Exponentially convergent lattice sums

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For any oblique incidence and arbitrarily high order, lattice sums for one-dimensional gratings can be expressed in terms of exponentially convergent series. The scattering Green's function can be efficiently evaluated also in the grating plane. Numerical implementation of the method is 200 times faster than for the previous best result. © 2001 Optical Society of America

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The study of efficient techniques for the calculation of the free-space periodic scattering Green's function for a one-dimensional (1D) periodic array of line sources or a 1D grating has a long history and has recently increased in intensity.[1–10] Knowledge of the Green's function and related lattice sums is a key to efficient numerical analysis of electromagnetic scattering by 1D periodic structures. However, even with the latest progress reported by Yasumoto and Yoshitomi[10], it takes 40 s on a SPARC workstation to compute the Green's function from lattice sums at a single point and frequency, in striking contrast to the calculation of exponentially convergent lattice sums for infinite two-dimensional (2D) lattices in two dimensions[11,12] and infinite three-dimensional (3D) lattices in three dimensions.[13] The 2D and 3D expressions, which seem to be largely unknown to some parts of optical community, result from the so-called complete Ewald summation[14] and are hybrid in the sense that they involve simultaneous summation over the spatial and spectral domains. For comparison, a variant of a single Korringa–Kohn–Rostocker program run,[15,16] which performs many other functions apart from the calculation of lattice sums with six-digit accuracy, requires, on a PC with a Pentium II processor, ≈0.03 s for a 2D photonic crystal[15] and ≈0.8 s for a 3D photonic crystal.[16] This indicates that the calculation of lattice sums for 1D gratings is far from being optimal. Surprisingly enough, it seems that many persons have not noticed that exponentially convergent lattice sums for 1D gratings can be derived by extension of Kambe's[17] treatment of scattering from a 2D grating in three dimensions to one dimension lower, resulting in significantly faster numerics and in expressions that can be directly incorporated into powerful scattering techniques developed within the context of diffraction and scattering of electron waves. This extension is the main achievement reported in this Letter.

Let Λ denote a simple 1D grating in two dimensions and Λ^* be the corresponding dual (momentum) lattice, i.e., $\mathbf{r}_n \cdot \mathbf{k}_s = 2\pi N$, where N is an integer, for any $\mathbf{r}_n \in \Lambda$ and $\mathbf{k}_s \in \Lambda^*$ (see Fig. 1). Let plane wave $\exp(i\mathbf{k} \cdot \mathbf{r})$ be incident upon Λ. Given a vector $\mathbf{r} = \mathbf{r}_\parallel + \mathbf{r}_\perp$ (wave vector $\mathbf{k} = \mathbf{k}_\parallel + \mathbf{k}$), one can define its respective parallel and perpendicular components $\mathbf{r}_\parallel$ and $\mathbf{r}_\perp$($\mathbf{k}_\parallel$ and $\mathbf{k}_\perp$) with respect to grating plane Λ (Λ^*) and its inward normal, which is defined to have a positive scalar product with $\mathbf{k}$. The incident plane wave is, according to general theory, diffracted (transmitted) to a set of plane waves, each with a wave vector $\mathbf{K}_s^-$ ($\mathbf{K}_s^+$), where $\mathbf{K}_s^\pm = (\mathbf{k}_\parallel + \mathbf{k}_s, \pm K_{\perp s})$,

$$K_{\perp s} = \begin{cases} (\sigma^2 - |\mathbf{k}_\parallel + \mathbf{k}_s|^2)^{1/2} & \sigma > |\mathbf{k}_\parallel + \mathbf{k}_s| \\ i(|\mathbf{k}_\parallel + \mathbf{k}_s|^2 - \sigma^2)^{1/2} & \sigma < |\mathbf{k}_\parallel + \mathbf{k}_s| \end{cases}, \quad (1)$$

$\mathbf{k}_s \in \Lambda^*$, and $|\mathbf{k}| = |\mathbf{K}_s^\pm| = \sigma$. In this definition, the surface projection $\mathbf{K}_{\parallel s} = \mathbf{k}_\parallel + \mathbf{k}_s$ is real but the normal projection $\mathbf{K}_{\perp s}$ can be either real (a propagating wave) or imaginary (an evanescent wave). Let $G_0(\sigma, \mathbf{r}, \mathbf{r}')$ be the free-space Green's function of the 2D Helmholtz equation. The corresponding periodic free-space Green's function of the Helmholtz equation is

$$G_{0\Lambda}\left(\sigma, \mathbf{k}_\parallel, \mathbf{R}\right) = \sum_{\mathbf{r}_s \in \Lambda} G_0(\sigma, \mathbf{R} + \mathbf{r}_s)\exp(-i\mathbf{k} \cdot \mathbf{r}_s), \quad (2)$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and $\mathbf{k}_\parallel$ is called the Bloch momentum. Obviously, $G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) = G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R})$

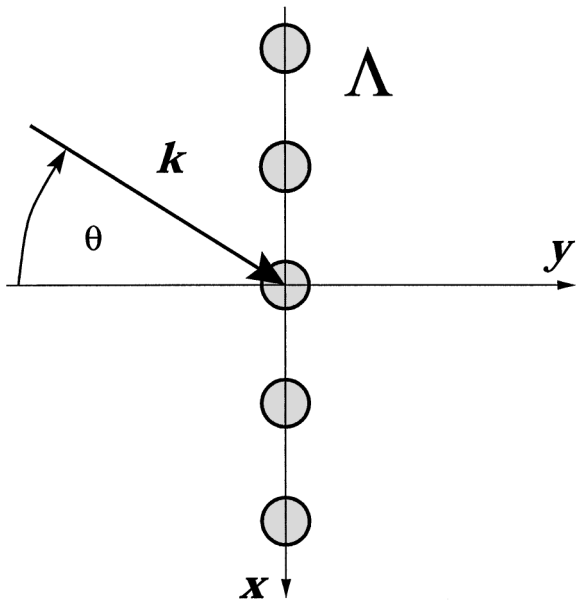

Fig. 1. Plane wave with wave vector $\mathbf{k}$ incident upon 1D grating Λ oriented along the x axis, with an incidence angle θ.

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and $G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) = G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R} + \mathbf{r}_s) = G_{0\Lambda}(\sigma, \mathbf{k} + \mathbf{k}_s, \mathbf{R})$ for any $\mathbf{r}_s \in \Lambda$, $\mathbf{k}_s \in \Lambda^*$. Let us specify to the scattering Green's functions in the scalar case. Then $G_0(\sigma, \mathbf{R}) = -iH_0^{(1)}(\sigma R)/4$, where $H_0^{(1)}$ is the cylindrical Hankel function.[18] Define

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

where $G_0{}^p(\sigma, \mathbf{R}) = N_0(\sigma R)/4$ (N_0 is the cylindrical Neumann function[18] and $R = |\mathbf{R}|$) denotes the real or principal (singular) part of $G_0(\sigma, \mathbf{R})$. Within a primitive cell of Λ, Green's functions $G_0{}^p$ and $G_{0\Lambda}$ differ only up to boundary conditions, and their respective singular parts are identical. Therefore D_Λ is regular for $\mathbf{R} \to 0$ and can be expanded in terms of the regular cylindrical Bessel functions $J_l(\sigma R)$:

$$D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = \sum_{l=-\infty}^{\infty} D_l(\sigma, \mathbf{k}_\parallel) J_{|l|}(\sigma R) Y_l(\mathbf{R}), \qquad (4)$$

where the $Y_l(\mathbf{u}) = (1/\sqrt{2\pi})\exp(il\phi_{\mathbf{u}})$ are the normalized cylindrical harmonics and $\phi_{\mathbf{u}}$ denotes the polar angle of vector $\mathbf{u}$. Expansion (4) is the defining equation for the lattice sums $D_l(\sigma, \mathbf{k}_\parallel)$, whose efficient calculation is the main purpose of this Letter. The values of D_l do not depend on $\mathbf{R}$. Consequently, by combining Eqs. (3) and (4) one can evaluate $G_{0\Lambda}$ at any observation point by using the same set of lattice sums.

Explicit calculation of D_l, following Kambe's analysis[17] for 2D gratings in three dimensions, involves two steps. First, an exponentially convergent expression for $G_{0\Lambda}$ is obtained. Second, the lattice sums are calculated as

$$D_l(\sigma, \mathbf{k}_\parallel) = \lim_{R\to 0} \frac{1}{J_{|l|}(\sigma R)} \oint Y_l{}^*(\mathbf{R}) D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) \mathrm{d}\Omega_{\mathbf{R}}, \qquad (5)$$

where $\oint \mathrm{d}\Omega_{\mathbf{R}}$ denotes the angular integration. The first step in the calculation is rather straightforward and follows the main steps of the complete Ewald summation.[14] As in three dimensions,[14,17] one begins with an appropriate contour integral representation for the free-space Green's function $G_0(\sigma, \mathbf{R})$ in Eq. (2). Subsequently, the integration contour is split at some point η into two parts, resulting in two separate integrals. Obviously, although each of the partial integrals depends on η, called the Ewald parameter, their sum does not. Using, in one of the partial integrals, the Jacobi ϑ-function identity to convert the sum over Λ into a sum over the dual lattice Λ^* results in an exponentially convergent representation of $G_{0\Lambda}$, which involves summation over both Λ and Λ^*.[17] This representation of $G_{0\Lambda}$ is then substituted back into Eq. (3), and the angular integration and limit $R \to 0$ in Eq. (5) are taken,[17] which are the most complicated parts of the calculation. The resultant D_l are conventionally written as a sum[13]:

$$D_l = D_l{}^{(1)} + D_l{}^{(2)} + D_l{}^{(3)}, \qquad (6)$$

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

$$D_l{}^{(1)}(\sigma, \mathbf{k}_\parallel) = -\frac{i^{|l|+1}|l|!}{\sqrt{2}\,\sigma v_0} \sum_{\mathbf{k}_s\in\Lambda^*} \sum_{n=0}^{[|l|/2]} \frac{1}{2^{2n} n!} \times \Gamma\left[1/2 - n, \exp(-\pi i)\frac{K_{\perp s}{}^2 \eta}{2}\right] \times \frac{(|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma)^{|l|-2n}(K_{\perp s}/\sigma)^{2n-1}}{(|l| - 2n)!} \times \begin{cases} \exp[-i(|l| - 2n)\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}] & l \geq 0 \\ \exp[i(|l| - 2n)\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}] & l < 0 \end{cases}, \qquad (7)$$

where v_0 is the lattice constant (the length of the primitive cell of Λ), $[|l|/2]$ stands for the integral part of $|l|/2$, and Γ is the incomplete gamma function [see Eq. (6.5.3) of Ref. 18],

$$D_l{}^{(2)}(\sigma, \mathbf{k}_\parallel) = -\frac{(-1)^{|l|}}{2^{|l|+1}\sqrt{2\pi}} {\sum_{\mathbf{r}_s\in\Lambda}}' \exp(-i\mathbf{k}_\parallel \cdot \mathbf{r}_s)(\sigma r_s)^{|l|} \times \exp(-il\phi_{\mathbf{r}_s}) \int_0^\alpha u^{-|l|-1} \exp\left(u - \frac{\sigma^2 r_s{}^2}{4u}\right) \mathrm{d}u, \qquad (8)$$

where $\alpha = \sigma^2\eta/2$, the prime over $\sum$ indicates that the term $\mathbf{r}_s = 0$ is omitted, and

$$D_l{}^{(3)}(\sigma) = -\frac{1}{2\sqrt{2\pi}}\left[\gamma + \ln(\sigma^2\eta/2) + \sum_{n=1}^{\infty} \frac{(\sigma^2\eta/2)^n}{n!n}\right]\delta_{l0}, \qquad (9)$$

where $\gamma = 0.577\,215\,6649$ is the Euler constant [see Eq. (6.1.3) of Ref. 17]. Note that, for Λ oriented along the x axis, $D_l{}^{(j)} = D_{-l}{}^{(j)}$, $j = 1, 2$, and hence $D_l = D_{-l}$, in accord with the fact that $G_{0\Lambda}$ depends only on y by means of $|y|$.[1–10]

Numerical implementation of the resultant formulas for $D_l{}^{(j)}$ is straightforward. The incomplete gamma function $\Gamma(b, x)$ in Eq. (7) is derived successively by recurrence formula $b\Gamma(b, x) = \Gamma(b + 1, x) - x^b \exp(-x)$ from the value for $n = 0$, which can be expressed in terms of the error function erfc [see Eq. (6.5.17) of Ref. 17]:

$$\Gamma(1/2, x) = \begin{cases} \sqrt{\pi} - 2\int_0^{\sqrt{x}} \exp(-t^2)\mathrm{d}t = \sqrt{\pi}\,\mathrm{erfc}(\sqrt{x}) & \arg x = 0 \\ \sqrt{\pi} + 2i\int_0^{\sqrt{-x}} \exp(t^2)\mathrm{d}t & \arg x = -\pi \end{cases}. \qquad (10)$$

Denoting by $U_{|l|}$ the integral in Eq. (8), one can determine $U_{|l|}$ if the values of U_0 and U_1 are known, from the recurrence

$$\left(\frac{\sigma r_s}{2}\right)^2 U_{|l|+1} = |l|U_{|l|} - U_{|l|-1} + \alpha^{-|l|} \times \exp[\alpha - \sigma^2 r_s{}^2/(4\alpha)], \qquad (11)$$

which is derived by means of a simple integration by parts. The invariance of D_l on the value of Ewald parameter η then serves as a check of correct numerical implementation.

To compare the speed of convergence, I investigated the case of a plane wave incident at an angle $\pi/8$ upon grating Λ oriented along the x axis. In this case, for wavelength $\lambda/v_0 = 0.23$ and fixed $x/v_0 = 0.2$, convergence results for $G_{0\Lambda}$ calculated in terms of the lattice sums have been presented in the literature for various values of y/v_0 (see Table III of Ref. 9 and Table IV of Ref. 10). The computational time required to reproduce a value of $G_{0\Lambda}$ in these tables within 8×10^{-15} of that obtained by direct summation turns out to be $\approx$0.2 s, in line with the respective $\approx$0.03 and $\approx$0.8 s for convergence times of sets of bulk 2D (Ref. 15) and 3D (Ref. 16) lattice sums with six-digit accuracy. These times should be compared with 1232 s of Nicorovici and McPhedran[9] or with 40 s of Yasumoto and Yoshitomi.[10] Ewald parameter η can often be varied by several orders of magnitude without affecting the result in a wide frequency window. However, for some singular values of η, one can enter a numerically unstable region: the $D_l^{(1)}$ and $D_l^{(2)}$ contributions have opposite signs and similar magnitude, which is several orders larger than the resultant D_l. 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.[11] Of the cases tested, the simplest case of a constant η was chosen, as was the case in Refs. 15 and 16; here the numerical instability limited η to the interval (0, 0.2).

To conclude, I have derived, for the first time to my knowledge, an exponentially convergent analytic representation of lattice sums for 1D gratings. The new representation [Eqs. (7)–(9)] (i) can be implemented numerically more simply and (ii) converges roughly 200 times faster than the previous best representation.[10] In addition, the present representation can be directly incorporated into powerful techniques developed within the context of diffraction and scattering of electron waves, which, as illustrated in Refs. 15 and 16, can also be applied to a variety of classic, including electromagnetic, waves. The result presented here in principle makes possible efficient investigations of the diffraction of light by (photonic crystal) gratings and of subtle phenomena that involve light–matter interaction in the presence of a single or a finite stack of 1D gratings. The FORTRAN 77 source code of my numerical implementation is available on request.

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