On the Efficient Evaluation of the Two Dimensional Periodic Green's Function for the Helmholtz Equation

Andrew Dienstfrey, Fengbo Hang, Jingfang Huang

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Abstract

Many algorithms that are currently used for the solution of the Helmholtz equation in periodic domains require the evaluation the Green's function, G_β. The fact that the canonical representation of G_β via the method of images gives rise to a conditionally convergent series whose direct evaluation is prohibitive has inspired the development of more efficient procedures for evaluating this Green's function. Recently, the evaluation of G_β through the "lattice sum" representation has proven to be both accurate and fast. As a consequence, the computation of the requisite, also conditionally convergent, lattice sums has become an active area of research. In the following paper we describe a new integral representation for these sums, and compare our results with other techniques for evaluating similar quantities.

1 Introduction

In this paper, we consider the evaluation of the Green's function for the Helmholtz equation on the unit square in two dimensions with periodic boundary conditions, ie. $B_1 = \{\vec{x} = (x, y) \in \mathbf{R}^2 | |x|, |y| < 1/2\}$, G_β is defined on $2 \cdot B_1$ and satisfies the following

$$\begin{cases} (\Delta + \beta^2) G_\beta(x, y) = \delta(x, y), \\ G_\beta(x - \frac{1}{2}, y) = G_\beta(x + \frac{1}{2}, y), -\frac{1}{2} < x < \frac{1}{2}, -1 < y < 1 \\ G_\beta(x, y - \frac{1}{2}) = G_\beta(x, y + \frac{1}{2}), -\frac{1}{2} < y < \frac{1}{2}, -1 < x < 1, \end{cases} \tag{1}$$

where $\delta(x, y)$ is the Dirac delta function at the origin. It is a standard fact that the spectrum for the periodic Laplacian operator on B_1 is the set

$$\sigma = \{s \in \mathbf{R} | \exists m, n \in \mathbf{Z}, s = (2\pi)\sqrt{m^2 + n^2}\}. \tag{2}$$

Below we will assume that $\beta \in \mathbf{R}^+ \setminus \sigma$ in which case G_β defined by (1) exists and is unique.

As periodic Helmholtz equations occur in numerous applications, there is considerable interest in developing algorithms to compute G_β both accurately and efficiently. A natural idea is to proceed via the method of images. Keeping in mind that the free-space Green's function is given by $\frac{i}{4} H_0(\beta|\vec{x}|)$ (H_0 is the zeroth-order Hankel function of the first-kind), we define the "lattice" $\Lambda = \mathbf{Z}^2 \setminus \vec{0}$ and write G_β as the formal sum

$$G_\beta(\vec{x}) = \frac{i}{4} H_0(\beta|\vec{x}|) + \frac{i}{4} \sum_{\vec{p} \in \Lambda} H_0(\beta|\vec{x} - \vec{p}|). \tag{3}$$

There are several problems with this representation. For one, $H_0(r) \sim e^{i(r-\pi/4)}r^{-1/2}$ which implies that the sum converges only conditionally. Therefore one must define a summation convention for (3) to make sense. Furthermore, with the convention specified, one may still anticipate that the convergence is so slow as to be computationally prohibitive.

A survey of efforts directed at evaluating sums of the form (3) is presented in the review articles by Linton (Ref. [11]) and by McPhedran, et. al. (Ref. [14]). The evaluation of such sums via Ewald's method was outlined in (Ref. [11]). Other early approaches focussed on the application of various summation acceleration techniques, also known as Kummer transformations, in which the principal parts of the asymptotic expansion of the conditionally convergent sums are subtracted from the summand term by term and added outside the summand analytically (e.g. Refs. [11], [12],and [16]). These procedures are effective. However, they are algebraically very involved, and do not allow for significant gains in computational efficiency. Since that time, other techniques have been attempted with various degrees of success (Refs. [4], [12], and [16]). Among these we isolate the so-called "Lattice-Sum" representation for discussion below.

The derivation of the Lattice-Sum representation for G_β is a simple consequence of a separation of variables result for H_0 (for the original idea in the context of the Laplace's Equation see Rayleigh, Ref. [21]). Assuming for the moment that $\vec{x}$ and $\vec{p} \in \Lambda$ are well-separated (see Section 3 for a discussion of this point), by Graf's Addition Theorem

$$H_0(\beta|\vec{x}-\vec{p}|) = \sum_{l=-\infty}^{l=\infty} J_l(\beta|\vec{x}|)e^{il\theta_{\vec{x}}} H_l(\beta|\vec{p}|)e^{-il\theta_{\vec{p}}}. \quad (4)$$

Substituting (4) into (3), collecting like terms, we are led to

$$\begin{aligned} G_\beta(\vec{x}) &= \frac{i}{4}H_0(\beta|\vec{x}|) + \frac{i}{4}\sum_{l=-\infty}^{\infty} S_l(\beta)J_l(\beta|\vec{x}|)e^{il\theta_{\vec{x}}}, \\ S_l(\beta) &= \sum_{\vec{p}\in\Lambda} H_l(\beta|\vec{p}|)e^{il\theta_{\vec{p}}}. \end{aligned} \quad (5)$$

(The sign of the exponential in (5) is irrelevant as the lattice is symmetric.) Restricting to a square lattice, one may check that the four-fold symmetry implies that $S_l = 0$ for l not divisible by four. Rearranging terms we write

$$G_\beta(\vec{x}) = \frac{i}{4}\left(H_0(\beta|\vec{x}|) + S_0(\beta)J_0(\beta|\vec{x}|) + 2\sum_{l=1}^{\infty} S_{4l}(\beta)J_{4l}(\beta|\vec{x}|)\cos(4l\theta_{\vec{x}})\right). \quad (6)$$

In applications, the summation (6) is truncated for $l < L$, leading to an evaluation procedure whose cost is proportional to L times the number of evaluation points. In practice this cost is significantly smaller than that necessary to obtain converged values of (3) even with the acceleration procedures (See Refs. [11] and [23]). In the literature on the subject one often finds statements to the effect that the representation (6) is superior only when the number of Green's function evaluations is sufficiently large. We feel this to be misleading as these numerical studies include the computation of (5) in their timings. Clearly, these sums may be precomputed. If one compares evaluation of G_β via (6) disregarding the cost of this precomputation, the breakeven is immediate.

In a series of papers by McPhedran, et. al. (Ref. [13], [16], [18], and [20]), these sums were evaluated by recognizing an identity between the so-called "spectral" and "spatial" representations of G_β, and considerable algebra. We take a different approach. Our main result is presented in the following theorem:

Theorem 1 *Given $\beta \in \mathbf{R}^+ \setminus \sigma$, we define the index*

$$J_\beta = \max\{j \in \mathbf{Z} | j \left(\frac{2\pi}{\beta}\right) < 1\} \tag{7}$$

Let $\vec{x} \in B_1$ be given by its polar coordinates $(|\vec{x}|, \theta_{\vec{x}})$, then $G_\beta(\vec{x})$ is given by the representation (6) where the lattice sums S_{4l} may be expressed as the sum of a "propagating" and an "evanescent" part which, in turn, are defined by

$$S_{4l}(\beta) = S_{4l}^e + S_{4l}^p \tag{8}$$

$$S_{4l}^e = -\frac{4i}{\pi}\int_0^\infty \frac{e^{-t}}{\sqrt{t^2+\beta^2}}\left(\frac{1+\cos\sqrt{t^2+\beta^2}}{1+e^{-2t}-2e^{-t}\cos\sqrt{t^2+\beta^2}}\right)\left(\left(\frac{\sqrt{t^2+\beta^2}-t}{\beta}\right)^{4l}+\left(\frac{\sqrt{t^2+\beta^2}+t}{\beta}\right)^{4l}\right) \tag{9}$$

$$S_{4l}^p = -\delta_{l,0} + 4i\sqrt{2}(-1)^l {\sum_{j=0}^{J_\beta}}' \frac{1}{\sqrt{\beta^2-2j^2\pi^2}} \cot\left(\frac{\sqrt{2}}{4}\sqrt{\beta^2-2j^2\pi^2}-\frac{j\pi}{2}\right)\cos\left(4l\arcsin\left(\frac{\sqrt{2}j\pi}{\beta}\right)\right) \tag{10}$$

Note: the prime on the summation indicates that the "0th-term" should be added with a factor of 1/2 and $\delta_{l,0}$ is the standard Kronecker delta symbol.

The new feature of Theorem 1 is the integral-sum representation for the coefficients S_{4l} ((8) through (10)). In the future, we intend to extend Theorem 1 to arbitrary, two dimensional lattices, and to derive analogous integral-sum representations for the corresponding lattice constants. Such formulae would have significant practical and theoretical interest. However, as the analysis and algebra for the square array is already considerable, we present only this case below. (See also Section 3 for further generalizations.) Clearly the integration corresponding to the evanescent contribution (9) must be performed numerically. However, as the integrand is exponentially decaying, this quadrature poses no problem. Finally, inspection of formulae (9), (10), reveals that, given a square array, there are symmetries which allow for further simplification of (6). Following McPhedran (Ref. [14]), we designate the real and imaginary parts of the lattice sum, $S_l = S_l^J(\beta) + iS_l^Y(\beta)$. The corresponding splitting of (9), (10) gives

$$S_{4l}^J(\beta) = -\delta_{l,0},$$

and $S_{4l}^Y(\beta)$ is given by the remaining integral and sum. Rearranging (6) we observe

$$G_\beta(\vec{x}) = -\frac{1}{4}\left(Y_0(\beta|\vec{x}|) + S_0^Y(\beta)J_0(\beta|\vec{x}|) + 2\sum_{l=1}^{\infty} S_{4l}^Y(\beta)J_{4l}(\beta|\vec{x}|)\cos(4l\theta_{\vec{x}})\right). \tag{11}$$

We refer to both S_l and S_l^Y as the "lattice sums" below.

We conclude this section with a brief outline of the rest of the paper. In Section 2 we derive Theorem 1 via a series of propositions and computations. The algebra is lengthy; however we feel it important to give as complete a sketch as possible. Therefore we include many of the details of our derivation. In this section we also address some of the more subtle technical points. In the interest of clarity we reserve the proofs for the Appendix.

These considerations not withstanding, the idea of the theorem is, in fact, quite clear. We begin by defining a summation convention for the lattice sums as they too are only conditionally convergent. For any integer $N \geq 1$, we define $\Lambda^N = \{(m,n)|(m,n) \in \Lambda, |m|, |n| \leq N-1\}$. We consider $G_\beta^N(\vec{x})$ as the partial summation (3) restricted to Λ^N. Again, employing the addition theorem (4) and collecting terms we are led to the corresponding partial lattice sums:

$$S_{4l}^N(\beta) = \sum_{\vec{p} \in \Lambda^N} H_{4l}(\beta|\vec{p}|)e^{i4l\theta_{\vec{p}}}. \tag{12}$$

In Section 2.1 we derive a standard plane-wave expansion for $H_l(|\vec{x}|)e^{il\theta_{\vec{x}}}$ from the classical plane-wave expansion for H_0 and a differential identity relating Hankel functions of different orders. Each expansion receives contributions from an exponentially decaying and an oscillatory integrand which we term the evanescent and propagating parts respectively. In both parts of this expansion, the centers $\{\vec{p} \in \Lambda^N\}$ in (12) appear in the exponents of the integrands. Thus the sum over centers maps to a geometric series that admits explicit summation. The evanescent integral must be evaluated numerically. However, as it contains exponentially decaying terms, this poses no problem. This is precisely the integral (9) above.

The propagating contribution is more involved. As these integrals contain a mixture of highly oscillatory terms and principal value-type singularities, the large-N limit must be taken with care. We evaluate this limit explicitly with the aid of Proposition 6 proved below. The result is surprising in that the limits do not exist in the classical sense but rather are oscillatory, ie.

$$S_{4l}^{p,N} \sim \sum_{j=-J_\beta}^{J_\beta} A_{4l}^j + \sum_{k=-K_\beta}^{K_\beta} B_{4l}^k e^{i\omega_k N}, \; \omega_k \in \mathbf{R}^+ \setminus 2\pi\mathbf{Z}.$$

(See Theorem 3.) This motivates consideration of the weak limit of the summation (Definition 7). It is simple matter to see that this standard limiting procedure annihilates the oscillatory terms.

Now, however, it is no longer obvious that the function defined by substituting these weak limits in the lattice sum representation (6) yields the desired periodic Green's function. Although we can prove that this weak-limiting procedure is valid, the details are tedious and omitted. We rely, instead, on numerical demonstration of this fact in Section 3. In the same section we compare the computation of the lattice sums via the integral-sum formulae (9), (10) with previous results existing in the literature.

We mention that the approach outlined above is similar in spirit to the computation of 1-D lattice sums performed by Yasumoto and Yoshitomi (Ref. [23]) and also, the computation of 2-D lattice sums for the harmonic equation by one of the authors (Ref. [10]).

2 Theory

2.1 Plane Wave representation for $H_l(\beta r)e^{il\theta}$

In this section we derive the integral representations for Hankel functions of arbitrary order. These representations are derived from a plane wave expansion of H_0, and a differentiation identity relating H_l to H_0.

The subject of plane wave representations for $H_0(\beta r)$ is classical. (Ref. [15]) These representations are typically derived via contour integration and Cauchy's Theorem. Hence it is natural that the contours employed depend on the location of the point (x, y). For our purposes it is convenient to divide $\mathbf{R}^2$ into four overlapping regions–North, South, East, West–corresponding to points $(x, y) \in R^2$ with $y > 0, y < 0, x > 0, x < 0$ respectively. Making the necessary arguments and performing some elementary algebra one arrives at the following

$$H_0(\beta r) = \begin{cases} \frac{1}{\pi}\int_0^{\pi} e^{i\beta(y\sin\theta - x\cos\theta)}d\theta + \frac{1}{i\pi}\int_0^{\infty} \frac{e^{-ty}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)x} + e^{-i\rho_\beta(t)x}\right)dt & \text{North} \\ \frac{1}{\pi}\int_0^{\pi} e^{i\beta(-y\sin\theta - x\cos\theta)}d\theta + \frac{1}{i\pi}\int_0^{\infty} \frac{e^{ty}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)x} + e^{-i\rho_\beta(t)x}\right)dt & \text{South} \\ \frac{1}{\pi}\int_0^{\pi} e^{i\beta(-y\cos\theta + x\sin\theta)}d\theta + \frac{1}{i\pi}\int_0^{\infty} \frac{e^{-tx}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)y} + e^{-i\rho_\beta(t)y}\right)dt & \text{East} \\ \frac{1}{\pi}\int_0^{\pi} e^{i\beta(-y\cos\theta - x\sin\theta)}d\theta + \frac{1}{i\pi}\int_0^{\infty} \frac{e^{tx}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)y} + e^{-i\rho_\beta(t)y}\right)dt & \text{West} \end{cases}$$

We next need to derive equivalent representations for the higher order Hankel functions H_l. This may be achieved using the following differential identity

$$H_l(\beta|\vec{x}|)e^{il\theta_{\vec{x}}} = \left(\frac{-1}{\beta}\right)^l \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^l H_0(\beta|\vec{x}|) \tag{13}$$

Readers are referred to Ref. [9] (p.127) or Refs. [7], [11], [23]. for a detailed discussion.

Theorem 2 *For a point (x, y) with polar coordinates (r, θ) in $\mathbf{R}^2$, we have the following integral representations.* $H_l(\beta r)e^{il\theta} =$

- **North:**

$$\begin{aligned} &\frac{i^l}{\pi}\int_0^{\pi} e^{i\beta(y\sin\theta - x\cos\theta)}e^{-il\theta}d\theta + \\ &\frac{(-i)^l}{i\pi}\int_0^{\infty} \frac{e^{-ty}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)x}\left(\frac{\rho_\beta(t) - t}{\beta}\right)^l + e^{-i\rho_\beta(t)x}\left(\frac{-\rho_\beta(t) - t}{\beta}\right)^l\right)dt \end{aligned} \tag{14}$$

- **South:**

$$\begin{aligned} &\frac{i^l}{\pi}\int_0^{\pi} e^{i\beta(-y\sin\theta - x\cos\theta)}e^{il\theta}d\theta + \\ &\frac{(-i)^l}{i\pi}\int_0^{\infty} \frac{e^{ty}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)x}\left(\frac{\rho_\beta(t) + t}{\beta}\right)^l + e^{-i\rho_\beta(t)x}\left(\frac{-\rho_\beta(t) + t}{\beta}\right)^l\right)dt \end{aligned} \tag{15}$$

- **East:**

$$\begin{aligned} &\frac{1}{\pi}\int_0^{\pi} e^{i\beta(x\sin\theta - y\cos\theta)}e^{il\theta}d\theta + \\ &\frac{(-1)^l}{i\pi}\int_0^{\infty} \frac{e^{-tx}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)y}\left(\frac{-\rho_\beta(t) - t}{\beta}\right)^l + e^{-i\rho_\beta(t)y}\left(\frac{\rho_\beta(t) - t}{\beta}\right)^l\right)dt \end{aligned} \tag{16}$$

- **West:**

$$\frac{(-1)^l}{\pi}\int_0^{\pi} e^{i\beta(-x\sin\theta - y\cos\theta)}e^{-il\theta}d\theta + \\ \frac{(-1)^l}{i\pi}\int_0^{\infty}\frac{e^{tx}}{\rho_\beta(t)}\left(e^{i\rho_\beta(t)y}\left(\frac{-\rho_\beta(t)+t}{\beta}\right)^l + e^{-i\rho_\beta(t)y}\left(\frac{\rho_\beta(t)+t}{\beta}\right)^l\right)dt \tag{17}$$

2.2 Integral Representations of the Lattice Sums

In this section we demonstrate Theorem 1. The idea is that after substituting the integral representations ((14) to (17)) into the partial summation (12), and summing the resulting geometric series, one obtains explicit integral representations for the lattice sums S_{4l}^N. Inspection of these integrals leads to the natural decomposition of the lattice sums into evanescent and propagating parts,

$$S_{4l}^N = S_{4l}^{e,N} + S_{4l}^{p,N},$$

corresponding to the exponentially decaying and oscillatory integrals respectively. Taking the suitable large N limit of the evanescent integral is straight-forward, giving the integral (9).

As mentioned previously, evaluation of the propagating contribution is more technical. With the aid of Proposition 6, we derive

Theorem 3 *Given $\beta \in \mathbf{R}^+ \setminus \sigma$, we define the indices*

$$\begin{cases} J_\beta = \max\{j \in \mathbf{Z} | j(\frac{2\pi}{\beta}) < 1\} \\ K_\beta = \max\{k \in \mathbf{Z} | k(\frac{2\pi}{\beta}) < \sqrt{2}/2\} \end{cases} \tag{18}$$

and the corresponding angles

$$\begin{cases} \sin(\theta_j^{(0)}) = \frac{1}{\sqrt{2}}\left(\frac{2\pi}{\beta}\right)j & 0 \le j < J_\beta,\ \{\theta_j^{(0)}\} \in [0, \frac{\pi}{4}] \\ \cos(\theta_k^{(1)}) = \left(\frac{2\pi}{\beta}\right)k & 0 \le k < K_\beta,\ \{\theta_k^{(1)}\} \in [\pi, \frac{\pi}{2}] \end{cases}. \tag{19}$$

Then, for large N, the propagating contribution to the lattice sums defined by the partial summation (12) can be expressed by the following formulae

$$\lim_{N\to\infty} S_{4l}^{p,N} \sim -\delta_{l,0} + i(-1)^l\left(\frac{4\sqrt{2}}{\beta}\right)\sum_{j=0}^{J_\beta}{}' \frac{\cos(4l\theta_j^{(0)})}{\cos\theta_j^{(0)}}\cot\left(\frac{\beta}{2}\cos(\theta_j^{(0)}+\frac{\pi}{4})\right) \tag{20}$$

$$-i\left(\frac{8}{\beta}\right)\sum_{k=0}^{K_\beta}{}' \frac{\cos(4l\theta_k^{(1)})}{\sin\theta_k^{(1)}}\left(\frac{e^{-\frac{i\beta}{2}\sin\theta_k^{(1)}}}{\sin\left(\frac{\beta}{2}\sin\theta_k^{(1)}\right)}\right)e^{Ni\beta\sin\theta_k^{(1)}} \tag{21}$$

where $\delta_{l,0}$ is the standard Kronecker delta symbol and we utilize the primed summation as in Theorem 1.

We draw attention to the oscillatory terms in (21). It is clear that the lattice sums defined by our partial summation do not converge in the classical sense due to these oscillations. Considering Cesaro summation of S_{4l} and the corresponding weak-limit (Definition 7), we have the following immediate corollary

Corollary 4 *Given* $\beta,\ J_\beta,\ \theta_j^{(0)}$ *as above,*

$$wk-\lim_{N\to\infty} S_{4l}^{p,N} = -\delta_{l,0} + i(-1)^l\left(\frac{4\sqrt{2}}{\beta}\right)\sum_{j=0}^{J_\beta}{}' \frac{\cos(4l\theta_j^{(0)})}{\cos\theta_j^{(0)}}\cot\left(\frac{\beta}{2}\cos(\theta_j^{(0)}+\frac{\pi}{4})\right)$$
$$= -\delta_{l,0} + i4\sqrt{2}(-1)^l\sum_{j=0}^{J_\beta}{}' \frac{1}{\sqrt{\beta^2-2j^2\pi^2}}\cot(\frac{\sqrt{2}}{4}\sqrt{\beta^2-2j^2\pi^2}-\frac{j\pi}{2})\cos(4l\arcsin(\frac{\sqrt{2}j\pi}{\beta}))$$

where the last identity follows from evaluating $\sin\theta_j^{(0)},\ \cos\theta_j^{(0)}$ *using the definition (19).*

Theorem 1 then follows from the substitution of the weak-limits of Corollary 4 in place of the oscillatory sums of Theorem 3. Prior to these computations we note some general considerations.

In considering sums over the truncated lattice Λ^N, we group the terms as follows ($\vec{x} = (x, y)$)

$$\sum_{\vec{x}\in\Lambda^N} f(x,y) = \sum_{n=1}^{N-1}\sum_{m=-n}^{n} f(n,m) + f(-n,m) + \sum_{n=1}^{N-1}\sum_{m=-n+1}^{n-1} f(m,n) + f(m,-n). \tag{22}$$

Employing the terminology from the previous section we see that the first two sums lie strictly in the East and West regions of $\mathbf{R}^2$ while the second two are in the North and South respectively. (The fact that the lattice points along the diagonal lines $x = \pm y$ are preferentially assigned to the East and West summations has no significance.)

Substituting the plane wave expansions for $H_l(\vec{p})e^{il\theta_{\vec{p}}}$ into the summation gives rise to certain geometric series. We record the following geometric summation for reference as it appears many times in the expressions below

$$\sum_{n=1}^{N-1} p^n\left(\sum_{m=-n}^{n} + \sum_{m=-n+1}^{n-1} q^m\right) = \left(\frac{1+q}{1-q}\right)\left[\frac{pq^{-1}}{1-pq^{-1}} - \frac{pq}{1-pq} - \frac{(pq^{-1})^N}{1-pq^{-1}} + \frac{(pq)^N}{1-pq}\right]. \tag{23}$$

As a final convention, we note that the partial summation of geometric series will give rise to functions that appear to have simple poles in the domain of integration. These singularities are removable in the sense that the terms in (23) are differences which cancel to first order at any apparent pole. However, we wish to consider the terms separately in which case the integration is to be taken in the principal value sense, eg. if $f(s)$ has a simple pole singularity at $s = s_0 \in (a, b)$, then by integration of f we mean

$$\int_a^b f(s)ds \equiv \lim_{\epsilon\to 0}\int_a^{s_0-\epsilon} + \int_{s_0+\epsilon}^b f(s)ds.$$

As a matter of convenience, we do not write a special integration symbol to denote this fact. As the location of the poles below will be independent of N, we leave it to the reader to check that our interpretation is consistent, ie. the integration of the difference of terms with a first order cancellation is equal to the difference of principal value integrals.

Returning to the lattice sums, we consider the evanescent term first. Upon grouping the terms (22), substituting the appropriate plane wave expansions for the Hankel functions ((14) through (17)), applying the geometric summation formulae (23), and performing some algebra we obtain,

$$\begin{aligned}
\rho_\beta(t) &= \sqrt{t^2+\beta^2} \\
S_{4l}^{e,N} &= \frac{2}{\pi i}\int_0^\infty \frac{1}{\rho_\beta(t)} \sum_{n=1}^{N-1} e^{-tn}\left(\sum_{m=-n}^{n} + \sum_{m=-n+1}^{n-1} e^{i\rho_\beta(t)m}\right)\left((\frac{\rho_\beta(t)+t}{\beta})^{4l} + (\frac{\rho_\beta(t)-t}{\beta})^{4l}\right) dt \\
&= +\frac{2}{\pi i}\int_0^\infty \frac{e^{-t}}{\rho_\beta(t)}\left(\frac{1+e^{-i\rho_\beta(t)}}{1-e^{-i\rho_\beta(t)}}\right)\left[\frac{e^{-i\rho_\beta(t)}}{1-e^{-t-i\rho_\beta(t)}} - \frac{e^{i\rho_\beta(t)}}{1-e^{-t+i\rho_\beta(t)}}\right]\left((\frac{\rho_\beta(t)+t}{\beta})^{4l} + (\frac{\rho_\beta(t)-t}{\beta})^{4l}\right) dt \\
&\quad -\frac{2}{\pi i}\int_0^\infty \frac{e^{-Nt}}{\rho_\beta(t)}\left(\frac{1+e^{-i\rho_\beta(t)}}{1-e^{-i\rho_\beta(t)}}\right)\left[\frac{e^{-i\rho_\beta(t)N}}{1-e^{-t-i\rho_\beta(t)}} - \frac{e^{i\rho_\beta(t)N}}{1-e^{-t+i\rho_\beta(t)}}\right]\left((\frac{\rho_\beta(t)+t}{\beta})^{4l} + (\frac{\rho_\beta(t)-t}{\beta})^{4l}\right) dt
\end{aligned}$$

We first note that for $\beta = 2\pi m, m \geq 0$, both integrands in the final expression above exhibit a dipole singularity as $t \to 0$. However, as such β are in σ (2), these values are excluded from the analysis. Turning to the N-dependent term, even with the restriction $\beta \neq 2\pi m$, there remain simple poles of the integrand for $\{t_n = \sqrt{(2\pi n)^2 - \beta^2}, n > 2\pi/\beta, n \in \mathbf{Z}^+\}$. Clearly, however, the principal value limit is uniform with respect to N. Therefore, we apply the Dominated Convergence Theorem and observe that this term goes to zero in the large N limit. Performing further algebraic simplifications we arrive at the following expression for the evanescent contribution

$$S_{4l}^{e} = \frac{4}{i\pi}\int_0^\infty \frac{e^{-t}}{\rho_\beta(t)}\left(\frac{1+\cos\rho_\beta(t)}{1+e^{-2t}-2e^{-t}\cos\rho_\beta(t)}\right)\left(\left(\frac{\rho_\beta(t)-t}{\beta}\right)^{4l} + \left(\frac{\rho_\beta(t)+t}{\beta}\right)^{4l}\right) dt$$

We next consider the propagating part. Prior to taking the large N limit, the analysis is similar to that for the evanescent terms. Without further ado we write

$$\begin{aligned}
X &= e^{i\beta\cos(\theta)} \\
Y &= e^{i\beta\sin(\theta)} \\
S_{4l}^{p,N} &= \frac{2}{\pi}\int_0^\pi \cos(4l\theta)\left(\sum_{n=1}^{N-1} Y^n \left(\sum_{m=-n}^{n} + \sum_{m=-n+1}^{n-1} X^m\right)\right) d\theta \\
&= +\frac{2}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+X}{1-X}\right)\left[\frac{YX^{-1}}{1-YX^{-1}} - \frac{YX}{1-YX}\right] d\theta \\
&\quad -\frac{2}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+X}{1-X}\right)\left[\frac{(YX^{-1})^N}{1-YX^{-1}} - \frac{(YX)^N}{1-YX}\right] d\theta \\
&= +\frac{4}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+X}{1-X}\right)\left[\frac{YX^{-1}}{1-YX^{-1}}\right] d\theta \qquad (24) \\
&\quad -\frac{4}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+X}{1-X}\right)\left[\frac{(YX^{-1})^N}{1-YX^{-1}}\right] d\theta, \qquad (25)
\end{aligned}$$

where in the final equality we have made the change of variables $\theta' = \pi - \theta$ which takes $X \rightarrow X^{-1}$ while leaving fixed: Y, $\cos(4l\theta)$, and the domain of integration.

We dispense with the N-independent term (24) in the following proposition

Proposition 5 *Given $\beta \in \mathbf{R}$, $l \in \mathbf{Z}$*

$$\frac{4}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+e^{i\beta\cos(\theta)}}{1-e^{i\beta\cos(\theta)}}\right)\left[\frac{e^{i\beta(\sin(\theta)-\cos(\theta))}}{1-e^{i\beta(\sin(\theta)-\cos(\theta))}}\right]d\theta = \begin{cases} -1 & l=0 \\ 0 & l=\pm1,\pm2,\ldots \end{cases}. \tag{26}$$

Proof:
See appendix.

Unlike the evanescent contributions, the N-dependence in (25) contributes to an oscillatory integrand, hence the large N limit requires some care. One observes that there are many values of $\theta \in [0,\pi]$ that will cause the integrands to become singular. As we demonstrate below, a subset of these singularities gives non-zero contributions to the lattice sums in the limit of infinite oscillations. Adding to the complexity of the problem, we will see that the integrals do not converge to a number but rather have well-defined limits of the form

$$S_{4l}^{p,N} \sim \sum_{j=-J_\beta}^{J_\beta} A_{4l}^j + \sum_{k=-K_\beta}^{K_\beta} B_{4l}^k e^{i\omega_k N},\ \omega_k = \beta\sin\theta_k^{(1)} \tag{27}$$

Note that $\omega_k \in \mathbf{R}^+$ and $\omega_k \neq 2\pi n$ as $\beta \notin \sigma$ (See (2)). Thus this term is always oscillatory. We introduce the weak convergence ideas below so as to eliminate the oscillations in (27).

The following result concerning asymptotics of oscillatory integrals facilitates the evaluation of (25). We reserve the proof for the Appendix.

Proposition 6 *Given functions $f(s), g(s), h(s)$ analytic in the interval $s \in [s_0, s_1]$ satisfying the following conditions:*

1. *h is real and $h' \neq 0$ on $[s_0, s_1]$.*

2. *g has a single simple zero at $s = a$ in the open interval (s_0, s_1).*

Then we have the following limits:

$$\lim_{N\to\infty}\int_{s_0}^{s_1} f(s)e^{iNh(s)}ds = 0 \tag{28}$$

$$\lim_{N\to\infty}\int_{s_0}^{s_1} \frac{f(s)e^{iNh(s)}}{g(s)}ds \sim \pi i\frac{f(a)}{g'(a)}e^{iNh(a)}sgn\left(h'(a)\right), \tag{29}$$

where $sgn(x) = x/|x| = \pm1$ for $x > 0$ or $x < 0$ respectively.

Proof:
See Appendix.

We wish to apply Proposition 6 to evaluate

$$\lim_{N\to\infty}\left(-\frac{4}{\pi}\right)\int_0^\pi \cos(4l\theta)\left(\frac{1+e^{i\beta\cos(\theta)}}{1-e^{i\beta\cos(\theta)}}\right)\left[\frac{e^{iN\beta(\sin(\theta)-\cos(\theta))}}{1-e^{i\beta(\sin(\theta)-\cos(\theta))}}\right]d\theta$$

For β fixed and $\theta \in [0,\pi]$, there are two possible types of singularities corresponding to $\beta(\sin\theta - \cos\theta) = 2\pi n$ or $\beta\cos\theta = 2\pi n$. Regarding the former, we will find it more convenient to make the change of variables $\theta = \theta - \pi/4$ which takes $\sin\theta - \cos\theta \to \sqrt{2}\sin\theta'$. Dropping the primes, we are led to consider the points

$$\left\{ \begin{array}{l} \sin(\theta_j^{(0)}) = \frac{1}{\sqrt{2}}\left(\frac{2\pi}{\beta}\right) j, \ \theta_j^{(0)} \in [-\frac{\pi}{4}, \frac{3\pi}{4}] \\ \cos(\theta_k^{(1)}) = \left(\frac{2\pi}{\beta}\right) k, \ \theta_k^{(1)} \in [0,\pi] \end{array} \right. , j,k \in \mathbf{Z}. \tag{30}$$

Inspection of (30) leads us to define the indices

$$\left\{ \begin{array}{l} J_\beta^* = \max\{j | j(\frac{2\pi}{\sqrt{2}\beta}) < 1\} \\ K_\beta^* = \max\{k | k(\frac{2\pi}{\beta}) < 1\} \end{array} \right. .$$

As we will see below, there is cancellation between some but **never all** of the pairs of these singularities, e.g. for $J_\beta < j \le J_\beta^*$ (J_β is defined below), the contribution from $\theta_{-j}^{(0)}$ will cancel that from $\theta_j^{(0)}$.

Turning to the set $\{\theta_k^{(1)}\}$, one may verify that the hypotheses of the Proposition 6 are met. Furthermore, in evaluating the limit it is sufficient to restrict the integration (25) to small neighborhoods of these singular points. We compute

$$\begin{aligned} &\lim_{N\to\infty}\left(-\frac{4}{\pi}\right)\int_{\theta_k^{(1)}-\epsilon}^{\theta_k^{(1)}+\epsilon} \cos(4l\theta)\left(\frac{1+e^{i\beta\cos(\theta)}}{1-e^{i\beta\cos(\theta)}}\right)\left[\frac{e^{iN\beta(\sin(\theta)-\cos(\theta))}}{1-e^{i\beta(\sin(\theta)-\cos(\theta))}}\right] d\theta \\ &= \pi i\left(-\frac{4}{\pi}\right)\cos(4l\theta_k^{(1)})\frac{2}{(1-e^{i\beta\sin\theta_k^{(1)}})}\frac{1}{i\beta\sin\theta_k^{(1)}} e^{iN\beta\sin\theta_k^{(1)}} sgn(\cos\theta_k^{(1)} + \sin\theta_k^{(1)}) \end{aligned} \tag{31}$$

where we have made repeated use of the fact that $\exp(i\beta\cos\theta_k^{(1)}) = 1$.

We next make use of the symmetry of the set $\{\theta_k^{(1)}\}$ about $\theta_0^{(1)} = \pi/2$. Clearly, for $0 \le k < K_\beta^*$, one observes that

$$\left\{ \begin{array}{l} \theta_{-k}^{(1)} = \frac{\pi}{2} - \Delta\theta_k^{(1)} \\ \theta_k^{(1)} = \frac{\pi}{2} + \Delta\theta_k^{(1)} \end{array} \right. \Longrightarrow \left\{ \begin{array}{rcl} \sin(\theta_{-k}^{(1)}) &=& \sin(\theta_k^{(1)}) \\ \cos(4l\theta_{-k}^{(1)}) &=& \cos(4l\theta_k^{(1)}) \end{array} \right.$$

yet

$$\left\{ \begin{array}{rcll} sgn(\sin\theta_{-k}^{(1)} + \cos\theta_{-k}^{(1)}) &=& sgn(\sin\theta_k^{(1)} + \cos\theta_k^{(1)}) & |\theta_k^{(1)} - \frac{\pi}{2}| < \frac{\pi}{4} \\ sgn(\sin\theta_{-k}^{(1)} + \cos\theta_{-k}^{(1)}) &=& -sgn(\sin\theta_k^{(1)} + \cos\theta_k^{(1)}) & |\theta_k^{(1)} - \frac{\pi}{2}| > \frac{\pi}{4} \end{array} \right.$$

as the cosine contribution is dominant. Looking at (31), we see that the sum of these two terms will add in the former case and cancel in the later. Therefore we define $K_\beta = \max\{k | k(\frac{2\pi}{\beta}) < \sqrt{2}/2\}$; this is index appearing in (21).

We next examine the singularities $\{\theta_j^{(0)}\}$. We perform a change of variables to bring the points into a more symmetric position. Considering $\theta' = \theta - \frac{\pi}{4}$ one observes that (again we employ the shorthand $X = \exp(i\beta\cos(\theta)),\ Y = \exp(i\beta\sin(\theta))$)

$$-\frac{4}{\pi}\int_0^\pi \cos(4l\theta)\left(\frac{1+X}{1-X}\right)\frac{(YX^{-1})^N}{1-YX^{-1}} d\theta$$

$$= \quad (-1)^{l+1}\frac{4}{\pi}\int_{-\frac{\pi}{4}}^{\frac{3\pi}{4}}\cos(4l\theta)\left(\frac{1+(XY^{-1})^{\frac{1}{\sqrt{2}}}}{1-(XY^{-1})^{\frac{1}{\sqrt{2}}}}\right)\frac{Y^{\sqrt{2}N}}{1-Y^{\sqrt{2}}}d\theta.$$

In this variable the singularities clearly are $\{\theta_j^{(0)}\}$ defined in (30). Applying Proposition 6 once again we see that

$$(-1)^{l+1}\left(\frac{4}{\pi}\right)\lim_{N\to\infty}\int_{\theta_j^{(0)}-\epsilon}^{\theta_j^{(0)}+\epsilon}\cos(4l\theta)\left(\frac{1+e^{i\beta(\cos(\theta)-\sin(\theta))/\sqrt{2}}}{1-e^{i\beta(\cos(\theta)-\sin(\theta))/\sqrt{2}}}\right)\left[\frac{e^{Ni\beta\sin(\theta)\sqrt{2}}}{1-e^{i\beta\sin(\theta)\sqrt{2}}}\right]d\theta$$
$$= \quad (-1)^{l+1}\left(\frac{4}{\pi}\right)\pi i\cos(4l\theta_j^{(0)})\left(\frac{1+e^{i\beta(\cos(\theta_j^{(0)}+\frac{\pi}{4}))}}{1-e^{i\beta(\cos(\theta_j^{(0)}+\frac{\pi}{4}))}}\right)\frac{1}{-\sqrt{2}i\beta\cos\theta_j^{(0)}}sgn(\cos\theta_j^{(0)}) \qquad (32)$$

Note that the set $\{\theta_j^{(0)}\}$ may be considered as two subsets $-\pi/4 < \theta_j^{(0)} < \pi/4$ symmetric about $\theta = 0$, and $\pi/4 < \theta_j^{(0)} < 3\pi/4$ symmetric about $\theta = \pi/2$. We observe that the sum of the contributions from the later cancel due to the change in sign of $sgn(\cos\theta_j^{(0)})$. Therefore, as before, we need only consider contributions from the singularities $\{\theta_j^{(0)}||j| < J_\beta\}$ where $J_\beta = \max\{j|j(\frac{2\pi}{\beta}) < 1\}$.

We collect the results, (31), (32), perform more algebra, and arrive at the statement of Theorem 3

$$\begin{aligned}\lim_{N\to\infty} S_{4l}^{p,N} \quad &\sim \quad -\delta_{l,0} + i(-1)^l\left(\frac{4\sqrt{2}}{\beta}\right)\sum_{j=0}^{J_\beta}{}'\frac{\cos(4l\theta_j^{(0)})}{\cos\theta_j^{(0)}}\cot\left(\frac{\beta}{2}\cos(\theta_j^{(0)}+\frac{\pi}{4})\right)\\ &-i\left(\frac{8}{\beta}\right)\sum_{k=0}^{K_\beta}{}'\frac{\cos(4l\theta_k^{(1)})}{\sin\theta_k^{(1)}}\left(\frac{e^{-\frac{i\beta}{2}\sin\theta_k^{(1)}}}{\sin\left(\frac{\beta}{2}\sin\theta_k^{(1)}\right)}\right)e^{Ni\beta\sin\theta_k^{(1)}}\end{aligned}$$

We will discard the oscillating terms above. Formally, this corresponds to interpreting S_{4l} as a weak-limit of S_{4l}^N, in the following sense

Definition 7 *Given a sequence $\{a_n\}$, we define the weak-limit by*

$$wk-\lim_{n\to\infty} a_n = \lim_{n\to\infty}\frac{\sum_{i=1}^n a_i}{n}.$$

It is an easy matter to check that

Proposition 8 *Given a sequence $\{b_n\}$ with $\lim\{b_n\} = b$ and $\omega \in \mathbf{R}\setminus 2\pi\mathbf{Z}$, then*

$$\begin{aligned} wk-\lim_{n\to\infty} b_n &= b\\ wk-\lim_{n\to\infty} b_n e^{i\omega n} &= 0\end{aligned}$$

Applying this proposition to the result for the lattice sums (Theorem 3) gives the statement of Corollary 4.

Table 1: Numerical values of $S_0(\beta), S_{12}(\beta),$ and $S_{24}(\beta)$ given by our method, and reported in Ref. [13]

	S_0		S_{12}		S_{24}	
β	Theorem 1	Ref. [13]	Theorem 1	Ref. [13]	Theorem 1	Ref. [13]
2	1.39962 10^0	1.39963 10^0	-5.47552 10^7	-5.47550 10^7	-3.43888 10^{22}	-3.43888 10^{22}
10.9548	-0.14189 10^0	-0.14187 10^0	-2.16949 10^0	-2.16950 10^0	-2.38213 10^5	-2.38225 10^5
20	6.46161 10^0	6.46161 10^0	-4.53737 10^0	-4.53738 10^0	-3.65184 10^0	-3.65184 10^0

3 Numerical Results

As a first test of our result, we compare the values of the lattice sums computed via Theorem 1 with the results of computations using a dual-lattice summation identity described in Ref. [13]. As the values of S_{4l} have been tabulated previously in the literature, we do not report an entire table here but, rather, only a general "cross-section" (Table 1). The two methods agree to four significant figures. At the time of writing, we have not performed any detailed convergence analysis of the quadrature of (9), therefore we are satisfied with this level of agreement. (The numerical value was computed in both Maple or Mathematica depending on the separate author's biases.)

Next we address the convergence of the sum representation of the periodic Green's function, Theorem 1. It is a standard fact that such an expansion converges only when there exists separation between the evaluation points and the images of the singular term at the origin, ie. $|\vec{x}| \leq c < 1$. This is a familiar situation for readers familiar with multipole-type codes. The remedy is simply to include more of the singular source terms explicitly in the formulae (5) and modify the lattice sums so as to reflect this, eg.

$$G_\beta(\vec{x}) = \frac{i}{4}\left(\sum_{\vec{p}\in\mathcal{N}} H_0(\beta|\vec{x}-\vec{p}|) + \tilde{S}_0(\beta)J_0(\beta|\vec{x}|) + 2\sum_{l=1}^{\infty}\tilde{S}_{4l}J_{4l}(\beta|\vec{x}|)\cos(4l\theta_{\vec{x}})\right)$$

where $\mathcal{N}$ denotes the origin and its nearest neighbors

$$\mathcal{N} = \{(-1,1),(0,1),(1,1),(-1,0),(0,0),(1,0),(-1,-1),(0,-1),(1,-1)\}.$$

and $\tilde{S}_{4l}(\beta)$ are defined by

$$\tilde{S}_{4l}(\beta) = \sum_{\vec{p}\in\mathbf{Z}^2-\mathcal{N}} H_{4l}(\beta|\vec{p}|)e^{i4l\phi_{\vec{p}}}.$$

We refer the reader to Refs. [2], [6], and [22]) for a detailed discussion of this type of acceleration procedure applied to a FMM periodic Laplace solver. To avoid this technical detail we evaluate $G_\beta(x,y)$ for $-1/4 < x < 1/4$, $-1/2 < y < 1/2$. Under this restriction on the domain, we have found that the representation (11) converges to four-digit accuracy with the infinite sum truncated after ten terms ($L = 10$).

With regards to the substitution of the lattice sums defined by (5) with the weak-limit of the partial summation (12), we have a rigorous proof that weak-limit of G_β^N converges to G_β, however the idea is standard and the estimates technical. Instead we adopt an empirical approach. For β not an eigenvalue of the periodic Laplace equation on B_1, G_β defined in (1) exists and is unique.

Table 2: Difference of $G_\beta(x-\frac{1}{2},y)$ and $G_\beta(x+\frac{1}{2},y)$ $-\frac{1}{4}<x<\frac{1}{4}$, $-\frac{1}{2}<y<\frac{1}{2}$, and $L=10$.

β	2.0		10.9548		20	
(x,y)	$G_\beta(x-\frac{1}{2},y)$	$G_\beta(x+\frac{1}{2},y)$	$G_\beta(x-\frac{1}{2},y)$	$G_\beta(x+\frac{1}{2},y)$	$G_\beta(x-\frac{1}{2},y)$	$G_\beta(x+\frac{1}{2},y)$
(0.194,0.002)	-0.243102	-0.243102	-0.0250198	-0.0250198	-0.422105	-0.422105
(0.214,-0.358)	-0.291333	-0.291333	-0.0253164	-0.0253161	0.350195	0.350195
(0.187,0.221)	-0.272955	-0.272955	-0.0559112	-0.0559112	-0.345961	-0.345961
(0.189,-0.456)	-0.302836	-0.302838	0.0054734	0.0054712	0.527526	0.527522
(0.250,0.480)	-0.297197	-0.297257	0.0466605	0.0465896	0.103749	0.103638
(0.189,0.290)	-0.284772	-0.284772	-0.0494379	-0.0494379	0.234581	0.234581
(0.175,0.384)	-0.299235	-0.299235	-0.0185029	-0.0185028	0.693037	0.693037
(0.151,0.460)	-0.306522	-0.306522	-0.0099674	-0.0099671	0.416608	0.416609

Subtracting the singular term, $H_0(\beta|\vec{x}|)$, from G_β, using the fact that $\{J_l(|\vec{x}|)e^{il\theta_{\vec{x}}}\}$ form a basis of smooth solutions to the Helmholtz equation, and employing the symmetries of the problem, one knows *a priori* that a representation of the form (6) also exists and is unique. Therefore, we need only check that the function defined by Theorem 1 is periodic. As the expression (11) is invariant under rotation by $\pi/2$, we need only test for periodicity in the x-variable

$$G_\beta(x-\frac{1}{2},y)=G_\beta(x+\frac{1}{2},y),\ \ x\in[-\frac{1}{2},\frac{1}{2}],y\in[-1,1].$$

We demonstrate this periodicity for a few points selected at random and selected values of β. Again we observe that G_β is periodic to four significant digits.

To our knowledge, the representation of $S_{4l}(\beta)$ as a closed-form integral and sum (9), (10) is new. We are in the process of exploring the analytical consequences implied by this representation. As a simple first step, one may simply enquire as to the relative strength of the two contributions to the total sum. In figure 1 we plot the value of $S_l^p(\beta)$ and $S_l^e(\beta)$ as a function of β for $l=0$. The eigenvalues $\beta=2\pi\sqrt{m^2+n^2}$ appear clearly as poles of S_0. Inspection of the formulae (9) reveals that for $\beta=2\pi n$, the evanescent integral (9) has a second-order singularity at $t=0$ which gives rise to a pole contribution to the lattice sum. The behavior of the propagating part is more subtle. As J_β (see Theorem 1) is defined by

$$J_\beta=\max\{j\in\mathbf{Z}|j(\frac{2\pi}{\beta})<1\},$$

one may check that

$$\begin{aligned}\lim_{\beta\to(2\pi n)_-}S^p(\beta)&<\infty\\ \lim_{\beta\to(2\pi n)_+}S^p(\beta)&=\infty,\end{aligned}$$

as, in the latter case, one may let $j=n$ in the summation (10). In contrast, for $\beta=2\pi\sqrt{m^2+n^2}$, the singularity is due only to the cotangent term in the propagating sum (10), and the evanescent integral is clearly finite. For all other values of β, the two contributions are comparable.

Finally, we address possible extensions of our analysis. One of the many physical problems that gives rise to a 2D, periodic Helmholtz equation is electromagnetic scattering by an array of

Figure 1: Comparison of the contribution of S^p (solid line) and S^e (dashed line) to the total lattice sum as a function of β.

infinite cylinders. In such an experiment, our analysis is equivalent to the requirement that the incident radiation is normal to the cylindrical axis. Scattering by off-axis radiation is accommodated by replacing the periodicity condition on G_β with a phase-shift or "quasi-periodicity" factor

$$G_\beta(\vec{x}+\mathbf{e}_i) = G_\beta(\vec{x})e^{-i\mathbf{e}_i\cdot\mathbf{k}^\perp}$$

where $\mathbf{k}^\perp$ is the xy-plane component of the incident light and $\mathbf{e}_i$ is a translation by a lattice generator. At the level of the lattice sums this exponential factor appears inside the summand (5). We are considering incorporating this term into our analysis. Furthermore, one may consider more general lattices. Although the Green's function representation under a general lattice must be modified in the case of large "aspect-ratio", the computation of the sums proceeds in an entirely analogous manner. We are currently considering this extension.

4 Appendix

4.1 Derivation of Proposition 5

We prove (26) of Proposition 5. Although not obvious at first glance, we choose to work with the integral prior to (24) as it is real-valued.

$$\begin{aligned}
&\frac{4}{\pi}\int_0^\pi \left(\frac{1+e^{i\beta\cos(t)}}{1-e^{i\beta\cos(t)}}\right)\left[\frac{e^{i\beta(\sin(t)-\cos(t))}}{1-e^{i\beta(\sin(t)-\cos(t))}}\right]\cos(4lt)dt \\
&= -\frac{2}{\pi}\int_0^\pi \left(\frac{1+e^{i\beta\cos(t)}}{1-e^{i\beta\cos(t)}}\right)\left[\frac{e^{i\beta(\sin(t)-\cos(t))}}{1-e^{i\beta(\sin(t)-\cos(t))}} - \frac{e^{i\beta(\sin(t)+\cos(t))}}{1-e^{i\beta(\sin(t)+\cos(t))}}\right]\cos(4lt)dt \\
&= \frac{2}{\pi}\int_0^\pi \frac{1+\cos(\beta\cos(t))}{\cos(\beta\cos(t))-\cos(\beta\sin(t))}\cos(4lt)dt
\end{aligned}$$

We define $f(t;\beta)$,

$$f(t;\beta) = \frac{1+\cos(\beta\cos(t))}{\cos(\beta\cos(t))-\cos(\beta\sin(t))}$$

We first show that the integral is independent of β.

$$\frac{\partial f}{\partial\beta} = \frac{(\cos(\beta\sin(t))+1)\cos(t)\sin(\beta\cos(t))}{(\cos(\beta\cos(t))-\cos(\beta\sin(t)))^2} - \frac{(1+\cos(\beta\cos(t)))\sin(t)\sin(\beta\sin(t))}{(\cos(\beta\cos(t))-\cos(\beta\sin(t)))^2}.$$

Performing the change of variable to shift the integration one finds,

$$\int_0^\pi \frac{\partial f}{\partial\beta}\cos(4lt)dt = +\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{(\cos(\beta\cos(t))+1)\sin(t)\sin(\beta\sin(t))}{(\cos(\beta\sin(t))-\cos(\beta\cos(t)))^2}\cos(4lt)dt$$

$$
\begin{aligned}
&- \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{(\cos(\beta\sin(t))+1)\cos(t)\sin(\beta\cos(t))}{(\cos(\beta\sin(t))-\cos(\beta\cos(t)))^2}\cos(4lt)dt \\
= \; &+ \int_{-\frac{\pi}{2}}^{0} + \int_{0}^{\frac{\pi}{2}} \frac{(\cos(\beta\cos(t))+1)\sin(t)\sin(\beta\sin(t))}{(\cos(\beta\sin(t))-\cos(\beta\cos(t)))^2}\cos(4lt)dt \\
&- \int_{-\frac{\pi}{2}}^{0} - \int_{0}^{\frac{\pi}{2}} \frac{(\cos(\beta\sin(t))+1)\cos(t)\sin(\beta\cos(t))}{(\cos(\beta\sin(t))-\cos(\beta\cos(t)))^2}\cos(4lt)dt \\
= \; & 0,
\end{aligned}
$$

as the integrals "cross-cancel", ie. changing $t' = t - \pi/2$ in the last integral cancels the first and similarly for the second and third.

Next we evaluate the integral in the limit of small β. First note that arguing as above, one observes that

$$
\int_0^{\pi} \frac{1}{\cos(\beta\cos(t)) - \cos(\beta\sin(t))}\cos(4lt)dt = 0
$$

Thus we may ignore constant terms appearing in the numerator. Assuming $\beta \to 0$ we obtain

$$
\begin{aligned}
\frac{2}{\pi}\int_0^{\pi} f(t;\beta)\cos(4lt)dt &= -\frac{2}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1+\cos(\beta\sin(t))}{\cos(\beta\cos(t))-\cos(\beta\sin(t))}\cos(4lt)dt \\
&= \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\beta^2\sin^2(t)+O(\beta^4)}{\cos(\beta\cos(t))-\cos(\beta\sin(t))}\cos(4lt)dt \\
&= \frac{2}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{-\sin^2(t)}{\cos^2(t)-\sin^2(t)}\cos(4lt)dt + O(\beta^2) \\
&= -\frac{1}{\pi}\left(\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos(4lt)dt - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\frac{1}{\cos^2(t)-\sin^2(t)}\cos(4lt)dt\right) \\
&= \begin{cases} -1 & l=0 \\ 0 & l=\pm 1, \pm 2, \dots \end{cases},
\end{aligned}
$$

as, once again, one may show that the second integral in the penultimate line evaluates to 0 by splitting the domain of integration and performing a change of variables. This is the desired identity.

4.2 Proof of Proposition 6

Formula (28) is simply a Corollary of the Riemann Theorem concerning asymptotics of Fourier coefficients. The idea is that non-vanishing condition on the derivative of h allows one to change the scale of the integration. Specifically, as $h'(s) \neq 0$ by the Inverse Function Theorem one may find an analytic inverse function $s = s(h)$. Pulling back the integration we see that

$$
\begin{aligned}
\lim_{N\to\infty}\int_{s_0}^{s_1} f(s)e^{iNh(s)}ds &= \lim_{N\to\infty}\int_{h(s_0)}^{h(s_1)} f(s(h))e^{iNh}s'(h)dh \\
&= \lim_{N\to\infty}\int_{h(s_0)}^{h(s_1)} \tilde{f}(h)e^{iNh}dh \\
&= 0
\end{aligned}
$$

To derive the second formula (29) we first consider smooth $f(s)$ and the simpler case,

$$\begin{aligned}
\lim_{N\to\infty}\int_{-\epsilon}^{+\epsilon}\frac{f(s)}{s}e^{iNs}ds &= \lim_{N\to\infty}\int_{-\epsilon}^{+\epsilon}\frac{f(0)+f'(0)s+O\left(s^2\right)}{s}e^{iNs}ds \\
&= f(0)\lim_{N\to\infty}\int_{-\epsilon}^{+\epsilon}\frac{1}{s}e^{iNs}ds \qquad (33)\\
&= f(0)\int_{-\infty}^{\infty}\frac{1}{s}e^{is}ds \\
&= \pi i f(0). \qquad (34)
\end{aligned}$$

Equation (33) follows from the fact that the remaining terms of the Taylor expansion give rise to a smooth integrand which, in the limit, evaluates to zero. Equality (34) is standard.

We turn to (29) or Proposition 6. First, one may multiply by a smooth "bump-function" supported in a neighborhood of the singularity $s = a$, apply (28), and thereby see that it's sufficient to consider the restriction of the integral to any neighborhood of a. Making use of analyticity, performing algebra, and applying (34), we see that

$$\begin{aligned}
\lim_{N\to\infty}\int_{s_0}^{s_1}\frac{f(s)}{g(s)}e^{iNh(s)}ds &= \lim_{N\to\infty}\int_{a-\epsilon}^{a+\epsilon}\frac{f(s)}{g(s)}e^{iNh(s)}ds \\
&= \lim_{N\to\infty}\int_{-\epsilon}^{+\epsilon}\frac{f(a)+f'(a)s+O\left(s^2\right)}{g'(a)s+O\left(s^2\right)}e^{iNh(a+s)}ds \\
&= \lim_{N\to\infty}\frac{f(a)}{g'(a)}e^{iNh(a)}\int_{-\epsilon}^{+\epsilon}\frac{1}{s}e^{iN(h(a+s)-h(a))}ds \\
&= \lim_{N\to\infty}\frac{f(a)}{g'(a)}e^{iNh(a)}\int_{h(a-\epsilon)-h(a)}^{h(a+\epsilon)-h(a)}\frac{1}{s(h)}e^{iNh}s'(h)dh \\
&= \lim_{N\to\infty}\frac{f(a)}{g'(a)}e^{iNh(a)}\int_{\epsilon_1}^{\epsilon_2}\frac{1}{s(h)}e^{iNh}s'(h)dh,
\end{aligned}$$

where $\epsilon_1 < 0 < \epsilon_2$ if $h'(a) > 0$, and $\epsilon_2 < 0 < \epsilon_1$ otherwise. We let $\tilde{\epsilon} = \min\{|\epsilon_1|, |\epsilon_2|\}$ and rearrange the integration limits according to the sign of this derivative. Finally we see

$$\begin{aligned}
\lim_{N\to\infty}\int_{s_0}^{s_1}\frac{f(s)}{g(s)}e^{iNh(s)}ds &= sgn(h'(a))\lim_{N\to\infty}\frac{f(a)}{g'(a)}e^{iNh(a)}\frac{1}{s'(0)}\int_{-\tilde{\epsilon}}^{\tilde{\epsilon}}\frac{1}{h}e^{iNh}s'(h)dh \\
&= sgn(h'(a))\lim_{N\to\infty}\frac{f(a)}{g'(a)}e^{iNh(a)}\frac{1}{s'(0)}\int_{-\tilde{\epsilon}}^{\tilde{\epsilon}}\frac{1}{h}e^{iNh}s'(h)dh \\
&\sim \pi i\frac{f(a)}{g'(a)}e^{iNh(a)}sgn(h'(a)).
\end{aligned}$$

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