Implementation of Ewald Summation in SCUFF-EM

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Contents

1 The Periodic Green's Function

Consider a 1D or 2D lattice consisting of a set of lattice vectors $\{\mathbf{L}\}$. We use the symbol $\mathbf{p}$ to denote a two-dimensional Bloch wavevector.

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

$$\overline{G}(\mathbf{p};\mathbf{x}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} G\Big(\big|\mathbf{x}-\mathbf{L}\big|\Big) \tag{1}$$

where the sum ranges over all lattice vectors $\mathbf{L}$ and

$$G(r) \equiv \frac{e^{ikr}}{4\pi r}. \tag{2}$$

Note that my notation here hides the dependence of $\overline{G}$ and G on the photon wavenumber k.

The $\overline{G}^{\textbf{ABI}}$ kernel

For computation of BEM matrix elements in SCUFF-EM we also need a version of $\overline{G}$ in which the contribution of the innermost lattice cells are excluded. [Here the "innermost" cells include the cell at the origin ($\mathbf{L}=0$) and all cells within one lattice vector of the origin in any direction.] I refer to this as the "all but innermost" (ABI) periodic Green's function.

For a one-dimensional lattice with lattice vector $\mathbf{L}_0$, $\overline{G}^{\text{ABI}}$ is given by the sum (1) with three terms excluded:

$$\overline{G}^{\text{ABI,1D}}(\mathbf{p};\mathbf{x}) \equiv \sum_{|n|>1} e^{i\mathbf{p}\cdot(n\mathbf{L}_0)} G\Big(\big|\mathbf{x}-n\mathbf{L}_0\big|\Big) \tag{3}$$

For a two-dimensional lattice with lattice vectors $\mathbf{L}_{01},\mathbf{L}_{02}$, the sum excludes 9 terms:

$$\overline{G}^{\text{ABI,2D}}(\mathbf{p};\mathbf{x}) \equiv \sum_{|n_1|>1,|n_2>1|} e^{i\mathbf{p}\cdot(n_1\mathbf{L}_{01}+n_2\mathbf{L}_{02})} G\Big(\big|\mathbf{x}-n_1\mathbf{L}_{01}-n_2\mathbf{L}_{02}\big|\Big) \tag{4}$$

Symmetries of $\overline{G}$ and $\overline{G}^{\textbf{ABI}}$

The 1D case

Consider a 1D lattice with lattice vector $\mathbf{L}_0 = L_0\hat{\mathbf{x}}$. Consider a point $\mathbf{x}=(x,\boldsymbol{\rho})$ whose x coordinate lies outside the unit cell. Write $x = mL_0 + \overline{x}$ where $\overline{x}$ lies within the unit cell. Then we have

$$\begin{aligned}
\overline{G}^{\text{1D}}(\mathbf{p};x,\rho) &= e^{im\mathbf{p}\cdot\mathbf{L}_0}\overline{G}^{\text{1D}}(\mathbf{p};\overline{x},\rho)\\
\overline{G}^{\text{ABI,1D}}(\mathbf{p};x,\rho) &= \sum_{|n|>1} e^{in\mathbf{p}\cdot\mathbf{L}} G\big(\overline{x}+(m-n)L_0,\rho\big)
\end{aligned}$$

Change variables to $n' = n - m$:

$$\begin{aligned}
\overline{G}^{\text{ABI,1D}}(\mathbf{p}; x, \rho) &= e^{im\mathbf{p}\cdot\mathbf{L}} \sum_{|n'+m|>1} e^{in'\mathbf{p}\cdot\mathbf{L}} G\big(\overline{x} - n'L_0, \rho\big) \\
&= e^{im\mathbf{p}\cdot\mathbf{L}} \sum_{|n'+m|>1} T_{n'}
\end{aligned}$$

[where $T_n \equiv e^{in\mathbf{p}\cdot\mathbf{L}} G(\overline{x} - nL_0, \rho)$]. For the special case $m = 1$ we have

$$\begin{aligned}
&= e^{im\mathbf{p}\cdot\mathbf{L}} \Big[\overline{G}^{\text{1D}} - T_{-2} - T_{-1} - T_0\Big] \\
&= e^{im\mathbf{p}\cdot\mathbf{L}} \Big[\overline{G}^{\text{ABI1D}} + T_1 - T_{-2}\Big].
\end{aligned}$$

For $m = -1$ we have instead

$$= e^{im\mathbf{p}\cdot\mathbf{L}} \Big[\overline{G}^{\text{ABI1D}} + T_{-1} - T_2\Big].$$

2 Ewald summation

2.1 Decompose kernel into short-range and long-range contributions

The kernel (2) exhibits two pathologies which, together, make it unwieldy to work with: **(a)** It decays slowly as $r \to \infty$, which ensures that the real-space sum (1) is slowly convergent. This suggests using the Poisson summation formula to rewrite the real-space sum as a Fourier-space sum. However, upon doing this we are stymied by the second pathology of (2), namely, **(b)** It is singular at $r = 0$, which makes it long-ranged in Fourier space and thus prevents naïve application of Poisson summation.

To address this difficulty, we split the bare kernel (2) into a "short-ranged" component which avoids pathology **(a)**, plus a "long-ranged" component which avoids pathology **(b)**:

$$G(r) = G^{\text{short}}(r) + G^{\text{long}}(r) \tag{5}$$

$$G^{\text{short}}(r) \equiv \frac{1}{2\pi^{3/2}} \int_{\mathcal{C}_2} e^{-u^2 r^2 + k^2/(4u^2)}\, du \tag{6}$$

$$G^{\text{long}}(r) \equiv \frac{1}{2\pi^{3/2}} \int_{\mathcal{C}_1} e^{-u^2 r^2 + k^2/(4u^2)}\, du \tag{7}$$

where $\{\mathcal{C}_1, \mathcal{C}_2\}$ are two branches of a certain contour in the complex plane (see Appendix). The periodic DGF naturally decomposes into a contribution arising primarily from nearby lattice cells plus a contribution arising primarily from distant lattice cells (where "nearby" and "distant" are reckoned relative to the evaluation point $\mathbf{x}$:

$$\overline{G}(\mathbf{p};\mathbf{x}) = \overline{G}^{\text{nearby}}(\mathbf{p};\mathbf{x}) + \overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x}) \tag{8}$$

$$\overline{G}^{\text{nearby}}(\mathbf{p};\mathbf{x}) = \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} G^{\text{short}}\Big(\big|\mathbf{x}-\mathbf{L}\big|\Big) \tag{9}$$

$$\overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x}) = \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} G^{\text{long}}\Big(\big|\mathbf{x}-\mathbf{L}\big|\Big). \tag{10}$$

2.2 Evaluate $\overline{G}^{\textbf{nearby}}$ in real space

The sum defining $\overline{G}^{\text{nearby}}$ is now rapidly convergent and may be evaluated directly via simple code. To this end it is convenient to invoke the identity (24) to write

$$G^{\text{short}}(r) = \frac{1}{8\pi r}\left\{ e^{ikr}\text{erfc}\left[\eta r + i\frac{k}{2\eta}\right] + e^{-ikr}\text{erfc}\left[\eta r - i\frac{k}{2\eta}\right]\right\} \tag{11}$$

$$\equiv \texttt{PH}(\eta, r, k) \tag{12}$$

where the last line defines a convenient shorthand notation for the function of the first line ("`PH`" stands for "partial Helmholtz"). Evaluation of $\overline{G}^{\text{nearby}}$ now proceeds by straightforward numerical summation of equation (9) using (11) to compute summand values:

$$\overline{G}^{\text{nearby}}(\mathbf{p};\mathbf{x}) = \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}}\,\mathtt{PH}\Big(\eta, |\mathbf{r}-\mathbf{L}|, k\Big). \tag{13}$$

Note that the form of this equation is the same for the 1D and 2D cases; only the dimension of the summation changes.

Typically the partial sum converges to 10 or more decimal places after summing ~ 10 terms (in the 1D case) or ~ 100 terms (in the 2D case).

2.3 Evaluate $\overline{G}^{\textbf{distant}}$ in Fourier space

On the other hand, the real-space sum defining $\overline{G}^{\text{distant}}$ is slowly convergent, but the non-singular behavior of G^{long} allows the use of Poisson summation to recast the sum (17) as a rapidly convergent sum in reciprocal space. This sum takes slightly different forms in the 1D and 2D cases.

2.3.1 The 1D case

We first consider the case in which the fundamental lattice vector is aligned with the $\hat{\mathbf{x}}$ direction, i.e. $\mathbf{L}_0 = L_{0x}\hat{\mathbf{x}}$. The extension to an arbitrary two-dimensional lattice vector $\mathbf{L}_0 = L_{0x}\hat{\mathbf{x}} + L_{0y}\hat{\mathbf{y}}$ is then immediate.

For a 1D lattice with basis vectors $\{\mathbf{L} = n_x L_{0x}\hat{\mathbf{x}}\}$ (for all $n_x \in \mathbb{Z}$) we have

$$\begin{aligned}\overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x}) &= \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} G^{\text{long}}\Big(\big|\mathbf{x}-\mathbf{L}\big|\Big)\\ &= \sum_{n=-\infty}^{\infty} e^{inp_x L_{0x}} G^{\text{long}}\Big(\sqrt{(x-nL_{0x})^2+\rho^2}\Big)\end{aligned}$$

with $\rho^2 = y^2 + z^2$. Introduce shorthand:

$$\equiv \sum_{n=-\infty}^{\infty} f(n) \tag{14}$$

Now just use Poisson summation:

$$= 2\pi \sum_{m=-\infty}^{\infty} \widetilde{f}\,(2\pi m) \tag{15}$$

where $\widetilde{f}(\nu)$ is the Fourier transform of $f(n)$ with respect to n. To figure out what this is, introduce the Fourier-synthesis representation of G^{long} [Appendix

A]:

$$f(n) = e^{inp_x L_{0x}} G^{\text{long}}\Big(\sqrt{(x-nL_{0x})^2+\rho^2}\Big)$$

$$\begin{aligned}
&= e^{inp_x L_{0x}} \int_{-\infty}^{\infty} \widetilde{G^{\text{long}}}(k_x;\rho) e^{ik_x(x-nL_{0x})}\,dk_x \\
&= \int_{-\infty}^{\infty} e^{ik_x x}\widetilde{G^{\text{long}}}(k_x;\rho) e^{i(p_x-k_x)n_x L_{0x}}\,dk_x
\end{aligned}$$

Change integration variables to $\nu = -(k_x - p_x)L_{0x}$:

$$= \int_{-\infty}^{\infty} \underbrace{\frac{1}{L_{0x}} e^{i(p_x - \frac{\nu}{L_{0x}})x} \widetilde{G^{\text{long}}}\left(p_x - \frac{\nu}{L_{0x}};\rho\right)}_{\widetilde{f}(\nu)} e^{i\nu n_x}\,d\nu$$

This identifies the Fourier transform of the function $f(n)$ that enters (14) as

$$\widetilde{f}(\nu) = \frac{1}{L_{0x}} e^{i(p_x-\frac{\nu}{L_{0x}})x} \widetilde{G^{\text{long}}}\Big(p_x - \frac{\nu}{L_{0x}};\rho\Big)$$

and hence the sum that defines the distant contribution to the periodic GF, equation (15), reads

$$\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) = \frac{2\pi}{L_{0x}}\sum_m e^{i(p_x - \frac{2\pi m}{L_{0x}})x}\widetilde{G^{\text{long}}}\Big(p_x - \frac{2\pi m}{L_{0x}};\rho\Big). \tag{16}$$

This derivation assumed that the fundamental lattice vector was aligned with the positive x-direction, i.e. I had $\mathbf{L}_0 = L_{0x}\hat{\mathbf{x}}$. A more general form which is valid for any lattice vector $\mathbf{L}$ is

$$\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) = \mathcal{V}_{\text{BZ}}\sum_m e^{i(\mathbf{p}-m\boldsymbol{\Gamma}_0)\cdot\mathbf{x}}\widetilde{G^{\text{long}}}\Big(\big|\mathbf{p}-m\boldsymbol{\Gamma}_0\big|;\rho\Big) \tag{17}$$

where $\boldsymbol{\Gamma}_0 = \frac{2\pi}{|\mathbf{L}_0|^2}\mathbf{L}_0$ is the fundamental lattice vector of the 1-dimensional Brillouin zone and $\mathcal{V}_{\text{BZ}} = |\boldsymbol{\Gamma}|$ is its volume; in (17) the quantity ρ must now be interpreted as the $\left|\mathbf{x} - \frac{(\mathbf{x}\cdot\mathbf{L})}{|\mathbf{L}|^2}\mathbf{L}\right|$.

2.3.2 The 2D case

For a square 2D lattice with basis vectors $\mathbf{L} = n_x L_{0x}\hat{\mathbf{x}} + n_y L_{0y}\hat{\mathbf{y}}$ (for all $n_x, n_y \in \mathbb{Z}$) we have

$$\begin{aligned}
\overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x}) &= \sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}} G^{\text{long}}\Big(\big|\mathbf{x}-\mathbf{L}\big|\Big) \\
&= \sum_{n_x,n_y=-\infty}^{\infty} e^{i(n_x p_x L_{0x} + n_y p_y L_{0y})} G^{\text{long}}\Big(\sqrt{(x-n_xL_{0x})^2+(y-n_yL_{0y})^2+z^2}\Big)
\end{aligned}$$

Again introduce shorthand:

$$\equiv \sum_{n_x,n_y=-\infty}^{\infty} f(n_x,n_y) \tag{18}$$

and again use Poisson summation:

$$= (2\pi)^2 \sum_{m_x,m_y=-\infty}^{\infty} \widetilde{f}(2\pi m_x, 2\pi m_y) \tag{19}$$

where $\widetilde{f}(\nu_x,\nu_y)$ is the two-dimensional Fourier transform of $f(n_x,n_y)$ with respect to n_x,n_y. To figure out what this is, introduce the Fourier-synthesis representation of G^{long} [Appendix A]:

$$f(n_x,n_y) = e^{i(n_x p_x L_{0x}+n_y p_y L_{0y})} G^{\text{long}}\Big(\sqrt{(x-n_xL_{0x})^2+(y-n_yL_{0y})^2+z^2}\Big)$$

$$= e^{i(n_x p_x L_{0x}+n_y p_y L_{0y})} \int \widetilde{G^{\text{long}}}(\mathbf{k};z) e^{ik_x(x-n_xL_{0x})+ik_y(y-n_yL_{0y})}\,d\mathbf{k}$$

Change integration variables to $\nu_i = (p_i - k_i)L_i$:

$$= \int \underbrace{\frac{1}{L_{0x}L_{0y}} e^{i(p_x-\frac{\nu_x}{L_{0x}})x+i(p_y-\frac{\nu_y}{L_{0y}})y} \widetilde{G^{\text{long}}}(p_x-\frac{\nu_x}{L_{0x}}, p_y-\frac{\nu_y}{L_{0y}}; z)}_{\widetilde{f}(\nu_x,\nu_y)} e^{i(\nu_x n_x+\nu_y n_y)}\,d\boldsymbol{\nu}$$

This identifies the Fourier transform of the function $f(n_x,n_y)$ that enters (18) as

$$\begin{aligned}\widetilde{f}(\nu_x,\nu_y) &= \frac{1}{L_{0x}L_{0y}} e^{i(p_x-\frac{\nu_x}{L_{0x}})x+i(p_y-\frac{\nu_y}{L_{0y}})y} \widetilde{G^{\text{long}}}(p_x-\frac{\nu_x}{L_{0x}}, p_y-\frac{\nu_y}{L_{0y}}; z)\\ &= \frac{1}{2\pi L_{0x}L_{0y}} e^{i(p_x-\frac{\nu_x}{L_{0x}})x+i(p_y-\frac{\nu_y}{L_{0y}})y} \texttt{PH}\Big(\frac{1}{2\eta}, \sqrt{k^2-(p_x-\frac{\nu_x}{L_{0x}})^2-(p_y-\frac{\nu_y}{L_{0y}})^2}, \frac{z}{2}\Big)\end{aligned}$$

and hence the sum that defines the distant contribution to the 2D periodic Green's function, equation (19), reads

$$\begin{aligned}&\overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x})\\ &= \frac{2\pi}{L_{0x}L_{0y}} \sum_{m_x,m_y} e^{i(p_x-m_x\Gamma_{0x})x+(p_y-m_y\Gamma_{0y})y} \texttt{PH}\left(\frac{1}{2\eta}, \sqrt{k^2+(p_x-m_x\Gamma_{0x})^2+(p_y-m_y\Gamma_{0y})^2}, \frac{z}{2}\right)\end{aligned}$$

where $\{\Gamma_{0x},\Gamma_{0y}\} = \left\{\frac{2\pi}{L_{0x}}, \frac{2\pi}{L_{0y}}\right\}$. I could alternatively write this equation as a sum over all 2D reciprocal lattice vectors $\boldsymbol{\Gamma}$:

$$\overline{G}^{\text{distant}}(\mathbf{p};\mathbf{x}) = \frac{1}{2\pi}\mathcal{V}_{BZ} \sum_{\boldsymbol{\Gamma}} e^{i(\mathbf{p}-\boldsymbol{\Gamma})\cdot\mathbf{x}}\, \texttt{PH}\left(\frac{1}{2\eta}, \sqrt{k^2+|\mathbf{p}-\boldsymbol{\Gamma}|^2}, \frac{z}{2}\right) \tag{20}$$

where $\mathcal{V}_{BZ}$ is the volume (really the area since we are in two dimensions) of the Brillouin zone.

Although we derived it above for the case of a square lattice, the result in the form (20) holds for any shape of lattice.

A Fourier Transforms of G^{long} in 1 and 2 Dimensions

A.1 1D

The Fourier-synthesized form of $G^{\text{long}}(r)$ at a point $r=\sqrt{x^2+\rho^2}$ (with $\rho^2 = y^2+z^2$) is

$$\begin{aligned} G^{\text{long}}(r) &= G^{\text{long}}\Big(\sqrt{x^2+\rho^2}\Big) \\ &= \int_{-\infty}^{\infty} \widetilde{G^{\text{long}}}(k_x;\rho)e^{ik_x x}\,dk_x \end{aligned}$$

where

$$\widetilde{G^{\text{long}}}(k_x;\rho) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G^{\text{long}}\Big(\sqrt{x^2+\rho^2}\Big)e^{-ik_x x}\,dx.$$

Insert (7):

$$\begin{aligned} &= \frac{1}{4\pi^{5/2}}\int_{\mathcal{C}_1} du\, e^{-u^2\rho^2+\frac{k^2}{4u^2}} \underbrace{\int_{-\infty}^{\infty} e^{-u^2x^2-ik_x x}\,dx}_{\sqrt{\pi}\cdot u^{-1}\cdot e^{-k_x^2/4u^2}} \\ &= \frac{1}{4\pi^2}\int_{\mathcal{C}_1} \frac{du}{u}\, e^{-u^2\rho^2+(k^2-k_x^2)/(4u^2)}. \end{aligned}$$

Now put $k_t^2 = k_x^2 - k^2$ and change variables to $t=\eta/u^2$, $dt=-2tdu/u$:

$$= \frac{1}{8\pi^2}\int_1^{\infty} \frac{dv}{v}\, e^{-\frac{k_t^2}{4\eta^2}-\frac{\rho^2\eta^2}{4t}}$$

Series-expand the quantity $e^{-(\rho^2\eta^2)/4t}$:

$$\begin{aligned} &= \frac{1}{8\pi^2}\sum_{q=0}^{\infty}\frac{1}{q!}\left(-\frac{\rho^2\eta^2}{4}\right)^q \underbrace{\int_1^{\infty}\frac{dt}{t^{1+q}}\, e^{-\frac{k_t^2}{4\eta^2}}}_{\mathrm{E}_{1+q}\left(\frac{k_t^2}{4\eta^2}\right)} \\ &= \frac{1}{8\pi^2}\sum_{q=0}^{\infty}\frac{1}{q!}\left(-\frac{\rho^2\eta^2}{4}\right)^q \mathrm{E}_{1+q}\left(\frac{k_t^2}{4\eta^2}\right) \qquad (21) \end{aligned}$$

where E_{1+q} is the exponential integral function of order $1+q$. In what follows we will also need the first and second partial derivatives of $\widetilde{G^{\text{long}}}$ with respect to ρ. These wind up being given by almost the same sum as (21), but with extra factors inserted into the summand:

$$\partial_\rho \widetilde{G^{\text{long}}}(k_x,\rho) = \frac{1}{8\pi^2}\sum_{q=1}^{\infty}\frac{1}{q!}\left(\frac{2q}{\rho}\right)\left(-\frac{\rho^2\eta^2}{4}\right)^q \mathrm{E}_{1+q}\left(\frac{k_t^2}{4\eta^2}\right)$$

$$\partial_\rho^2 \widetilde{G^{\text{long}}}(k_x,\rho) = \frac{1}{8\pi^2}\sum_{q=1}^{\infty}\frac{1}{q!}\left(\frac{2q(2q-1)}{\rho^2}\right)\left(-\frac{\rho^2\eta^2}{4}\right)^q \mathrm{E}_{1+q}\left(\frac{k_t^2}{4\eta^2}\right)$$

Computation in the large-ρ regime

The series (21) is poorly convergent for large ρ (where "large" means "large compared to $1/\eta$."). However, this is the regime in which $G^{\text{long}}(r)$ is nearly equal[1] to the full Helmholtz Green's function $G^{\text{full}}(r) = \frac{e^{ikr}}{4\pi r}$, so we may approximate $\widetilde{G^{\text{long}}}$ by the 1D Fourier transform of G^{full}:

$$\widetilde{G^{\text{full}}}(k_x;\rho) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{ik\sqrt{x^2+\rho^2}}}{4\pi\sqrt{x^2+\rho^2}}\,e^{-ik_x x}\,dx$$

Insert the Fourier representation of G^{full}, which reads $\frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|} = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{|\mathbf{q}|^2-k^2}$:

$$\begin{aligned}
&= \frac{1}{2\pi}\int dx \int \frac{d\mathbf{q}}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{r}-ik_x x}}{\mathbf{q}^2-k^2} \\
&= \int \frac{d\mathbf{q}}{(2\pi)^3}\frac{e^{i(q_y y+q_z z)}}{\mathbf{q}^2-k^2}\cdot \underbrace{\frac{1}{2\pi}\int dx\, e^{i(q_x-k_x)x}}_{\delta(q_x-k_q)} \\
&= \int \frac{d\mathbf{q}_\perp}{(2\pi)^3}\frac{e^{i\mathbf{q}_\perp\cdot\boldsymbol{\rho}}}{k_x^2+\mathbf{q}_\perp^2-k^2} \\
&= \int_0^\infty \frac{q\,dq}{(2\pi)^3(k_x^2+q^2-k^2)}\underbrace{\int_0^{2\pi} e^{iq\rho\cos\theta}\,d\theta}_{2\pi J_0(q\rho)} \\
&= \int_0^\infty \frac{qJ_0(q\rho)dq}{(2\pi)^2(k_x^2+q^2-k^2)} \\
&= \frac{1}{4\pi^2}K_0\Big([k_x^2-k^2]^{1/2}\rho\Big)
\end{aligned}$$

where K_0 is a Bessel function.

Derivatives:

[1]By my calculations, $G^{\text{long}}(r)$ and $G^{\text{full}}(r)$ seem to agree to 9 or more digits whenever $r > 4.5\eta$.

$$\begin{aligned}\partial_\rho \widetilde{G^{\text{full}}}(k_x;\rho) &= -\frac{k_t K_1(k_t\rho)}{4\pi^2}\\ \partial_\rho^2 \widetilde{G^{\text{full}}}(k_x;\rho) &= \frac{k_t^2\Big[K_0(k_t\rho)+K_2(k_t\rho)\Big]}{8\pi^2}\end{aligned}$$

where

$$k_t^2 = k_x^2 - k^2.$$

A.2 2D

The Fourier-synthesized form of $G^{\text{long}}(r)$ at a point $r=\sqrt{x^2+y^2+z^2}$ is

$$\begin{aligned}G^{\text{long}}(r) &= G^{\text{long}}\Big(\sqrt{x^2+y^2+z^2}\Big)\\ &= \int_{-\infty}^{\infty} \widetilde{G^{\text{long}}}(\mathbf{k};z)e^{i\mathbf{k}\cdot\mathbf{x}}\,d\mathbf{k}\end{aligned}$$

where $\mathbf{x}=(x,y)$, $\mathbf{k}=(k_x,k_y)$, and

$$\begin{aligned}\widetilde{G^{\text{long}}}(\mathbf{k};z) &= \frac{1}{(2\pi)^2}\int G^{\text{long}}\Big(\sqrt{x^2+y^2+z^2}\Big)e^{-i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}\\ &= \frac{1}{(2\pi)^2}\int_0^\infty \rho\,d\rho\int_0^{2\pi} d\theta\, G^{\text{long}}\Big(\sqrt{\rho^2+z^2}\Big)e^{-i|\mathbf{k}|\rho\cos\theta}\\ &= \frac{1}{2\pi}\int_0^\infty \rho J_0(|\mathbf{k}|\rho)G^{\text{long}}\Big(\sqrt{\rho^2+z^2}\Big)\,d\rho\\ &= \frac{1}{4\pi^{5/2}}\int_{\mathcal{C}_1} du\, e^{-u^2z^2+k^2/(4u^2)}\underbrace{\int_0^\infty \rho J_0(|\mathbf{k}|\rho)e^{-u^2\rho^2}\,d\rho}_{\frac{1}{2u^2}e^{-|\mathbf{k}|^2/(4u^2)}}\\ &= \frac{1}{8\pi^{5/2}}\int_{\mathcal{C}_1}\frac{du}{u^2}\,e^{-u^2z^2+(k^2-|\mathbf{k}|^2)/(4u^2)}\end{aligned}$$

Change variables to $s=1/(2u)$:

$$\begin{aligned}&= \frac{1}{4\pi^{5/2}}\int_{\mathcal{C}_2} e^{-(k^2-|\mathbf{k}|^2)s^2+z^2/(4s^2)}\,ds\\ &= \frac{1}{2\pi}\mathtt{PH}\Big(\frac{1}{2\eta}, i\sqrt{k^2-|\mathbf{k}|^2}, \frac{z}{2}\Big).\end{aligned}$$

A.3 3D

$$\begin{aligned}G^{\text{long}}(r) &= G^{\text{long}}\Big(\sqrt{x^2+y^2+z^2}\Big)\\ &= \int_{-\infty}^{\infty}\widetilde{G^{\text{long}}}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\,d\mathbf{k}\end{aligned}$$

where $\mathbf{x} = (x, y, z)$, $\mathbf{k} = (k_x, k_y, k_y)$, and

$$\widetilde{G^{\text{long}}}(\mathbf{k}; z) = \frac{1}{(2\pi)^3} \int G^{\text{long}}\Big(\sqrt{x^2 + y^2 + z^2}\Big) e^{-i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{x}.$$

Insert (7):

$$= \frac{1}{16\pi^{9/2}} \int_{\mathcal{C}_1} du\, e^{\frac{k^2}{4u^2}} \underbrace{\Big[\int_{-\infty}^{\infty} e^{-u^2x^2 - ik_x x}\, dx\Big]}_{\sqrt{\pi}\cdot u^{-1}\cdot e^{-k_x^2/4u^2}} \underbrace{\Big[\int_{-\infty}^{\infty} e^{-u^2y^2 - ik_x y}\, dy\Big]}_{\sqrt{\pi}\cdot u^{-1}\cdot e^{-k_y^2/4u^2}} \underbrace{\Big[\int_{-\infty}^{\infty} e^{-u^2z^2 - ik_z z}\, dy\Big]}_{\sqrt{\pi}\cdot u^{-1}\cdot e^{-k_z^2/4u^2}}$$

$$= \frac{1}{16\pi^3} \int_{\mathcal{C}_1} \frac{du}{u^{3/2}} e^{\frac{k^2 - |\mathbf{k}|^2}{(4u^2)}}$$

B Short-distance behavior of G^{long} in real space

For computations of the "all-but-3" or "all-but-9" kernels we need to compute the contributions of the innermost 3 or 9 lattice cells to $\overline{G}^{\text{distant}}$ (so that we may subtract these real-space contributions from the Fourier-space sum that computes the sum over all real-space lattice cells). This involves evaluating the kernel G^{long} in real space. Unfortunately, it seems there is no formula equivalent to (11) for convenient evaluation of G^{long} in real space. Instead, we compute $G^{\text{long}}(r)$ as follows:

1. For r not close to zero, we simply set

$$G^{\text{long}}(r) = \frac{e^{ikr}}{4\pi r} - G^{\text{short}}(r) \tag{22}$$

   with G^{short} computed by equation (11).

2. In the limit $r \to 0$, both terms in (22) diverge, but the difference tends to a finite constant—that is to say, $G^{\text{long}}(r=0)$ is nonzero and finite. With a little work one obtains the following small-r expansion:

$$G^{\text{long}}(r) = C_0 + C_2 r^2 + C_4 r^4 + O(r^6)$$

$$C_0 = \frac{\eta}{2\pi^{3/2}} e^{k^2/(4\eta^2)} + \frac{ik}{4\pi}\left[1 + \text{erf}\left(\frac{ik}{2\eta}\right)\right]$$

$$C_2 = -\frac{\eta(2\eta^2 + k^2)}{12\pi^{3/2}} e^{k^2/(4\eta^2)} - \frac{ik^3}{24\pi}\left[1 + \text{erf}\left(\frac{ik}{2\eta}\right)\right]$$

$$C_4 = \frac{\eta(12\eta^4 + 2\eta^2 k^2 + k^4)}{240\pi^{3/2}} e^{k^2/(4\eta^2)} + \frac{ik^5}{480\pi}\left[1 + \text{erf}\left(\frac{ik}{2\eta}\right)\right]$$

   where again $\zeta = e^{-i\pi/4}$.

C Reference identities

Contour-integral expression for the Helmholtz kernel

$$\frac{e^{ikr}}{4\pi r} \equiv \frac{1}{2\pi^{3/2}} \int_{\mathcal{C}} e^{-r^2u^2+k^2/(4u^2)}\, du \tag{23}$$

where $\mathcal{C}$ is a contour like that pictured in Figure **??**; the key features of this contour are the following:

1. Over the interval $[0, \eta]$ on the real axis, the contour dips down into the lower half-plane with slope γ.
2. Over the interval $[\eta, \infty]$ on the real axis, the contour pokes up into the upper half-plane.
3. The slope at the origin, γ, lies in the range $0 \le \gamma \le \left(\frac{\pi}{4} - \arg k\right)$ where $\arg k$ is the phase angle of the complex wavenumber (Helmholtz parameter).
4. The variable substitution $z \to 1/z$ transforms integrals over $\mathcal{C}_1$ into integrals over $\mathcal{C}_2$.

Property (3) here is required to ensure that the integrand remains well-behaved as we approach $u = 0$ along $\mathcal{C}$. Indeed, in the vicinity of the origin we have

$$u \approx e^{-i\gamma} t$$

for a real-valued variable t approaching $t \to 0$. The exponent of the integrand in (23) then approaches

$$\text{exponent} \approx \frac{k^2}{4u^2} \to |k|^2 e^{2(\arg\, k+\gamma)} \cdot \frac{1}{4t^2}$$

and we need the real part of this quantity to tend to *negative* infinity so that the exponential as a whole tends to zero instead of blowing up, i.e. we require

$$\text{Re } e^{2(\arg\, k+\gamma)} < 0 \qquad \Longrightarrow \qquad \frac{\pi}{2} < 2(\arg\, k + \gamma) > \frac{3\pi}{2}$$

Since we always have $0 \le \arg\, k \le \pi/2$ and we want to choose γ in the range $0 \le \gamma \le \frac{\pi}{2}$, this translates into the requirement that

$$\gamma > \frac{\pi}{4} - \arg\, k.$$

Short-ranged Helmholtz kernel

$$\begin{aligned}\texttt{PH}(\eta,r,k) &\equiv \frac{1}{2\pi^{3/2}}\int_{\mathcal{C}_2} e^{ir^2u^2+i\frac{k^2}{4u^2}}\,du \\ &= \frac{1}{8\pi r}\left\{e^{ikr}\text{erfc}\left[\eta r+i\frac{k}{2\eta}\right]+e^{-ikr}\text{erfc}\left[\eta r-i\frac{k}{2\eta}\right]\right\} \end{aligned} \tag{24}$$

(Here $\mathcal{C}_2$ is the portion of the contour that covers the real-axis interval $[\eta,\infty]$.) I call this function the "partial Helmholtz" function because $\texttt{PH}(\eta,r,k)$ is a sort of partial version of the Helmholtz kernel $e^{ikr}/(4\pi r)$.

C.1 Example contour [COMPLETE ME]

One example of such a contour that satisfies the requirements enumerated in Section is

$$\mathcal{C}=\{\text{Re }z,\text{Im }z\}=\left\{t,-4\eta\gamma\sin\left(4\,\text{atan}\frac{t}{\eta}\right)\right\},\qquad 0\le t\le\infty$$

where $\mathcal{C}_1$ and $\mathcal{C}_2$ corresponding to the parameter ranges $t\in[0,\eta]$ and $t\in[\eta,\infty]$.

To demonstrate that this contour satisfies in particular property (4) in Section C.1, go like this:

$$\mathcal{I}=\int_{\mathcal{C}_1} f(z)dz=\int_0^\eta f\Big[z(t)\Big]z'(t)\,dt$$

where

$$z(t)=t-i\gamma\sin\left(4\,\text{atan}\frac{t}{\eta}\right),\qquad z'(t)=1-i\frac{16\gamma\eta^2\cos\left(4\text{atan}\frac{t}{\eta}\right)}{t^2+\eta^2}.$$

Now change variables to $s=\frac{\eta^2}{t},-\frac{\eta^2}{s^2}ds=dt$. The integral becomes

$$\mathcal{I}=\int_\eta^\infty f\Big[z(s)\Big]z'(s)\frac{\eta^2}{s^2}ds.$$

First note that

$$\text{atan}\frac{t}{\eta}=\text{atan}\frac{\eta}{s}=\frac{\pi}{2}-\text{atan}\frac{s}{\eta}$$

and hence

$$\sin\left(4\,\text{atan}\frac{t}{\eta}\right)=-\sin\left(4\,\text{atan}\frac{s}{\eta}\right),\qquad \cos\left(4\,\text{atan}\frac{t}{\eta}\right)=+\cos\left(4\,\text{atan}\frac{s}{\eta}\right).$$

Thus

$$z'(s)=1-\frac{\eta^2}{s}+i\gamma\left(4\,\text{atan}\frac{s}{\eta}\right)$$

Also,

$$z(t) = \frac{\eta^2}{s} + i\gamma\left(4\,\mathrm{atan}\frac{s}{\eta}\right)$$

$$G^{\mathrm{long}}(\mathbf{r}) = \frac{1}{2\pi^{3/2}}\int_0^\eta e^{-u^2(t)r^2+k^2/(4u^2(t))}\left[1 - i\frac{4\gamma\eta\cos\left(4\,\mathrm{atan}\frac{t}{\eta}\right)}{t^2+\eta^2}\right]dt$$

$$G^{\mathrm{short}}(\mathbf{r}) = \frac{1}{2\pi^{3/2}}\int_\eta^\infty e^{-u^2(t)r^2+k^2/(4u^2(t))}\left[1 - i\frac{4\gamma\eta\cos\left(4\,\mathrm{atan}\frac{t}{\eta}\right)}{t^2+\eta^2}\right]dt$$

where $u(t) = t - i\gamma\sin\left(4\,\mathrm{atan}\frac{t}{\eta}\right)$.

D Derivatives

D.1 Derivatives of $\overline{G}^{\text{nearby}}$

$$\frac{d}{dx_i}\overline{G}^{\text{nearby}}(\mathbf{p};\mathbf{x}) = \frac{x_i}{r}\sum_{\mathbf{L}} e^{i\mathbf{p}\cdot\mathbf{L}}\,\frac{\partial}{\partial r}\texttt{PH}\Big(\eta, r, k\Big)\Big|_{r=|\mathbf{r}-\mathbf{L}|}$$

D.2 Derivatives of $\overline{G}^{\text{distant}}$: 1D

In this section I assume the lattice basis vector points in the $\hat{\mathbf{x}}$ direction so that $\overline{G}^{\text{distant}}$ is is defined by the sum (16).

$$\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) = \frac{2\pi}{L_{0x}}\sum_m e^{iQ_m x}\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)$$

where

$$Q_m \equiv p_x - \frac{2m\pi}{L_{0x}}, \qquad \rho = \sqrt{x^2+y^2}.$$

$$\begin{aligned}
\partial_x\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\sum_m (iQ_m)e^{iQ_m x}\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_y\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{y}{\rho}\right)\sum_m e^{iQ_m x}\partial_\rho\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_z\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{z}{\rho}\right)\sum_m e^{iQ_m x}\partial_\rho\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_x\partial_y\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{y}{\rho}\right)\sum_m (iQ_m)e^{iQ_m x}\partial_\rho\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_x\partial_z\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{z}{\rho}\right)\sum_m (iQ_m)e^{iQ_m x}\partial_\rho\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_y\partial_z\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{yz}{\rho^2}\right)\sum_m e^{iQ_m x}\Big(\partial^2_{\rho\rho}-\frac{1}{\rho}\partial_\rho\Big)\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)\\
\partial_x\partial_y\partial_z\overline{G}^{\text{distant}}(\mathbf{p},\mathbf{x}) &= \frac{2\pi}{L_{0x}}\left(\frac{yz}{\rho^2}\right)\sum_m (iQ_m)e^{iQ_m x}\Big(\partial^2_{\rho\rho}-\frac{1}{\rho}\partial_\rho\Big)\widetilde{G^{\text{long}}}\Big(Q_m;\rho\Big)
\end{aligned}$$

where

D.3 Derivatives of $\overline{G}^{\text{distant}}$: 2D