Journal of Electromagnetic Waves and Applications

ISSN: 0920-5071 (Print) 1569-3937 (Online) Journal homepage: http://www.tandfonline.com/loi/tewa20

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To cite this article: A. Moroz (2002) On the Computation of the Free-Space Doubly-Periodic Green's Function of the Three-Dimensional Helmholtz Equation, Journal of Electromagnetic Waves and Applications, 16:4, 457-465, DOI: 10.1163/156939302X00372

To link to this article: http://dx.doi.org/10.1163/156939302X00372

Published online: 03 Apr 2012.

J. of Electromagn. Waves and Appl., Vol. 16, No. 4, 457–465, 2002

ON THE COMPUTATION OF THE FREE-SPACE DOUBLY-PERIODIC GREEN'S FUNCTION OF THE THREE-DIMENSIONAL HELMHOLTZ EQUATION

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Abstract—In a recent article [1] the performances of several methods used for the computation of the free-space doubly-periodic Green's function $G_{0\Lambda}$ of the three-dimensional (3D) Helmholtz equation were investigated. The existence of an alternative method that is superior to those discussed in that article is pointed out. The alternative method can have accuracy close to machine precision and is more efficient (at least 12 times faster for an identical convergence test). It yields a fast convergent result for any z, i.e., also for $z = 0$, where the series discussed by Guérin, Enoch, and Tayeb are only conditionally convergent.

1 Introduction

2 Kambe's Formulas for Lattice Sums

3 Discussion

4 Conclusion

Acknowledgment

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1. INTRODUCTION

Let Λ be a two-dimensional (2D) simple (Bravais) periodic lattice in three dimensions (3D) (the condition of a simple lattice can be relaxed to an arbitrary periodic lattice [4, 5]). Let Λ^* be the corresponding dual (momentum) lattice, i.e., for any $\mathbf{r}_n \in \Lambda$ and $\mathbf{k}_s \in \Lambda^*$ one has $\mathbf{r}_n \cdot \mathbf{k}_s = 2\pi N$, where N is an integer. Let $\mathbf{k}_\parallel$ be the projection of wavevector $\mathbf{k}$ of an incident monochromatic wave onto $\Lambda(\Lambda^*)$. Let

$$G_0(\sigma, \mathbf{r}, \mathbf{r}') = G_0(\sigma, \mathbf{R}) = -\frac{\exp(i\sigma R)}{4\pi R}, \tag{1}$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and $R = |\mathbf{R}|$, denote a free-space scattering Green's function of the 3D scalar Helmholtz equation at the points $\mathbf{r}$ and $\mathbf{r}'$ and at $\sigma = \omega n_h / c_0$, where ω is angular frequency, n_h is the host refractive index, and c_0 is the speed of light in vacuum. The free-space periodic Green's function $G_{0\Lambda}$ is defined as

$$G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = \sum_{\mathbf{r}_s \in \Lambda} G_0(\sigma, \mathbf{R} - \mathbf{r}_s) e^{i\mathbf{k}_\parallel \cdot \mathbf{r}_s} = \sum_{\mathbf{r}_s \in \Lambda} G_0(\sigma, \mathbf{R} + \mathbf{r}_s) e^{-i\mathbf{k}_\parallel \cdot \mathbf{r}_s}, \tag{2}$$

where the projection $\mathbf{k}_\parallel$ is usually called the Bloch momentum. For any $\mathbf{r}_s \in \Lambda$, $\mathbf{k}_s \in \Lambda^*$, $G_{0\Lambda}$ satisfies the following trivial properties, $G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R} + \mathbf{r}_s) = G_{0\Lambda}(\sigma, \mathbf{k}_\parallel + \mathbf{k}_s, \mathbf{R})$.

In a recent article by Guérin, Enoch, and Tayeb [1], the performances of several methods used for the computation of the free-space doubly-periodic Green's function $G_{0\Lambda}$ of the 3D scalar Helmholtz wave equation (Eq. (12) below) were investigated. It was stated that (i) only a few works concern this problem, (ii) for a large range of parameters (position in space, wavelength, periods, etc.), none of the methods is satisfactory, regarding accuracy and computing time criteria. Contrary to these claims, we would like to point out that there is a whole thriving industry of numerical techniques which efficiently and satisfactorily deal with the issue raised in [1] and which are based on a method superior to those discussed by Guérin, Enoch, and Tayeb [1]. The alternative method is based on the (complete) Ewald summation [2, 3] and yields an exponentially convergent representations of $G_{0\Lambda}$ and its lattice sums. These representations were first derived by Kambe as early as in 1967 [2, 3].

2. KAMBE'S FORMULAS FOR LATTICE SUMS

The lattice sums D_{lm} of $G_{0\Lambda}$ are defined as the expansion coefficients of

$$D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) \equiv G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) - G_0^p(\sigma, \mathbf{R}) \tag{3}$$

into regular spherical waves [3, 6],

$$D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = \sum_{lm} D_{lm}(\sigma, \mathbf{k}_\parallel) j_l(\sigma R) Y_{lm}(\mathbf{R}). \tag{4}$$

Here $l \geq 0$ and $-l \leq m \leq l$ are the angular-momentum numbers, $G_0^p = -\cos(\sigma R)/(4\pi R)$ denotes the real or principal (singular) part of the free-space Green's function G_0, j_l are the regular spherical Bessel functions [7], and Y_{lm} are the conventional spherical harmonics. The very possibility of the expansion (4) follows from the fact that D_Λ is regular for $\mathbf{R} \to 0$ [6]. Indeed, within a primitive cell of a lattice Λ, Green's functions G_0 and $G_{0\Lambda}$ only differ up to boundary conditions and their respective singular parts are identical [6]. Therefore, D_Λ is regular for $\mathbf{R} \to 0$ and as such it can be expanded in terms of the regular spherical waves [6]. The lattice sums are conventionally written as a sum [3]

$$D_{lm} = D_{lm}^{(1)} + D_{lm}^{(2)} + D_{lm}^{(3)}, \tag{5}$$

where $D_{lm}^{(1)}(D_{lm}^{(2)})$ involves a sum over Λ^* (all $\mathbf{r}_s \neq 0$ of Λ). $D_{lm}^{(3)}$ is the term which combines $G_0^p(\mathbf{R})$ and the $\mathbf{r}_s = 0$ contribution of the direct lattice sum, and is only nonzero for $l = m = 0$ [3]. Explicitly,

$$\begin{aligned} D_{lm}^{(1)} = & -\frac{1}{\sigma v_0} \frac{i^{-m+1}}{2^l} [(2l+1)(l+|m|)!(l-|m|)!]^{1/2} \sum_{\mathbf{k}_s \in \Lambda^*} e^{-im\phi_{\mathbf{k}_\parallel + \mathbf{k}_s}} \\ & \times \sum_{n=0}^{(l-|m|)/2} \Gamma\left(\frac{1}{2} - n, e^{-\pi i} \frac{K_{\perp s}^2 \eta}{2}\right) \\ & \times \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma]^{l-2n} [K_{\perp s}/\sigma]^{2n-1}}{n![(l-|m|)/2-n]![(l+|m|)/2-n]!}, \end{aligned} \tag{6}$$

$$\begin{aligned} D_{lm}^{(2)} = & -\frac{\sigma}{4\pi} \frac{(-1)^{l+(l+m)/2}}{2^{2l}} \frac{[(2l+1)(l-|m|)!(l+|m|)!]^{1/2}}{[(l-|m|)/2]![(l+|m|)/2]!} \\ & \times {\sum_{\mathbf{r}_s \in \Lambda}}' e^{-i\mathbf{k}_\parallel \cdot \mathbf{r}_s - im\phi_{\mathbf{r}_s}} (\sigma r_s)^l \int_0^{\sigma^2 \eta/2} u^{-l-3/2} \exp\left[u - \frac{\sigma^2 r_s^2}{4u}\right] du, \end{aligned} \tag{7}$$

where prime in $\sum'$ indicates that the term with $r_s = 0$ is omitted, and

$$D_{lm}^{(3)} = -\frac{\sigma}{2\pi} \sum_{n=0}^{\infty} \frac{(\sigma^2\eta/2)^{n-1/2}}{n!(2n-1)} \delta_{lm,00}. \tag{8}$$

Here, v_0 is the volume of the primitive cell of the direct lattice Λ, $\phi_{\mathbf{u}}$ is the polar angle of the vector $\mathbf{u}$ in the plane containing $\Lambda(\Lambda^*)$, Γ is the incomplete gamma function [7], the normal projection $\mathbf{K}_{\perp s}$ can be either real (a propagating wave) or imaginary (an evanescent wave),

$$K_{\perp s} = \begin{cases} \left[\sigma^2 - |\mathbf{k}_\parallel + \mathbf{k}_s|^2\right]^{1/2}, & \sigma > |\mathbf{k}_\parallel + \mathbf{k}_s| \\ i\left[|\mathbf{k}_\parallel + \mathbf{k}_s|^2 - \sigma^2\right]^{1/2}, & \sigma < |\mathbf{k}_\parallel + \mathbf{k}_s|, \end{cases} \tag{9}$$

and $\delta_{lm,l'm'}$ is the Kronecker delta function, which is equal to one for $(l,m) = (l',m')$ and otherwise is zero. The parameter η in Eqs. (6)–(8) is the so-called Ewald parameter [3]. Invariance of D_{lm} (Eq. (5)) on the value of the Ewald parameter η serves as a check of a correct numerical implementation. However, for some values of η, one can enter a numerically instable region: the $D_{lm}^{(1)}$ and $D_{lm}^{(2)}$ contributions have opposite sign and similar magnitude, which is several orders larger than the resultant D_{lm}. This instability can easily be remedied by choice of some other value of η, or, one can make η depend on σ and l and prevent numerical instability completely [8, 9]. For moderate values of σ, Kambe recommended [3]

$$\eta = \frac{v_0}{2\pi}. \tag{10}$$

A numerical implementation of Eqs. (6)–(8) is facilitated by the fact that, assuming standard spherical coordinates, for a lattice Λ embedded in the $z = 0$ plane the lattice sums are only nonzero if $l - |m|$ is *even*, i.e.,

$$D_{lm}^{(j)} \equiv 0, \qquad l - |m| \text{ odd}. \tag{11}$$

Therefore, $(l-|m|)/2$, which is the upper limit of a sum over integers in Eq. (6) and which also enters factorials and an exponent in Eqs. (6)–(7), is always an integer. Obviously, whenever $D_{lm} \neq 0$ then $(l+|m|)/2$ in Eqs. (6)–(7) is also an integer. Some other tricks facilitating numerical implementation, for instance, use of recurrence relations, are discussed in [3]. Corresponding lattice sums and $G_{0\Lambda}$ for a complex (non-Bravais) lattice (for instance, a diamond lattice) are calculated in [5].

3. DISCUSSION

The exponentially convergent representation of the lattice sums, given in Eqs. (6)–(8), was first derived by Kambe in 1967 [3]. Since then it became an integral and indispensable part of numerical programs based on the layer Korringa-Kohn-Rostocker (LKKR) method [10–17] and low-energy electron-diffraction (LEED) theory [12, 13, 18] which describe scattering and diffraction of quantum and classical waves off (a finite stack of) 2D lattice(s) in 3D. The LKKR and LEED based numerical programs have been successfully tested for various physical problems since the early seventies of the last century. The last decade they have been incorporated into acoustic, elastic, and electromagnetic variants of the LKKR theories [14–17]. Indeed, it is interesting to note that, to a large extent, the scalar case also covers the case of vector and tensorial waves, provided (such as in the case of acoustic, elastic, and electromagnetic waves) each field component ψ_j independently obeys the scalar Helmholtz equation,

$$[\Delta + \sigma^2]\psi_j = 0. \tag{12}$$

For several reasons, it has been rather surprising to find out that the Kambe's results (6)–(8) were not included in the analysis of Ref. [1]. First, given σ and $\mathbf{k}_{\|}$, an identical set of lattice sums is used in Eq. (4) to calculate Eqs. (3)–(4) the Green's function $G_{0\Lambda}$ anywhere, i.e., also in the lattice ($z = 0$) plane, as long as $\mathbf{r} \neq \mathbf{r}'(\mathbf{R} \neq 0)$. (Note that in the lattice plane, i.e., for $z = 0$, the series in Ref. [1] are only conditionally convergent and their convergence properties were only investigated in the region $|z| \geq 10^{-6}$.) Second, there is no problem to calculate $G_{0\Lambda}$ close to machine accuracy. Third, compared to variants of the spectral domain representation of $G_{0\Lambda}$ discussed in [1], Kambe's expressions (6)–(8) provide an unparallel speed of convergence for $G_{0\Lambda}$. Indeed, after initial calculation of the lattice sums D_{lm} up to a cutoff value l_{max}, any further evaluation of $G_{0\Lambda}$ for a given σ and $\mathbf{k}_{\|}$ only requires a straightforward evaluation of regular Bessel functions and spherical harmonics, and performing the sum in Eq. (4) with the same set of the D_{lm}'s. Let the respective T_1 and T_{10000} denote the time needed to calculate $G_{0\Lambda}$ at a single and at 10.000 points. For fixed $\sigma = 2\pi$ and $\mathbf{k}_{\|} = (\sigma \sin(\pi/4), 0)$ (the same parameters as in Ref. [1]), the convergence times T_1 and T_{10000} are summarized in Table 1 as a function of l_{max}. The lattice sums were calculated with 8 digits accuracy. The Ewald parameter was taken according to Eq. (10). F77 program was compiled without any optimalization and run on a standard PC with Pentium II processor. Bessel functions and spherical harmonics were calculated using routines from Numerical Recipes [22].

Table 1. Convergence times T_1 and T_{10000} as a function of l_{max} for fixed $\sigma = 2\pi$ and $\mathbf{k}_{\|} = (\sigma \sin(\pi/4), 0)$.

l_{max}	7	8	9	10	11	12	13	14	18	22
$10000 * T_1$	92	116	144	265	311	350	410	460	760	2800
T_{10000}	4	5	7	8	9	11	13	14	19	25

The number of lattice sums increases quadratically with a cutoff value l_{max} in the summation over l and m in Eq. (4): for a given l_{max}, there are $(l_{max}+1) \times (l_{max}+2)/2$ independent lattice sums (see the constraint (11)) [12]. Therefore, both T_1 and T_{10000} increase with l_{max}. The speed of convergence of the Ewald-Kambe summation shown in Table 1 is in line with the so-called bulk case (d-dimensional lattice in a d-dimensional space). A single run of an entire photonic KKR program [19], which performs many other functions apart from a calculation of the lattice sums with 6 digits accuracy, takes on a PC with Pentium II processor, ≈ 0.03 s for a 2D photonic crystal in 2D for $l_{max} = 22$ [20] and ≈ 0.8 s for a 3D photonic crystal in 3D for $l_{max} = 8$ [21]. Given $\mathbf{R}$ and $s = \sigma|\mathbf{R}|$, $G_{0\Lambda}$ is calculated with the accuracy of lattice sums, provided a suitable value of the cutoff l_{max} is taken. Since, according to Eqs. (9.3.1) and (10.1.1) of [7], one has

$$j_l(s) \sim \sqrt{e/8}\left(\frac{es}{2}\right)^l (l+1/2)^{-l-1} \qquad (l \gg s), \tag{13}$$

with e being the Euler number, a rapid convergence of series in Eq. (4) is ensured after some $l_0 > s$. Often the cutoff value

$$l_{max} \approx \sigma R + 4(\sigma R)^{1/3} + 2$$

is large enough [23]. The largest value of $|\mathbf{R}|(s)$ for which $G_{0\Lambda}$ was calculated in Ref. [1] was $R_{max} = \sqrt{3}\,(s_{max} \approx 11)$. Therefore, $l_{max} \approx 22$ should be large enough to ensure convergence over entire scanned region in Ref. [1]. Keeping l_{max} fixed to its maximal value 22, the convergence times T_1 and T_{10000} do not depend on $\mathbf{R}$ in the scanned region of Ref. [1]. Even with such an unoptimized procedure, Kambe's Eqs. (6)–(8) yield, according to Table 1, roughly 12 times faster convergence for $G_{0\Lambda}$ than the methods in [1] (see Table V there). (Unfortunately, in [1] there is no description of a computer on which the speed of convergence was tested. A reliable comparison would of course require to test the programs on the same computer.)

For 1D periodicity (e.g., along the x-axis) in 2D, Kambe-like expressions for $y = 0.03$ (a z-like coordinate there), have been found

to yield 20 times faster convergence time T_1 than the spectral domain form of $G_{0\Lambda}$ [24]. Only as y (z in the current case) increases further, the respective T_1 times are expected to converge to the same value. This indicates for the current case that an optimized program employing the Kambe expressions (6)–(8) can yield even faster convergence. Obviously, the speed of convergence in the current case can be enhanced by a trivial modification: after storing the values of D_{lm}'s up to $l_{max} \approx 22$, the actual number of generated Bessel functions and spherical harmonics to be used in Eq. (4) is made $|\mathbf{R}|$-dependent. However, the main goal of the article was rather to point out the existence of Kambe's expressions (6)–(8) [2, 3, 5] than to discuss properties of the most optimized program employing these expressions.

4. CONCLUSION

We have pointed out the existence of an alternative method for the calculation of the free-space periodic Green's function $G_{0\Lambda}$ that is superior to those discussed by Guérin, Enoch, and Tayeb [1]. The alternative method, which is based on Kambe's Eqs. (6)–(8) [2, 3, 5], can have accuracy close to machine precision and is more efficient (at least 12 times faster for the same test as that in Ref. [1]). It yields a fast convergent result for any z, i.e., also for $z = 0$, where the series discussed by Guérin, Enoch, and Tayeb [1] are only conditionally convergent. Therefore, it deserves full attention of electromagnetic waves community.

A comprehensive review of exponentially convergent lattice sums of the free-space periodic Green's functions of the Helmholtz equation for all physical situations can be found in [25]. Numerical F77 codes implementing Eqs. (6)–(8) can be found in a book by Pendry [12], or, can be downloaded from Comp. Phys. Commun. [26, 27]. They are also available upon request from the author.

ACKNOWLEDGMENT

I would like to thank Prof. A. van Blaaderen for careful reading of the manuscript and useful comments. Financial support by Breedte Strategie is gratefully acknowledged.

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