast f(g)$$

(146)

and thus from Proposition [18] that

$$\hat{H}_0[\hat{f}](\rho) = (|S| + \alpha_0)\hat{f}(\rho) - \sum_{g \in S} \rho(g)\hat{f}(\rho).$$

(147)
The problem then becomes to diagonalize the operator $\hat{H}_0$ in Fourier space by finding suitable eigenfunctions of $[147]$. Using the properties of the Fourier transform outlined above we can then find the corresponding eigenfunctions of $H_0$ in $\ell^2(G)$.

For ease of exposition, let $M(\rho) = \sum_{g \in S} \rho(g)$ in which case we have the following useful lemma.

**Lemma 19.** If $M(\rho) = \sum_{g \in S} \rho(g)$ where $\rho$ is a representation of a finite group, $G$, then $M(\rho)$ is diagonalizable.

**Proof.** We begin by noting that since $G$ is finite, $\rho$ is equivalent to a representation $\rho'$ such that $\rho'(g)$ is unitary for all $g \in G$. In particular, there exists a $d_\rho \times d_\rho$ matrix $B$ such that

$$
M(\rho) = BM(\rho')B^{-1}.
$$

(148)

Since $\rho'(g)$ is unitary observe that $\rho'(g^{-1}) = \rho'(g)^{-1} = \rho'(g)^*$, where $*$ once again denotes the adjoint of a matrix. Furthermore, we note that since $S$ is symmetric, if $g \in S$ then $g^{-1} \in S$ so that

$$
M(\rho') = \frac{1}{2} \sum_{g \in S} \left[ \rho'(g) + \rho'(g^{-1}) \right].
$$

(149)

It follows immediately that

$$
M(\rho')^* = \left[ \sum_{g \in S} \rho'(g) \right]^* = \frac{1}{2} \sum_{g \in S} \left[ \rho'(g) + \rho'(g^{-1}) \right]^* = \frac{1}{2} \sum_{g \in S} \left[ \rho'(g) + \rho'(g)^* \right]^* = M(\rho'),
$$

(150)

and so $M(\rho')$ is Hermitian. Since $M(\rho)$ is similar to $M(\rho')$ it follows that it too is diagonalizable. 

Fixing a maximal set of inequivalent irreducible representations $\hat{G} = \{\rho_1, \ldots, \rho_L\}$, let $v^i_j$ be the $j$th eigenvector of $M(\rho_i)$ with eigenvalue $\nu^i_j$. Furthermore, let $H^i_{jk}$ be the $d_{\rho_i} \times d_{\rho_i}$ zero matrix with the $k$th column replaced by $v^i_j$. We then define the function $f^i_{jk}: \rho \in \hat{G} \to \mathbb{C}^{d_{\rho_i}} \times \mathbb{C}^{d_{\rho_i}}$ by

$$
f^i_{jk}(\rho) = \delta_{\rho_i}(\rho)H^i_{jk}
$$

(151)

where $\delta_{\rho_i}(\rho)$ is 1 if $\rho = \rho_i$ and zero otherwise. We remark that the function $f$ has only been defined on the set of representations $\hat{G}$ though it has a natural, and unique, extension, $\tilde{f}$, to all representations of $G$ by requiring the following two conditions hold:
i) if $\rho$ and $\rho'$ are equivalent representations such that $\rho = B \rho'(g) B^{-1}$ for all $g \in G$ then 
\[ \tilde{f}_{jk}^i(\rho) = B^{-1} f_{jk}^i(\rho') B, \]
and

ii) if $\rho = \rho_1 \oplus \rho_2$ then 
\[ \tilde{f}_{jk}^i(\rho) = f_{jk}^i(\rho_1) \oplus f_{jk}^i(\rho_2). \]

The following proposition is an immediate consequence of the previous definitions.

**Proposition 20.** The function $f_{jk}^i(\rho)$ defined in (151) is an eigenfunction of the operator $\hat{H}_0$ with corresponding eigenvalue \( \lambda^i_{jk} = |S| + \alpha_0 - \nu_j^i. \) \( (152) \)

for all $i = 1, \ldots, L$ and $1 \leq j, k \leq d_{\rho_i}$.

Notice that Proposition 20 tells us that given the irreducible representations of $G$ we can reduce the problem of finding the eigenfunctions and eigenvalues of the operator $\hat{H}_0$ to that of finding the eigenvectors and eigenvalues of the matrices $\{M(\rho_i)\}_{i=1}^L$. To find the corresponding eigenfunctions of the operator $H_0$ we observe that

\[ H_0[f](g) = F^{-1} [H_0 F[f]] (g) \] \( (153) \)

from which it follows that $H_0$ has eigenfunctions $u_{jk}^i = F^{-1} f_{jk}^i$ with eigenvalues $\lambda^i_{jk}$. Proceeding in this way will generate $\sum_{\rho \in \hat{G}} d_{\rho}^2$ distinct eigenfunctions of $H_0$. However, we know that \( n = |G| = \sum_{\rho \in G} d_{\rho}^2 \) \( (154) \)

and so the above procedure will produce a complete set of eigenfunctions for the operator $H_0$. Since $H_0$ is Hermitian we can use Gram-Schmidt orthogonalization to produce a complete orthonormal set of eigenvectors $\phi_{jk}^i$, with eigenvalues once again given by $\lambda^i_{jk}$, from which it follows that

\[ G_0 = \sum_{i=1}^L \sum_{1 \leq j, k \leq d_{\rho_i}} \frac{1}{\lambda^i_{jk}} \phi_{jk}^i \phi_{jk}^i*. \] \( (155) \)

As an illustration of this procedure we now consider the background Green’s function for the permutohedron of order 4, shown in Figure 15, though the following analysis generalizes to permutohedra of arbitrary order.

We begin by noting that the permutohedron of order $n$ is isomorphic to the Cayley graph $X(S_n, S)$, where $S_n$ is the symmetric group on $n$ letters and $S$ is the symmetric set of generators consisting of all transpositions which interchange neighbouring elements \[2].

For each irreducible representation $\rho$ of $S_n$ we can construct the matrix $M(\rho)$, given by

\[ M(\rho) = \sum_{g \in S} \rho(g). \] \( (156) \)
Next, for each non-equivalent irreducible representation $\rho$, we diagonalize the matrix $M(\rho)$ and form the eigenvectors of $\hat{H}_0$ using (151). Taking the inverse Fourier transform of each of these eigenvectors yields eigenvectors of the original operator $H_0$, with corresponding eigenvalues (152). After normalizing the eigenvectors we construct the background Green’s function using (155). The matrix given by this procedure, plotted in Figure 16, agrees to within machine precision with the inverse of $H_0$ calculated numerically.

6 Point Absorbers

In scattering theory a classic problem is to consider a medium which is entirely homogeneous except for a few small inhomogeneities referred to as point absorbers. For convenience we typically assume that the inhomogeneities are sufficiently far apart relative to their diameters, so that each can be thought of as being supported on a single point.

6.1 A single point absorber

As above let $\Sigma = (V, E)$ be a graph with vertex boundary $\delta V$. If a single point absorber is present then $\eta : (V + \delta V) \to \mathbb{R}$ is of the form

$$\eta(x) = \kappa \delta_{x,y},$$

(157)

where $y \in V$ is the location of the point absorber and $\kappa$ is a positive constant. If $G_0$ is the Green’s function for the diffusion equation (8) we find from Propositions 3 and 4 that the
Figure 16: The background Green’s function for the permutohedron of order 4, with $\alpha_0 = 0.1$.

Green’s function corresponding to the diffusion equation (29) is

$$B = \sum_{n=0}^{\infty} (-\alpha_0 G_0 \tilde{\eta})^n G_0,$$

provided that the series on the right-hand side of (158) converges in norm. By rearranging the above equation and using (157) we obtain

$$B - G_0 = \alpha_0 \kappa G_0 \delta_{x,y} \left[ \sum_{n=0}^{\infty} (-\alpha_0 \kappa)^n (G_0 \delta_{x,y})^n \right] G_0.$$

(159)
If we let $G_0(\cdot, y) = (G_0(x_1, y), \ldots, G_0(x_{n+k}, y))^*$ then it is clear from the proof of Proposition 4 that

$$G_0 - B = \alpha_0 \kappa G_0(\cdot, y) \left[ \sum_{n=0}^{\infty} (-\alpha_0 \kappa)^n G_0(y, y)^n \right] G_0(\cdot, y)^*. \quad (160)$$

The series on the right-hand side of (160) is geometric, which converges if

$$|\alpha_0 \kappa G_0(y, y)| < 1, \quad (161)$$

in which case

$$G_0 - B = \frac{\alpha_0 \kappa}{1 + \alpha_0 \kappa G(y, y)} G_0(\cdot, y) G_0(\cdot, y)^*. \quad (162)$$

For example, consider the infinite path whose background Green’s function is given in Corollary 8. If the point absorber is located at the vertex $k$ then equation (162) yields

$$(G_0 - B)(i, j) = \frac{\alpha_0 \kappa}{1 + \alpha_0 \kappa \alpha} e^{-\log(r) (|i-k|+|j-k|)} \gamma^2 \sigma^2 (\sigma - 1)^2(\sigma - 1 + d)^2, \quad (163)$$

where $i, j \in \delta V$, $\gamma = 1/(1 + t)$ and $\sigma = 2 + \alpha_0 - \gamma$.

**6.2 Multiple point absorbers**

We now consider the case where there are $m$ identical point scatterers located at the vertices $\{x_{k1}, \ldots, x_{km}\} \subset V$. We begin by defining the $m \times m$ matrix

$$(G_R)_{i,j} = G(x_i, x_j), \quad 1 \leq i, j \leq m, \quad (165)$$

and the $m \times (|V| + |\delta V|)$ matrix

$$T_{i,j} = \delta_{ki,j}, \quad 1 \leq i \leq m, \quad 1 \leq j \leq |V| + |\delta V|, \quad (166)$$
so that
\[ G_{0,\Lambda} = T^* G_R T, \]  
(167)
where \( G_{0,\Lambda} \) is the matrix defined by Proposition 4 with \( \Lambda = \{x_{k_1}, \ldots, x_{k_t}\} \). Further note that \( TT^* = I_{k \times k} \), the \( k \times k \) identity matrix. It follows immediately from Proposition 4 that
\[ G_0 - B = \alpha_0 \kappa G_0 T^* \left( \sum_{\ell=0}^{\infty} (-\alpha_0 \kappa)^\ell G_R^\ell \right) T G_0. \]  
(168)
In particular, since \( G_R \) is Hermitian it is diagonalizable and can be written as
\[ G_R = V^* D_R V, \]  
(169)
where \( V \) is the unitary matrix containing the eigenvectors of \( G_R \) and \( D_R \) is the diagonal matrix whose entries \( \{\lambda_1, \ldots, \lambda_m\} \) are the corresponding eigenvalues of \( G_R \). Thus
\[ G_0 - B = \alpha_0 \kappa G_0 T^* V^* \left( \sum_{\ell=0}^{\infty} (-\alpha_0 \kappa)^\ell D_R^\ell \right) V T G_0. \]  
(170)
In particular, if \( \alpha_0 \kappa \max_{1 \leq \ell \leq m} |\lambda_\ell| < 1 \) and
\[ \left( \tilde{D}_R \right)_{i,j} = \frac{1}{1 + \alpha_0 \kappa \lambda_i} \delta_{i,j}, \quad 1 \leq i, j \leq m, \]  
(171)
then
\[ G_0 - B = \alpha_0 \kappa G_0 T^* V^* \tilde{D}_R V T G_0. \]  
(172)
As an example, we once again consider the infinite path and suppose there are two point absorbers located at the vertices corresponding to \( k_1 \) and \( k_2 \). Thus
\[ G_R = \frac{1}{2 \sinh \log r} \begin{pmatrix} 1 & e^{-\log(r)|k_2-k_1|} \\ e^{-\log(r)|k_2-k_1|} & 1 \end{pmatrix}, \]  
(173)
and
\[ V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad D_R = \frac{1}{2 \sinh \log r} \begin{pmatrix} 1 + e^{-\log(r)|k_2-k_1|} & 0 \\ 0 & 1 - e^{-\log(r)|k_2-k_1|} \end{pmatrix}. \]  
(174)
A straightforward calculation yields
\[ V T G_0 e_i = \frac{1}{2 \sqrt{2} \sinh \log r} \begin{pmatrix} e^{-\log(r)|i-k_1|} + e^{-\log(r)|i-k_2|} \\ e^{-\log(r)|i-k_1|} - e^{-\log(r)|i-k_2|} \end{pmatrix} \]  
(175)
and hence if we let $f_{i,j} = e^{-\log(r)|i-j|}/2\sinh\log r$ and $s = \sinh(\log(r))$ then

$$e_j^*(G_0 - B)e_i = \frac{1}{2} \left( f_{j,k_1} + f_{j,k_2} f_{j,k_1} - f_{j,k_2} \right) \left( \begin{array}{cc} \frac{\alpha_0 \kappa}{1+\alpha_0 \kappa (s^{-1}+f_{k_1,k_2})} & 0 \\ 0 & \frac{\alpha_0 \kappa}{1+\alpha_0 \kappa (s^{-1}-f_{k_1,k_2})} \end{array} \right) \times \left( \begin{array}{c} f_{i,k_1} + f_{i,k_2} \\ f_{i,k_1} - f_{i,k_2} \end{array} \right).$$

(176)

Observe that in the limit as $|k_1-k_2| \to \infty$, $f_{k_1,k_2} = o(1)$ and hence equation (176) becomes

$$e_j^*(G_0 - B)e_i \approx \frac{\alpha_0 \kappa}{2(1+\alpha_0 \kappa s^{-1})} \left( f_{j,k_1} + f_{j,k_2} f_{j,k_1} - f_{j,k_2} \right) \left( f_{i,k_1} + f_{i,k_2} f_{i,k_1} - f_{i,k_2} \right) \quad \text{(177)}$$

where $G_1(i,j;k)$ is the Green’s function for one point absorber located at the point $k$. Thus as the separation of the two point absorbers increases, the Green’s function tends toward the sum of the Green’s functions for two non-interacting point absorbers. Sample plots are shown in Figure [17] for the infinite path with two point absorbers equidistant from a point source located at the origin. Here $u_0$ represents the solution to the homogeneous problem and $u$ denotes the solution to the full time-independent diffusion equation.
Figure 17: Plots of $u_0 - u$ for the infinite path with two identical point scatterers equidistant from a point source located at the origin with $\alpha_0 = 0.001$ and $\kappa = 100$. 
As a second example we consider the scattering from two point absorbers on the infinite two-dimensional lattice. An analysis of the scattering properties of this system requires an expression for the Green’s function of the diffusion equation (8) on \( \mathbb{Z} \times \mathbb{Z} \), an integral formula for which was found in Proposition 14. For simplicity we specialize to the case in which the are two point absorbers are positioned on the y-axis and the source and detector are located on the x-axis as in Figure 18.

![Figure 18: A diagrammatic representation of the geometry of the point absorbers (blue circles), source (green diamond) and detector (red square) used to study the scattering properties of the two point absorber system on the infinite square lattice.](image)

If we assume the source is located at \((s,0)\) the detector is at \((j,0)\), and the point absorbers are located at \((0,k_1)\), and \((0,k_2)\), then an analogous calculation to the one performed for the one-dimensional case yields

\[
e_j^*(G_0 - B)e_s = \frac{1}{2} \left( f_{j,k_1} + f_{j,k_2} \quad f_{j,k_1} - f_{j,k_2} \right) \begin{pmatrix} \frac{\alpha \kappa}{1 + \alpha \kappa \lambda^+} & 0 \\ \frac{0}{1 + \alpha \kappa \lambda^-} & \frac{\alpha \kappa}{1 + \alpha \kappa \lambda^-} \end{pmatrix} \begin{pmatrix} f_{s,k_1} + f_{s,k_2} \\ f_{s,k_1} - f_{s,k_2} \end{pmatrix}.
\]

(178)
where

\[ \lambda_{\pm} = g(0, 0) \pm g(0, k_2 - k_1) \]

\[ = \frac{1}{\pi a} K \left( \frac{1}{a^2} \right) \pm \frac{1}{2\pi} \int_0^\pi \frac{\cos[(k_2 - k_1) v] \cos v |k_2 - k_1|}{(a + \sqrt{a^2 - \cos^2 v})^{|k_2 - k_1|} \sqrt{a^2 - \cos^2 v}} \, dv \]  

(179)

and \( f_{s,k} = g(|s|, |k|) \). Results for \(-s = j = 1\) and \(k_1 = -k_2\) are shown in Figure 19 for various values of the point absorber separation \(|k_2 - k_1|\) with \(\alpha_0 = 10^{-3}\) and \(\kappa = 10^3\). Note that due to the nature of our expression for the isotropic Green’s function we cannot evaluate equation (178) exactly and must make use of numerical integration both to evaluate \(g(|s|, |k|)\) and to find values for the integrals in (179).

Figure 19: Plots of \(u_0 - u\) for the infinite path with two identical point scatterers equidistant from a point source located at \((-1, 0)\) and detector located at \((1, 0)\) with \(\alpha_0 = 10^{-3}\) and \(\kappa = 10^3\).
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