Discrete scattering theory: Green’s function for a square lattice

P.A. Martin *

Department of Mathematical and Computer Sciences, Colorado School of Mines, Golden, CO 80401-1887, USA

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Abstract

It is well known that, under certain circumstances, discrete plane waves can propagate through lattices. Waves can also be generated by oscillating one point in the lattice: the corresponding solution of the governing partial difference equations is the discrete Green’s function, \( g_{mn} \). The far-field behaviour of \( g_{mn} \) is obtained using three methods: textbook derivations are corrected and a formula for \( g_{nn} \) as a Legendre function is derived. The low-frequency behaviour of \( g_{mn} \) is also obtained using Mellin transforms. These results are useful in the development of a discrete scattering theory.

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1. Introduction

Partial difference equations have been studied extensively. One motivation was the development of finite-difference approximations to partial differential equations. For example, one might try to compute \( u_{mn} \) for integer \( m \) and \( n \) by solving some partial difference equations, where \( u_{mn} \) is supposed to be an approximation to \( u(mh, nh) \) and \( u(x, y) \) solves a partial differential equation. The parameter \( h \) is the constant mesh spacing, so that one would want to know if the approximation converges to \( u \) as \( h \to 0 \) [12]. Further applications occur in mechanics, where the ‘continuum limit’ of lattice models has a large literature; see [25] for a recent review.

We are interested in methods for solving the discrete problem for fixed, finite \( h \), especially when the governing partial difference equations can support waves: this topic is known as lattice dynamics. Analogous static problems also arise; see, for example, [29] for a study of lattice defects and [10, Chapter IV] for an application to the interpolation of data given on an integer mesh. The classic applications of lattice dynamics are in solid-state physics [20]. There, one considers a periodic arrangement of interacting cells; each cell contains the same arrangement of interacting atoms. The propagation of waves through such a perfect lattice is a textbook subject [3]. If the lattice contains a defect, waves will be scattered. The corresponding scattering theory for a point defect was instigated by I.M. Lifshitz in the late 1940’s; see [16, 17, 18] and [20, pp. 376–381]. A key role in this theory is played by the lattice Green’s function; this is the main subject of the present paper.
We consider the simplest problem, with a two-dimensional, square lattice. We envisage that each lattice point can move out of the plane of the lattice, and that each point is connected to its neighbours by springs; only nearest-neighbour interactions are included. This leads to a system of partial difference equations. The same equations are obtained if the two-dimensional Helmholtz equation is discretized using the central-difference approximation for the Laplacian. The corresponding lattice Green’s function, \( g_{mn} \), can be written down as a Fourier integral over a square, \( B_1 \). If propagating lattice waves can exist (this is the situation of most interest), then the integrand is singular along a certain closed curve within \( B_1 \); this singularity must be treated properly in order that \( g_{mn} \) be ‘outgoing’ at infinity. This leads to a far-field analysis of \( g_{mn} \).

We describe three methods for calculating the far-field behaviour of \( g_{mn} \). The first method (see Section 4.1) is due to Koster [15]. It begins by writing \( g_{mn} \) as a three-dimensional integral followed by a stationary-phase argument. This approach is described in textbooks, but the argument given is incomplete; we show how this can be remedied, and then use the three-dimensional method of stationary phase (as described in the book of Bleistein and Handelsman [2]).

Second, in Section 4.2, we describe a method that goes back to Lifshitz [16]. (We have not found a description in English of his method.) The basic idea is to make a change of variables in the double integral for \( g_{mn} \). The inner integral is non-singular, and can be estimated by the standard one-dimensional method of stationary phase. The outer integral is replaced by a double integral, which is then estimated using the two-dimensional method of stationary phase.

Third, in Section 4.3, we use an integral representation for \( g_{mn} \) as a single infinite integral of Lipschitz–Hankel type (the integrand contains the product of an exponential and two Bessel functions). This is convenient along the diagonal, where \( m = n \), because it yields an explicit formula for \( g_{mn} \) as a single Legendre function of the second kind. The far-field behaviour of this function is shown to agree precisely with that obtained using the other two methods.

In Section 5, we obtain the low-frequency behaviour of \( g_{mn} \), using Mellin-transform techniques. Once the behaviour of \( g_{mn} \) is known, we can begin to build a discrete scattering theory. Thus, we can use discrete versions of Green’s theorems [8, 6] and discrete layer potentials [14, 22] in order to study the interaction of lattice waves with finite-sized defects in the lattice: this is the subject of ongoing work.

2. Lattice dynamics

Consider the two-dimensional wave equation. For time-harmonic solutions, with a time dependence of \( e^{-\imath \omega t} \), we obtain the Helmholtz equation,

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\omega^2}{c^2} u = 0,
\]

for \( u(x,y) \), where \( \epsilon \) is a constant.

Now, consider a uniform mesh (or lattice) and write

\[
u_{mn} = u(mh, nh),
\]

where \( h \) is a constant and \( m \) and \( n \) are integers. Then, using central-difference approximations for the partial derivatives in Eq. (1), we obtain

\[
(\Delta u)(m, n) \equiv u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{mn} + k^2 u_{mn} = 0,
\]

where \( k = \omega h/c \).

Suppose that Eq. (2) holds for all integers \( m \) and \( n \); we write \( (m, n) \in \mathbb{Z}^2 \), the set of all points in the plane with integer coordinates. Then, solutions of Eq. (2) are given by

\[
u_{mn} = \exp\{\imath(m\xi + n\eta)\},
\]

where \( \xi \) and \( \eta \) solve

\[
\sigma(\xi, \eta; k) = 0
\]

and the symbol, \( \sigma \), is given by
\[\sigma(\zeta, \eta; k) = k^2 - 4 + 2 \cos \zeta + 2 \cos \eta \]
\[= k^2 - 4 \sin^2 \frac{1}{2} \zeta - 4 \sin \frac{1}{2} \eta \]
\[= k^2 - 8 + 4 \cos^2 \frac{1}{2} \zeta + 4 \cos^2 \frac{1}{2} \eta \]
\[= k^2 - 8 + 4 \cos((\zeta + \eta)/2) \cos((\zeta - \eta)/2); \]

evidently, there are no real solutions when \(k^2 > 8\). When \(k^2 = 8\), the solution Eq. (3) reduces to \(u_{mn} = (-1)^{m+n}\). When they exist, solutions Eq. (3) are called lattice waves [3, §24]. For more details, see [4] and [23, §4].

The solution Eq. (3) is \(2\pi\)-periodic with respect to \(\zeta \) and \(\eta\), so we can suppose that
\[-\pi < \zeta \leq \pi \quad \text{and} \quad -\pi < \eta \leq \pi;\]
this is known as the first Brillouin zone (later, we denote this square by \(B_1\)).

Suppose that \((\zeta, \eta) = (\zeta_0, \eta_0)\) solves Eq. (4) with \(k^2 < 8\). Then, \((-\zeta_0, \eta_0), (\zeta_0, -\eta_0)\) and \((-\zeta_0, -\eta_0)\) are also solutions. Hence, we can assume that
\[0 \leq \zeta_0 \leq \pi \quad \text{and} \quad 0 \leq \eta_0 \leq \pi. \tag{9}\]

Denote this square by \(B_4\); it has corners at \(A(\pi, 0), B(\pi, \pi), C(0, \pi)\) and \(O(0, 0)\) in the \(\zeta-\eta\) plane. Notice that the term \(\cos((\zeta - \eta)/2)\) in Eq. (8) is non-negative in \(B_4\).

The solutions of Eq. (4) define a closed curve in \(B_1\). This curve can be parametrized easily. We identify two cases, depending on the value of \(k^2\):

Case 1: \(k^2 \leq 4\). Eq. (6) shows that solutions of Eq. (4) in \(B_4\) are given by
\[\sin \frac{1}{2} \zeta = \frac{1}{2} k \cos \theta \quad \text{and} \quad \sin \frac{1}{2} \eta = \frac{1}{2} k \sin \theta \tag{10}\]
for \(0 \leq \theta \leq \frac{1}{4} \pi\). Examination of the sign of \(\cos((\zeta + \eta)/2)\) in Eq. (8) shows that all solutions lie in the triangle \(OAC\); there are no solutions in the other half of \(B_4\).

Case 2: \(4 < k^2 < 8\). Eq. (7) shows that solutions of Eq. (4) in \(B_4\) are given by
\[\cos \frac{1}{2} \zeta = \frac{1}{2} \sqrt{8 - k^2} \cos \theta' \quad \text{and} \quad \cos \frac{1}{2} \eta = \frac{1}{2} \sqrt{8 - k^2} \sin \theta' \]
for \(0 \leq \theta' \leq \frac{1}{4} \pi\). These solutions lie in the triangle \(ABC\).

3. Lattice Green’s function

In Section 2, we considered solutions of \((\mathscr{A}u)(m, n) = 0\) for all \((m, n) \in \mathbb{Z}^2\). Now, we suppose that the lattice is forced at one grid point. This point can be taken to be the origin because of the periodicity of the lattice. Thus, we consider
\[\mathcal{G}(\zeta, \eta) = \delta_{0m} \delta_{0n} \quad \text{for all } (m, n) \in \mathbb{Z}^2, \tag{11}\]
where \(\delta_{ij}\) is the Kronecker delta; any solution \(g_{mn}\) may be called a lattice Green’s function. Define a function \(\mathcal{G}\) by
\[\mathcal{G}(\zeta, \eta) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} g_{mn} e^{-i(m\zeta + n\eta)} \]
for \(-\pi < \zeta \leq \pi \) and \(-\pi < \eta \leq \pi\). Thus,
\[g_{mn} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \mathcal{G}(\zeta, \eta) e^{i(m\zeta + n\eta)} d\zeta d\eta \]
and
\[\langle \mathcal{G} \rangle (m, n) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \sigma(\zeta, \eta; k) \mathcal{G}(\zeta, \eta) e^{i(m\zeta + n\eta)} d\zeta d\eta, \]
where $\sigma$ is defined by Eq. (5). This equation and Eq. (11) imply that $\sigma \theta = 1$, whence

$$g_{mn} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{e^{i(m\xi + n\eta)}}{\sigma(\xi, \eta; k)} \, d\xi \, d\eta. \tag{12}$$

As $\sigma(\xi, \eta; k)$ is even in $\xi$ and in $\eta$, we obtain

$$g_{mn} = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{\cos m\xi \cos n\eta}{\sigma(\xi, \eta; k)} \, d\xi \, d\eta,$$

which shows that $g_{mn}$ is even in $m$ and in $n$; hence, we can assume that $m \geq 0$ and $n \geq 0$. Also, interchanging $m$ and $n$, and $\xi$ and $\eta$, shows that $g_{mn} = g_{nm}$.

The formula Eq. (12) is well known. See, for example, [11, Eq. (5.31)].

The Green’s function for a discrete waveguide, with $g_{nn} = 0$ at $m = \pm M$ for all $n$ and a finite positive integer $M$, has been used by Glaser [13]. Such a $g_{nn}$ can be called an exact Green’s function, as it satisfies some additional boundary conditions. For the calculation of some static exact Green’s functions, see [27].

4. The far-field behaviour of $g_{nn}$

In order to build a scattering theory, we need to know the far-field behaviour of the Green’s function. Thus, we require the behaviour of $g_{nn}$ as $R \to \infty$ where $R = \sqrt{m^2 + n^2}$.

Now, formulas such as Eq. (12) have been studied extensively: changes in the difference relation Eq. (2) lead to different symbols. The far-field properties of the corresponding Green’s function depend crucially on the zeros of $\sigma$ within the square of integration, $B_1$. If $\sigma \neq 0$ in $B_1$, then $g_{nn}$ decays exponentially with $R$ [9, p. 404, 10, p. 82]; this is our situation when $k^2 > 8$.

More generally, $\sigma$ will vanish at places within $B_1$, implying that the integrand in Eq. (12) has singularities. For certain equations, including the discrete form of Laplace’s equation (put $k = 0$ in Eq. (2)), $\sigma$ has a non-integrable singularity at the origin, and so the formula Eq. (12) must be modified [28, 21].

Returning to our specific $g_{nn}$, suppose that $k^2 < 8$. Then $\sigma$ in Eq. (12) vanishes along certain curves in $B_1$. We have to specify how to handle the corresponding singularities. Physically, we seek a solution for $g_{nm}$ that is outgoing at infinity.

4.1. The method of Koster

One standard approach begins by giving the wavenumber a small positive imaginary part: replace $k^2$ by

$$k^2 + i\delta, \quad \text{with } 0 < \delta \ll 1, \tag{13}$$

and let $\delta \to 0$ at the end of the calculation. Then, use an integral representation for $(\sigma + i\delta)^{-1}$, where $\sigma(\xi, \eta; k^2)$ is real. Koster [15] used the formula

$$\frac{1}{\sigma + i\delta} = -i \int_0^\infty e^{i(\sigma + i\delta)\zeta} \, d\zeta \tag{14}$$

in Eq. (12), giving

$$g_{nn} = \frac{1}{i(2\pi)^2} \lim_{\delta \to 0+} \int_{-\pi}^\pi \int_{-\pi}^\pi \int_0^\infty e^{-\delta\zeta} e^{iR(\xi \cos \alpha + \eta \sin \alpha) + i\zeta} \, d\xi \, d\zeta \, d\eta, \tag{15}$$

where $m = R\cos \alpha$ and $n = R\sin \alpha$; we can assume that $0 \leq \alpha \leq \frac{1}{2}\pi$. Then, Koster ‘follows the method of stationary phases and assumes that the principal contribution to the integral comes from that region where the variation of the exponent is small’ [15, p. 1440]. However, it is not immediately clear how to justify this assumption, because the large parameter $R$ is not a factor in the exponent. Instead, we simply replace Eq. (14) by

$$\frac{1}{\sigma + i\delta} = -iR \int_0^\infty e^{iR(\sigma + i\delta)\zeta} \, d\zeta;$$
when substituted in Eq. (12), we obtain

$$g_{mn} = \frac{R}{i(2\pi)^2} \lim_{\varepsilon \to 0^+} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{0}^{\infty} e^{-\varepsilon \sigma} e^{iR\Phi(\xi, \eta, \zeta)} d\xi d\eta,$$

(16)

where

$$\Phi(\xi, \eta, \zeta) = \xi \cos \alpha + \eta \sin \alpha + \xi \sigma(\xi, \eta, k^2)$$

is real and we have put

$$\delta = \varepsilon / R \text{ with } 0 < \varepsilon \ll 1.$$  

The integral in Eq. (16) is amenable to the three-dimensional method of stationary phase. Thus, from [2, Eq. (8.4.44)], we obtain

$$g_{mn} \sim \frac{R}{i(2\pi)^2} \left( \frac{2\pi}{R} \right)^{3/2} \exp \left\{ iR\Phi(x_0) + \frac{i}{2} \pi \text{sign} A \right\} \sqrt{|\det A|},$$

as $R \to \infty$, where $x_0 = (\xi_0, \eta_0, \zeta_0)$ is a relevant point of stationary phase, the $3 \times 3$ matrix $A$ has entries

$$A_{ij} = \frac{\partial^2 \Phi}{\partial \xi_i \partial \xi_j} \text{ evaluated at } x_0,$$

with $\xi_1 = \xi$, $\xi_2 = \eta$ and $\xi_3 = \zeta$, and $\text{sign} A$ is the signature of $A$ (equal to the number of positive eigenvalues of $A$ minus the number of negative eigenvalues).

To find $x_0$, we put $\partial \Phi / \partial \xi_i = 0$ for $i = 1, 2, 3$, giving three equations,

$$\sigma(\xi_0, \eta_0, k^2) = 0, \quad \cos \alpha - 2\xi_0 \sin \xi_0 = 0, \quad \sin \alpha - 2\xi_0 \sin \eta_0 = 0.$$  

(17)

The first of these shows that the pair $(\xi_0, \eta_0)$ corresponds to a propagating lattice wave; see Eq. (4). Hence, $R\Phi(x_0) = m\xi_0^2 + m\eta_0$. The other two equations in Eq. (17) determine the (artificial) parameter, $\xi_0$, and the direction of propagation: the direction of observation (given by $\alpha$) coincides with the direction of the group velocity. Thus,

$$2\xi_0 = (\sin^2 \xi_0 + \sin^2 \eta_0)^{-1/2} \text{ and } \sin \alpha \sin \xi_0 = \cos \alpha \sin \eta_0.$$  

(18)

Relevant points $x_0$ have $\xi_0 > 0$, so that Eq. (17)$_{2,3}$ give $\sin \xi_0 \geq 0$ and $\sin \eta_0 \geq 0$. (Recall that $0 \leq \alpha \leq \frac{1}{2} \pi$.) Given a solution $x_0$ with $0 \leq \xi_0 < \pi$ and $0 \leq \eta_0 < \pi$, we see that Eq. (17)$_{2,3}$ are also satisfied if we replace $\xi_0$ by $\pi - \xi_0$, or $\eta_0$ by $\pi - \eta_0$, or both; however, these replacements do not satisfy Eq. (17)$_1$. Consequently, there is only one relevant point of stationary phase, $x_0$. For $A$, we obtain

$$A = -2 \begin{pmatrix} \zeta_0 \cos \zeta_0 & 0 & \sin \zeta_0 \\ 0 & \zeta_0 \cos \eta_0 & \sin \eta_0 \\ \sin \zeta_0 & \sin \eta_0 & 0 \end{pmatrix},$$

whence $\det A = 8\zeta_0(\cos \zeta_0 + \cos \eta_0)(1 - \cos \zeta_0 \cos \eta_0)$. We notice that $\det A = 0$ when $k^2 = 4$, so that the stationary-phase calculation must be modified for this special case.

The eigenvalues of $A$, $\lambda_i$ with $i = 1, 2, 3$, are given by solving the cubic, $\det(A - \lambda I) = 0$. They are all real. The product $\lambda_1 \lambda_2 \lambda_3 = \det A$. Elementary considerations show that $\text{sign} A = -1$ when $0 < k^2 < 4$ and $\text{sign} A = 1$ when $4 < k^2 < 8$.

For more explicit results, suppose that $0 < k^2 < 4$ so that we can use Eq. (10),

$$2 \sin \frac{1}{2} \zeta_0 = k \cos \theta_0 \quad \text{and} \quad 2 \sin \frac{1}{2} \eta_0 = k \sin \theta_0.$$

Then, $\theta_0$ is determined from Eq. (18)$_2$:

$$\tan \theta_0 = \sqrt{-\lambda + \sqrt{\lambda^2 + \tan^2 \alpha}} \text{ with } \lambda = \frac{2(1 - \tan^2 \alpha)}{4 - k^2}.$$  

(19)

We find that $\det A > 0$,
\[ \det A = k(4 - k^2)(2 - k^2 \sin^2 \theta_0 \cos^2 \theta_0)\{4 - k^2(\cos^4 \theta_0 + \sin^4 \theta_0)\}^{-1/2}. \]

Finally, we obtain
\[ g_{mm} \sim -\frac{e^{i(m\xi_0 + n\eta_0)}}{\sqrt{2\pi kR}} \frac{e^{i/4\{4 - k^2(\cos^4 \theta_0 + \sin^4 \theta_0)\}^{1/4}}}{\sqrt{(4 - k^2)(2 - k^2 \sin^2 \theta_0 \cos^2 \theta_0)}} \quad \text{as } R \to \infty. \tag{20} \]

Apart from a constant multiplicative factor, the formula Eq. (20) agrees with one on p. 84 of Economou’s book [11], where a paper by Callaway [5] is cited. In fact, Callaway’s paper contains the analogous result for a three-dimensional cubic lattice. See also [26] and [20, pp. 376–381].

The approximation Eq. (20) simplifies on the diagonal, where \( m = n \). Then, \( R = n\sqrt{2}, \theta_0 = \pi/4, \xi_0 = \eta_0, \cos \xi_0 = (4 - k^2)/4 \) and
\[ \cos 2\xi_0 = 1 - k^2 + k^4/8, \]
so that Eq. (20) reduces to
\[ g_{mm} \sim -\frac{e^{i\xi_0 \xi_0}}{\sqrt{\pi kn(4 - k^2)(8 - k^2)^{1/4}}} \quad \text{as } n \to \infty. \tag{21} \]

4.2. The method of Lifshitz

For an alternative method, return to Eq. (12), the double integral over the square \( B_1 \). Let \( B' \) denote the smaller square, with corners at \( (\xi, \eta) = (\pm \pi, 0) \) and \( (0, \pm \pi) \), and put \( B'' = B_1 \setminus B' \). Suppose that \( 0 < k^2 < 4 \) so that all zeros of \( \sigma \) are in \( B'' \) and not in \( B' \). Then,
\[ g_{mm} = g'_{mn} + g''_{mn}, \]
where
\[ g'_{mn} = \frac{1}{(2\pi)^2} \int_{B'} \frac{e^{i(m\xi + n\eta)}}{\sigma(\xi, \eta; k)} \, d\xi d\eta \quad \text{and} \quad g''_{mn} = \frac{1}{(2\pi)^2} \int_{B''} \frac{e^{i(m\xi + n\eta)}}{\sigma(\xi, \eta; k)} \, d\xi d\eta. \]

As \( \sigma \neq 0 \) in \( B'' \), it follows that \( g''_{mn} = O(R^{-1}) \) as \( R \to \infty \). (This is the two-dimensional method of stationary phase when there are no points of stationary phase; see [2, Eq. (8.4.2)].) For \( g'_{mn} \), we make a change of variables, motivated by Eq. (10):
\[ 2 \sin \frac{1}{2} \xi = r \cos \theta \quad \text{and} \quad 2 \sin \frac{1}{2} \eta = r \sin \theta. \]

With these variables, \( \sigma = k^2 - r^2 \). Taking account of the Jacobian, we obtain
\[ g'_{mn} = \frac{1}{\pi^2} \int_0^2 \frac{F(r; R)r}{k^2 - r^2} \, dr = \frac{R}{\pi^2} \lim_{\epsilon \to 0} \int_0^\infty \int_0^2 e^{-\epsilon \xi} F(r; R)e^{i(R(k^2-r^2)\xi)} r \, dr \, d\xi, \tag{22} \]
with
\[ F(r; R) = \int_0^\pi \frac{e^{i\Psi(r, \theta)}}{\sqrt{(4 - r^2 \cos^2 \theta)(4 - r^2 \sin^2 \theta)}} \, d\theta \tag{23} \]
and \( \Psi(r, \theta) = \xi \cos \theta + \eta \sin \theta \). Note that \( F \) is real.

The idea of changing the variables was used by Lifshitz [16]; see also \([17, \text{p. 721}, 18, \text{p. 233}] \) and [1]. To estimate \( F(r, R) \) for large \( R \), we use the ordinary one-dimensional method of stationary phase. We have
\[ \frac{\partial \Psi}{\partial \theta} = \frac{2r \cos \theta \sin x}{\sqrt{4 - r^2 \sin^2 \theta}} - \frac{2r \sin \theta \cos x}{\sqrt{4 - r^2 \cos^2 \theta}}. \]

(24)

This vanishes at \( \theta_0(r) \) and \( \theta_0(r) - \pi \), with \( 0 \leq \theta_0(r) < \frac{\pi}{2} \). Thus, there are two points of stationary phase within the range of integration. Also,

\[ \frac{\partial^2 \Psi}{\partial \theta^2} = 2(r^2 - 4) \left( \frac{\cos \theta \cos x}{(4 - r^2 \cos^2 \theta)^{3/2}} + \frac{\sin \theta \sin x}{(4 - r^2 \sin^2 \theta)^{3/2}} \right) \equiv \Psi_{\theta \theta}(r, \theta). \]

(25)

Let \( \mathcal{P}_0(r) = \Psi_{\theta \theta}(r, \theta_0(r)) \). Then,

\[ \mathcal{P}_0(r) < 0 \quad \text{and} \quad \Psi_{\theta \theta}(r, \theta_0(r) - \pi) = -\mathcal{P}_0(r) > 0. \]

Hence, from \([2, \text{Eq. (6.1.5)}]\),

\[ F(r; R) \sim \frac{\sqrt{2\pi}}{\sqrt{-R\mathcal{P}_0(r)}} \frac{e^{ir\Psi_0(r) - iz/4} + e^{-ir\Psi_0(r) + iz/4}}{\sqrt{(4 - r^2 \cos^2 \theta_0(r))(4 - r^2 \sin^2 \theta_0(r))}} \]

as \( R \to \infty \), for \( 0 < r < 2 \), where \( \Psi_0(r) = \Psi(r, \theta_0(r)) \). Then, Eq. (22) gives

\[ g'_{mn} \sim \frac{\sqrt{2\pi R}}{\pi^2} \lim_{\epsilon \to 0} \int_0^\infty \int_0^2 f(r)e^{-\epsilon \zeta} \left\{ e^{i\Phi_+(r, \zeta)}e^{-iz/4} + e^{i\Phi_-(r, \zeta)}e^{iz/4} \right\} r \, dr \, d\zeta, \]

(26)

where

\[ f(r) = \left\{ -\mathcal{P}_0(r) [4 - r^2 \cos^2 \theta_0(r)] [4 - r^2 \sin^2 \theta_0(r)] \right\}^{-1/2} \]

(27)

and

\[ \Phi_\pm(r, \zeta) = (k^2 - r^2)\zeta \pm \Psi(r, \theta_0(r)). \]

We now estimate the remaining double integral in Eq. (26) using the two-dimensional method of stationary phase. We have

\[ \frac{\partial \Phi_\pm}{\partial \zeta} = k^2 - r^2 = 0, \]

so that relevant points of stationary phase have \( r = k \). Then

\[ \frac{\partial \Phi_\pm}{\partial r} = -2r_\zeta \pm \frac{\partial \Psi}{\partial r} \bigg|_{\theta = \theta_0} \pm \frac{\partial \Psi}{\partial \theta} \bigg|_{\theta = \theta_0} \frac{d\theta_0}{dr} = 0. \]

(28)

The last term vanishes because of the definition of \( \theta_0(r) \). Also

\[ \frac{\partial \Psi}{\partial r} = \frac{2 \sin \theta \sin x}{\sqrt{4 - r^2 \sin^2 \theta}} + \frac{2 \cos \theta \cos x}{\sqrt{4 - r^2 \cos^2 \theta}}, \]

which is positive at \( \theta = \theta_0(r) \). Thus, to obtain a positive \( \zeta \), we must take the ‘+’ in Eq. (28): the term in Eq. (26) involving \( \Phi_- \) gives a negligible contribution compared to the \( \Phi_+ \) term. Notice that

\[ R\Phi_+(k, \zeta) = R\Psi(k, \theta_0) = m\zeta_0 + m\eta_0, \]

where \( \zeta_0, \eta_0 \) and \( \theta_0 \equiv \theta(k) \) are the same as in Section 4.1.

Thus, from \([2, \text{Eq. (8.4.44)}]\), we obtain

\[ g'_{mn} \sim \frac{2\pi}{\pi^2} \frac{f(k)k}{R} \frac{1}{\sqrt{|\det A|}} \exp\{iR\Phi_+(k, \zeta) - i\pi(1 - \text{sgn}A)/4\} \]

as \( R \to \infty \), where the \( 2 \times 2 \) matrix \( A \) has entries...
with \( \zeta_1 = r \) and \( \zeta_2 = \zeta \). We find
\[
A = \begin{pmatrix} A_{11} & -2k \\ -2k & 0 \end{pmatrix}
\]
so that \( \det A = -4k^2 \) and \( \text{sgn} A = 0 \). (The eigenvalues of \( A \) are real and their product equals \( \det A \); fortunately, we do not need to calculate \( A_{11} \).) Hence
\[
g_{mn} \sim \frac{\sqrt{2}}{\sin \pi R} e^{i(m \omega_0 + n \omega_0)} e^{-i \pi / 4} f(k) \text{ as } R \to \infty. \tag{29}
\]
Now, from Eq. (24), we have
\[
\cos \theta_0 \sin \varphi \sqrt{4 - k^2 \cos^2 \theta_0} = \sin \theta_0 \cos \varphi \sqrt{4 - k^2 \sin^2 \theta_0}
\]
which gives
\[
\frac{\cos \varphi}{\cos \theta_0} = \frac{\sqrt{4 - k^2 \cos^2 \theta_0}}{\sqrt{4 - k^2 (\cos^4 \theta_0 + \sin^4 \theta_0)}}.
\]
Then, using \( \varphi_0(k) = \varphi_{\omega_0}(k, \theta_0) \), Eqs. (25) and (27), some calculation gives
\[
f(k) = \frac{\{4 - k^2 (\cos^4 \theta_0 + \sin^4 \theta_0)\}^{1/4}}{2 \sqrt{k} \sqrt{(4 - k^2)(2 - k^2 \sin^2 \theta_0 \cos^2 \theta_0)}}.
\]
It follows that Eqs. (29) and (20) agree precisely.

4.3. An integral representation

As a by-product of Eq. (15), we can derive an integral representation for \( g_{mn} \) as a single integral. Thus, using Eq. (5) and the formula
\[
\int_{-\pi}^{\pi} e^{imz} e^{2iz \cos \zeta} d\zeta = 2\pi i^n J_m(2\zeta),
\]
twice, we obtain
\[
g_{mn} = i^{m+n-1} \lim_{\delta \to 0+} \int_{0}^{\infty} e^{i(k^2 - 4 + i\delta)J_m(2\zeta)J_n(2\zeta)} d\zeta, \tag{30}
\]
where \( J_m \) is a Bessel function. This formula is [7, Eq. (A1)]. The corresponding formula for \( k^2 > 8 \) is older; see [31, p. 368] or [30].

On the diagonal, where \( m = n \), the integral in Eq. (30) can be evaluated in terms of a Legendre function [32, p. 389],
\[
g_{nn} = \frac{(-1)^n}{2\pi i} \lim_{\delta \to 0+} Q_{n-1/2}(Z).
\]
Here, the complex quantity \( Z \) is given by
\[
Z = 1 + [\delta + i(4 - k^2)]^2 / 8
\]
\[
\simeq 1 - (4 - k^2)^2 / 8 + i\delta(4 - k^2) / 4
\]
for \( 0 < \delta \ll 1 \). Thus, for \( 0 < k^2 < 8 \), \( |\text{Re}Z| \ll 1 \) and \( \text{sgn}(\text{Im}Z) = \text{sgn}(4-k^2) \).
The function $Q_\nu(Z)$ is defined in the complex $Z$-plane, with a cut between $Z = -1$ and $Z = +1$. Thus, we require $Q_{n - 1/2}(\cos \varphi + i0)$ for $0 < k^2 < 4$ and $Q_{n - 1/2}(\cos \varphi - i0)$ for $4 < k^2 < 8$, where $\cos \varphi = 1 - (4 - k^2)^2/8$ so that $0 < \varphi < \pi/4$.

Suppose that $0 < k^2 < 4$ and $n$ is large. Then

$$g_{mn} = \frac{(-1)^n}{2\pi i} Q_{n-1/2}(\cos \varphi + i0)$$

and for $k > 4$ we obtain

$$H_0^{(2)}(z) = \frac{(-1)^n}{2\pi i} \frac{\pi}{2i} \left( \frac{\varphi}{\sin \varphi} \right)^{1/2} H_0^{(2)}(n\varphi)$$

as $n \to \infty$, where $H_0^{(2)}$ is a Hankel function and we have used the asymptotic approximation on p. 472 of Olver’s book [24]. Since

$$H_0^{(2)}(x) \sim \sqrt{2/(\pi x)} e^{-i(x-\pi/4)}$$

we obtain

$$g_{mn} \sim \frac{e^{i(x-\varphi)}}{2\sqrt{2\pi n \sin \varphi}}$$

as $n \to \infty$. (31)

As $\cos \varphi = 1 - (4 - k^2)^2/8$, we have

$$\cos(\pi - \varphi) = 1 - k^2 + k^4/8 \quad \text{and} \quad \sin \varphi = (k/8)(4 - k^2) \sqrt{8 - k^2}$$

Then, we see that Eq. (31) agrees precisely with Eq. (21).

5. The low-frequency behaviour of $g_{mn}$

It is well known that the integral Eq. (12) defining $g_{mn} \equiv g_{mn}(k^2)$ diverges when $k^2 = 0$. Here, we investigate this divergence, using Mellin-transform techniques [2]. Put $\kappa = k^2$ and consider

$$\tilde{g}(z) = \int_0^\infty \kappa^{z-1} g_{mn}(\kappa) \, d\kappa.$$ 

This defines an analytic function of $z$ within the strip $0 < \text{Re} \, z < 1$. The inversion contour lies in this strip. We shall see that there is a double pole at $z = 0$, implying that $g_{mn}$ is logarithmically singular at $k = 0$. We find that

$$\tilde{g}(z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} \int_{-\pi}^{+\pi} e^{i(m\xi+n\eta)} I(\xi, \eta; z) \, d\xi \, d\eta,$$

where

$$I(\xi, \eta; z) = \lim_{\delta \to 0} \frac{\kappa^{z-1}}{\kappa - z + i\delta}$$

and we have used Eqs. (6) and (13). A standard contour-integral calculation gives

$$I(\xi, \eta; z) = -\frac{\pi e^{i\xi}}{\sin \pi z} \gamma^{-1},$$

so that

$$\tilde{g}(z) = -\frac{\pi e^{i\xi}}{\sin \pi z} \tilde{h}(z)$$

with

$$\tilde{h}(z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} \int_{-\pi}^{+\pi} e^{i(m\xi+n\eta)} \gamma^{-1} \, d\xi \, d\eta.$$
We see that \( \tilde{h}(0) \) is divergent. This divergence is caused by the behaviour of the integrand near \( \zeta = \eta = 0 \), where \( \gamma \approx \xi^2 + \eta^2 = \varrho^2 \), say. We consider a small disc \( \varrho < a \) (inside \( B_1 \)) and put \( \zeta = \varrho \cos \vartheta \) and \( \eta = \varrho \sin \vartheta \). This gives

\[
\tilde{h}(z) \approx \frac{1}{(2\pi)^2} \int_0^a \int_0^{2\pi} e^{iR\varrho \cos(\vartheta - z)} \varrho^{2(z-1)} \varrho \, d\vartheta \, d\varrho
\]

\[
= \frac{1}{2\pi} \int_0^a J_0(R\varrho) \varrho^{2z-1} \, d\varrho
\]

\[
\approx \frac{1}{2\pi} J_1(aR)
\]

for \( z \) near zero. Letting \( a \to 0 \) gives the approximation \( \tilde{h}(z) \approx (4\pi)^{-1} \), so that

\[
\tilde{g}(z) \approx -\frac{e^{iz\pi}}{4\pi \sin \pi z} \approx -\frac{1}{4\pi^2} \text{ near } z = 0.
\]

Finally, moving the inversion contour to the left, we pick up the residue at the pole giving

\[
g_{nn} \sim \frac{1}{2\pi} \log k \text{ as } k \to 0.
\]  

\[1\]

6. Discussion

We have investigated properties of the lattice Green’s function, \( g_{nn} \), for the simplest square lattice. The far-field behaviour is given by

\[
g_{nn} \sim (KR)^{-1/2} e^{iR(\zeta_0 \cos x + \eta_0 \sin x)} \tilde{G}(x; k^2) \text{ as } R = \sqrt{m^2 + n^2} \to \infty,
\]  

\[33\]

where \( m = R \cos x \) and \( n = R \sin x \), so that \( x \) gives the observation direction; the quantities \( \zeta_0, \eta_0 \) and \( \tilde{G} \) are known in terms of \( x \) and \( k^2 \). A corresponding Green’s function for the Helmholtz equation, Eq. (1), is

\[
G(x, y) = H_0^{(1)}(KR),
\]  

\[34\]

with \( K = \omega/c = k/h \) and \( R = \sqrt{x^2 + y^2} \); its far-field behaviour is given by

\[
G(x, y) \sim (KR)^{-1/2} e^{KR0} G_0 \text{ as } R \to \infty,
\]  

\[35\]

where \( x = \Re \cos \varphi, y = \Re \sin \varphi \) and \( G_0 \) is a known constant.

There are evident similarities and differences between Eqs. (33) and (35). For example, we see the same inverse square-root decay, but the lattice Green’s function is anisotropic: the behaviour of \( G \) does not depend on the direction \( x \).

From Eq. (34), we have \( G \approx \log(KR) \) as \( KR \to 0 \), so that \( G \) has a logarithmic singularity with respect to \( K \) and with respect to \( R \). On the other hand, \( g_{nn} \) is also logarithmically singular as \( k \to 0 \) (see Section 5) but \( g_{00} \) is finite (for \( k \neq 0 \)).

The methods described in Sections 4.1 and 4.2 generalize to more complicated lattices. In such generalizations, the associated curve (or curves or surfaces) in \( B_1 \) (see Section 2) may also become more complicated, and then it may become more difficult to identify the desired ‘outgoing’ solution; this issue was discussed in some detail by Maradudin [19, Appendix D].

In Section 4.3, we obtained an expression for \( g_{nn} \) as a Legendre function. Using the formula

\[
Q_n(x \pm i0) = Q_n(x) + \frac{1}{2\pi} \pi P_{n-1/2}(\cos \varphi) + 2i Q_{n-1/2}(\cos \varphi)
\]  

\[36\]

for \( 0 < k^2 < 4 \), where \( \cos \varphi = 1 - (4 - k^2)^2/8 \). This gives the real and imaginary parts of \( g_{nn} \) explicitly. For example,
\[ \text{Im}(g_{nn}) = (2\pi)^{-1}(-1)^{n+1} Q_{n-1/2}(\cos \varphi) \sim (2\pi)^{-1}(-1)^n \log(4 - k^2) \]  
(37)

as \( k^2 \to 4^+ \), using the approximation \( Q_n(x) \sim -\frac{1}{2} \log(1 - x) \) as \( x \to 1^- \) [24, p. 186, Eq. (15.08)]. The logarithmic behaviour seen in Eq. (37) is well known in solid-state physics, where it is identified with the van Hove singularities of the frequency spectrum; see [20, Chapter IV] for more information on this topic. Notice also that the properties

\[ g_{nn} = g_{|m|,|n|} = g_{mn} \]

combined with the definition Eq. (11) mean that we can construct \( g_{nn} \) recursively once we know \( g_{nn} \) for \( n = 0, 1, 2, \ldots \), and these values are given by Eq. (36).

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