

# A New Method with Exponential Convergence to Evaluate the Periodic Green Function †

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## 1. Introduction

The Green function method is very effective in the analysis of doubly periodic systems in the three-dimensional space (e.g. frequency selective surfaces [1]). In important cases, it allows reducing the domain of the problem to a single unit cell with a significant diminution of the computational effort. The “periodic Green function”  $\Phi_H$  is the dynamic potential from a two-dimensional array of point sources at the lattice points  $\mathbf{r}_{\bar{\mathbf{I}}} = i_1 \mathbf{a}_1 + i_2 \mathbf{a}_2$ , being  $\mathbf{a}_1$  and  $\mathbf{a}_2$  the primitive vectors [2, 3]. The phase-shift between the point sources is determined by the wave vector  $\mathbf{k}$ . The Green function satisfies (assuming without loss of generality that the source point is the origin):

$$\nabla^2 \Phi_H + \beta^2 \Phi_H = - \sum_{\bar{\mathbf{I}}} \delta(\mathbf{r} - \mathbf{r}_{\bar{\mathbf{I}}}) e^{-j\mathbf{k} \cdot \mathbf{r}} \quad (1)$$

where  $\beta$  is the wave number, and  $\bar{\mathbf{I}} = (i_1, i_2)$  is a generic double-index of integers. The efficient computation of the periodic Green function can greatly reduce the computation time in the analysis of doubly periodic structures. Different mathematical representations for the Green function are known [2, 3]. To our best knowledge, only Jordan’s representation [3] has exponential convergence (independently of the observation point). However, Jordan’s representation requires the evaluation of the complex error function in the complex plane, which is computationally demanding and decisively worsens its global efficiency. Besides that, the evaluation of the error function in the complex plane poses some difficulties of implementation.

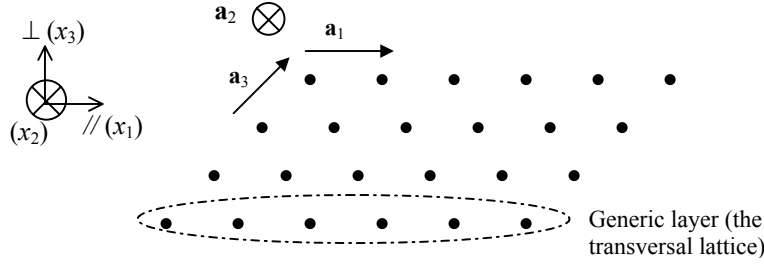
In this paper, we propose a new representation for the Green function with exponential convergence rate. The computational effort required to evaluate the new representation is comparable to that of the Jordan’s *et al* representation [3]. However, our representation is much easier to implement numerically. The idea is that the double-array defined by the vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  can be regarded as a sub-lattice of the array defined by the vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$  and a third arbitrary vector  $\mathbf{a}_3$ . This concept is illustrated in Fig.1. The potential from the triple-array of point sources is by definition the “lattice Green function”. The lattice Green function is pseudo-periodic in 3 independent directions of space, in contrast with the periodic Green function, which is pseudo-periodic in 2 directions. The lattice Green function,  $\Phi_p$ , satisfies:

$$\nabla^2 \Phi_p + \beta^2 \Phi_p = - \sum_{\mathbf{I}} \delta(\mathbf{r} - \mathbf{r}_{\mathbf{I}}) e^{-j\mathbf{k} \cdot \mathbf{r}} \quad (2)$$

where  $\mathbf{r}_{\mathbf{I}} = i_1 \mathbf{a}_1 + i_2 \mathbf{a}_2 + i_3 \mathbf{a}_3$ , and  $\mathbf{I} = (i_1, i_2, i_3)$  is a generic triple-index of integers.

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**Fig. 1** The two-dimensional array of point sources defined by the primitive vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , can be regarded as a sub-lattice of a three-dimensional array.

As shown in previous work [4, 5] we can easily relate the potentials  $\Phi_p$  and  $\Phi_H$ . The idea is to write the potential  $\Phi_p$  as a superimposition of the potentials from the different sub-lattices (“layers”). The potential from each layer is written in terms of the spectral representation of  $\Phi_H$  [2]. It turns out that the sum of the layer potentials corresponds to two geometrical series that can be summed in closed analytical form. In this way, we obtain that [4, 5]:

$$\Phi_p(\mathbf{r}) = \sum_{\bar{\mathbf{J}}} \frac{1}{A_{\text{cell}}} \frac{1}{2\gamma_{\bar{\mathbf{J}}}} \left( e^{-\gamma_{\bar{\mathbf{J}}}|r_{\perp}|} + \sum_{\pm} \frac{e^{\pm\gamma_{\bar{\mathbf{J}}}r_{\perp}}}{e^{|a_{3\perp}|(\gamma_{\bar{\mathbf{J}}}\pm jk_{\bar{\mathbf{J},\perp})} - 1}} \right) e^{-j\mathbf{k}_{\bar{\mathbf{J}},//}\cdot\mathbf{r}}, \quad |r_{\perp}| < |a_{3\perp}| \quad (3)$$

where  $A_{\text{cell}} = |\mathbf{a}_1 \times \mathbf{a}_2|$  is the area of the transversal lattice,  $\bar{\mathbf{J}} = (j_1, j_2)$  is a double-index of integers,  $\mathbf{k}_{\bar{\mathbf{J}}} = \mathbf{k} + j_1\mathbf{b}_1 + j_2\mathbf{b}_2$ , and  $\mathbf{b}_1$ ,  $\mathbf{b}_2$ , and  $\mathbf{b}_3$  are the reciprocal lattice primitive vectors, defined by  $\mathbf{a}_n \cdot \mathbf{b}_m = 2\pi \delta_{n,m}$ ,  $n, m=1,2,3$ . We define  $\mathbf{k}_{\bar{\mathbf{J}},//}$  as the projection of  $\mathbf{k}_{\bar{\mathbf{J}}}$  onto the transversal lattice (defined by the primitive vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ ), and  $k_{\bar{\mathbf{J},\perp}$ ,  $a_{3\perp}$  and  $r_{\perp}$  as the projections of  $\mathbf{k}_{\bar{\mathbf{J}}}$ ,  $\mathbf{a}_3$ , and  $\mathbf{r}$  onto a unit vector normal to the transversal lattice, respectively. We put  $\gamma_{\bar{\mathbf{J}}} = \sqrt{|\mathbf{k}_{\bar{\mathbf{J}},//}|^2 - \beta^2}$ . In (3) the sum with index “ $\pm$ ” is a shorthand notation for the sum of two terms: one with “+” sign and the other with “-” sign. We refer to (3) as the “spectral-like” representation of the lattice Green function relative to the transversal lattice defined by  $\mathbf{a}_1$  and  $\mathbf{a}_2$ . The formula is valid only for  $|r_{\perp}| < |a_{3\perp}|$ . Nevertheless, since the lattice Green function is pseudo-periodic, it is possible to evaluate  $\Phi_p$  in an arbitrary point of space by reducing the observation point to the unit cell [4, 5]. In (3), it is easy to recognize that the series associated to the first term in brackets is the spectral-representation of the periodic Green function. Thus, we can write that:

$$\Phi_H(\mathbf{r}) = \Phi_p(\mathbf{r}) - \sum_{\bar{\mathbf{J}}} \frac{1}{A_{\text{cell}}} \frac{1}{2\gamma_{\bar{\mathbf{J}}}} \left( \sum_{\pm} \frac{e^{\pm\gamma_{\bar{\mathbf{J}}}r_{\perp}}}{e^{|a_{3\perp}|(\gamma_{\bar{\mathbf{J}}}\pm jk_{\bar{\mathbf{J},\perp})} - 1}} \right) e^{-j\mathbf{k}_{\bar{\mathbf{J}},//}\cdot\mathbf{r}}, \quad |r_{\perp}| < |a_{3\perp}| \quad (4)$$

The above equation relates  $\Phi_p$  and  $\Phi_H$ . Notice that the left-hand side is independent of the primitive vector  $\mathbf{a}_3$ . The second parcel in the right-hand side is a double series with exponential convergence rate. Thus, provided we can evaluate  $\Phi_p$  efficiently we also can evaluate  $\Phi_H$  efficiently. In the next section, we obtain a mixed-domain representation for  $\Phi_p$  with Gaussian convergence.

## 2. The lattice Green function

The lattice Green function is utilized in solid state-physics for computing the electronic structure of solids, in [6] for calculating the Coulomb interaction energy of a lattice of ions, and in [4] for computing the band structure of artificial materials. Spatial and spectral representations for the Green function are well known. These representations converge slowly. In [6], Ewald derived a mixed-domain representation for the Green function with Gaussian convergence rate. However, Ewald's representation requires computing the error function in the complex plane, which is numerically efficient (we refer here parenthetically that Jordan's representation for the periodic Green function is derived directly from Ewald's result). Next, we obtain a new representation for the lattice Green function that does not suffer from that shortcoming. To begin with, we note that the lattice Green function can be written as:

$$\Phi_p(\mathbf{r}) = \sum_{\mathbf{r}_1} \frac{1}{4\pi} \frac{\cos(\beta \rho_1)}{\rho_1} g(\rho_1) e^{-j\mathbf{k}\cdot\mathbf{r}_1} + \sum_{\mathbf{r}_1} \frac{1}{4\pi} \frac{\cos(\beta \rho_1)}{\rho_1} (1 - g(\rho_1)) e^{-j\mathbf{k}\cdot\mathbf{r}_1} \quad (5)$$

where  $\rho_1 = |\mathbf{r} - \mathbf{r}_1|$  and  $g = g(\rho)$  is an arbitrary real function. The above expression is obviously independent of  $g$  and corresponds to the spatial representation of the Green function. Notice that  $\Phi_0 = \cos(\beta|\mathbf{r}|)/4\pi|\mathbf{r}|$  is a fundamental solution of the Helmholtz's equation ( $\Phi_0$  does not satisfy the Sommerfeld's radiation condition; this is irrelevant since  $\Phi_p$ , unlike  $\Phi_H$ , is not required to satisfy any particular boundary condition at infinite). The idea to accelerate the convergence rate of (5) is applying the Poisson summation formula to the first series in the right-hand side of (5). The Poisson formula transforms a sum in the spatial domain into a sum in the spectral domain. We have that:

$$\sum_{\mathbf{r}_1} \frac{1}{4\pi} \frac{\cos(\beta \rho_1)}{\rho_1} g(\rho_1) e^{-j\mathbf{k}\cdot\mathbf{r}_1} = \frac{1}{V_{\text{cell}}} \sum_{\mathbf{J}} \tilde{f}(-\mathbf{k}_{\mathbf{J}}) e^{-j\mathbf{r}\cdot\mathbf{k}_{\mathbf{J}}} \quad (6)$$

where  $V_{\text{cell}} = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|$  is the volume of the unit cell,  $\mathbf{k}_{\mathbf{J}} = \mathbf{k} + j_1 \mathbf{b}_1 + j_2 \mathbf{b}_2 + j_3 \mathbf{b}_3$ , and  $\mathbf{J} = (j_1, j_2, j_3)$  is a generic triple-index. In the above  $\tilde{f}$  is the (triple) Fourier transform of  $g(|\mathbf{r}|)\cos(\beta|\mathbf{r}|)/4\pi|\mathbf{r}|$ . Since this function only depends on  $|\mathbf{r}|$ ,  $\tilde{f}$  can be easily reduced to an integral over the positive real axis. A careful analysis shows that function  $g$  must be chosen such that it is an odd function that converges exponentially to unity as  $\rho$  approaches infinity, and such that  $\tilde{f}$  can be calculated in closed form. An adequate choice for  $g$  is:

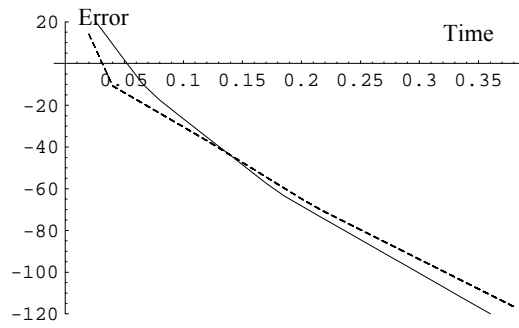
$$g(\rho) = \text{erf}(E\rho) ; \quad \tilde{f}(\mathbf{k}) = \frac{1}{2|\mathbf{k}|} \sum_{\pm} \frac{e^{-(|\mathbf{k} \pm \beta|^2)/4E^2}}{|\mathbf{k} \pm \beta|} \quad (7)$$

In the above, "erf" is the error function, and the sum with index " $\pm$ " is a shorthand notation for the sum of two terms: one with "+" sign and the other with "-" sign. The parameter  $E$  is an arbitrary positive number that defines the relative convergence rate of the two series in (5). An appropriate choice for  $E$  is  $E = \sqrt{\pi}/V_{\text{cell}}^{1/3}$ . Inserting (6) in (5), we obtain a mixed-domain representation for the lattice Green function with Gaussian convergence. Unlike the representation proposed in [6], our representation only requires the evaluation of the error function in the real axis.

### 3. Results and Conclusions

We suggest the following strategy to compute the periodic Green function in an arbitrary point  $\mathbf{r}$ . If  $|r_{\perp}| > 0.5\sqrt{A_{\text{cell}}}$ , the periodic Green function can be efficiently computed using the spectral representation [2], and thus no acceleration technique is required. On the other hand, if  $|r_{\perp}| < 0.5\sqrt{A_{\text{cell}}}$ , the Green function is computed using (4), with  $\mathbf{a}_3$  chosen in such a way that (4) converges as fast as possible. An adequate choice is  $\mathbf{a}_3 = \sqrt{A_{\text{cell}}} \hat{\mathbf{u}}_{\perp}$ , where  $\hat{\mathbf{u}}_{\perp}$  is a unit vector normal to the transversal lattice defined by  $\mathbf{a}_1$  and  $\mathbf{a}_2$ . Since the periodic Green function is independent of  $k_{\perp}$ , we can assume that the wave vector  $\mathbf{k}$  is transversal. Within the considered hypothesis, (4) is valid for  $|r_{\perp}| < \sqrt{A_{\text{cell}}}$ . In (4), the lattice Green function is computed using the mixed-domain representation derived in the previous section.

We compare the computation time between (4) and Jordan's et al formula [3]. In the numerical simulation, we admit that the point sources are arranged into a square lattice in the  $x_1 \times x_2$  plane. The lattice constant is  $a$ . The observation point is  $\mathbf{r} = (0.1, 0, 0)a$  and the wave vector is  $\mathbf{k} = (0.5\pi/a, 0, 0)$ . The wave number is  $\beta = 2\pi/(0.6a)$ . We implemented the numerical algorithms in the commercial software application MATHEMATICA. In Fig. 2, we depict the relative error in percentage for both representations (as a function of the computation time). Note that the vertical axis is in logarithmic units. In spite of Jordan's representation being a double series and representation (4) being a triple series, the computation time for the same accuracy is approximately the same. The simulated results show that the efficiency of both representations is comparable. However, as representation (4) is easier to implement numerically, we conclude that in spite of involving the calculation of a triple series, it is of great relevance and may contribute for the improvement of the existent electromagnetic solvers.



**Fig. 2**  $10\log_{10}$ (relative error in percentage) as function of the computation time (normalized to arbitrary units). Full line: our results. Dashed Line: Jordan's et al formula.

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