ASYMPTOTIC EXPANSIONS OF LATTICE GREEN'S FUNCTIONS

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Abstract. We derive asymptotic expansions for the Green's functions associated with coercive difference equations on general lattices. These expansions lead to rigorous methods for approximating the lattice Green's functions by polyharmonic rational functions.

1. Introduction

1.1. **Background.** Periodic lattice models are central to crystal physics (Maradudin [12]) and they are frequently encounterd in analysis of light-weight structures (Noor [14]) and materials (Gibson and Ashby [6]). Difference equations defined on periodic lattices also arise naturally in numerical analysis of partial differential equations (Babuška [1], and Fix and Strang [3, 4]).

Equations associated with lattices typically involve a local and coercive convolution operator that relates the unknown potential to the given load. In such a case the solution can be written as the convolution between the load and a lattice Green's function that is typically non-local. Even though one can easily obtain an explicit representation for this Green's function in terms of a Fourier integral, see [2, 12], it is in general not possible to express it in terms of elementary functions. Nevertheless, some results in this direction are given by Joyce, [9, 10, 11], and Glasser and co-workers, [7].

In this paper we derive approximations for the lattice Green's function in terms of rational, poly-harmonic functions. Our methods apply to linear scalar equations defined on an arbitrary lattice. The approximation procedure is systematic enough that the derivation of the approximate Green's function can be automated using symbolic algebra software. In many respects, the work presented here is a generalization of the results provided by Duffin [2].

Although the asymptotic expansions we provide are interesting in their own right and shed light on the nature of the lattice equations, our primary motivation is that such expansions are central to fast solution methods for lattice equations. In later work we will utilize these expansions to develop translation theorems that will allow the extension of the Fast Multipole algorithm, by Greengard and Rokhlin, [8], to lattice equations.

Before proceeding to the general case we give a brief review on how the lattice Green's functions arise and illustrate the ideas of the paper with a simple example.

1.2. **Lattice Green's Functions.** Consider the equation

$$[\mathfrak{A}\mathfrak{u}](n) = \mathfrak{f}(n), \qquad \forall\, n \in \mathbb{Z}^3, \tag{1.1}$$

where $\mathfrak{A}$ is a local difference operator of the form

$$[\mathfrak{A}\mathfrak{u}](n) = \sum_{j=1}^{b} \alpha_j \big(-\mathfrak{u}(n - m_j) + 2\mathfrak{u}(n) - \mathfrak{u}(n + m_j)\big), \tag{1.2}$$

for some positive scalars α_j and vectors $m_j \in \mathbb{Z}^3$ that span $\mathbb{R}^3$. Given a load $\mathfrak{f}$ such that $\sum_n |\mathfrak{f}(n)| < \infty$ we look for a solution $\mathfrak{u}$ that has finite energy, $\sum_n [\mathfrak{A}\mathfrak{u}(n)]\mathfrak{u}(n) < \infty$. We will demonstrate how to construct a Green's function whereby a solution can be constructed explicitly.

Introducing the discrete Fourier transform

$$\tilde{\mathfrak{u}}(\xi) = \mathfrak{F}[\mathfrak{u}](\xi) = \sum_{n \in \mathbb{Z}^3} e^{\mathrm{i}n\cdot\xi}\mathfrak{u}(n),$$

we can diagonalize Equation (1.2),

$$\sigma(\xi)\tilde{\mathfrak{u}}(\xi) = \tilde{\mathfrak{f}}(\xi), \qquad \forall\, \xi \in (-\pi,\, \pi)^3 =: I^3,$$

where we defined the Fourier representation, or *symbol*, of $\mathfrak{A}$ by

$$\sigma(\xi) = \mathfrak{F}\,\mathfrak{A}\,\mathfrak{F}^{-1} = \sum_{j=1}^{b} 4\alpha_j \sin^2 \frac{\xi_j}{2}. \tag{1.3}$$

It is easy to show that for $\xi \in I^3$, the symbol satisfies $\sigma(\xi) \geq c|\xi|^2$ for some positive constant c. Since $\tilde{\mathfrak{f}}$ is bounded (recall that we assumed that $\mathfrak{f}$ is summable), this implies that $\tilde{\mathfrak{f}}/\sigma$ is integrable over I^3 and thus a solution to Equation (1.2) is provided by

$$\mathfrak{u}(n) = \mathfrak{F}^{-1}\left[\frac{\tilde{\mathfrak{f}}}{\sigma}\right](n) = \frac{1}{(2\pi)^3}\int_{I^3} e^{-\mathrm{i}n\cdot\xi}\frac{\tilde{\mathfrak{f}}(\xi)}{\sigma(\xi)}\,d\xi.$$

Next we note that $\mathfrak{F}^{-1}[\tilde{\mathfrak{f}}/\sigma] = (\mathfrak{F}^{-1}[1/\sigma]) * \mathfrak{f}$. By setting

$$\mathfrak{G}(n) := \mathfrak{F}^{-1}\left[\frac{1}{\sigma}\right](n) = \frac{1}{(2\pi)^3}\int_{I^3} e^{-\mathrm{i}n\cdot\xi}\frac{1}{\sigma(\xi)}\,d\xi, \tag{1.5}$$

we can thus write the solution

$$\mathfrak{u}(n) = [\mathfrak{G} * \mathfrak{f}](n) = \sum_{m \in \mathbb{Z}^3} \mathfrak{G}(n-m)\mathfrak{f}(m).$$

It can be shown that this solution is unique up to a constant, see [13].

We will later show that the asymptotic behaviour of $\mathfrak{G}(n)$ for large n is governed by the $O(|\xi|^{-2})$ singularity of $\sigma^{-1}(\xi)$ at the origin. This can be explained heuristically by noting that the function $\sigma^{-1}(\xi)$ is analytic for $\xi \neq 0$, thus contributions to the integral in (1.5) from any domain bounded away from the origin decay faster than any inverse polynomial. Hence, in order to approximate $\mathfrak{G}(n)$ for large n, we will approximate $\sigma^{-1}(\xi)$ by a rational function that captures the singularity at the origin. Then we use the Fourier transform of that function to approximate the exact Green's function. We will illustrate these ideas with a simple example.

Example: Consider heat conduction on the simple cubic lattice obtained by connecting each node $n \in \mathbb{Z}^3$ to its six nearest neighbours. In this case $\mathfrak{u}(n)$ represents the temperature of the node n and $\mathfrak{f}(n)$ is an external heat source. Letting e_j denote the canonical unit vectors (so that for instance $e_1 = (1,0,0)$) the equilibrium equations read

$$\sum_{j=1}^{3}\big(-\mathfrak{u}(n-e_j) + 2\mathfrak{u}(n) - \mathfrak{u}(n+e_j)\big) = \mathfrak{f}(n), \qquad \forall\, n \in \mathbb{Z}^3. \tag{1.6}$$

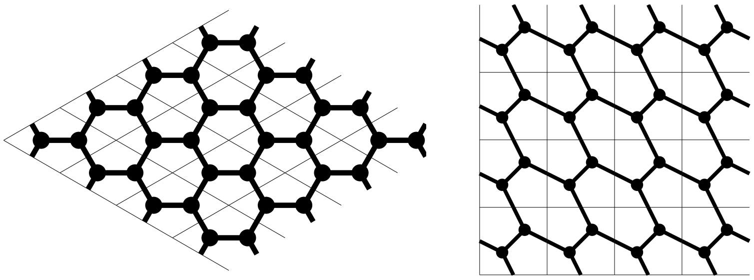

FIGURE 1. The lattice to the left can be transformed to the lattice to the right, which has a square irreducible cell, by an affine transformation.

In this case

$$\sigma(\xi) = 4\sin\frac{\xi_1}{2} + 4\sin\frac{\xi_2}{2} + 4\sin\frac{\xi_3}{2}. \tag{1.7}$$

The singularity of $\sigma^{-1}(\xi)$ at the origin can be captured by a rational function,

$$\frac{1}{\sigma(\xi)} = \frac{1}{|\xi|^2} + \frac{1}{12}\frac{\xi_1^4 + \xi_2^4 + \xi_3^4}{|\xi|^4} + O(|\xi|^2), \tag{1.8}$$

whence a continuum approximation G to $\mathfrak{G}$ can be constructed as follows:

$$\mathfrak{G}(n) = \frac{1}{(2\pi)^3}\int_{I^3} e^{-\mathrm{i}n\cdot\xi}\frac{1}{\sigma(\xi)}\,d\xi \approx \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-\mathrm{i}n\cdot\xi}\left(\frac{1}{|\xi|^2} + \frac{1}{12}\frac{\xi_1^4+\xi_2^4+\xi_3^4}{|\xi|^4}\right)d\xi =: G(n).$$

The integral on the right hand side is not absolutely convergent but as we will show it can be given a well-defined meaning in the context of tempered distributions. It evaluates to

$$G(x) = \frac{1}{4\pi|x|} + \frac{1}{16\pi}\frac{x_1^4 + x_2^4 + x_3^4 - 3x_1^2x_2^2 - 3x_1^2x_3^2 - 3x_2^2x_3^2}{|x|^7}.$$

The first term in the expansion is the fundamental solution of Poisson's equation, which is not surprising since the left-hand side of Equation (1.6) is a common discretization of the Laplace operator. We will demonstrate later that there exists a constant C such that

$$|\mathfrak{G}(n) - G(n)| \le \frac{C}{|n|^5} \qquad \forall\, n \in \mathbb{Z}^3. \tag{1.9}$$

Any order of accuracy can be obtained by including more terms in (1.8). □

The ideas presented easily extend to general lattices on $\mathbb{R}^d$, including lattices that have more than one node in the unit cell. For notational convenience we will restrict attention to lattices with a cubic unit cell. Note that this restriction is insignificant since a lattice with a general parallel-epipede can be mapped easily to one with a cubic unit cell, as illustrated in Figure 1.

1.3. **Outline.** The manuscript is structured as follows. In Section 2 we derive the asymptotic expansion of Green's functions associated with equations on mono-atomic lattices in three dimensions. These results are extended to two dimensions and multi-atomic lattices in sections 3 and 4, respectively. In Section 5 we present a numerical example that indicates that the constants appearing in the bounds are small.

2. Mono-atomic lattices in three dimensions

Synopsis: *In this section we derive the asymptotic expansion of the lattice Green's function defined by Equation (1.5). We start by showing how the appropriate series expansion of $\sigma^{-1}(\xi)$ can be derived from the expansion of $\sigma(\xi)$, then we formally define the approximate Green's function from the expansion of $\sigma^{-1}(\xi)$. Finally we bound the remainder term.*

The symbol defined in Equation (1.3) has a series expansion of the form $\sigma(\xi) = \xi \cdot (M\xi) + O(|\xi|^4)$, where M is a positive definite matrix. For the moment we assume that this matrix is the identity matrix, $M = I$. At the end of the section we demonstrate how this assumption can be relaxed. Thus, by letting Π^k denote the set of multinomials of degree exactly k, we assume that

$$\sigma(\xi) = |\xi|^2 + \sum_{j=2}^{\infty} b_j(\xi), \quad \text{for} \quad b_j \in \Pi^{2j}. \tag{2.1}$$

The following result shows how to capture the singulary of $\sigma^{-1}(\xi)$ by a rational function.

Proposition 2.1. *Suppose that $\sigma(\xi)$ is given by (2.1). Then for any non-negative integer Q,*

$$\frac{1}{\sigma(\xi)} = \sum_{q=0}^{Q} \frac{a_{2q}(\xi)}{|\xi|^{2q+2}} + \hat{R}_Q(\xi),$$

where $a_{2q} \in \Pi^{4q}$, and

$$\hat{R}_Q(\xi) = \frac{\sum_{j=2Q+2}^{\infty} c_j^Q(\xi)}{|\xi|^{2Q+2}\sigma(\xi)} \tag{2.2}$$

for some $c_j^Q \in \Pi^{2j}$. In particular, if Ω is a compact set such that $\sigma(\xi) > 0$ for $\xi \in \Omega \backslash \{0\}$, then $|\hat{R}_Q(\xi)| \leq C|\xi|^{2Q}$ for $\xi \in \Omega$.

This proposition is easily proved by induction. One finds that the multinomials a_{2j} and c_j^Q can be determined recursively from the b_j's by the following formulae,

$$\begin{aligned} a_0(\xi) &= 1, & c_j^0(\xi) &= -b_j(\xi), \\ a_{2q}(\xi) &= c_{2q}^{q-1}(\xi), & c_j^q(\xi) &= -b_{j-2q}(\xi)c_{2q}^{q-1}(\xi) + |\xi|^2 c_{j-1}^{q-1}(\xi). \end{aligned} \tag{2.3}$$

Letting $\mathcal{F}$ denote the continuous Fourier transform, we use the approximation of $\sigma^{-1}(\xi)$ to define an approximation for $\mathfrak{G}$ by

$$G_Q := \mathcal{F}^{-1}\left[\sum_{q=0}^{Q} \frac{a_{2q}(\xi)}{|\xi|^{2q+2}}\right]. \tag{2.4}$$

The inverse continuous Fourier transform is defined by

$$\mathcal{F}^{-1}[\varphi](x) = \frac{1}{(2\pi)^3}\int_{I^3} e^{-\mathrm{i}x\cdot\xi}\varphi(\xi)\,d\xi$$

for $\varphi \in L^1$. This definition can be extended to tempered distributions using the standard variational methods, see [5], and it is in this sense that we interpret the definition (2.4). Although we need to use this abstract framework to prove our main statements, it is actually a simple matter to compute G_Q, as the following result shows.

Proposition 2.2. *Given a function $a_{2q} \in \Pi^{4q}$ we have, for $q \geq 1$,*

$$g_q(x) := \mathcal{F}^{-1}\left[\frac{a_{2q}(\xi)}{|\xi|^{2q+2}}\right](x) = \frac{(-1)^q}{\pi\, 2^{2q+2}\, q!\,(2q-1)!!} a_{2q}(\partial)|x|^{2q-1},$$

where $\partial = (\partial_1, \partial_2, \partial_3)$ is the vector of first order partial differential operators.

Proof: We first use induction to show that the function $f_q(x) := \alpha_q |x|^{2q-1}$, where $\alpha_0 = (4\pi)^{-1}$ and $\alpha_q = (-1)^q(\pi 2^{q+2}\, q!\,(2q-1)!)^{-1}$ for $q \geq 1$, solves the distributional equation

$$(-\Delta)^{q+1} f_q(x) = \delta(x). \tag{2.5}$$

It is well known that this is true for $q = 0$. Next suppose that it is true for all integers up to $(q-1)$. Then, recalling that the product rule for differentiation holds for distributions of the type $p \cdot F$, where p is a multi-nomial and F is any distribution, we find that

$$\begin{aligned}
(-\Delta)^{q+1} f_q(x) &= -\,(-\Delta)^q \alpha_q \left[(\Delta|x|^{2q})|x|^{-1} + 2(\nabla|x|^{2q})\cdot(\nabla|x|^{-1}) + |x|^{2q}(\Delta|x|^{-1})\right] \\
&= -\,(-\Delta)^q \alpha_q \left[2q(2q+1)|x|^{2q-3} - 4q|x|^{2q-3} - 4\pi|x|^{2q}\delta(x)\right] \\
&= -\,(-\Delta)^q \alpha_q (4q^2 - 2q)|x|^{2q-3}.
\end{aligned} \tag{2.6}$$

At this point we apply the induction assumption which completes the proof of (2.5).

Applying the Fourier transform to Equation (2.5) we find that $|\xi|^{2q+2}\hat{f}_q(\xi) = 1$ and so

$$|\xi|^{-(2q+2)} = \hat{f}_q(\xi) + \hat{\varphi}(\xi) \tag{2.7}$$

where $\varphi(x)$ is a distribution such that $|\xi|^{2q+2}\hat{\varphi}(\xi) = 0$. This implies that $\mathrm{supp}(\hat{\varphi}) = \{0\}$ and since $\hat{\varphi}$ is a tempered distribution we then know that $\hat{\varphi}(\xi)$ is a finite sum of delta-functions and derivatives of delta-functions, all supported at the origin. This in turn means that φ is a finite multi-nomial. Multiplying Equation (2.7) by $a_{2q}(\xi)$ and taking inverse Fourier transforms we find that

$$g_q(x) = a_{2q}(\partial) f_q(x) + a_{2q}(\partial)\varphi(x).$$

It remains to prove that the last term on the right hand side vanishes. Since it is a multi-nomial it is sufficient to prove that it tends to zero as $|x| \to \infty$. The term $a_{2q}(\partial) f_q$ clearly decays in this fashion so we only need to prove that g_q decays. To this end fix a compactly supported, infinitely differentiable function ψ such that $\psi(x) \equiv 1$ in some neighbourhood of the origin and set $g_q' := \mathcal{F}^{-1}[\psi \hat{g}_q]$ and $g_q'' := \mathcal{F}^{-1}[(1-\psi)\hat{g}_q]$ so that $g_q = g_q' + g_q''$. Then

$$|x|^{2q} g_q'(x) = |x|^{2q}\mathcal{F}^{-1}[\psi\hat{g}_q](x) = \mathcal{F}^{-1}[(-\Delta)^q(\psi\hat{g}_q)](x),$$

which is uniformly bounded since $(-\Delta)^q(\psi\hat{g}_q) \in L^1$. The proof for g_q'' is analogous. □

We are now prepared to state and prove a bound on the truncation error.

Theorem 2.3. *Let $\mathfrak{G}$ be defined by (1.5) and G_Q by (2.4). Then*

$$|\mathfrak{G}(n) - G_Q(n)| \leq \frac{C}{|n|^{2Q+3}}, \qquad \forall\, n \in \mathbb{Z}^3,$$

where C depends on Q but not on n.

Proof: First note that, with g_q defined in Proposition 2.2,

$$\mathfrak{G} - G_Q = \mathfrak{G} - G_{Q+1} + g_{Q+1}.$$

By Proposition 2.2, $g_{Q+1}(n) = O(|n|^{-2Q-3})$. Therefore we only need to prove that $|\mathfrak{G}(n) - G_{Q+1}(n)| \leq C|n|^{-2Q-3}$. This reformulation is necessary because our technique for bounding the remainder term does not give a sharp bound.

Fix an infinitely differentiable function ψ such that $\psi(\xi) \equiv 1$ for $|\xi| \leq 1$ and $\psi(\xi) \equiv 0$ for $|\xi| \geq 2$. Using that $\mathfrak{F}^{-1}[\psi\varphi] = \mathcal{F}^{-1}[\psi\varphi]$ for any φ, we obtain the representation

$$\begin{aligned} \mathfrak{G} - G_{Q+1} =& \mathfrak{F}^{-1}[\sigma^{-1}] - \mathcal{F}^{-1}[\hat{G}_{Q+1}] \\ =& \mathfrak{F}^{-1}[\sigma^{-1}] - \mathfrak{F}^{-1}[\psi\,\hat{G}_{Q+1}] + \mathcal{F}^{-1}[\psi\,\hat{G}_{Q+1}] - \mathcal{F}^{-1}[\hat{G}_{Q+1}] \\ =& \mathfrak{F}^{-1}[\sigma^{-1} - \psi\,\hat{G}_{Q+1}] + \mathcal{F}^{-1}[(\psi - 1)\hat{G}_{Q+1}] =: E_1 + E_2. \end{aligned} \tag{2.8}$$

We start by bounding E_1. Set $R = \sigma^{-1} - \psi\,\hat{G}_{Q+1}$ so that $E_1 = \mathfrak{F}^{-1}[R]$. Note that R is I^3-periodic, has partial derivatives of all orders away from the origin, and that $|\partial^\alpha R(\xi)| \leq C|\xi|^{2Q+2-|\alpha|}$. Then

(2.9)

$$|n|^{2Q+4}E_1(n) = \frac{1}{(2\pi)^3}\int_{I^3}\left[(-\Delta)^{Q+2}e^{-\mathrm{i}n\cdot\xi}\right]R(\xi)\,d\xi = \lim_{\varepsilon\to 0}\frac{1}{(2\pi)^3}\int_{I^3\setminus B_\varepsilon}\left[(-\Delta)^{Q+2}e^{-\mathrm{i}n\cdot\xi}\right]R(\xi)\,d\xi.$$

where B_ε is the ball of radius ε around the origin. We use Green's theorem to move all the derivatives onto R. The volume integrals will then contain a $|\xi|^{-2}$ singularity at the origin and the surface integrals a $|\xi|^{-1}$ singularity. Consequently the integral is bounded as $\varepsilon \to 0$, which means that $|n|^{2Q+4}|E_1(n)|$ is uniformly bounded in n.

To bound E_2, we use that for any positive integer p

$$|n|^{2p}E_2(n) = |n|^{2p}\mathcal{F}^{-1}[(\psi - 1)\hat{G}_{Q+1}](n) = \mathcal{F}^{-1}[(-\Delta)^p(\psi - 1)\hat{G}_{Q+1}](n).$$

Note that the function $(\psi - 1)\hat{G}_{Q+1}$ is infinitely differentiable and that it equals a rational function outside the sphere $|\xi| = 2$. This means that for sufficiently large p, the function $(-\Delta)^p(\psi - 1)\hat{G}_{Q+1}$ is integrable and thus $E_2(n)$ decays faster than any inverse polynomial. $\square$

Remark: If the series expansion of the symbol has the general form $\sigma(\xi) = \xi\cdot(M\xi) + O(|\xi|^4)$ so that (2.1) does not hold, then set $\xi' := M^{1/2}\xi$ and change variables in (1.5) so that

$$\mathfrak{G}(n) = \frac{1}{(2\pi)^3\sqrt{\det M}}\int_{M^{-1/2}I^3} e^{-\mathrm{i}(M^{-1/2}n)\cdot\xi'}\frac{1}{\sigma(M^{-1/2}\xi')}\,d\xi'.$$

Since the function $\xi' \mapsto \sigma(M^{-1/2}\xi')$ does have the series expansion (2.1) all asymptotic expansion results can be applied to approximate this integral. $\square$

3. Mono-atomic lattices in two dimensions

Synopsis: *In this section we show how the analysis of Section 2 should be adjusted for the two dimensional case. This case is singled out becuase the $O(|\xi|^{-2})$ singularity at the origin is not integrable in two dimensions.*

Consider the two-dimensional counterpart of the basic lattice equation, (1.1), namely

$$\begin{cases} [\mathfrak{A}\mathfrak{u}](n) = \mathfrak{f}(n), & \forall\, n \in \mathbb{Z}^2, \\ \sum_{n\in\mathbb{Z}^2}\big([\mathfrak{A}\mathfrak{u}](n)\big)\mathfrak{u}(n) < \infty, & \end{cases} \tag{3.1}$$

where the lattice operator $\mathfrak{A}$ is of the form (1.2). As in the three-dimensional case, we require that $\sum_n |\mathfrak{f}(n)| < \infty$ but now we must also ask that the load is equilibriated,

$$\sum_{n\in\mathbb{Z}^2} \mathfrak{f}(n) = 0.$$

Under these conditions Equation (3.1) is guaranteed to have a solution that is unique up to a constant. Using the fact that $\mathfrak{f}$ sums to zero one can easily verify that a solution is given by

$$\mathfrak{u}(n) = [\mathfrak{G} * \mathfrak{f}](n) = \sum_{m\in\mathbb{Z}^2} \mathfrak{G}(n-m)\mathfrak{f}(m),$$

where the lattice Green's function is now defined by

$$\mathfrak{G}(n) = \frac{1}{(2\pi)^2}\int_{I^2}\left[e^{-\mathrm{i}n\cdot\xi}\frac{1}{\sigma(\xi)} - \frac{1}{\sigma(\xi)}\right] d\xi. \tag{3.2}$$

Note that we needed to insert a regularising term since the $O(|\xi|^{-2})$ singularity at the origin is not integrable in two dimensions. This singularity is fundamental and cannot be overcome by defining the integral in a distributional sense.

Let b_j and a_j be defined as in Section 2 and assume (without loss of generality) that $\sigma(\xi) = |\xi|^2 + O(|\xi|^4)$. We then define the first term in the approximation of $\mathfrak{G}$ by

$$g_0(x) := \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\left[\frac{e^{-\mathrm{i}x\cdot\xi}}{|\xi|^2} - \frac{\chi(\xi)}{\sigma(\xi)}\right] d\xi, \tag{3.3}$$

where χ is the characteristic function for the square I^2. Strictly speaking this definition is made in a distributional sense so that for φ a Schwartz' function we set

$$\langle g_0, \varphi\rangle := \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\frac{\hat{\varphi}(-\xi) - \chi(\xi)\hat{\varphi}(0)}{|\xi|^2} d\xi.$$

For $q \geq 1$ the terms are straight-forwardly defined by $g_q = \mathcal{F}^{-1}[a_{2q}(\xi)/|\xi|^{2q+2}]$ and then

$$G_Q(x) := \sum_{q=0}^{Q} g_q(x). \tag{3.4}$$

The next two results provide elementary methods for calculating G_Q given the symbol.

Proposition 3.1. *The function g_0 defined by (3.3) evaluates to*

$$g_0(x) = -\frac{1}{2\pi}\log|x| + C_{\mathrm{fund}} + \frac{1}{(2\pi)^2}\int_{I^2}\left[\frac{1}{|\xi|^2} - \frac{1}{\sigma(\xi)}\right] d\xi,$$

where C_{fund} does not depend on σ. Numerically, $C_{\mathrm{fund}} = -0.18124942796\cdots$

Proof: We rewrite the definition of g_0 as follows

$$g_0(x) = G_{\mathrm{fund}}(x) + \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\left[\frac{\chi(\xi)}{|\xi|^2} - \frac{\chi(\xi)}{\sigma(\xi)}\right] d\xi,$$

where

$$G_{\mathrm{fund}}(x) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\frac{e^{-\mathrm{i}x\cdot\xi} - \chi(\xi)}{|\xi|^2} d\xi.$$

Since the integral defining G_{fund} is not absolutely convergent, we have to define it as a tempered distribution. For $\varphi \in \mathcal{S}$ (the set of Schwartz functions) we set

$$\langle G_{\text{fund}}, \varphi \rangle = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \varphi(x) \frac{e^{-\mathbf{i}x\cdot\xi} - \chi(\xi)}{|\xi|^2} \, dx \, d\xi = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\hat{\varphi}(-\xi) - \hat{\varphi}(0)\chi(\xi)}{|\xi|^2} \, d\xi, \tag{3.5}$$

where $\hat{\varphi}$ is the Fourier transform of φ, as usual.

First we demonstrate that $-\Delta G_{\text{fund}} = \delta$,

$$\langle -\Delta G_{\text{fund}}, \varphi \rangle = \langle G_{\text{fund}}, -\Delta \varphi \rangle = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{|\xi|^2 \hat{\varphi}(\xi) - 0 \cdot \hat{\varphi}(0)\chi(\xi)}{|\xi|^2} \, d\xi = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \hat{\varphi}(\xi) \, d\xi = \varphi(0).$$

Define $h \in \mathcal{S}'$ by $h(x) = G_{\text{fund}}(x) + (2\pi)^{-1} \log |x|$ so that $\Delta h = 0$. Then h is a harmonic multi-nomial. Since G_{fund} is a radial function, so is h. Finally note that all radial harmonic multi-nomials are constant and thus there exists a constant C_{fund} such that $G_{\text{fund}}(x) = -(2\pi)^{-1} \log |x| + C_{\text{fund}}$. $\square$

Remark: Note that the function $G_{\text{fund}} \in \mathcal{S}'$ that was defined in Equation (3.5), is a viable candidate for a distributional fundamental solution to Poisson's equation on $\mathbb{R}^2$. $\square$

Proposition 3.2. *For any $a_{2q} \in \Pi^{4q}$*

$$\mathcal{F}^{-1} \left[\frac{a_{2q}(\xi)}{|\xi|^{2q+2}} \right] = -\frac{1}{2\pi (q!)^2 (-4)^q} a_{2q}(\partial) |x|^{2q} \log |x|.$$

The proof of this result is completely analogous to the proof of Proposition 2.2. The final result of this section also mimics its three-dimensional counterpart and we omit the proof.

Theorem 3.3. *Let $\mathfrak{G}$ be defined by (3.2) and G_Q by (3.4). Then*

$$|\mathfrak{G}(n) - G_Q(n)| \le \frac{C}{|n|^{2Q+2}}, \qquad \forall \, n \in \mathbb{Z}^2,$$

where C depends on Q but not on n.

4. Multi-atomic lattices

Synopsis: *We show that the asymptotic expansion of the Green's function for a multi-atomic lattice can be obtained from the expansion of the Green's function of a fictitious mono-atomic lattice.*

For a multi-atomic lattice, the potential associated with the cell $n \in \mathbb{Z}^d$ forms a vector $\mathfrak{u}(n) = [\mathfrak{u}_1(n), \dots, \mathfrak{u}_q(n)]$, and likewise $\mathfrak{f}(n) = [\mathfrak{f}_1(n), \dots, \mathfrak{f}_q(n)]$, where q is the number of nodes in the irreducible cell. We can still write the Fourier representation of the lattice equations in the form $\sigma(\xi)\tilde{\mathfrak{u}}(\xi) = \tilde{\mathfrak{f}}(\xi)$ but now the symbol $\sigma(\xi)$ is a $q \times q$-matrix. Defining the Green's function $\mathfrak{G}(n)$ as a $q \times q$-matrix with the ij entry

$$\mathfrak{G}_{ij}(n) = \frac{1}{(2\pi)^d} \int_{I^d} e^{-\mathbf{i}n\cdot\xi} [\sigma^{-1}(\xi)]_{ij} \, d\xi,$$

we can still write the solution in the form $\mathfrak{u} = \mathfrak{G} * \mathfrak{f}$. In two dimensions the integral needs to be normalized as shown in the previous section. Before studying $\mathfrak{G}$ closer we give a simple example.

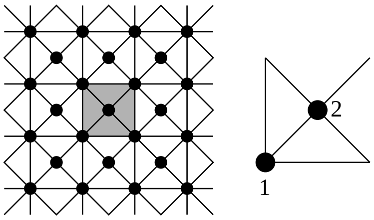

FIGURE 2. A bi-atomic lattice. The unit cell is exhibited to the left.

Example: Consider heat conduction through the lattice illustrated in Figure 2, with the nodes labeled as illustrated. The equilibrium equations read

$$\begin{aligned} \mathfrak{f}_1(n) =& 8\mathfrak{u}_1(n) - \mathfrak{u}_1(n-e_1) - \mathfrak{u}_1(n+e_1) - \mathfrak{u}_1(n-e_2) - \mathfrak{u}_1(n+e_2) \\ & - \mathfrak{u}_2(n) - \mathfrak{u}_2(n-e_1) - \mathfrak{u}_2(n-e_1-e_2) - \mathfrak{u}_2(n-e_2), \\ \mathfrak{f}_2(n) =& 4\mathfrak{u}_2(n) - \mathfrak{u}_1(n) - \mathfrak{u}_1(n+e_1) - \mathfrak{u}_1(n+e_1+e_2) - \mathfrak{u}_1(n+e_2). \end{aligned} \tag{4.1}$$

The symbol then takes the form

$$\sigma(\xi) = \begin{bmatrix} 4\sin^2\frac{\xi_1}{2} + 4\sin^2\frac{\xi_2}{2} + 4 & -1 - e^{\mathbf{i}\xi_1} - e^{\mathbf{i}\xi_2} - e^{\mathbf{i}(\xi_1+\xi_2)} \\ -1 - e^{-\mathbf{i}\xi_1} - e^{-\mathbf{i}\xi_2} - e^{-\mathbf{i}(\xi_1+\xi_2)} & 4 \end{bmatrix}.$$

The determinant of the symbol is given by

$$\det\sigma(\xi) = \left[24\sin^2\frac{\xi_1}{2} + 24\sin^2\frac{\xi_2}{2} + 4\sin^2\frac{(\xi_1+\xi_2)}{2} + 4\sin^2\frac{(\xi_1-\xi_2)}{2}\right],$$

and the inverse is given by

$$\sigma^{-1}(\xi) = \frac{1}{\det\sigma(\xi)} \begin{bmatrix} 4 & 1 + e^{\mathbf{i}\xi_1} + e^{\mathbf{i}\xi_2} + e^{\mathbf{i}(\xi_1+\xi_2)} \\ 1 + e^{-\mathbf{i}\xi_1} + e^{-\mathbf{i}\xi_2} + e^{-\mathbf{i}(\xi_1+\xi_2)} & 4\sin^2\frac{\xi_1}{2} + 4\sin^2\frac{\xi_2}{2} + 4 \end{bmatrix}. \tag{4.2}$$

Two points are noteworthy. First, the determinant of the symbol has exactly the same type of second-order singularity at the origin as the symbol for a mono-atomic lattice. Second, all codeterminants of $\sigma(0)$ are equal. These points are valid for general multi-atomic lattices. □

Proposition 4.1. *Let σ be the symbol of a multi-atomic lattice. Then there exists a positive definite matrix M such that $\det\sigma(\xi) = \xi \cdot M\xi + O(|\xi|^4)$. Furthermore, the codeterminants of $\sigma(0)$ are all equal and positive.*

This proposition (which is proved in [13]) has the important consequence that $\det\sigma(\xi)$ is the symbol for some fictitious mono-atomic lattice, which we call the *associated lattice.* Setting

$$\mathfrak{G}_{\mathrm{H}}(n) := \mathcal{F}^{-1}\left[\frac{1}{\det\sigma(\xi)}\right], \tag{4.3}$$

we thus know that the asymptotic expansions we derived in Sections 2 and 3 all apply to $\mathfrak{G}_{\mathrm{H}}$. The main result of this section states that the full Green's function of the multi-atomic lattice is given by adding up a finite number of shifts of $\mathfrak{G}_{\mathrm{H}}$.

Theorem 4.2. *Given a general lattice Green's function $\mathfrak{G}$, let $\mathfrak{G}_{\mathrm{H}}$ be the associated Green's function defined by (4.3). Then there exists a local convolution operator $\mathfrak{D}$ such that $\mathfrak{G} = \mathfrak{G}_{\mathrm{H}} * \mathfrak{D}$.*

Proof: Start with Cramer's rule,

$$[\sigma^{-1}(\xi)]_{ij} = \frac{p_{ij}(e^{\mathbf{i}\xi})}{\det \sigma(\xi)},$$

where p_{ij} is a multinomial of the form

$$p_{ij}(e^{\mathbf{i}\xi}) = \sum_{m\in\mathbb{D}_{ij}} c_{ij,m} e^{\mathbf{i}m\cdot\xi}.$$

for some finite sets $\mathbb{D}_{ij} \subset \mathbb{Z}^d$ and constants $\{c_{ij,m}\}_{m\in\mathbb{D}_{ij}}$. Then for any lattice function $\mathfrak{v}$,

$$\mathfrak{F}^{-1}[p_{ij}(e^{\mathbf{i}\xi})\tilde{\mathfrak{v}}(\xi)](n) = \sum_{m\in\mathbb{D}_{ij}} c_{ij,m}\mathfrak{v}(n-m) =: [\mathfrak{D}_{ij} * \mathfrak{v}](n),$$

which defines the ij component of the convolution operator $\mathfrak{D}$. We can now evaluate $\mathfrak{G}_{ij}$,

$$\mathfrak{G}_{ij} = \mathfrak{F}^{-1}\left[\frac{p_{ij}(e^{\mathbf{i}\xi})}{\det\sigma(\xi)}\right] = \mathfrak{D}_{ij} * \mathfrak{F}^{-1}\left[\frac{1}{\det\sigma(\xi)}\right] = \mathfrak{D}_{ij} * \mathfrak{G}_{\mathrm{H}} = \mathfrak{G}_{\mathrm{H}} * \mathfrak{D}_{ij},$$

which proves the claim. □

Remark: Proposition 4.1 states that for any ij we have $\sum c_{ij,m} = c_0$ for some positive constant. This means that to lowest order all components of $\mathfrak{G}$ are identical. □

5. A Numerical Example

Synopsis: *We compute the asymptotic expansion for the simple square lattice in two dimensions and show numerically that for this case the numbers $C = C(Q)$ in Theorem 3.3 are small.*

Consider the two-dimensional square lattice $\mathbb{Z}^2$ where each node is connected to its four nearest neighbours so that the lattice operator equals the five-point discrete Laplace operator. Then

$$\sigma(\xi) = 4\sin^2\frac{\xi_1}{2} + 4\sin^2\frac{\xi_2}{2}.$$

Using Proposition 2.1 we compute the series expansion of the inverse symbol and find that

$$\frac{1}{\sigma(\xi)} = \frac{1}{|\xi|^2} + \frac{1}{|\xi|^4}\left(\frac{\xi_1^4}{12} + \frac{\xi_2^2}{12}\right) + \frac{1}{|\xi|^6}\left(\frac{\xi_1^8}{240} - \frac{\xi_1^6\xi_2^2}{360} + \frac{\xi_1^4\xi_2^4}{72} - \frac{\xi_1^2\xi_2^6}{360} + \frac{\xi_2^8}{240}\right) +$$
$$\frac{1}{|\xi|^8}\left(\frac{\xi_1^{12}}{6048} - \frac{11\xi_1^{10}\xi_2^2}{30240} + \frac{\xi_1^8\xi_2^4}{756} - \frac{\xi_1^6\xi_2^6}{1080} + \frac{\xi_1^4\xi_2^8}{756} - \frac{11\xi_1^2\xi_2^{10}}{30240} + \frac{\xi_2^{12}}{6048}\right) + O(|\xi|^6).$$

By virtue of Propositions 3.1 and 3.2 we can now compute the $g_q(x)$'s, which are most easily given in polar coordinates, $(x_1, x_2) = r(\cos\theta, \sin\theta)$,

$$\begin{aligned}
g_0(x) &= -\frac{1}{2\pi}\log r + C, \quad \text{where } C = -0.2573434264137\cdots \\
g_1(x) &= \left(\frac{\partial_1^4}{12} + \frac{\partial_2^4}{12}\right)\frac{1}{8\pi}|x|^2\log|x| = \frac{1}{24\pi}\frac{x_1^4 - 6x_1^2x_2^2 + x_2^4}{|x|^6} = \frac{1}{24\pi}\frac{\cos(4\theta)}{r^2}, \\
g_2(x) &= \cdots = \frac{1}{480\pi}\frac{25\cos(8\theta) + 18\cos(4\theta)}{r^4} \\
g_3(x) &= \cdots = \frac{1}{2016\pi}\frac{490\cos(12\theta) + 459\cos(8\theta)}{r^6}.
\end{aligned} \tag{5.1}$$

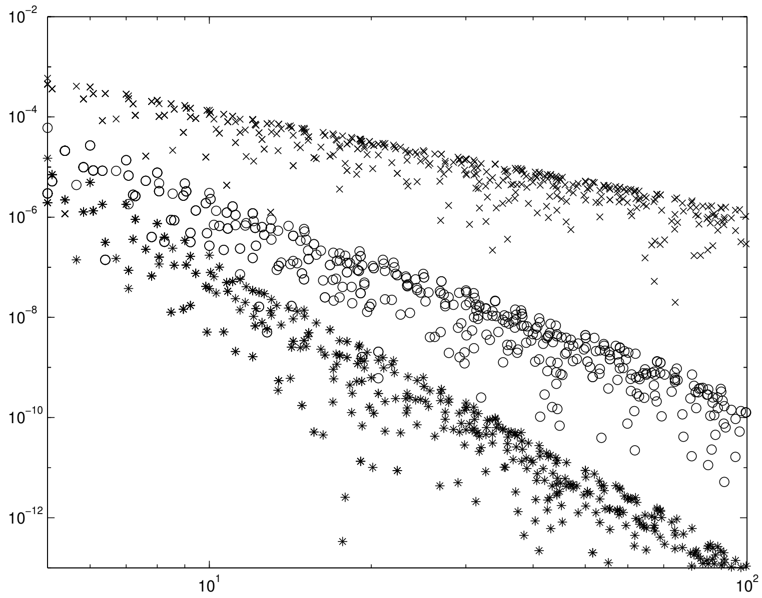

FIGURE 3. The absolute error $|E_Q(n)|$ plotted versus $|n|$. $|E_0|$ is marked with $\mathtt{x}$, $|E_1|$ with $\mathtt{o}$ and $|E_2|$ with $*$.

and set $G_Q = \sum_{q=0}^{Q} g_q$.

In order to estimate the approximation error

$$E_Q(n) := \mathfrak{G}(n) - G_Q(n)$$

we randomly distributed 500 points $n \in \mathbb{Z}^2$ in the annulus $5 \leq |n| \leq 100$. For each point we computed the error and plotted $|E_Q(n)|$ versus $|n|$ in a log-log diagram, see Figure 3. Note that the remainder terms are very small, and that they seem to decay as Theorem 3.3 claimed; $|E_Q(n)| \leq C(Q)|n|^{-(2Q+2)}$. In order to estimate $C(Q)$ numerically we plotted $|n|^{2Q+2}|E_Q(n)|$ versus $|n|$, see Figure 4. We estimate that for $|n| \geq 20$, the bound in the theorem is valid with the constants

$$C(0) \approx 0.015, \qquad C(1) \approx 0.03, \qquad C(2) \approx 0.15.$$

These numbers indicate that for large n, the remainder term $E_Q(n)$ is entirely dominated by the next term in the asymptotic expansion g_{Q+1} since

$$\sup_x |x|^2 |g_1(x)| \approx 0.013, \qquad \sup_x |x|^4 |g_2(x)| \approx 0.029, \qquad \sup_x |x|^6 |g_3(x)| \approx 0.15.$$

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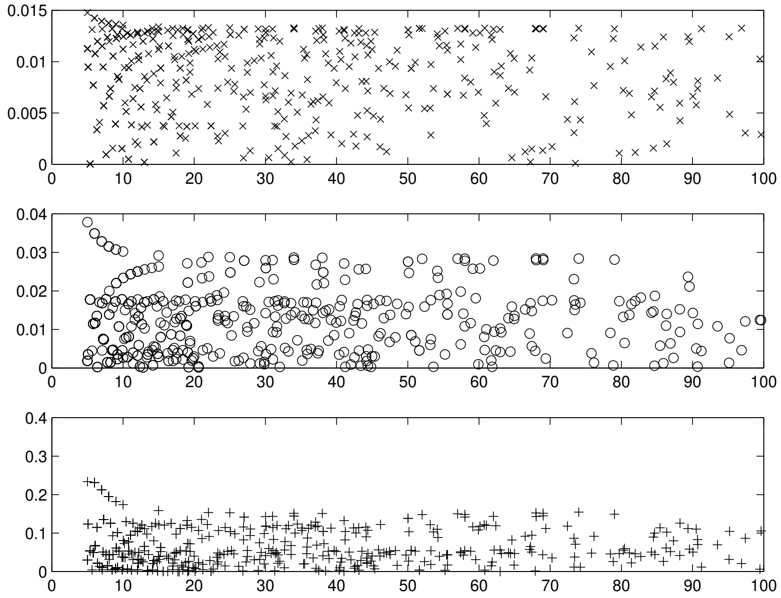

FIGURE 4. Plots of $|n|^{2Q+2}|E_Q(n)|$ versus $|n|$ for $Q = 0, 1, 2$, respectively.

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