Available online at www.sciencedirect.com
ScienceDirect
Wave Motion 43 (2006) 619–629
WAVE MOTION
www.elsevier.com/locate/wavemoti

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

Received 11 October 2005; received in revised form 23 May 2006; accepted 25 May 2006
Available online 7 July 2006

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.

Keywords: Lattice Green's function; Partial difference equations; Method of stationary phase; Mellin transforms

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.

* Tel.: +1 3032733895; fax: +1 3032733875.
E-mail address: pamartin@mines.edu.

0165-2125/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.wavemoti.2006.05.006

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_{nn} 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 $e^{-i\omega t}$, we obtain the Helmholtz equation,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\omega^2}{c^2} u = 0, \tag{1}$$

for $u(x,y)$, where c 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

$$(\mathscr{A}u)(m,n) \equiv u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{mn} + k^2 u_{mn} = 0, \tag{2}$$

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

$$u_{mn} = \exp\{i(m\xi + n\eta)\}, \tag{3}$$

where ξ and η solve

$$\sigma(\xi, \eta; k) = 0 \tag{4}$$

and the *symbol*, σ, is given by

$$\sigma(\xi,\eta;k) = k^2 - 4 + 2\cos\xi + 2\cos\eta \quad (5)$$
$$= k^2 - 4\sin^2\tfrac{1}{2}\xi - 4\sin^2\tfrac{1}{2}\eta \quad (6)$$
$$= k^2 - 8 + 4\cos^2\tfrac{1}{2}\xi + 4\cos^2\tfrac{1}{2}\eta \quad (7)$$
$$= k^2 - 4 + 4\cos([\xi+\eta]/2)\cos([\xi-\eta]/2); \quad (8)$$

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 2π-periodic with respect to ξ and η, so we can suppose that

$$-\pi < \xi \leqslant \pi \quad \text{and} \quad -\pi < \eta \leqslant \pi;$$

this is known as the *first Brillouin zone* (later, we denote this square by B_1).

Suppose that $(\xi,\eta) = (\xi_0,\eta_0)$ solves Eq. (4) with $k^2 < 8$. Then, $(-\xi_0,\eta_0)$, $(\xi_0,-\eta_0)$ and $(-\xi_0,-\eta_0)$ are also solutions. Hence, we can assume that

$$0 \leqslant \xi_0 \leqslant \pi \quad \text{and} \quad 0 \leqslant \eta_0 \leqslant \pi. \quad (9)$$

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 ξ-η plane. Notice that the term $\cos([\xi-\eta]/2)$ 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: $k^2 \leqslant 4$. Eq. (6) shows that solutions of Eq. (4) in B_4 are given by

$$\sin\tfrac{1}{2}\xi = \tfrac{1}{2}k\cos\theta \quad \text{and} \quad \sin\tfrac{1}{2}\eta = \tfrac{1}{2}k\sin\theta \quad (10)$$

for $0 \leqslant \theta \leqslant \frac{1}{2}\pi$. Examination of the sign of $\cos([\xi+\eta]/2)$ 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

$$\cos\tfrac{1}{2}\xi = \tfrac{1}{2}\sqrt{8-k^2}\cos\theta' \quad \text{and} \quad \cos\tfrac{1}{2}\eta = \tfrac{1}{2}\sqrt{8-k^2}\sin\theta'$$

for $0 \leqslant \theta' \leqslant \frac{1}{2}\pi$. 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

$$(\mathscr{A}g)(m,n) = \delta_{0m}\delta_{0n} \text{ for all } (m,n) \in \mathbb{Z}^2, \quad (11)$$

where δ_{ij} is the Kronecker delta; any solution g_{mn} may be called a *lattice Green's function*. Define a function $\mathscr{G}$ by

$$\mathscr{G}(\xi,\eta) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} g_{mn}\mathrm{e}^{-\mathrm{i}(m\xi+n\eta)}$$

for $-\pi < \xi \leqslant \pi$ and $-\pi < \eta \leqslant \pi$. Thus,

$$g_{mn} = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\mathscr{G}(\xi,\eta)\mathrm{e}^{\mathrm{i}(m\xi+n\eta)}\,\mathrm{d}\xi\,\mathrm{d}\eta$$

and

$$(\mathscr{A}g)(m,n) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\sigma(\xi,\eta;k)\mathscr{G}(\xi,\eta)\mathrm{e}^{\mathrm{i}(m\xi+n\eta)}\,\mathrm{d}\xi\,\mathrm{d}\eta,$$

where σ is defined by Eq. (5). This equation and Eq. (11) imply that $\sigma\mathscr{G} = 1$, whence

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

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

$$g_{mn} = \frac{1}{\pi^2}\int_{0}^{\pi}\int_{0}^{\pi}\frac{\cos m\xi\cos n\eta}{\sigma(\xi,\eta;k)}\,\mathrm{d}\xi\,\mathrm{d}\eta,$$

which shows that g_{mn} is even in m and in n; hence, we can assume that $m \geqslant 0$ and $n \geqslant 0$. Also, interchanging m and n, and ξ and η, 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 $g_{mn} = 0$ at $m = \pm M$ for all n and a finite positive integer M, has been used by Glaser [13]. Such a g_{mn} 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_{mn}

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_{mn} 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 σ within the square of integration, B_1. If $\sigma \neq 0$ in B_1, then g_{mn} decays exponentially with R [9, p. 404, 10, p. 82]; this is our situation when $k^2 > 8$.

More generally, σ 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)), σ has a non-integrable singularity at the origin, and so the formula Eq. (12) must be modified [28, 21].

Returning to our specific g_{mn}, suppose that $k^2 < 8$. Then σ 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_{mn} 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

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

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

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

in Eq. (12), giving

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

where $m = R\cos\alpha$ and $n = R\sin\alpha$; we can assume that $0 \leqslant \alpha \leqslant \frac{1}{2}\pi$. 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

$$\frac{1}{\sigma+\mathrm{i}\delta} = -\mathrm{i}R\int_0^\infty \mathrm{e}^{\mathrm{i}R(\sigma+\mathrm{i}\delta)\zeta}\mathrm{d}\zeta;$$

when substituted in Eq. (12), we obtain

$$g_{mn} = \frac{R}{\mathrm{i}(2\pi)^2} \lim_{\varepsilon\to 0+} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{0}^{\infty} \mathrm{e}^{-\varepsilon\zeta} \mathrm{e}^{\mathrm{i}R\Phi(\xi,\eta,\zeta)} \mathrm{d}\zeta\,\mathrm{d}\xi\,\mathrm{d}\eta, \tag{16}$$

where

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

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

$$g_{mn} \sim \frac{R}{\mathrm{i}(2\pi)^2} \left(\frac{2\pi}{R}\right)^{3/2} \frac{\exp\{\mathrm{i}R\Phi(\mathbf{x}_0) + \frac{1}{4}\mathrm{i}\pi\,\mathrm{sig}A\}}{\sqrt{|\det A|}}$$

as $R \to \infty$, where $\mathrm{x}_0 = (\xi_0, \eta_0, \zeta_0)$ is a relevant point of stationary phase, the 3×3 matrix A has entries

$$A_{ij} = \frac{\partial^2\Phi}{\partial\xi_i\partial\xi_j} \text{ evaluated at } \mathbf{x}_0,$$

with $\xi_1 = \xi$, $\xi_2 = \eta$ and $\xi_3 = \zeta$, and sig$A$ 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,

$$\sigma(\xi_0,\eta_0;k^2) = 0, \quad \cos\alpha - 2\zeta_0\sin\xi_0 = 0, \quad \sin\alpha - 2\zeta_0\sin\eta_0 = 0. \tag{17}$$

The first of these shows that the pair (ξ_0, η_0) corresponds to a propagating lattice wave; see Eq. (4). Hence, $R\Phi(\mathbf{x}_0) = m\xi_0 + n\eta_0$. The other two equations in Eq. (17) determine the (artificial) parameter, ζ_0, and the direction of propagation: the direction of observation (given by α) coincides with the direction of the group velocity. Thus,

$$2\zeta_0 = (\sin^2\xi_0 + \sin^2\eta_0)^{-1/2} \text{ and } \sin\alpha\sin\xi_0 = \cos\alpha\sin\eta_0. \tag{18}$$

Relevant points $\mathbf{x}_0$ have $\zeta_0 > 0$, so that Eq. $(17)_{2,3}$ give $\sin\xi_0 \geqslant 0$ and $\sin\eta_0 \geqslant 0$. (Recall that $0 \leqslant \alpha \leqslant \frac{1}{2}\pi$.) Given a solution $\mathbf{x}_0$ with $0 \leqslant \xi_0 < \pi$ and $0 \leqslant \eta_0 < \pi$, we see that Eq. $(17)_{2,3}$ are also satisfied if we replace ξ_0 by $\pi - \xi_0$, or η_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, $\mathbf{x}_0$. For A, we obtain

$$A = -2\begin{pmatrix} \zeta_0\cos\xi_0 & 0 & \sin\xi_0 \\ 0 & \zeta_0\cos\eta_0 & \sin\eta_0 \\ \sin\xi_0 & \sin\eta_0 & 0 \end{pmatrix},$$

whence $\det A = 8\zeta_0(\cos\xi_0 + \cos\eta_0)(1 - \cos\xi_0\cos\eta_0)$. 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, λ_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 $\mathrm{sig}A = -1$ when $0 < k^2 < 4$ and $\mathrm{sig}A = 1$ when $4 < k^2 < 8$.

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

$$2\sin\tfrac{1}{2}\xi_0 = k\cos\theta_0 \quad \text{and} \quad 2\sin\tfrac{1}{2}\eta_0 = k\sin\theta_0.$$

Then, θ_0 is determined from Eq. $(18)_2$:

$$\tan\theta_0 = \sqrt{-\lambda + \sqrt{\lambda^2 + \tan^2\alpha}} \text{ with } \lambda = \frac{2(1 - \tan^2\alpha)}{4 - k^2}. \tag{19}$$

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

$$g_{mn} \sim -\frac{\mathrm{e}^{\mathrm{i}(m\xi_0+n\eta_0)}}{\sqrt{2\pi kR}}\frac{\mathrm{e}^{\mathrm{i}\pi/4}\{4-k^2(\cos^4\theta_0+\sin^4\theta_0)\}^{1/4}}{\sqrt{(4-k^2)(2-k^2\sin^2\theta_0\cos^2\theta_0)}} \text{ as } R\to\infty. \tag{20}$$

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

$$g_{nn} \sim -\frac{\mathrm{e}^{2\mathrm{i}n\xi_0}\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{\pi kn(4-k^2)}(8-k^2)^{1/4}} \text{ as } n\to\infty. \tag{21}$$

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 σ are in B' and not in B''. Then,

$$g_{mn} = g'_{mn} + g''_{mn},$$

where

$$g'_{mn} = \frac{1}{(2\pi)^2}\int_{B'}\frac{\mathrm{e}^{\mathrm{i}(m\xi+n\eta)}}{\sigma(\xi,\eta;k)}\mathrm{d}\xi\mathrm{d}\eta \text{ and } g''_{mn} = \frac{1}{(2\pi)^2}\int_{B''}\frac{\mathrm{e}^{\mathrm{i}(m\xi+n\eta)}}{\sigma(\xi,\eta;k)}\mathrm{d}\xi\,\mathrm{d}\eta.$$

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):

$$2\sin\tfrac{1}{2}\xi = r\cos\theta \quad \text{and} \quad 2\sin\tfrac{1}{2}\eta = r\sin\theta.$$

With these variables, $\sigma = k^2 - r^2$. Taking account of the Jacobian, we obtain

$$\begin{aligned} g'_{mn} &= \frac{1}{\pi^2}\int_0^2 \frac{F(r;R)r}{k^2-r^2}\mathrm{d}r \\ &= \frac{R}{\mathrm{i}\pi^2}\lim_{\varepsilon\to 0}\int_0^\infty\int_0^2 \mathrm{e}^{-\varepsilon\zeta}F(r;R)\mathrm{e}^{\mathrm{i}R(k^2-r^2)\zeta}r\,\mathrm{d}r\,\mathrm{d}\zeta, \end{aligned} \tag{22}$$

with

$$F(r;R) = \int_{-\pi}^{\pi}\frac{\mathrm{e}^{\mathrm{i}R\Psi(r,\theta)}\mathrm{d}\theta}{\sqrt{(4-r^2\cos^2\theta)(4-r^2\sin^2\theta)}} \tag{23}$$

and $\Psi(r,\theta) = \xi\cos\alpha + \eta\sin\alpha$. Note that F is real.

The idea of changing the variables was used by Lifshitz [16]; see also [17, p. 721, 18, p. 233] and [1].

To estimate $F(r; R)$ for large R, we use the ordinary one-dimensional method of stationary phase. We have

$$\frac{\partial \Psi}{\partial \theta} = \frac{2r\cos\theta\sin\alpha}{\sqrt{4 - r^2\sin^2\theta}} - \frac{2r\sin\theta\cos\alpha}{\sqrt{4 - r^2\cos^2\theta}}. \tag{24}$$

This vanishes at $\theta_0(r)$ and $\theta_0(r) - \pi$, with $0 \leqslant \theta_0(r) < \frac{1}{2}\pi$. Thus, there are two points of stationary phase within the range of integration. Also,

$$\frac{\partial^2 \Psi}{\partial \theta^2} = 2r(r^2 - 4)\left\{\frac{\cos\theta\cos\alpha}{(4 - r^2\cos^2\theta)^{3/2}} + \frac{\sin\theta\sin\alpha}{(4 - r^2\sin^2\theta)^{3/2}}\right\} \equiv \Psi_{\theta\theta}(r,\theta). \tag{25}$$

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

$$\mathscr{P}_0(r) < 0 \text{ and } \Psi_{\theta\theta}(r, \theta_0(r) - \pi) = -\mathscr{P}_0(r) > 0.$$

Hence, from [2, Eq. (6.1.5)],

$$F(r;R) \sim \frac{\sqrt{2\pi}}{\sqrt{-R\mathscr{P}_0(r)}} \frac{\mathrm{e}^{\mathrm{i}R\Psi_0(r) - \mathrm{i}\pi/4} + \mathrm{e}^{-\mathrm{i}R\Psi_0(r) + \mathrm{i}\pi/4}}{\sqrt{(4 - r^2\cos^2\theta_0(r))(4 - r^2\sin^2\theta_0(r))}}$$

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

$$g'_{mn} \sim \frac{\sqrt{2\pi R}}{\mathrm{i}\pi^2} \lim_{\varepsilon \to 0} \int_0^\infty \int_0^2 f(r)\mathrm{e}^{-\varepsilon\zeta}\{\mathrm{e}^{\mathrm{i}R\Phi_+(r,\zeta)}\mathrm{e}^{-\mathrm{i}\pi/4} + \mathrm{e}^{\mathrm{i}R\Phi_-(r,\zeta)}\mathrm{e}^{\mathrm{i}\pi/4}\} r\,\mathrm{d}r\,\mathrm{d}\zeta, \tag{26}$$

where

$$f(r) = \left\{-\mathscr{P}_0(r)\left[4 - r^2\cos^2\theta_0(r)\right]\left[4 - r^2\sin^2\theta_0(r)\right]\right\}^{-1/2} \tag{27}$$

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

$$\frac{\partial \Phi_\pm}{\partial r} = -2r\zeta \pm \left.\frac{\partial \Psi}{\partial r}\right|_{\theta=\theta_0} \pm \left.\frac{\partial \Psi}{\partial \theta}\right|_{\theta=\theta_0} \frac{\mathrm{d}\theta_0}{\mathrm{d}r} = 0. \tag{28}$$

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

$$\frac{\partial \Psi}{\partial r} = \frac{2\sin\theta\sin\alpha}{\sqrt{4 - r^2\sin^2\theta}} + \frac{2\cos\theta\cos\alpha}{\sqrt{4 - r^2\cos^2\theta}},$$

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

$$R\Phi_+(k,\zeta) = R\Psi(k,\theta_0) = m\xi_0 + n\eta_0,$$

where ξ_0, η_0 and $\theta_0 \equiv \theta_0(k)$ are the same as in Section 4.1.

Thus, from [2, Eq. (8.4.44)], we obtain

$$g'_{mn} \sim \frac{\sqrt{2\pi R}}{\mathrm{i}\pi^2} \frac{2\pi}{R} \frac{f(k)k}{\sqrt{|\det A|}} \exp\{\mathrm{i}R\Phi_+(k,\zeta) - \mathrm{i}\pi(1 - \mathrm{sig}A)/4\}$$

as $R \to \infty$, where the 2×2 matrix A has entries

$$A_{ij} = \frac{\partial^2 \Phi_+}{\partial \xi_i \partial \xi_j} \text{ evaluated at } r = k,$$

with $\xi_1 = r$ and $\xi_2 = \zeta$. We find

$$A = \begin{pmatrix} A_{11} & -2k \\ -2k & 0 \end{pmatrix}$$

so that $\det A = -4k^2$ and $\operatorname{sig} A = 0$. (The eigenvalues of A are real and their product equals $\det A$; fortunately, we do not need to calculate A_{11}.) Hence

$$g_{mn} \sim \frac{\sqrt{2}}{\mathrm{i}\sqrt{\pi R}} \mathrm{e}^{\mathrm{i}(m\xi_0 + n\eta_0)} \mathrm{e}^{-\mathrm{i}\pi/4} f(k) \text{ as } R \to \infty. \tag{29}$$

Now, from Eq. (24), we have

$$\cos\theta_0 \sin\alpha \sqrt{4 - k^2 \cos^2\theta_0} = \sin\theta_0 \cos\alpha \sqrt{4 - k^2 \sin^2\theta_0}$$

which gives

$$\frac{\cos\alpha}{\cos\theta_0} = \frac{\sqrt{4 - k^2\cos^2\theta_0}}{\sqrt{4 - k^2(\cos^4\theta_0 + \sin^4\theta_0)}}.$$

Then, using $\mathscr{P}_0(k) = \Psi_{\theta\theta}(k, \theta_0)$, 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

$$\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}m\xi} \mathrm{e}^{2\mathrm{i}\zeta\cos\xi} \mathrm{d}\xi = 2\pi \mathrm{i}^m J_m(2\zeta),$$

twice, we obtain

$$g_{mn} = \mathrm{i}^{m+n-1} \lim_{\delta \to 0+} \int_0^\infty \mathrm{e}^{\mathrm{i}\zeta(k^2 - 4 + \mathrm{i}\delta)} J_m(2\zeta) J_n(2\zeta) \mathrm{d}\zeta, \tag{30}$$

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],

$$g_{nn} = \frac{(-1)^n}{2\pi\mathrm{i}} \lim_{\delta \to 0+} Q_{n-1/2}(Z).$$

Here, the complex quantity Z is given by

$$\begin{aligned} Z &= 1 + [\delta + \mathrm{i}(4 - k^2)]^2/8 \\ &\simeq 1 - (4 - k^2)^2/8 + \mathrm{i}\delta(4 - k^2)/4 \end{aligned}$$

for $0 < \delta \ll 1$. Thus, for $0 < k^2 < 8$, $|\mathrm{Re} Z| \leqslant 1$ and $\operatorname{sgn}\{\mathrm{Im} Z\} = \operatorname{sgn}(4 - k^2)$.

The function $Q_\nu(Z)$ is defined in the complex Z-plane, with a cut between $Z = -1$ and $Z = +1$. Thus, we require $Q_{n-1/2}(\cos\varphi + \mathrm{i}0)$ for $0 < k^2 < 4$ and $Q_{n-1/2}(\cos\varphi - \mathrm{i}0)$ for $4 < k^2 < 8$, where $\cos\varphi = 1 - (4 - k^2)^2/8$ so that $0 < \varphi < \frac{1}{2}\pi$.

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

$$\begin{aligned} g_{nn} &= \frac{(-1)^n}{2\pi\mathrm{i}} Q_{n-1/2}(\cos\varphi + \mathrm{i}0) \\ &\sim \frac{(-1)^n}{2\pi\mathrm{i}} \frac{\pi}{2\mathrm{i}} \left(\frac{\varphi}{\sin\varphi}\right)^{1/2} H_0^{(2)}(n\varphi) \end{aligned}$$

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

$$H_0^{(2)}(x) \sim \sqrt{2/(\pi x)}\mathrm{e}^{-\mathrm{i}(x-\pi/4)} \text{ as } x \to \infty,$$

we obtain

$$g_{nn} \sim -\frac{\mathrm{e}^{\mathrm{i}n(\pi-\varphi)}\mathrm{e}^{\mathrm{i}\pi/4}}{2\sqrt{2\pi n \sin\varphi}} \text{ as } n \to \infty. \tag{31}$$

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

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

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

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

This defines an analytic function of z within the strip $0 < \mathrm{Re}\, z < 1$. 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

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

where

$$I(\xi, \eta; z) = \lim_{\delta\to 0} \int_0^\infty \frac{\kappa^{z-1}\, \mathrm{d}\kappa}{\kappa - \gamma + \mathrm{i}\delta},$$

$\gamma = 4\sin^2\frac{1}{2}\xi + 4\sin^2\frac{1}{2}\eta$ and we have used Eqs. (6) and (13). A standard contour-integral calculation gives

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

so that

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

with

$$\tilde{h}(z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m\xi+n\eta)} \gamma^{z-1}\, \mathrm{d}\xi\, \mathrm{d}\eta.$$

We see that $\tilde{h}(0)$ is divergent. This divergence is caused by the behaviour of the integrand near $\xi = \eta = 0$, where $\gamma \simeq \xi^2 + \eta^2 = \varrho^2$, say. We consider a small disc $\varrho < a$ (inside B_1) and put $\xi = \varrho \cos\vartheta$ and $\eta = \varrho \sin\vartheta$. This gives

$$\begin{aligned}\tilde{h}(z) &\simeq \frac{1}{(2\pi)^2}\int_0^a \int_0^{2\pi} e^{iR\varrho\cos(\vartheta-\alpha)}\varrho^{2(z-1)}\varrho \, d\vartheta \, d\varrho \\ &= \frac{1}{2\pi}\int_0^a J_0(R\varrho)\varrho^{2z-1} \, d\varrho \\ &\simeq \frac{1}{2\pi z}\frac{J_1(aR)}{aR},\end{aligned}$$

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

$$\tilde{g}(z) \simeq -\frac{e^{i\pi z}}{4z\sin\pi z} \simeq -\frac{1}{4\pi z^2} \text{ near } z = 0.$$

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

$$g_{mn} \sim \frac{1}{2\pi}\log k \text{ as } k \to 0. \tag{32}$$

6. Discussion

We have investigated properties of the lattice Green's function, g_{mn}, for the simplest square lattice. The far-field behaviour is given by

$$g_{mn} \sim (kR)^{-1/2} \, e^{iR(\xi_0\cos\alpha+\eta_0\sin\alpha)}\mathscr{F}(\alpha;k^2) \text{ as } R = \sqrt{m^2+n^2} \to \infty, \tag{33}$$

where $m = R\cos\alpha$ and $n = R\sin\alpha$, so that α gives the observation direction; the quantities ξ_0, η_0 and $\mathscr{F}$ are known in terms of α and k^2. A corresponding Green's function for the Helmholtz equation, Eq. (1), is

$$G(x,y) = H_0^{(1)}(K\mathscr{R}), \tag{34}$$

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

$$G(x,y) \sim (K\mathscr{R})^{-1/2} \, e^{iK\mathscr{R}}G_0 \text{ as } \mathscr{R} \to \infty, \tag{35}$$

where $x = \mathscr{R}\cos\alpha$, $y = \mathscr{R}\sin\alpha$ 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 α.

From Eq. (34), we have $G \simeq \log(K\mathscr{R})$ as $K\mathscr{R} \to 0$, so that G has a logarithmic singularity with respect to K and with respect to $\mathscr{R}$. On the other hand, g_{mn} 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 $Q_\nu(x \pm i0) = Q_\nu(x) \mp \frac{1}{2}\pi i P_\nu(x)$, we obtain

$$g_{nn} = \frac{(-1)^{n+1}}{4\pi}\{\pi P_{n-1/2}(\cos\varphi) + 2i \, Q_{n-1/2}(\cos\varphi)\} \tag{36}$$

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,

$$\mathrm{Im}(g_{nn}) = (2\pi)^{-1}(-1)^{n+1}\mathrm{Q}_{n-1/2}(\cos\varphi) \sim (2\pi)^{-1}(-1)^{n}\log(4-k^2) \tag{37}$$

as $k^2 \to 4-$, using the approximation $\mathrm{Q}_\nu(x) \sim -\frac{1}{2}\log(1-x)$ 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

$$g_{mn} = g_{|m|,|n|} = g_{nm}$$

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

Acknowledgements

This work started with a lecture from G.J. Rodin. I am grateful to A.Y. Grosberg, A.A. Maradudin and V.K. Tewary for their electronic correspondence, especially on the work of I.M. Lifshitz.

References

[1] F. Bentosela, Scattering from impurities in a crystal, Commun. Math. Phys. 46 (1976) 153–166.
[2] N. Bleistein, R.A. Handelsman, Asymptotic Expansions of Integrals, Dover, New York, 1986.
[3] M. Born, K. Huang, Dynamical Theory of Crystal Lattices, Clarendon Press, Oxford, 1954.
[4] W.A. Bowers, H.B. Rosenstock, On the vibrational spectra of crystals, J. Chem. Phys. 18 (1950) 1056–1062, Erratum: 21 (1953) 1607.
[5] J. Callaway, Theory of scattering in solids, J. Math. Phys. 5 (1964) 783–798.
[6] W.C. Chew, Electromagnetic theory on a lattice, J. Appl. Phys. 75 (1994) 4843–4850.
[7] P.-L. Chow, Wave propagation in a random lattice. II, J. Math. Phys. 14 (1973) 1364–1373.
[8] R. Courant, K. Friedrichs, H. Lewy, On the partial difference equations of mathematical physics, IBM J. Res. Dev. 11 (1967) 215–234, Translated from the original German paper, Mathematische Annalen 100 (1928) 32–74.
[9] C. de Boor, K. Höllig, S. Riemenschneider, Fundamental solutions for multivariate difference equations, Am. J. Math. 111 (1989) 403–415.
[10] C. de Boor, K. Höllig, S. Riemenschneider, Box Splines, Springer, New York, 1993.
[11] E.N. Economou, Green's Functions in Quantum Physics, second ed., Springer, Berlin, 1983.
[12] G.E. Forsythe, W.R. Wasow, Finite-Difference Methods for Partial Differential Equations, Wiley, New York, 1960.
[13] J.I. Glaser, Numerical solution of waveguide scattering problems by finite-difference Green's functions, IEEE T. Microw. Theory Tech. MTT-18 (1970) 436–443.
[14] K. Gürlebeck, A. Hommel, On finite difference potentials and their applications in a discrete function theory, Math. Method. Appl. Sci. 25 (2002) 1563–1576.
[15] G.F. Koster, Theory of scattering in solids, Phys. Rev. 95 (1954) 1436–1443.
[16] I.M. Lifšic, The scattering of short elastic waves in a crystal lattice, Akad. Nauk SSSR. Zhurnal Eksper. Teoret. Fiz. 18 (1948) 293–300 [in Russian].
[17] I.M. Lifšic, Some problems of the dynamic theory of non-ideal crystal lattices, Il Nuovo Cimento. Supplemento 3 (1956) 716–733.
[18] I.M. Lifshitz, A.M. Kosevich, The dynamics of a crystal lattice with defects, Rep. Prog. Phys. 29 (1966) 217–254.
[19] A.A. Maradudin, Phonons and lattice imperfections, in: T.A. Bak (Ed.), Phonons and Phonon Interactions, W.A. Benjamin, New York, 1964, pp. 424–504.
[20] A.A. Maradudin, E.W. Montroll, G.H. Weiss, I.P. Ipatova, Theory of Lattice Dynamics in the Harmonic Approximation, second ed., Academic Press, New York, 1971.
[21] P.-G. Martinsson, G.J. Rodin, Asymptotic expansions of lattice Green's functions, P. Roy. Soc. A 458 (2002) 2609–2622.
[22] P.-G. Martinsson, G.J. Rodin, Boundary algebraic equations for lattice problems, in: A.B. Movchan (Ed.), IUTAM Symposium on Asymptotics, Singularities and Homogenisation in Problems of Mechanics, Kluwer, Dordrecht, 2003, pp. 191–198.
[23] E.W. Montroll, Frequency spectrum of vibrations of a crystal lattice, Am. Math. Monthly 61, No. 7, Part 2 (1954) 46–73.
[24] F.W.J. Olver, Asymptotics and Special Functions, A.K. Peters, Natick, Massachusetts, 1997.
[25] M. Ostoja-Starzewski, Lattice models in micromechanics, Appl. Mech. Rev. 55 (2002) 35–60.
[26] B. Preziosi, Causality conditions in crystals, Il Nuovo Cimento 6B (1971) 131–138.
[27] J. Schiøtz, A.E. Carlsson, Calculation of elastic Green's functions for lattices with cavities, Phys. Rev. B 56 (1997) 2292–2294.
[28] V. Thomée, Discrete interior Schauder estimates for elliptic difference operators, SIAM J. Numer. Anal. 5 (1968) 626–645.
[29] R. Thomson, S.J. Zhou, A.E. Carlsson, V.K. Tewary, Lattice imperfections studied by use of lattice Green's functions, Phys. Rev. E 46 (1992) 10613–10622.
[30] B. van der Pol, The finite-difference analogy of the periodic wave equation and the potential equation, Appendix IV in: M. Kac, Probability and Related Topics in Physical Sciences, Interscience, London, 1959, pp. 237–257.
[31] B. van der Pol, H. Bremmer, Operational Calculus Based on the Two-sided Laplace Integral, third ed., Chelsea, New York, 1987.
[32] G.N. Watson, Theory of Bessel Functions, second ed., Cambridge University Press, Cambridge, 1944.