# Implementation of Ewald Summation in SCUFF-EM

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## Contents

# 1 The Periodic Dyadic Green's Function

Consider a two-dimensional lattice consisting of a set of lattice vectors $\{\mathbf{L} = (L_x, L_y)\}$. We use the symbol $\mathbf{p} = (p_x, p_y)$ to denote a two-dimensional Bloch wavevector.

The Bloch-periodic version of the scalar Helmholtz Green's function is

$$\overline{G}(k;\mathbf{p};\mathbf{x}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} \frac{e^{ik|\mathbf{x}+\mathbf{L}|}}{4\pi|\mathbf{x}+\mathbf{L}|} \tag{1}$$

# 2 Evaluation by Ewald Summation: The JRS Method

To evaluate the sum in (**??**) efficiently, we use a method outlined by Jordan, Richter, and Sheng (JRS)[1] based on the original ideas of Ewald[2]. For completeness, I will briefly recapitulate the key ideas of this approach.

The starting point is the identity

$$\frac{e^{ikr}}{4\pi r} \equiv \frac{1}{4\pi}\cdot\frac{2}{\sqrt{\pi}}\int_{\mathcal{C}} e^{-z^2r^2+\frac{k^2}{4z^2}}\,dz$$

where $\mathcal{C}$ is a contour in the complex plane running from the origin to $\infty$ and satisfying certain conditions depending on $k$. One choice of $\mathcal{C}$ that suffices for $k$ in the upper-right quadrant is a straight line running from the origin to infinity at an angle of $-\pi/4$ from the positive real axis, i.e.

$$z = \zeta s, \qquad 0 \le s \le \infty, \qquad \zeta = e^{-i\pi/4}$$

in terms of which our identity becomes

$$\frac{e^{ikr}}{4\pi r} \equiv \frac{1}{4\pi}\cdot\frac{2}{\sqrt{\pi}}\cdot\zeta\cdot\int_0^\infty e^{+is^2r^2+\frac{ik^2}{4s^2}}\,ds.$$

## Split the sum into direct-lattice-local and reciprocal-lattice-local contributions

$$\overline{G}(k;\mathbf{p};\mathbf{x}) = \overline{G}^{(1)}(k;\mathbf{p};\mathbf{x}) + \overline{G}^{(2)}(k;\mathbf{p};\mathbf{x}) \tag{2}$$

$$\overline{G}^{(1)}(k;\mathbf{p};\mathbf{x}) = \frac{1}{4\pi}\cdot\frac{2}{\sqrt{\pi}}\cdot\zeta\cdot\sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}}\int_0^E e^{is^2|\mathbf{x}+\mathbf{L}|^2+\frac{ik^2}{4s^2}}\,ds \tag{3}$$

$$\overline{G}^{(2)}(k;\mathbf{p};\mathbf{x}) = \frac{1}{4\pi}\cdot\frac{2}{\sqrt{\pi}}\cdot\zeta\cdot\sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}}\int_E^\infty e^{is^2|\mathbf{x}+\mathbf{L}|^2+\frac{ik^2}{4s^2}}\,ds \tag{4}$$

[1] K. E. Jordan, G. R. Richter, and P. Sheng, "An Efficient Numerical Evaluation of the Green's Function for the Helmholtz Operator on Periodic Structures," *Journal of Computational Physics* **63** 222 (1986). `http://dx.doi.org/10.1016/0021-9991(86)90093-8`

[2]

## Evaluate $\overline{G}^{(2)}$ in real space

The first step is to tackle the sum in (**??**) head-on. The integral in that equation may be evaluated in closed form in terms of the complex error function:

$$\frac{2}{\sqrt{\pi}}\cdot\zeta\int_E^\infty e^{is^2R^2+\frac{ik^2}{4s^2}}ds=\frac{1}{2R}\left\{e^{ikR}\,\text{Erfc}\,\left[RE\zeta+\frac{ik}{2E\zeta}\right]+e^{-ikR}\,\text{Erfc}\,\left[RE\zeta-\frac{ik}{2E\zeta}\right]\right\} \tag{5}$$

Plugging into (**??**), the real-space sum is

$$\begin{aligned}\overline{G}^{(2)}(k;\mathbf{p};\mathbf{x})=\frac{1}{8\pi}\sum_{\mathbf{L}}\frac{e^{i\mathbf{p}\cdot\mathbf{L}}}{|\mathbf{x}+\mathbf{L}|}\Bigg\{&e^{ik|\mathbf{x}+\mathbf{L}|}\text{Erfc}\,\left[R|\mathbf{x}+\mathbf{L}|+\frac{ik}{2E}\right]\\&+e^{-ik|\mathbf{x}+\mathbf{L}|}\text{Erfc}\,\left[R|\mathbf{x}+\mathbf{L}|-\frac{ik}{2E}\right]\Bigg\}\end{aligned}$$

This sum converges very rapidly in real space. Indeed, as soon as $|\mathbf{r}+\mathbf{L}|$ is greater than a few times $E$, the Erfc factors begin to bite down *doubly exponentially* on the summand, and the contribution of distant lattice sites becomes utterly negligible. In practice, for a 2D lattice we achieve 8 or more digits of accuracy by retaining only $\approx$ terms in the sum. Thus we consider this term done, and move on to $\overline{G}^{(1)}$.

## Evaluate $\overline{G}^{(1)}$ in reciprocal space

We would next like to do for $\overline{G}^{(1)}$ what we just did for $\overline{G}^{(2)}$, but this requires a little more work.

First, the integral in (**??**) involves the lower range of the $s$ integral (from $s=0$ to $E$), but the nice closed-form expression we have, equation (**??**), is for the upper range of the integral ($s=E$ to $\infty$). This difficulty was circumvented by Ewald in an ingenious way by appealing to the properties of the classical *Jacobi theta function*, which is defined as

$$\theta(s)=\sum_{n=-\infty}^{\infty}e^{-n^2\pi s} \tag{6}$$

and which satisfies the amazing and bizarre functional identity

$$\theta(s)=\sqrt{\frac{1}{s}}\cdot\theta\left(\frac{1}{s}\right). \tag{7}$$

We will need a slightly more complicated version of this identity, obtained by generalizing (**??**) in two ways: **(a)** we consider a more general summand in which the exponent contains a term linear in $n$ besides the quadratic term in (**??**), and **(b)** instead of summing over all integers $n$ (which we may think of as a sum over a one-dimensional lattice) we instead sum over a *two-dimensional* lattice. The result is that the sum over lattice vectors $\mathbf{L}$ that enters into our equation (**??**) is converted into a sum over *reciprocal lattice* vectors $\mathbf{\Gamma}$:

$$\frac{1}{4\pi}\cdot\frac{2}{\sqrt{\pi}}\sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} e^{-s^2|\mathbf{x}+\mathbf{L}|^2+\frac{k^2}{4s^2}}$$

$$= \frac{1}{s^2}\cdot\frac{A_{\mathbf{\Gamma}}}{8\pi^{5/2}}\sum_{\mathbf{\Gamma}} e^{i(\mathbf{\Gamma}-\mathbf{p})\cdot\mathbf{x}} e^{-\frac{1}{4s^2}\left[|\mathbf{\Gamma}-\mathbf{p}|^2-k^2\right]-z^2s^2} \tag{8}$$

Here the sum is over all vectors $\mathbf{\Gamma}$ that satisfy $\mathbf{\Gamma}\cdot\mathbf{L}=2\pi$ for some lattice vector $\mathbf{L}$, and $A_{\mathbf{\Gamma}}$ is the area of Brillouin zone of the reciprocal lattice.[3] Inserting (**??**) in (**??**), we have

$$\overline{G}^{(1)}(k;\mathbf{p};\mathbf{x}) = \frac{\zeta A_{\mathbf{\Gamma}}}{8\pi^{5/2}}\sum_{\mathbf{\Gamma}} e^{i(\mathbf{\Gamma}-\mathbf{p})\cdot\mathbf{x}}\int_0^E \frac{ds}{s^2} e^{\frac{i}{4s^2}\left[|\mathbf{\Gamma}-\mathbf{p}|^2-k^2\right]+iz^2s^2}$$

Change integration variables according to $s\to\frac{1}{2s}$:

$$= \frac{\zeta A_{\mathbf{\Gamma}}}{4\pi^{5/2}}\sum_{\mathbf{\Gamma}} e^{i(\mathbf{\Gamma}-\mathbf{p})\cdot\mathbf{x}}\int_{\frac{1}{2E}}^{\infty} ds e^{is^2\left[|\mathbf{\Gamma}-\mathbf{p}|^2-k^2\right]+\frac{iz^2}{4s^2}}$$

Evaluate the integral using (**??**):

$$= \frac{A_{\mathbf{\Gamma}}}{16\pi^2}\sum_{\mathbf{\Gamma}}\frac{e^{i(\mathbf{\Gamma}-\mathbf{p})\cdot\mathbf{x}}}{Q(\mathbf{\Gamma},\mathbf{p},k)}\Bigg\{e^{+Qz}\,\mathrm{Erfc}\left[\frac{Q(\mathbf{\Gamma},\mathbf{p},k)}{2E\zeta}+E\zeta z\right] \tag{9}$$
$$+ e^{-Qz}\,\mathrm{Erfc}\left[\frac{Q(\mathbf{\Gamma},\mathbf{p},k)}{2E\zeta}-E\zeta z\right]\Bigg\}$$

where we put

$$Q(\mathbf{\Gamma},\mathbf{p},k)=\sqrt{(\mathbf{\Gamma}-\mathbf{p})^2-k^2}.$$

[3] For a simple rectangular lattice with basis vectors

$$\mathbf{L}_1 = L_x\hat{\mathbf{x}},\qquad \mathbf{L}_2 = L_y\hat{\mathbf{y}},$$

a basis for the reciprocal lattice is

$$\mathbf{\Gamma}_1 = \frac{2\pi}{L_x}\hat{\mathbf{x}},\qquad \mathbf{\Gamma}_2 = \frac{2\pi}{L_y}\hat{\mathbf{y}}$$

and we have $A_{\mathbf{\Gamma}}=\frac{4\pi^2}{L_xL_y}$.
For a hexagonal lattice with basis vectors

$$\mathbf{L}_1 = L\hat{\mathbf{x}},\qquad \mathbf{L}_2 = \frac{L}{2}\hat{\mathbf{x}}+\frac{L\sqrt{3}}{2}\hat{\mathbf{y}}$$

a basis for the reciprocal lattice is

$$\mathbf{\Gamma}_1 = \frac{2\pi}{L}\hat{\mathbf{x}}+\frac{2\pi}{L\sqrt{3}}\hat{\mathbf{y}},\qquad \mathbf{\Gamma}_2 = \frac{4\pi}{\sqrt{3}L}\hat{\mathbf{y}}$$

and we have $A_{\mathbf{\Gamma}}=\frac{8\pi^2}{L^2\sqrt{3}}$.

# The 1D Case

In the 1D case, equations (**??**) and (**??**) take the form