

An Efficient Numerical Evaluation of the Green's Function for the Helmholtz Operator on Periodic Structures

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Numerical methods which are based on boundary integral formulations require the numerical evaluation of the Green's function associated with the problem. In the case of periodic structures, the Green's function is often an infinite series. This infinite series may converge slowly, making numerical evaluation expensive. Here, we present a practical computer implementation of a technique which dramatically speeds up the convergence of the infinite series Green's function associated with the Helmholtz operator. To show the consequences of using this technique, we include some numerical examples. © 1986 Academic Press, Inc.

1. INTRODUCTION

In this article, we present a practical computer implementation for the numerical evaluation of the Green's function associated with the Helmholtz operator on a periodic structure. In a somewhat simpler form, this Green's function also appears in the calculation of Coulomb interaction energy for a lattice of ions, an application which motivated Ewald [1] to develop a very elegant procedure for its evaluation. Here, we show how to apply the basic formulas of Ewald's method to the problem of evaluating the Green's function for the Helmholtz equation on a periodic lattice. For this problem, we demonstrate the efficacy of Ewald's method. We also indicate

how to choose optimal values for the parameters in our numerical implementation of Ewald's method.

Ewald studied techniques for speeding up convergence of series appearing in certain lattice sums. He relied on the theory of periodic functions in a lattice, obtaining a Fourier series representation for the original series. The Fourier coefficients in this case can be explicitly evaluated. As Ewald published his method in 1921, he had not considered the practical implementation of his method on high speed computers. However, D. Meiron implemented Ewald's method on a computer [2]. Meiron used Ewald's method to speed up the convergence of the Green's function associated with the Laplace operator. We, on the other hand, apply Ewald's method to a more general problem, that of Maxwell's equations with pseudo-periodic boundary conditions.

In Section 2, we briefly motivate our need for Ewald's method for efficient numerical evaluation of the series which represents the Green's function in the boundary integral equation formulation of Maxwell's equations. As we wish to solve Maxwell's equations in a region composed of different media, we obtain through the boundary integral formulation a coupled system of integral equations. We present the relevant equations from Ewald's paper in Section 3. Also there, we show how we choose the optimal point at which to split the infinite interval of integration. Section 4 contains the numerical results. We show that Ewald's method produces a dramatic improvement in convergence, most notably in cases where the basic series converges slowly. Even in the most favorable case for convergence of the basic series, that of a dielectric constant with large negative real part and small imaginary part, Ewald's method still required only approximately the same number of terms for comparable accuracy. Hence, in solving our coupled system of integral equations, we always apply Ewald's method to evaluate the Green's function and its derivatives. Section 5 summarizes the results and gives some general observations.

2. THE GREEN'S FUNCTION

To give some motivation, we briefly describe the problem for which we apply Ewald's method. We are interested in the three-dimensional Maxwell's equations defined on a doubly periodic domain with interfaces between media of differing dielectric constants. In the absence of charges or currents and in the case of time-harmonic electromagnetic wave, the electric field vector \mathbf{E} defined in a medium in Maxwell's equations satisfies the Helmholtz equation of the form

$$\Delta \mathbf{E} + \epsilon k_0^2 \mathbf{E} = 0 \quad (2.1)$$

subject to pseudo-periodic boundary conditions and interface conditions between adjacent media. Here ϵ is the complex dielectric constant and k_0 is the free space wave number. We obtain a system of Helmholtz equations which are coupled through the interface conditions.

This coupled system of Helmholtz equations can be reformulated using the vector form of the Helmholtz-Kirchoff integral theorem (cf. Jackson [3]) in terms of a coupled system of boundary integral equations. Of course the boundary integral method assumes that one can obtain a suitable Green's function for the problem. For our case, following the development in Morse and Feshbach [4], it is a straightforward task to derive the Green's function with the following form:

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \exp[-i(\mu m D_x + \nu n D_y)] \frac{\exp(i\sqrt{\varepsilon} k_0 R_{mn})}{R_{mn}}. \quad (2.2)$$

Here

$$\mu = k_0 \sin \theta \cos \varphi,$$

$$\nu = k_0 \sin \theta \sin \varphi,$$

and

$$R_{mn} = [(x - x' + m D_x)^2 + (y - y' + n D_y)^2 + (z - z')^2]^{1/2}.$$

The angles θ, φ are the polar and azimuthal angles, respectively, of the incident plane wave; D_x and D_y are the periodic distances in the x and y directions, respectively; ε and k_0 are as defined above. We note that equation (2.2) in essence is the superposition of fundamental solutions to the Helmholtz equation (2.1) modified by an appropriate phase factor which takes into account the pseudo-periodic boundary conditions.

The accurate and efficient evaluation of the series given in Eq. (2.2) is of fundamental importance for numerically solving the coupled system of boundary integral equations. In order to obtain an accurate and efficient evaluation of this Green's function, we have derived and implemented on the computer an appropriately modified version of Ewald's method.

The significance of speeding up the convergence of Eq. (2.2) becomes apparent in the case when the dielectric constant for one media is 1. That is, the case of air being a medium. In particular, if we have normal incidence, $\theta = 0$, the phase factor is no longer present in the Green function and (2.2) reduces to

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \frac{\exp(ik_0 R_{mn})}{R_{mn}}. \quad (2.3)$$

Equation (2.3) is exceedingly slow to converge (for arbitrary d , the number of terms having magnitude 10^{-d} is of order 10^{+2d}) making numerical evaluation by truncating the series difficult and computationally expensive.

3. EWALD'S METHOD

For the purpose of this article, we restrict ourselves to the case of a periodic structure whose unit cell in the xy plane is a rectangle. It would be a straightforward task to generalize to a periodic structure whose unit cell in the xy plane is a parallelogram, a case of interest to us. However, such a generalization adds nothing to the presentation of Ewald's method and merely complicates the mathematical expressions.

We begin with Eq. (2.2) for the Green's function. Following Ewald [1], we note that the second part of the term under the summation signs can be rewritten as

$$\frac{\exp(i\sqrt{\varepsilon}k_0R_{mn})}{R_{mn}} = (2/\sqrt{\pi}) \int_0^\infty \exp\left(-R_{mn}^2s^2 + \frac{\varepsilon k_0^2}{4s^2}\right) ds \quad (3.1)$$

for a suitably chosen path of integration. Here s is a complex variable.

For validity of (3.1), the path of integration must be such that the integrand remains bounded as $s \rightarrow 0$ and decays as $s \rightarrow \infty$. Thus as

$$s \rightarrow \infty, \quad \arg(s) \in [\beta/2 - 3\pi/4, \beta/2 - \pi/4]$$

and as

$$s \rightarrow 0, \quad \arg(s) \in [-\pi/4, \pi/4], \quad \text{where } \beta \equiv \arg(\varepsilon).$$

Actually, we shall want to restrict our attention to contours for which $\arg(s)$ lies in the intersection of these two regions as $s \rightarrow 0$ or ∞ ; i.e., as $s \rightarrow 0$ or $s \rightarrow \infty$,

$$\arg(s) \in \begin{cases} [-\pi/4, \beta/2 - \pi/4], & \beta \in [0, \pi], \\ [\beta/2 - 3\pi/4, \pi/4], & \beta \in [\pi, 2\pi]. \end{cases}$$

For any such contour (see Fig. 1 for an example), the change of variable $s' = 1/s$ leads to a contour of the same type in s' . This will be important later.

The Green's function as given by Eq. (2.2) can be written in two parts by using Eq. (3.1) and splitting the path of integration at E in Eq. (3.1). Thus we define

$$G(\mathbf{x}, \mathbf{x}') = G_1(\mathbf{x}, \mathbf{x}') + G_2(\mathbf{x}, \mathbf{x}'), \quad (3.2)$$

where

$$G_1(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \exp[-i(\mu m D_x + \nu n D_y)] (2/\sqrt{\pi}) \times \int_0^E \exp\left[-R_{mn}^2s^2 + \frac{\varepsilon k_0^2}{4s^2}\right] ds \quad (3.3)$$

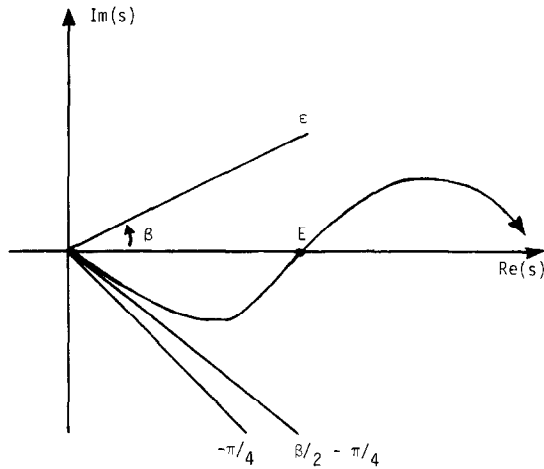


FIG. 1. Path of integration.

and

$$G_2(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \exp[-i(\mu m D_x + \nu n D_y)] (2/\sqrt{\pi}) \\ \times \int_E^{\infty} \exp\left[-R_{mn}^2 s^2 + \frac{\varepsilon k_0^2}{4s^2}\right] ds, \quad (3.4)$$

with ν , μ , and R_{mn} as in Eq. (2.2). For the integral in Eq. (3.4), Ewald's formulae apply directly. More precisely, following Ewald's paper, one can write the integral as

$$(2/\sqrt{\pi}) \int_E^{\infty} \exp\left[-R_{mn}^2 s^2 + \frac{\varepsilon k_0^2}{4s^2}\right] ds \\ = \frac{1}{2R_{mn}} \left(\exp[i\sqrt{\varepsilon} k_0 R_{mn}] \operatorname{erfc}\left(R_{mn} E + \frac{i\sqrt{\varepsilon} k_0}{2E}\right) \right. \\ \left. + \exp[-i\sqrt{\varepsilon} k_0 R_{mn}] \operatorname{erfc}\left(R_{mn} E - \frac{i\sqrt{\varepsilon} k_0}{2E}\right) \right). \quad (3.5)$$

This identity is the key to our evaluation of the Green's function. Applying (3.5) to (3.4), G_2 becomes

$$G_2(\mathbf{x}, \mathbf{x}') = \frac{1}{8\pi} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \frac{\exp[-i(\mu m D_x + \nu n D_y)]}{R_{mn}} \\ \times \sum_{\pm} \exp[\pm i\sqrt{\varepsilon} k_0 R_{mn}] \operatorname{erfc}\left(R_{mn} E \pm \frac{i\sqrt{\varepsilon} k_0}{2E}\right). \quad (3.6)$$

The summation over \pm is a shorthand notation for the right-hand side of Eq. (3.5). We will use this notation throughout the remainder of the paper. Before reformulating G_1 so that we can apply Eq. (3.5), we need the following identity:

$$\begin{aligned} & \sum_{l=-\infty}^{\infty} \exp[-(\Delta s)^2(l+g)^2 - i \Delta dl] \\ &= (\sqrt{\pi/\Delta s}) \exp[-d^2/4s^2] \\ & \times \sum_{l=-\infty}^{\infty} \exp\left[\frac{-(\pi l/\Delta)^2 - (\pi l/\Delta)d}{s^2} + 2\pi ilg\right] \exp[i \Delta dg]. \end{aligned} \tag{3.7}$$

This may be obtained from an identity of Ewald, (Eq. 13 in [1]):

$$\begin{aligned} & \sum_{l=-\infty}^{\infty} \exp[-\tau(l+g)^2 + 2(l+g)] \\ &= \sqrt{\pi/\tau} \exp[u^2/\tau] \sum_{l=-\infty}^{\infty} \exp[-(\pi^2/\tau)l^2 - 2\pi il(u/\tau - g)] \end{aligned}$$

by making the following replacements:

$$\begin{aligned} \tau & \text{ by } (\Delta s)^2, \\ u & \text{ by } -\frac{i \Delta d}{2}. \end{aligned}$$

If we interchange summation and integration in the definition of G_1 , Eq. (3.3) becomes

$$G_1(\mathbf{x}, \mathbf{x}') = \frac{1}{2\pi^{3/2}} \int_0^E \left\{ \exp\left[\frac{\epsilon k_0^2}{4s^2} - (z-z')^2 s^2\right] A(s) \right\} ds, \tag{3.8}$$

where

$$\begin{aligned} A(s) &= \sum_{n=-\infty}^{\infty} \exp\left[-(D_y s)^2 \left(n + \frac{(y-y')}{D_y}\right)^2 - i\nu n D_y\right] \\ & \times \sum_{m=-\infty}^{\infty} \exp\left[-(D_x s)^2 \left(m + \frac{x-x'}{D_x}\right)^2 - i\mu m D_x\right]. \end{aligned} \tag{3.9}$$

Consider the inner sum in Eq. (3.9). By applying identity (3.7) to it, interchanging summations, and then apply (3.7) again to the new inner sum, Eq. (3.9) is reduced to

$$\begin{aligned}
A(s) &= \frac{\pi}{D_x D_y s^2} \exp[i\mu(x-x') + \nu(y-y')] \exp\left[-\frac{\mu^2 - \nu^2}{4s^2}\right] \\
&\times \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \exp\left[\frac{-(\pi m/D_x)^2 - (\pi m/D_x)\mu - (\pi n/D_y)^2 - (\pi n/D_y)\nu}{s^2}\right] \\
&\times \exp\left[2\pi i \left(\frac{m(x-x')}{D_x} + \frac{n(y-y')}{D_y}\right)\right]. \tag{3.10}
\end{aligned}$$

Let us define α_{mn} such that

$$\alpha_{mn}^2 = \left(\frac{\pi m}{D_x}\right)^2 + \left(\frac{\pi n}{D_y}\right)^2 + \left(\frac{\pi m}{D_x}\right)\mu + \left(\frac{\pi n}{D_y}\right)\nu + \frac{1}{4}(\mu^2 + \nu^2 - \varepsilon k_0^2). \tag{3.11}$$

If further we define

$$\xi = x - x', \tag{3.12a}$$

$$\eta = y - y', \tag{3.12b}$$

$$\zeta = z - z', \tag{3.12c}$$

then Eq. (3.8) takes the form

$$\begin{aligned}
G_1 &= \exp\left[\frac{i(\mu\xi + \nu\eta)}{2\sqrt{\pi} D_x D_y}\right] \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \int_0^E \\
&\times \exp\left[-\frac{\alpha_{mn}^2}{s^2} - \zeta^2 s^2\right] \exp\left[2\pi i \left(\frac{m\xi}{D_x} + \frac{n\eta}{D_y}\right)\right] \frac{ds}{s^2}. \tag{3.13}
\end{aligned}$$

Making the change of variable $s = 1/s_1$ we arrive at

$$\begin{aligned}
G_1 &= \exp\left[\frac{i(\mu\xi + \nu\eta)}{2\sqrt{\pi} D_x D_y}\right] \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \int_{1/E}^{\infty} \\
&\times \exp\left[-\alpha_{mn}^2 s_1^2 - \frac{\zeta^2}{s_1^2}\right] \exp\left[2\pi i \left(\frac{m\xi}{D_x} + \frac{n\eta}{D_y}\right)\right] ds_1. \tag{3.14}
\end{aligned}$$

Now, Eq. (3.14) is in the desired form to use (3.5) and we find

$$\begin{aligned}
G_1 &= \frac{\exp[i(\mu\xi + \nu\eta)]}{8D_x D_y} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{\pm} \\
&\times \frac{\exp(\pm 2\zeta) \operatorname{erfc}(\alpha_{mn}/E \pm \zeta E)}{\alpha_{mn}} \exp\left[2\pi i \left(\frac{m\xi}{D_x} + \frac{n\eta}{D_y}\right)\right]. \tag{3.15}
\end{aligned}$$

This equation and Eq. (3.6) are combined to give the numerical value of the Green's function. The complimentary error function which appears in both series,

Eqs. (3.6) and (3.15), makes these series converge rapidly. This is a consequence of the fact that $\operatorname{erfc}(z)$ behaves asymptotically like

$$\exp(-z^2)/(\sqrt{\pi z}) \quad \text{as } z \rightarrow \infty \text{ for } |\arg z| < 3\pi/4.$$

In the next section, we will show through our numerical results that for several places of accuracy, the number of terms required is small.

4. NUMERICAL RESULTS

In this section, we describe some numerical results for the algorithm developed in the previous section. The particular dielectric constants we chose for the evaluation of the Green's functions were motivated by the application for which the coupled system of integral equations was developed. For the most part, the dielectric constants used in this section are those associated with either air, amorphous silicon, or silver.

We first compare evaluating the Green's function using Eq. (2.2) versus Eqs. (3.6) and (3.15). Two different dielectric constants are used; $\epsilon_{\text{Ag}} = (-9.5, 0.309)$, dielectric constant for silver with wavelength 0.5μ , and $\epsilon_{\text{Air}} = (1, 0)$. Figures 2A and 3A show the exponents of the terms in (2.2) for ϵ_{Ag} and ϵ_{Air} for m and n in the range $-10 \leq m \leq 10$, $-10 \leq n \leq 10$. The evaluation point was taken as $\mathbf{R} = (0.1, 0.2, 0.3)$ with $D_x = D_y = 0.25$. Note that for ϵ_{Ag} , the number of terms in this range of m and n with magnitude exceeding 10^{-10} was 22, while the corresponding figure for ϵ_{Air} was 441 (all the terms). Application of Ewald's method to these two cases yielded the results depicted in Figures 2B and 3B.

Note that in the case of ϵ_{Ag} , both formulations give the same value of the Green's function to all digits printed. Here Ewald's method yields 26 terms of magnitude greater than 10^{-10} , as opposed to 22 for the basic series. This is the case most favorable for rapid convergence of the basic series: a dielectric constant with large negative real part and small imaginary part. It produces rapid exponential decay in (2.2).

The case least favorable for the basic series is an ϵ lying on the positive real axis, e.g., ϵ_{Air} , where the terms in (2.2) lose their exponential decay, as illustrated in Fig. 3A. On the other hand, the rate of convergence of G_1 and G_2 are affected relatively little by the value of ϵ , as indicated in Fig. 3B. In fact, for ϵ lying in the general proximity of the positive real axis, using Ewald's method rather than the basic series typically results in a speed up of an order of magnitude or more in evaluating G . Moreover, for no value of ϵ is Ewald's method appreciably less economical than summing the basic series.

We now address the question of how to select E . We remark that E multiplies R_{mn} in the complementary error function in Eq. (3.6) while the reciprocal of E multiplies α_{mn} in Eq. (3.15).

TABLE I
Choice of Splitting Point E ; $\epsilon_{Ag} = (-9.5, 0.309)$, $\mathbf{R} = (0.1, 0.2, 0.3)^a$

E	Terms in G_1	Terms in G_2	Total terms in Ewald's method	Value of G from Ewald
3	0	19	19	(0.23208[-4], 0.3965[-5])
4	1	19	20	(0.23208[-4], 0.3965[-5])
5	5	17	23	(0.23208[-4], 0.3965[-5])
6	9	14	23	(0.23208[-4], 0.3965[-5])
7	9	10	19	(0.23208[-4], 0.3965[-5])
8	13	7	20	(0.23208[-4], 0.3965[-5])
9	13	6	19	(0.23208[-4], 0.3965[-5])
15	21	0	21	(0.23208[-4], 0.3965[-5])

^a Terms included in sums if magnitude $> 1 \times 10^{-10}$. Terms in basic series: 19. Value of G from basic: (0.23208[-4], 0.3965[-5]).

Thus increasing E has the effect of making the terms in G_1 decay faster while making those in G_2 decay more slowly. From the standpoint of efficiency, the best choice of E is that which balances the rate of decay of the two series as $([m] + [n]) \rightarrow \infty$, making G_1 and G_2 contribute an equal number of terms to the final value of $G_1 + G_2$. Comparing the terms in the two series for large m and n and using the asymptotic expansion for erfc, we obtain

$$E = \pi / \sqrt{D_x D_y} \tag{4.1}$$

as an approximation to the optimal value of E .

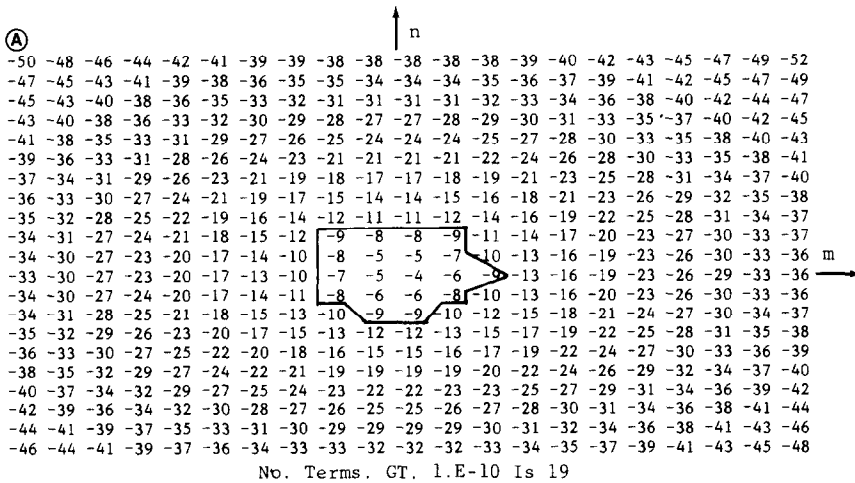


FIG. 2. Terms in the basic series; $\epsilon_{Ag} = (-9.546, 0.309)$, $\mathbf{R} = (0.1, 0.2, 0.3)$. (A) $G = (0.22633[-4], 0.38566[-5])$, (B) $G_1 = (0.11775[-4], 0.24874[-5])$, $G_2 = (0.10857[-4], 0.13692[-5])$.

The suitability of this cutoff has been verified computationally for a wide range of values of the parameters on which the Green's function depends. Table I summarizes one such computational experiment. Here $\epsilon = \epsilon_{Ag}$, $D_x = D_y = 0.25$ and $R = (0.1, 0.2, 0.3)$. Equation (4.1) yields a value 7.1 for the optimal E , and it is clear from the table that this value is well prescribed. Table II describes a similar experiment with $\epsilon = \epsilon_{Air}$. We note that formulas (3.6) and (3.15) remain valid for complex E . In general, however, moving E off the positive real axis increased the number of terms needed to attain a given accuracy.

Terms in First Part of G

(B)	↑ n																		m
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	

No. Terms. GT. 1.E-10 Is 9

Terms in Second Part of G

↑ n																		m
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
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-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
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-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	
-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	-99	

No. Terms. GT. 1E-10 Is 10

FIG. 2—Continued.

TABLE II
Choice of Splitting point $E: \epsilon_{\text{Air}} = (1., 0.), \mathbf{R} = (0.1, 0.2, 0.3)^a$

E	Terms in G_1	Terms in G_2	Total terms in Ewald's method	Value of G from Ewald
5	9	35	44	(-0.11325, 0.79199)
6	9	22	31	(-0.11325, 0.79199)
7	13	14	27	(-0.11325, 0.79199)
8	21	12	33	(-0.11325, 0.79199)
9	21	7	28	(-0.11325, 0.79199)
15	21	0	21	(-0.11325, 0.79199)

^a Terms included in sums if magnitude $> 1 \times 10^{-10}$. Terms in basic series: 441. Value of G from basic: (-0.92732[-1], -0.78613).

We include in Table III several values of the dielectric constants for silver (the first 5 dielectric constants) and for silicon (the last 5). In those cases where the basic series converged to 10^{-10} within the 441 terms computed, the value of the Green's function from the basic series and from Ewald's method agree to several digits. In all cases in the table, E was 7. Here $\mathbf{R} = (0.15, 0.15, 0.15)$ which is a slightly more stringent case than in the previous tables as we are closer to the singularity. The number of terms with magnitude greater than 10^{-10} is recorded. We see once again that with $E = 7$ the number of terms contributing to G_1 in Ewald's method, i.e., contributing to G_1 and G_2 is roughly equal.

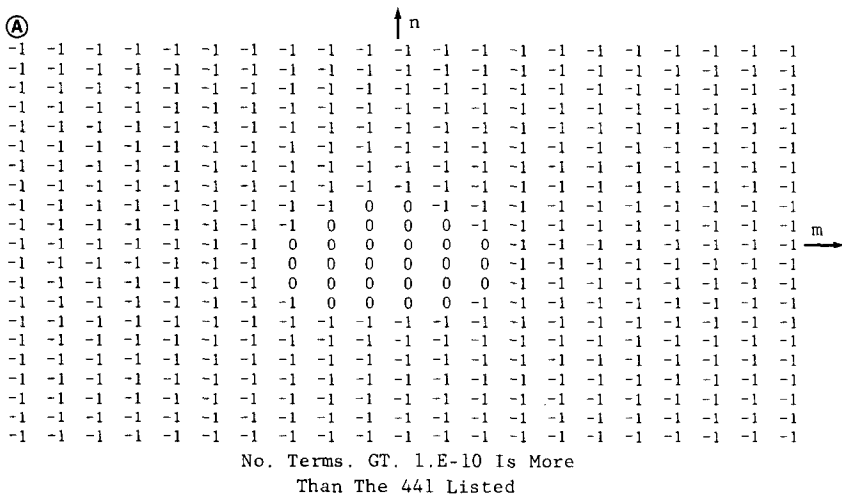


FIG. 3. Terms in the basic series; $\epsilon_{\text{Air}} = (1.0, 0.0), \mathbf{R} = (0.1, 0.2, 0.3)$. (A) $G = (-0.92732[-1], -0.78613)$, (B) $G_1 = (0.11424, 0.79199), G_2 = (0.99425[-3], 0.0)$.

5. SUMMARY AND CONCLUSIONS

We have applied Ewald's method to speed up the convergence of the series which is the Green's function for the Helmholtz operator on a periodic structure. We have shown that pseudo-periodic boundary conditions poses no difficulty for Ewald's methods. In addition, we have indicated that the unit cell of the periodic structure may be a parallelogram. Such a unit cell complicates the mathematical expressions

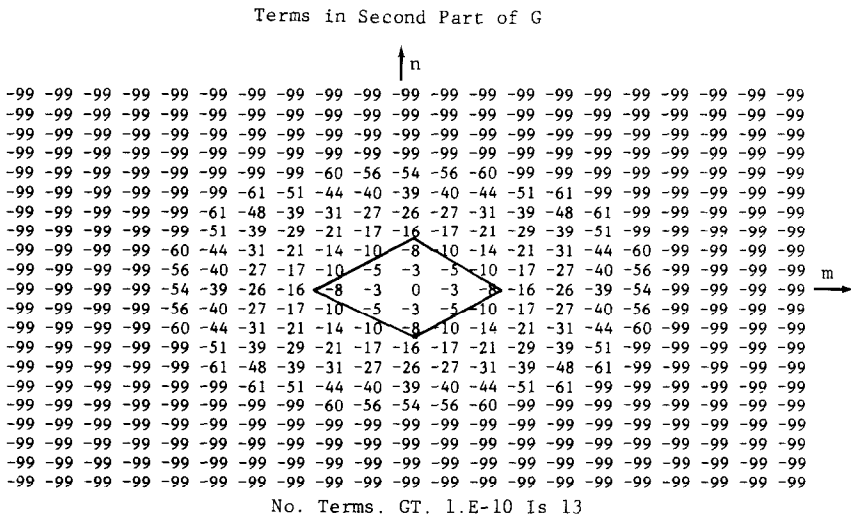
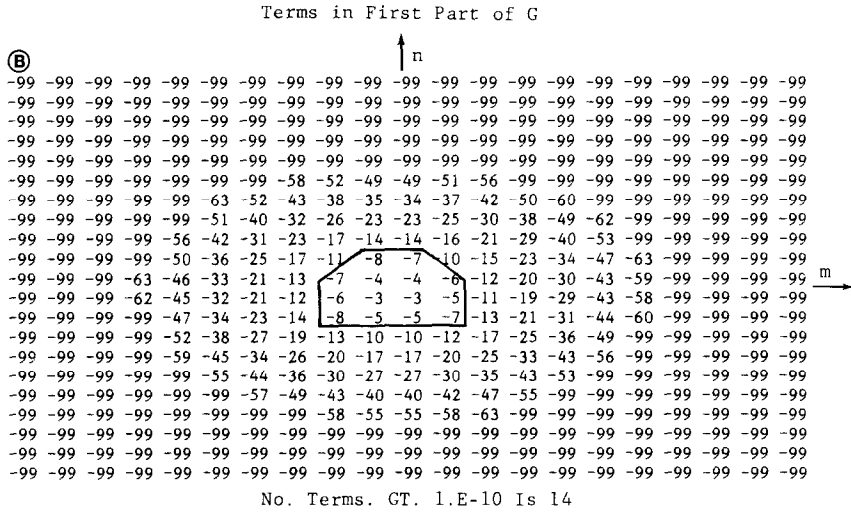


FIG. 3—Continued.

TABLE III
 $R = (0.15, 0.15, 0.15), E = 7$

δ	Terms in G_1	Terms in G_2	Value of G from Ewald's method	Terms in basic series	Basic series value
(-4.28, 0.207)	13	16	(0.123251[-1], 0.1418511[-2])	50	(0.123251[-1], 0.1418511[-2])
(-9.5, 0.309)	13	13	(0.126111[-2], 0.1409908[-3])	22	(0.126111[-2], 0.1409908[-3])
(-16.04, 0.441)	9	12	(0.1647765[-3], 0.1995575[-4])	13	(0.1647765[-3], 0.1995575[-4])
(-23.4, 0.387)	5	8	(0.2700259[-4], 0.2346362[-5])	10	(0.270026[-4], 0.2346362[-5])
(-30.97, 0.4)	1	4	(0.5618820[-5], 0.4350652[-6])	4	(0.5618821[-5], 0.4350654[-6])
(20.3, 15.89)	25	30	(-0.3004464[-2], -0.19198281[-1])	75	(-0.299157[-2], -0.1906592[-1])
(20.8, 5.49)	25	30	(-0.2967531[-1], -0.1940261)	462	(-0.2974047[-1], -0.1941308)
(16., 1.072)	25	26	(-0.9381068, -0.4154008)	441	(-0.9342341, -0.4108271)
(14.44, 0.0912)	25	26	(-0.2036177[+1], -0.5259123[-1])	441	(-0.2024578[+1], 0.1958743)
(13.18, 0.00116)	21	26	(-0.3067228[+1], -0.2106425[+1])	441	(-0.3387392[+1], 0.2957335[+1])

which must be evaluated numerically but does not affect the theoretical results. In those cases where the dielectric constant is such that the basic series for the Green's function converged rapidly, the series from Ewald's methods also converged to the same value with similar number of terms. However, in those cases of slow convergence for the basic series, Ewald's method converged in significantly fewer terms. Here the computational benefits are obvious, a mere 25 to 50 terms are computed compared with hundreds or even thousands of terms for the basic series.

The impact of Ewald's method is much greater when one considers the use we have in mind. We wish to solve a coupled system of integral equations. In the course of deriving an approximating system to be solved by the computer, we must compute the value of the Green's function numerous times. Ewald's method allows us to do this accurately and efficiently. We have also applied Ewald's method to the derivatives of the Green's function.

Ewald's method gives two series as a result of splitting an infinite interval of integration. The choice of where to split the interval of integration affects the number of terms that contribute to the value of the Green's function. We have provided a formula for the optimal value of this cutoff point and demonstrated its efficiency in computational experiments.

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