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One- and two-dimensional lattice sums for the three-dimensional Helmholtz equation

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ABSTRACT

The accurate and efficient computation of lattice sums for the three-dimensional Helmholtz equation is considered for the cases where the underlying lattice is one- or two-dimensional. We demonstrate, using careful numerical computations, that the reduction method, in which the sums for a two-dimensional lattice are expressed as a sum of one-dimensional lattice sums leads to an order-of-magnitude improvement in performance over the well-known Ewald method. In the process we clarify and improve on a number of results originally formulated by Twersky in the 1970s.

1. Introduction

Lattice sums of the type considered in this paper arise naturally in two different ways. On the one hand, problems involving scattering by either a sheet or a line of spheres can be reduced to linear systems of equations in which the elements of the coefficient matrix involve lattice sums. Alternatively, lattice sums can used as part of an efficient scheme for the computation of the quasi-periodic Green's function which is required when solving more general scattering problems using integral equations. An example of this second use (for three-dimensional lattices) can be found in [1].

Our particular interest is in the lattice sums which arise when considering acoustic scattering by a sheet of spheres, a problem first considered over 30 years ago by Twersky [2–4]. No numerical results were presented in these papers (the focus was on deriving analytic properties of the solutions and approximate formulas valid for small spheres or low frequencies) and, moreover, the machinery that Twersky uses is elaborate and (in our opinion) difficult to follow. The equivalent electromagnetic problem has also been considered in the context of low energy electron diffraction (e.g., [5]) and a formulation based on lattice sums is given in [6] and used in [7]. However, the computation of the lattice sums was not emphasised; instead reference was made to FORTRAN codes published in [8].

Lattice sums have independent mathematical interest and since the papers above were published, considerable progress has been made in devising efficient methods for their computation. Calculating lattice sums accurately and efficiently is still something of a challenge, but as computing power increases and new analytic representations are developed, their usefulness in practical applications becomes more and more apparent. A unified treatment of lattice sums in two and three dimensions, for the cases where the lattice dimension is less than the dimension of the underlying space, is given in [9]. Particular focus is given there to the method of Ewald summation, which yields exponentially convergent series representations for the

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lattice sums. For the case of a two-dimensional lattice in three dimensions this representation involves the incomplete Gamma function with negative real argument, the evaluation of which is not trivial [10].

An alternative approach, and the one we pursue here, is to express the two-dimensional lattice sum as an infinite sum of one-dimensional sums. This idea, which we call lattice reduction, has received considerable attention in recent years (e.g., [11–13]) and appears to have a number of advantages. In fact it was used by Twersky [3] (though Twersky's paper is not cited in any of the above). One-dimensional lattice sums have received much less attention than two-dimensional ones, largely because the associated physical problems do not lead so easily to applications. However, such applications do exist [14,15]. In [12], these lattice sums are represented as infinite, exponentially convergent contour integrals, but simpler expressions are available, again based on earlier work by Twersky [16].

In this article we have attempted to draw together much of this earlier work and present an accurate and efficient method for computing two-dimensional lattice sums when the governing equation is the three-dimensional Helmholtz equation. Many of the expressions that we use can be found in Twersky's papers, but these do not appear to be widely read (they are certainly difficult to follow) and, more importantly, the results do not appear to be widely known.

The plan of the paper is as follows. We begin in Section 2 with a description of our notation and conventions. This is a vital aspect of this type of work since poor notation leads to significant confusion for those trying to follow. We have been very careful to define precisely spherical harmonics and associated Legendre functions, as different authors use different definitions. We also describe some of the basic properties of lattice sums. In Section 3 we examine one-dimensional sums and show that they can be written as rapidly convergent series. Two-dimensional sums are treated in Section 4 and we begin by stating Ewald formulas, which we use to check our numerical calculations. Then we show how lattice reduction can be used to express these two-dimensional sums in terms of one-dimensional sums. Interestingly, when we sum over these one-dimensional sums we are led to lattice sums which are appropriate for one-dimensional lattices in two dimensions, and these can be computed efficiently, again using results of Twersky [17]. Lattice sums possess singularities (these correspond in a physical scattering problem to combinations of frequency and incident wave angle where modes cut on and off, which in turn lead to the observed Wood anomalies [18], and the places where these occur differ for one- and two-dimensional lattices. These singularities are made explicit in our analysis as this can greatly facilitate the calculation of the response at or near these resonances (see, e.g., [19]). Care must be taken when using lattice reduction as this introduces artificial singularities and we show how these can be successfully removed. Numerical results are presented in Section 5 and concluding remarks can be found in Section 6.

2. Preliminaries

2.1. Wave functions

We are concerned with time-harmonic waves governed by the three-dimensional Helmholtz equation

$$(\nabla^2 + k^2)u = 0, \tag{2.1}$$

where $k = \omega/c$ with ω the angular frequency and c the speed of sound. A solution to (2.1) is termed a wave function. In particular we will use the notation

$$\mathcal{J}_n^m(\mathbf{r}) = j_n(kr)Y_n^m(\hat{\mathbf{r}}), \quad \mathcal{Y}_n^m(\mathbf{r}) = y_n(kr)Y_n^m(\hat{\mathbf{r}}) \quad \text{and} \quad \mathcal{H}_n^m(\mathbf{r}) = h_n(kr)Y_n^m(\hat{\mathbf{r}}), \tag{2.2}$$

for, respectively, regular, singular, and outgoing spherical wave functions. Here $\mathbf{r} = r\hat{\mathbf{r}}$, $j_n(\cdot)$, $y_n(\cdot)$ and $h_n(\cdot) \equiv h_n^{(1)}(\cdot)$ are, respectively, spherical Bessel functions of the first and second kind, and spherical Hankel functions of the first kind, and Y_n^m are spherical harmonics defined by

$$Y_n^m(\hat{\mathbf{r}}) \equiv Y_n^m(\theta,\phi) = (-1)^m \lambda_{nm} P_n^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}, \quad n \geqslant |m| \geqslant 0, \tag{2.3}$$

where

$$\lambda_{nm} = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}}. \tag{2.4}$$

Care needs to be taken over the definition of the associated Legendre functions $P_n^m(\cdot)$; the conventions we use are described in Appendix A.

We note that

$$\overline{Y_n^m(\hat{\mathbf{r}})} = (-1)^m Y_n^{-m}(\hat{\mathbf{r}}), \quad Y_n^m(-\hat{\mathbf{r}}) = (-1)^n Y_n^m(\hat{\mathbf{r}}), \tag{2.5}$$

$$\int_\Omega Y_n^m \overline{Y_\nu^\mu}\,\mathrm{d}\Omega = \delta_{n\nu}\delta_{m\mu}, \tag{2.6}$$

the integral being over the unit sphere, and we have the expansion [20, Theorem 3.16]

$$\mathcal{H}_0^0(\mathbf{r}-\mathbf{r}') = 4\pi\sum_{n,m}(-1)^m \mathcal{J}_n^m(\mathbf{r})\mathcal{H}_n^{-m}(\mathbf{r}'), \quad |\mathbf{r}| < |\mathbf{r}'|, \tag{2.7}$$

where we have introduced the shorthand notation

$$\sum_{n,m} \equiv \sum_{n=0}^{\infty} \sum_{m=-n}^{n}.$$

2.2. Lattices

A lattice Λ of dimension d is defined by the position vectors

$$\mathbf{R}_n = \sum_{i=1}^{d} n_i \mathbf{a}_i, \quad n_i \in \mathbb{Z}. \tag{2.8}$$

Here $n = (n_1, \ldots, n_d)$ is a multi-index. We will only be concerned here with the cases $d = 1$ and $d = 2$. If $d = 2$, the vectors $\mathbf{a}_i$ are not necessarily orthogonal (though they are linearly independent) and need not have the same length. In the $d = 1$ case we will drop the subscripts and $a = |\mathbf{a}|$ is the spacing between the lattice points. Reciprocal lattice vectors are

$$\mathbf{K}_n = 2\pi \sum_{i=1}^{d} n_i \mathbf{b}_i, \quad n_i \in \mathbb{Z}, \tag{2.9}$$

where

$$\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}, \quad i,j = 1, \ldots, d. \tag{2.10}$$

If $d = 1$, we have $\mathbf{b} = \mathbf{a}/a^2$ and in all cases

$$\mathbf{R}_n \cdot \mathbf{K}_m = 2N\pi \text{ for some integer } N. \tag{2.11}$$

The reciprocal lattice will be denoted by Λ^*. If we have a lattice Λ then we can define a quantity $\mathcal{A}$ as the length ($d = 1$) or area ($d = 2$) of a unit cell. Explicitly

$$\mathcal{A} = \begin{cases} |\mathbf{a}| & d = 1 \\ |\mathbf{a}_1 \times \mathbf{a}_2| & d = 2. \end{cases} \tag{2.12}$$

The length (area) of a unit cell of the reciprocal lattice is, in each case, $\mathcal{A}^{-1}$.

2.3. Quasi-periodic Green's functions

A point source at $\mathbf{r}'$ will be represented by $G_0(\mathbf{r};\mathbf{r}')$. Thus

$$G_0(\mathbf{r};\mathbf{r}') = -\frac{\exp(\mathrm{i}k\rho)}{4\pi\rho} = -\frac{\mathrm{i}k}{4\pi} h_0(k\rho) = -\frac{\mathrm{i}k}{4\pi} \mathcal{H}_0^0(\mathbf{r} - \mathbf{r}'), \tag{2.13}$$

where $\rho = |\mathbf{r} - \mathbf{r}'|$, and we have

$$(\nabla^2 + k^2) G_0 = \delta(\mathbf{r} - \mathbf{r}'), \tag{2.14}$$

with G_0 behaving like an outgoing wave as $|\mathbf{r}| \to \infty$.

A quasi-periodic Green's function is an array of such sources modulated by a phase factor governed by the vector $\boldsymbol{\beta}$. We write this formally as

$$G_\Lambda(\mathbf{r};\boldsymbol{\beta}) = \sum_{\mathbf{R}_n \in \Lambda} G_0(\mathbf{r};\mathbf{R}_n) \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_n}. \tag{2.15}$$

Without loss of generality, we can assume that $\boldsymbol{\beta}$ lies in the space spanned by the lattice vectors $\mathbf{a}_i$. Moreover, it follows from (2.11) that we can restrict $\boldsymbol{\beta}$ to a single cell of the reciprocal lattice. If $\mathbf{R}_n \in \Lambda$,

$$G_\Lambda(\mathbf{r} + \mathbf{R}_n;\boldsymbol{\beta}) = \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_n} G_\Lambda(\mathbf{r};\boldsymbol{\beta}), \tag{2.16}$$

illustrating the quasi-periodic nature of G_Λ. We also define

$$\boldsymbol{\beta}_n = \boldsymbol{\beta} + \mathbf{K}_n, \quad \beta_n = |\boldsymbol{\beta}_n|, \quad \alpha_n = \arg \boldsymbol{\beta}_n, \quad R_n = |\mathbf{R}_n|. \tag{2.17}$$

2.4. Lattice sums

We define lattice sums σ_n^m formally by

$$\sigma_n^m(\boldsymbol{\beta}) = \sum_{\mathbf{R}_j \in \Lambda}{}' \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_j} \mathcal{H}_n^m(\mathbf{R}_j) = (-1)^n \sigma_n^m(-\boldsymbol{\beta}). \tag{2.18}$$

The dash on the summation sign indicates that the $\mathbf{R}_j = 0$ term is to be omitted. The effect at the origin of a phased array of wave functions at all the lattice sites other than the origin, the phase factor at $\mathbf{R}_j$ being $\exp(\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_j)$, is then $\sigma_n^m(-\boldsymbol{\beta})$ (to see this simply replace $\mathbf{R}_j$ by $-\mathbf{R}_j$ in the definition). The summation in (2.18) is conditionally convergent and so the order in which this is carried out is potentially critical. In one dimension the order is implied but in two dimensions it is not and if numerical computations were to be made from (2.18) this would be a serious issue (see, e.g., [21]). For particular values of $\boldsymbol{\beta}$ and k the sums are in fact singular due to phase cancellation; these singularities will be considered in detail later.

The lattice sums can also be thought of as the coefficients in the expansion about the origin of the regular part of the quasi-periodic Green's function. Thus, it can be shown from (2.15), using (2.7), that for $r < \xi \equiv \min_{\mathbf{R}_j\in\Lambda,\mathbf{R}_j\neq 0} R_j$

$$G_\Lambda(\mathbf{r};\boldsymbol{\beta}) - G_0(\mathbf{r};0) = -\mathrm{i}k\sum_{n,m}(-1)^m\sigma_n^{-m}(\boldsymbol{\beta})\mathcal{J}_n^m(\mathbf{r}). \tag{2.19}$$

Note that the lattice sums (unlike G_Λ and G_0) depend on the choice of polar axis for the spherical harmonics. The representation (2.19) can be used to evaluate G_Λ if the lattice sums can be evaluated easily. This is particularly useful in cases where the value of G_Λ is required at many different spatial points since the lattice sums are independent of position.

We have, using the orthogonality of the spherical harmonics (2.6),

$$\sigma_n^m(\boldsymbol{\beta})j_n(kr) = \frac{\mathrm{i}}{k}\int_{\Omega(\hat{\mathbf{r}})}(G_\Lambda(\mathbf{r};\boldsymbol{\beta}) - G_0(\mathbf{r};0))Y_n^m(\hat{\mathbf{r}})\mathrm{d}\Omega, \tag{2.20}$$

the integral being over the unit sphere.

It will be useful to introduce the associated $\mathcal{J}$- and $\mathcal{Y}$-series defined by

$$\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta}) = {\sum_{\mathbf{R}_j\in\Lambda}}' \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_j}\mathcal{J}_n^m(\mathbf{R}_j), \quad \sigma_n^{m\mathcal{Y}}(\boldsymbol{\beta}) = {\sum_{\mathbf{R}_j\in\Lambda}}' \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_j}\mathcal{Y}_n^m(\mathbf{R}_j), \tag{2.21}$$

so that

$$\sigma_n^m = \sigma_n^{m\mathcal{J}} + \mathrm{i}\sigma_n^{m\mathcal{Y}}. \tag{2.22}$$

A simple calculation reveals that

$$2\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta}) = \sigma_n^m(\boldsymbol{\beta}) + (-1)^{n+m}\overline{\sigma_n^{-m}(\boldsymbol{\beta})}, \tag{2.23}$$

$$2\mathrm{i}\sigma_n^{m\mathcal{Y}}(\boldsymbol{\beta}) = \sigma_n^m(\boldsymbol{\beta}) - (-1)^{n+m}\overline{\sigma_n^{-m}(\boldsymbol{\beta})}. \tag{2.24}$$

3. One-dimensional lattice sums

If $d = 1$ we can choose the lattice to lie on the axis of the spherical coordinate system (defined by the unit vector $\mathbf{e}_z$) so that on the lattice, $\theta = 0$ or π. In that case $Y_n^m(\hat{\mathbf{R}}_j) = 0$ unless $m = 0$ (see (A.6) and so

$$\sigma_n^m(\boldsymbol{\beta}) = 0, \quad \text{if} \quad m\neq 0. \tag{3.1}$$

We set $\boldsymbol{\beta} = \beta\mathbf{e}_z$ and write $\ell_n(\beta)$ for $\sigma_n^0(\boldsymbol{\beta})$. This will aid clarity since the one-dimensional sums will appear later in our representation for the two-dimensional sums. The non-zero lattice sums are

$$\ell_n(\beta) = {\sum_{j\in\mathbb{Z}}}' \mathrm{e}^{\mathrm{i}\beta aj}\mathcal{H}_n^0(aj\mathbf{e}_z) = \lambda_{n0}\sum_{j=1}^{\infty}h_n(kaj)(\mathrm{e}^{\mathrm{i}\beta aj} + (-1)^n\mathrm{e}^{-\mathrm{i}\beta aj}) \tag{3.2}$$

with λ_{n0} defined in (2.4). We introduce the quantities

$$\beta_p = \beta + 2p\pi/a, \quad p\in\mathbb{Z} \tag{3.3}$$

and when $|\beta_p| \leqslant k$ we define $\psi_p \in [0,\pi]$ via

$$\cos\psi_p = \beta_p/k. \tag{3.4}$$

Then it is known [16] that, provided $|\beta_p|\neq k$ for any p,

$$\ell_n^{\mathcal{J}}(\beta) \equiv \lambda_{n0}\sum_{j=1}^{\infty}j_n(kaj)(\mathrm{e}^{\mathrm{i}\beta aj} + (-1)^n\mathrm{e}^{-\mathrm{i}\beta aj}) = -\frac{\delta_{n0}}{\sqrt{4\pi}} + \frac{\pi\mathrm{i}^n\lambda_{n0}}{ka}\sum_{|\beta_p|<k}P_n(\cos\psi_p) \tag{3.5}$$

which expresses $\ell_n^{\mathcal{J}}$ as a finite sum over propagating modes. The derivation of this result in [16] is by no means transparent, involving as it does various scattering operators defined via infinite contour integrals. Here we present a more direct derivation.

Using the Poisson summation formula in the form $\sum_j f(j) = \sum_p \int_{-\infty}^{\infty} f(x)\exp(2p\pi\mathrm{i}x)\mathrm{d}x$ we can show that, for $n \geqslant 0$,

$$\sum_{j\in\mathbb{Z}}\frac{j_n(ka\sqrt{j^2+\epsilon^2})}{(j^2+\epsilon^2)^{n/2}}\mathrm{e}^{\mathrm{i}\beta aj} = \frac{\pi}{k^{n+1}a\epsilon^n}\sum_{|\beta_p|<k}(k^2-\beta_p^2)^{n/2}J_n\left(a\epsilon\sqrt{k^2-\beta_p^2}\right), \tag{3.6}$$

where we have used [22, 6.726(2)]. Taking the limit as $\epsilon \to 0$ leads to

$$\frac{(ka)^n}{(2n+1)!!} + \sum_{j\in\mathbb{Z}}{}' \frac{j_n(ka|j|)}{|j|^n} e^{i\beta aj} = \frac{\pi a^n}{2^n n! k^{n+1} a} \sum_{|\beta_p|<k} (k^2 - \beta_p^2)^n. \tag{3.7}$$

This is a special case of a more general formula given in [23]. The sum on the left-hand side is absolutely convergent for $n \geqslant 1$ and we can differentiate n times with respect to β to yield

$$\mathrm{i}^n \sum_{j\in\mathbb{Z}}{}' j_n(kaj) e^{i\beta aj} = \frac{\pi}{2^n n! k^{n+1} a} \sum_{|\beta_p|<k} \left(\frac{d}{d\beta}\right)^n (k^2 - \beta_p^2)^n, \quad n \geqslant 1 \tag{3.8}$$

$$= \frac{\pi(-1)^n}{ka} \sum_{|\beta_p|<k} P_n(\cos\psi_p), \tag{3.9}$$

using (A.1). This and (3.7) with $n = 0$ yield (3.5).

Rapidly convergent series representations for the sums $\ell_n^{\mathcal{Y}}$ can be derived as follows. Using [24, 10.1.16] we have

$$\ell_n(\beta) = \lambda_{n0}(-\mathrm{i})^{n+1} \sum_{s=0}^{n} c_{ns}(L_s^+(\beta) + (-1)^n L_s^-(\beta)), \tag{3.10}$$

where

$$c_{ns} = \frac{(n+s)!}{2^s s!(n-s)!} \quad \text{and} \quad L_s^{\pm}(\beta) = \mathrm{i}^s \sum_{j=1}^{\infty} \frac{e^{i(k\pm\beta)aj}}{(kaj)^{s+1}}. \tag{3.11}$$

Then

$$2\mathrm{i}\ell_n^{\mathcal{Y}}(\beta) = \ell_n(\beta) - (-1)^n \overline{\ell_n(\beta)} \tag{3.12}$$

$$= 2\lambda_{n0}(-\mathrm{i})^{n+1} \sum_{s=0}^{n} \frac{c_{ns}\Omega_s}{(ka)^{s+1}} [Cl_{s+1}(ka+\beta a) + (-1)^n Cl_{s+1}(ka-\beta a)], \tag{3.13}$$

where

$$\Omega_s = \begin{cases} \mathrm{i}^s & s \text{ even}, \\ \mathrm{i}^{s+1} & s \text{ odd}, \end{cases} \tag{3.14}$$

and $Cl_s(\cdot)$ are the Clausen functions

$$Cl_{2m}(x) = \sum_{j=1}^{\infty} \frac{\sin jx}{j^{2m}}, \quad Cl_{2m+1}(x) = \sum_{j=1}^{\infty} \frac{\cos jx}{j^{2m+1}}. \tag{3.15}$$

Exponentially convergent series representations for these functions are given in Appendix B.

The lattice sum $\ell_0(\beta)$ has a particularly simple representation:

$$\ell_0(\beta) = \frac{1}{ka\sqrt{4\pi}}(M\pi - ka + \mathrm{i}\log[2|\cos\beta a - \cos ka|]), \tag{3.16}$$

where M is the number of integers p for which $|\beta_p| < k$, which corresponds to the number of scattered modes in a diffraction problem.

3.1. Singularities

From (3.13) and (3.15) it is clear that the sums $\ell_n(\beta)$ are singular when either $ka \pm \beta a$ is an integer multiple of 2π. Note that both cases can occur simultaneously if ka is an integer multiple of π. Eq. (3.5) shows that $\ell_n^{\mathcal{J}}(\beta)$ is finite for all β, though it is discontinuous at the singularities of $\ell_n^{\mathcal{Y}}(\beta)$ since the number of terms in the finite sum changes at these points. On the other hand, from (3.13) and (B.1),

$$\ell_n^{\mathcal{Y}}(\beta) = \frac{\mathrm{i}^n \lambda_{n0}}{2ka}((-1)^n \log[2 - 2\cos(ka+\beta a)] + \log[2 - 2\cos(ka-\beta a)]) + \widehat{\ell}_n^{\mathcal{Y}}(\beta), \tag{3.17}$$

where $\widehat{\ell}_n^{\mathcal{Y}}(\beta)$ is non-singular.

4. Two-dimensional lattice sums

4.1. Ewald representation

If we choose coordinates such that the lattice lies in the plane $\theta = \pi/2$, then for any lattice vector $\mathbf{R}_{pq}$, $Y_n^m(\hat{\mathbf{R}}_{pq}) = 0$ if $n+m$ is odd (see (A.7)), and so we have

$$\sigma_n^m(\boldsymbol{\beta}) = 0, \quad n+m \text{ odd}. \tag{4.1}$$

Here and in what follows we have written the two lattice indices p and q explicitly rather than using a muti-index as in Section 2.2.

Ewald representations for σ_n^m date back to the 1960s [25] and are fairly standard in the solid-state physics literature where they are used to evaluate so-called structure constants in electron scattering theory [26, Chapter 15]; see also [9,27]. The representations below make extensive use of the incomplete Gamma function $\Gamma(\mu, z)$ which, unless μ is a positive integer, has a branch cut along the negative real axis. For negative real z we use the definition

$$\Gamma(\mu, z) = \lim_{\epsilon \to 0} \Gamma(\mu, z - \mathrm{i}\epsilon). \tag{4.2}$$

We can thus write

$$\sigma_n^m = \sigma_n^{m(0)} + \sigma_n^{m(1)} + \sigma_n^{m(2)}, \tag{4.3}$$

where each of the terms on the right-hand side depends on an Ewald parameter $\eta > 0$, though their sum does not. In our notation, we have, for $n+m$ even,

$$\sigma_n^{m(0)} = \delta_{n0}\delta_{m0}\left(-\frac{1}{\sqrt{4\pi}} + \frac{\mathrm{i}}{2\pi}\sum_{j=0}^{\infty}\frac{(k/2\eta)^{2j-1}}{j!(1-2j)}\right) = \frac{\delta_{n0}\delta_{m0}}{4\pi}\Gamma\left(-\frac{1}{2}, -\frac{k^2}{4\eta^2}\right), \tag{4.4}$$

$$\begin{aligned}\sigma_n^{m(1)} = &-\frac{\mathrm{i}^{n+1}}{2k^2\mathcal{A}}(-1)^{(n+m)/2}\sqrt{(2n+1)(n-m)!(n+m)!}\\ &\times \sum_{\mathbf{K}_{pq}\in\Lambda^*}\sum_{j=0}^{[(n-|m|)/2]}\frac{(-1)^j(\beta_{pq}/2k)^{n-2j}\mathrm{e}^{\mathrm{i}m\alpha_{pq}}\Gamma_{j,pq}}{j!(\frac{1}{2}(n-m)-j)!(\frac{1}{2}(n+m)-j)!}\left(\frac{\gamma_{pq}}{2}\right)^{2j-1},\end{aligned} \tag{4.5}$$

$$\sigma_n^{m(2)} = -\frac{2^{n+1}\mathrm{i}}{k^{n+1}\sqrt{\pi}}\sum_{\mathbf{R}_{pq}\in\Lambda}{}' R_{pq}^n \mathrm{e}^{\mathrm{i}\boldsymbol{\beta}\cdot\mathbf{R}_{pq}} Y_n^m(\hat{\mathbf{R}}_{pq})\int_\eta^\infty \mathrm{e}^{-R_{pq}^2\xi^2}\mathrm{e}^{k^2/4\xi^2}\xi^{2n}\mathrm{d}\xi, \tag{4.6}$$

where

$$\gamma_{pq} = \gamma(\beta_{pq}/k), \quad \Gamma_{j,pq} = \Gamma\left(\frac{1}{2} - j, \frac{k^2\gamma_{pq}^2}{4\eta^2}\right), \tag{4.7}$$

and $\gamma(\cdot)$ is defined in (A.9). The first exponential in the integral in (4.6) can be expanded as a power series to reduce the integral to a sum involving incomplete Gamma functions, but we prefer to use direct quadrature of the (exponentially convergent) integral. If $nk \geqslant R_{pq}$, the integrand has extrema for real ξ and the uppermost of these occurs at the point $\xi = \xi_0$, where

$$\xi_0^2 = \frac{n + \sqrt{n^2 - R_{pq}^2 k^2}}{2R_{pq}^2}. \tag{4.8}$$

If $\eta < \xi_0$, separate quadratures are applied on the intervals $[\eta, \xi_0]$ and $[\xi_0, \infty)$. A single integration by parts yields a recurrence relation that can be used to increase efficiency when calculating σ_n^m for more than one value of n.

Since $\Gamma(\mu, z) \sim z^{\mu-1}\mathrm{e}^{-z}$, the Ewald method involves exponentially convergent two-dimensional sums, which is attractive. On the other hand the computation of the incomplete Gamma function with negative real argument is not straightforward. When $|x| < 2$ we use a series expansion (the second series in equation (2) of [10]) for $\Gamma(\mu, x)$ which converges monotonically provided $|x| < 1$ but cannot be used effectively for large $|x|$. Since the modulus of any negative real argument in (4.7) is always less than $k^2/4\eta^2$, this puts a restriction on the Ewald parameter η. When $|x| \geqslant 2$ the incomplete Gamma function is computed using the NAG library routine S14BAF if $\mu > 0$ and via direct quadrature of the integral definition when $\mu \leqslant 0$. This may not be optimal, but it is hard to see how it could be improved on significantly.

The Ewald method involves the numerical evaluation of two-dimensional sums and the order in which the terms are taken needs to be addressed. The natural ordering of terms is such that β_{pq} or R_{pq} increases monotonically, but arranging terms in this way is computationally expensive, and so we use an alternative approach, the essence of which is as follows. For a lattice with basis vectors $\mathbf{c}_1$ and $\mathbf{c}_2$ we define the sequence of perimeters $\mathcal{P}_n$ (each of which is a set of lattice points) via

$$\mathcal{P}_n = \{j\mathbf{c}_1 + p\mathbf{c}_2 : \quad j \leqslant n, \quad p \leqslant n, \quad (j-n)(p-n) = 0\} \tag{4.9}$$

and then sum around $\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3, \ldots$.

To improve the efficiency in evaluating $\sigma_n^{m(2)}$ we can derive an upper bound for the magnitude of the contribution from each point using the fact that

$$\left|R_{pq}^n\int_\eta^\infty e^{-R_{pq}^2\xi^2}e^{k^2/4\xi^2}\xi^{2n}d\xi\right| \leqslant R_{pq}^n e^{k^2/4\eta^2}\int_\eta^\infty e^{-R_{pq}^2\xi^2}\xi^{2n}d\xi = \frac{e^{k^2/4\eta^2}}{2R_{pq}^{n+1}}\Gamma\left(n+\frac{1}{2},R_{pq}^2\eta^2\right). \tag{4.10}$$

The expression on the right-hand side is monotonically decreasing in R_{pq} and hence if (4.10) predicts that a term is negligible (by which we mean that its magnitude relative to the sum is smaller than machine precision), then all terms with larger values of R_{pq} are also negligible. A similar approach can be used when computing $\sigma_n^{m(1)}$. There are a finite number of terms for which γ_{pq} is not real and these must always be included in the summation. For the other terms we can obtain an upper bound on the summand by noting that for $j \geqslant 0$ and $x > 0$,

$$\Gamma\left(\frac{1}{2}-j,x\right) = \int_x^\infty t^{-j-1/2}e^{-t}dt \leqslant x^{-j-1/2}\int_x^\infty e^{-t}dt = x^{-j-1/2}e^{-x}. \tag{4.11}$$

In this case, the upper bound (as a function of β_{pq}) has turning points and these must be taken into account when using the bound to discard subsequent terms.

The value of the parameter η has a significant effect on the performance of the Ewald representation. The exponential convergence in (4.6) is due to the term $\exp(-R_{pq}^2\xi^2)$ that appears in the integrand, and since the lower limit for ξ is η, we can estimate that the convergence rate of the two-dimensional sum for $\sigma_n^{m(2)}$ is proportional to $\exp(-R_{pq}^2\eta^2)$. Similarly, in (4.5), if we assume that $k\gamma_{pq} \approx \beta_{pq}$, we see that the convergence rate for $\sigma_n^{m(1)}$ can be estimated as $\exp(-\beta_{pq}^2/(4\eta^2))$. Thus, increasing η improves the convergence in (4.6) but is detrimental to that in (4.5). Ideally, we should choose the Ewald parameter to balance the two convergence rates, but this is difficult given the two-dimensional nature of the summations. Instead, we set the value using the shorter of the lattice basis vectors; thus

$$\eta = \sqrt{\pi b_m/a_m}, \tag{4.12}$$

where

$$a_m = \min\{a_1,a_2\} \quad \text{and} \quad b_m = \min\{b_1,b_2\}. \tag{4.13}$$

Note that the integrals in (4.6) are independent of m, whereas the incomplete Gamma functions in (4.5) are independent of both m and n. Furthermore, if we change $\mathbf{R}_{pq}$ to $-\mathbf{R}_{pq}$ and m to $-m$ in (4.6) and then take the complex conjugate we see that

$$\sigma_n^{m(2)} = -\overline{\sigma_n^{-m(2)}} \tag{4.14}$$

in view of (2.5). As it is usual in applications to have to calculate σ_n^m for all n and m such that $0 \leqslant |m| \leqslant n \leqslant N$ for some fixed N, these facts can be used to gain a considerable increase in efficiency. For small k (low frequency), $\sigma_n^{m(1)}$ also satisfies (4.14) because if $\gamma_{pq}^2 \geqslant 0$, then $\Gamma_{j,pq} \in \mathbb{R}$.

4.2. Regular lattice sums

Another check on our computations is provided by the identity

$$\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta}) = -\frac{\delta_{n0}\delta_{m0}}{\sqrt{4\pi}} + \frac{2\pi i^n}{k\mathcal{A}}\sum_{\beta_{pq}<k}\frac{Y_n^m(\hat{\zeta}_{pq})}{\sqrt{k^2-\beta_{pq}^2}}, \quad n+m \text{ even}, \tag{4.15}$$

where $k\hat{\zeta}_{pq} = \boldsymbol{\beta}_{pq} + \sqrt{k^2-\beta_{pq}^2}\mathbf{e}_z$ and the coordinates are as in Section 4.1. Equivalent versions of this formula can be found in [3,12]; we will not re-derive it here. From (2.23) we then get, for $n+m$ even

$$\sigma_n^m(\boldsymbol{\beta}) + \overline{\sigma_n^{-m}(\boldsymbol{\beta})} = -\frac{\delta_{n0}\delta_{m0}}{\sqrt{\pi}} + \frac{4\pi i^n}{k\mathcal{A}}\sum_{\beta_{pq}<k}\frac{Y_n^m(\hat{\zeta}_{pq})}{\sqrt{k^2-\beta_{pq}^2}}. \tag{4.16}$$

4.3. Lattice reduction

The basic idea here is to express the two-dimensional lattice sum as a sum of one-dimensional sums. We choose to make the polar axis of the spherical coordinate system parallel to one of the lattice vectors so that the reduced one-dimensional lattice sum takes a particularly simple form. Thus we write $\mathbf{a}_1 = a_1\mathbf{e}_z$ and $\mathbf{a}_2 = \eta_1\mathbf{e}_z + \eta_2\mathbf{e}_y$, with $\eta_2 > 0$. The reciprocal lattice vectors are then $\mathbf{b}_1 = (1/a_1\eta_2)(\eta_2\mathbf{e}_z - \eta_1\mathbf{e}_y)$ and $\mathbf{b}_2 = (1/\eta_2)\mathbf{e}_y$. We set $\boldsymbol{\beta} = \xi_1\mathbf{e}_z + \xi_2\mathbf{e}_y$ and we have

$$\mathbf{R}_{pq} = (pa_1 + q\eta_1)\mathbf{e}_z + q\eta_2\mathbf{e}_y, \quad \boldsymbol{\beta}_{pq} = \xi_{1p}\mathbf{e}_z + \frac{1}{\eta_2}(w_p + 2q\pi)\mathbf{e}_y, \tag{4.17}$$

where we have written

$$\xi_{1p} = \xi_1 + \frac{2p\pi}{a_1}, \quad w_p = \xi_2\eta_2 - \frac{2p\pi\eta_1}{a_1}. \tag{4.18}$$

Then, from (2.18),

$$\sigma_n^m(\boldsymbol{\beta}) = \sum_{p=-\infty}^{\infty}{}' e^{i\boldsymbol{\beta}\cdot\mathbf{R}_{p0}}\mathcal{H}_n^m(\mathbf{R}_{p0}) + \sum_{q=-\infty}^{\infty}{}' \sum_{p=-\infty}^{\infty} e^{i\boldsymbol{\beta}\cdot\mathbf{R}_{pq}}\mathcal{H}_n^m(\mathbf{R}_{pq}) \tag{4.19}$$

$$= \ell_n(\xi_1)\delta_{m0} + \sum_{q=-\infty}^{\infty}{}' e^{iq(\xi_1\eta_1+\xi_2\eta_2)} \sum_{p=-\infty}^{\infty} e^{ip\xi_1 a_1}\mathcal{H}_n^m(\mathbf{R}_{pq}), \tag{4.20}$$

where $\ell_n(\xi_1)$ is a one-dimensional lattice sum as in Section 3.

The lattice sums σ_n^m considered this section are not the same as the sums σ_n^m considered in Section 4.1 due to the different orientation of the spherical coordinate system in the two cases. However, we can reconstruct one from the other using rotation matrices; see Appendix C. For $q\neq 0$, the azimuthal angle of the lattice vector $\mathbf{R}_{pq}$ is either $-\pi/2$ or $+\pi/2$ depending on whether $q > 0$ or $q < 0$, respectively, and it follows that in this case $\mathcal{H}_n^{-m}(\mathbf{R}_{pq}) = \mathcal{H}_n^m(\mathbf{R}_{pq})$. Thus the lattice sums considered in this section have the property that

$$\sigma_n^m(\boldsymbol{\beta}) = \sigma_n^{-m}(\boldsymbol{\beta}). \tag{4.21}$$

We now insert into the sum over p in (4.20) the integral representation

$$h_n(kr)P_n^m(\cos\theta) = \frac{(-i)^{n+1}}{\pi}\int_{-\infty}^{\infty} e^{ikzt}K_m(k\rho\gamma(t))P_n^m(t)dt, \tag{4.22}$$

where $\rho = \sqrt{r^2 - z^2} > 0$, $\gamma(\cdot)$ is as defined in (A.8), $K_m(\cdot)$ is a modified Bessel function, and we have used (A.10). This follows from, for example, [28, Thm A1] (note the extra $(-1)^m$ in the definition of P_n^m used in that paper). Our choice of definition for $P_n^m(z)$ is largely motivated by the simple form that this representation now takes. The sum over p becomes

$$(-i)^{n+m+1}(\operatorname{sgn}q)^m\frac{\lambda_{nm}}{\pi}\sum_{p=-\infty}^{\infty} e^{ip\xi_1 a_1}\int_{-\infty}^{\infty} e^{ikt(pa_1+q\eta_1)}K_m(k\eta_2|q|\gamma(t))P_n^m(t)dt$$

$$= -\frac{2i^{n+m+1}}{ka_1}(\operatorname{sgn}q)^m\lambda_{nm}\sum_{p=-\infty}^{\infty} e^{-i\xi_{1p}q\eta_1}K_m(k\eta_2|q|\gamma_p)P_n^m(\xi_{1p}/k), \tag{4.23}$$

on using the Poisson summation formula. Here $\gamma_p = \gamma(\xi_{1p}/k)$. Then (4.20) becomes

$$\sigma_n^m(\boldsymbol{\beta}) = \ell_n(\xi_1)\delta_{m0} - \frac{2i^{n+m+1}}{ka_1}\lambda_{nm}\sum_{p=-\infty}^{\infty} P_n^m(\xi_{1p}/k)\sum_{q=1}^{\infty}[e^{iqw_p} + (-1)^m e^{-iqw_p}]K_m(k\eta_2 q\gamma_p). \tag{4.24}$$

The reduction (4.24) is equivalent to that carried out in [3, Section 2B] for the rectangular lattice.

If $|\xi_{1p}| \leqslant k$ we define the angles $\chi_p \in [0, \pi]$ via

$$\cos\chi_p = \xi_{1p}/k. \tag{4.25}$$

Then if we separate the contributions from the propagating ($|\xi_{1p}| < k$) and evanescent modes we have

$$\sigma_n^m(\boldsymbol{\beta}) = \ell_n(\xi_1)\delta_{m0} + \mathrm{H}_n^m + \mathrm{K}_n^m, \tag{4.26}$$

where (using [24, 9.6.4] to write the modifed Bessel function of imaginary argument in terms of the Hankel function of the first kind $H_n \equiv H_n^{(1)}$),

$$\mathrm{H}_n^m = \frac{\pi i^n}{ka_1}(-1)^m\lambda_{nm}\sum_{|\xi_{1p}|<k} P_n^m(\cos\chi_p)\sum_{q=1}^{\infty}[e^{iqw_p} + (-1)^m e^{-iqw_p}]H_m(k\eta_2 q\sin\chi_p) \tag{4.27}$$

$$= \frac{\pi i^{n-m}}{ka_1}\sum_{|\xi_{1p}|<k} Y_n^m(\zeta_p)S_m(w_p, k\eta_2\sin\chi_p), \tag{4.28}$$

with $\zeta_p = \sin\chi_p\mathbf{e}_y + \cos\chi_p\mathbf{e}_z$, and

$$\mathrm{K}_n^m = -\frac{2i^{n+m+1}}{ka_1}\lambda_{nm}\sum_{|\xi_{1p}|>k} P_n^m(\xi_{1p}/k)\sum_{q=1}^{\infty}[e^{iqw_p} + (-1)^m e^{-iqw_p}]K_m(k\eta_2 q\gamma_p). \tag{4.29}$$

Since [24, 9.7.2] $K_m(x) \sim \sqrt{\pi/2x}\exp(-x)$, the sums in (4.29) decay exponentially with respect to both $|p|$ and q. The sum S_m in (4.28) (which is a type of Schlömilch series, [29, Chap. XIX]) is in the form of a one-dimensional lattice sum for the two-dimensional Helmholtz equation and can be evaluated efficiently using expressions originally derived in [17]; see Appendix D. Note that the Schlömilch series in (4.28) and the sums over q in (4.29) are independent of n.

From (2.23) and (4.26) we can obtain an expression for $\sigma_n^{m\mathcal{J}}$ as a finite sum. It is easy to show that $(-1)^{n+m}\overline{\mathrm{K}_n^{-m}} = -\mathrm{K}_n^m$ and $\ell_n + (-1)^n\overline{\ell_n} = 2\ell_n^{\mathcal{J}}$, where $\ell_n^{\mathcal{J}}$ is given as a finite sum in (3.5). We also have

$$\mathrm{H}_n^m + (-1)^{n+m}\overline{\mathrm{H}_n^{-m}} = \frac{\pi \mathrm{i}^{n-m}}{ka_1}\sum_{|\xi_{1p}|<k} Y_n^m(\boldsymbol{\zeta}_p)(S_m + (-1)^m\overline{S_m}), \tag{4.30}$$

the arguments of the sums being as in (4.28). It follows from (D.2,D.4) and (D.5) that

$$S_m + (-1)^m\overline{S_m} = -2\delta_{m0} + 4\mathrm{i}^m \sum_{\beta_{pq}<k} \frac{\cos m\Delta_{pq}}{\eta_2\sqrt{k^2-\beta_{pq}^2}}, \tag{4.31}$$

where Δ_{pq} is defined by

$$\cos\Delta_{pq} = \frac{w_p + 2q\pi}{k\eta_2\sin\chi_p}, \quad \sin\Delta_{pq} = \frac{\sqrt{k^2-\beta_{pq}^2}}{k\sin\chi_p}. \tag{4.32}$$

The contribution that comes from the Kronecker delta in (4.31) cancels with the sum from (3.5) and we find that

$$\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta}) = -\frac{\delta_{m0}\delta_{n0}}{\sqrt{4\pi}} + \frac{2\pi \mathrm{i}^{n-m}\lambda_{nm}}{ka_1\eta_2}\sum_{|\xi_{1p}|<k} P_n^m(\xi_{1p}/k)\sum_{\beta_{pq}<k}\frac{\cos m\Delta_{pq}}{\sqrt{k^2-\beta_{pq}^2}}. \tag{4.33}$$

Since $|\xi_{1p}| < k$ is necessarily true if $\beta_{pq} < k$, this can be simplified to

$$\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta}) = -\frac{\delta_{m0}\delta_{n0}}{\sqrt{4\pi}} + \frac{2\pi \mathrm{i}^{n-m}\lambda_{nm}}{ka_1\eta_2}\sum_{\beta_{pq}<k}\frac{P_n^m(\xi_{1p}/k)\cos m\Delta_{pq}}{\sqrt{k^2-\beta_{pq}^2}}. \tag{4.34}$$

4.4. Singularities

From (4.15) it is easy to see that the two-dimensional sums $\sigma_n^{m\mathcal{J}}(\boldsymbol{\beta})$ are singular whenever there are integers p and q such that $\beta_{pq} = k$. It turns out that these are the only singularities of $\sigma_n^m(\boldsymbol{\beta})$, though this is not immediately apparent. On the other hand, it is clear from the representation (4.26) that the individual terms on the right-hand side have other singularities, which must therefore cancel out. The series used to define H_n^m and K_n^m are both singular if $|\xi_{1p}| = k$ for some p (since $\sin\chi_p = \mathrm{i}\gamma_p = 0$ at these points). These singularities must cancel with those from $\ell_n(\xi_1)$.

In order to determine the singular behaviour of H_n^m and K_n^m near these points we make a slight change in definition. Thus instead of splitting the sum over p in (4.24) into parts for which $|\xi_{1p}|$ is greater or less than k, we write

$$\mathrm{H}_n^m = \frac{\pi \mathrm{i}^n}{ka_1}(-1)^m\lambda_{nm}\sum_{|\xi_{1p}|<k+\epsilon} P_n^m(\xi_{1p}/k)S_m(w_p, \mathrm{i}k\eta_2\gamma_p), \tag{4.35}$$

where $0 < \epsilon < 2p\pi/a_1$. In this way all the singularities are in the H_n^m terms. Likewise, in (4.29), the limits for the sum over p are now $|\xi_{1p}| \geqslant k+\epsilon$ and so this series (which we write as $\widehat{\mathrm{K}}_n^m$) is exponentially convergent for all parameter values. Note that $\mathrm{i}\gamma_p$ is either positive real or positive imaginary, but the series given in Appendix D are valid in either case.

The quantity Θ_q, defined in (D.3), when $\lambda = w_p$ and $\mu = \mathrm{i}k\eta_2\gamma_p$, is given by

$$\mathrm{i}[(w_p + 2q\pi)^2 + \eta_2^2(\xi_{1p}^2 - k^2)]^{1/2} = \mathrm{i}\eta_2(\beta_{pq}^2 - k^2)^{1/2} \tag{4.36}$$

(either positive real or positive imaginary) and this clearly vanishes whenever there are integers p and q such that $\beta_{pq} = k$, just as in (4.15). These are the actual singularities of σ_n^m.

The sums S_m with $m > 0$ in (4.35) have singularities as $\gamma_p \to 0$ which come from the finite sums in (D.4) and (D.5) and which are $O(\gamma_p^{-m})$. However, these singularities are cancelled by the factor γ_p^m which comes from the associated Legendre functions; see (A.10). In view of this, the only other singularities of H_n^m come from the logarithmic terms in the series for S_0 and so we choose to write

$$\mathrm{H}_n^m = \widehat{\mathrm{H}}_n^m - \delta_{m0}\frac{\mathrm{i}^{n+1}}{ka_1}\lambda_{n0}\sum_{|\xi_{1p}|<k+\epsilon} P_n(\xi_{1p}/k)\log\left[\frac{\eta_2^2}{16\pi^2}(k^2-\xi_{1p}^2)\right], \tag{4.37}$$

where $\widehat{\mathrm{H}}_n^m$ is bounded in the limit $|\xi_{1p}| \to k$. The imaginary part of the logarithm is either 0 or π.

Finally, we collect together our results and rewrite (4.26) using (3.5,3.17) and (4.37):

$$\sigma_n^m(\boldsymbol{\beta}) = \widehat{\mathrm{H}}_n^m + \widehat{\mathrm{K}}_n^m + \delta_{m0}\left(-\frac{\delta_{n0}}{\sqrt{4\pi}} + \mathrm{i}\widehat{\ell}_n^{\mathcal{Y}}(\xi_1) + \frac{\mathrm{i}^{n+1}\lambda_{n0}}{2ka_1}\mathrm{Q}_n\right), \tag{4.38}$$

where

$$Q_n = (-1)^n \log[2-2\cos(ka_1+\xi_1 a_1)] + \log[2-2\cos(ka_1-\xi_1 a_1)] - \sum_{|\xi_{1p}|<k+\epsilon} 2P_n(\xi_{1p}/k)\log\left[\frac{\eta_2^2}{16\pi^2}(k^2-\xi_{1p}^2)\right] - 2\pi\mathrm{i}\sum_{|\xi_{1p}|<k} P_n(\xi_{1p}/k), \tag{4.39}$$

which is regular for all values of ξ_1. Contributions from the imaginary part of the logarithm in the first sum on the right-hand side (from terms for which $k < |\xi_{1p}| < k+\epsilon$) can be included in the second sum. After simplification we obtain

$$Q_n = (-1)^n \log[2-2\cos(ka_1+\xi_1 a_1)] + \log[2-2\cos(ka_1-\xi_1 a_1)] - \sum_{|\xi_{1p}|<k+\epsilon} P_n(\xi_{1p}/k)\left\{2\pi\mathrm{i} + \log\left[\left(\frac{\eta_2}{4\pi}\right)^4 (k^2-\xi_{1p}^2)^2\right]\right\}, \tag{4.40}$$

where all the logarithms are now real.

There is a decision to make in choosing the parameter ϵ, arising from the fact that any term with $|\xi_{1p}| > k$ can be included either in (4.29) or (4.35). We use $\epsilon = 1/\eta_2$ which ensures rapid convergence in all of the sums over q in (4.29).

5. Numerical results

Numerical calculations for lattice sums over sheets of spheres have been performed by Enoch et al. [12], though the authors report only limited accuracy due to time restrictions brought about by their use of *Mathematica*. By contrast, our program code is written entirely in Fortran 2003 and can rapidly calculate the lattice sums with great precision. In addition, Enoch et al. noted a significant decrease in precision in calculating σ_n^m as n is increased; our program codes exhibit no such deficiency. Table 1 shows selected values of σ_n^m. The parameters are taken from Enoch et al. but the results are typical of those that our program codes generate. The values shown are for the case where the axis of the spherical coordinate system is orthogonal to the lattice, and so $\sigma_n^m = 0$ if $n+m$ is odd, and in addition $\sigma_n^{-m} = -\overline{\sigma_n^m}$ for $n > 0$. In the first column we have reproduced the values given by Enoch et al. and in the second we give our calculations to 10 significant figures in both the real and imaginary parts. The error estimate in the final column is the percentage by which the our computations using the Ewald formula differ from those using the reduction formula. This is a fairly rigorous test of accuracy, given the fact that the two methods are entirely different.

Fig. 1 shows performance data for the Ewald and reduction formulae. The quantity plotted is the logarithm of the reciprocal of the time taken to evaluate all non-zero values of σ_n^m with $n \leqslant 5$ (of which there are 36) for fixed values of $\mathbf{a}_1$, $\mathbf{a}_2$ and $\boldsymbol{\beta}$, with varying k. Calculations were repeated many times to get an accurate measurement of performance. The program was run in double precision on a 2.1 GHz machine and the largest percentage discrepancy between the Ewald and reduction methods encountered in any calculation was 0.28×10^{-8}. In both cases, the Ewald method performs consistently, for $k < 4.6$. For $k > 4.6$, (4.12) gives $\eta < k/\sqrt{8}$, which in turn leads to the necessity of evaluating $\Gamma(\mu, x)$ with $x < -2$, and we choose not to permit this. Instead, the value $\eta = k/\sqrt{8}$ is used, and the performance begins to deteriorate as the convergence rate of the series for $\sigma_n^{m(1)}$ slows.

The dominant factor in determining the performance of the reduction method was found to be the number of Schlömilch series that must be evaluated when computing (4.35). Thus, the dashed vertical lines in the figure show where a term is transferred from (4.29) to (4.35). Best performance is observed to the left of the first line, where (4.35) has no terms. The subsequent peak at $k = 1.8$ corresponds to a removable singularity; here the infinite series in (D.4) and (D.5) disappear, unless $m = 0$, in which case an exact evaluation in terms of the polygamma function is available. Given that the removable singularities are logarithmic in nature, the value $1/\eta_2$ that we used for ϵ in (4.35) could be considered too con-

Table 1
Selected values of σ_n^m for $\mathbf{a}_1 = [1, 0]$, $\mathbf{a}_2 = [0.65, 0.81]$, $k = 2\pi/7.69$ and $\boldsymbol{\beta} = [0.37, 0.79]$. The results shown are for the case where the axis of the spherical coordinate system is orthogonal to the lattice.

n	m	σ_n^m [Enoch et al.]		σ_n^m		% error
0	0	−0.282095	−7.30057i	−0.2820947918	−7.300570977i	7.0×10^{-12}
1	1	−4.37786	−9.49568i	−4.377846777	−9.495715723i	4.4×10^{-12}
2	0		8.03245i		8.033506836i	3.2×10^{-12}
2	2	−10.9071	−7.05139i	−10.90806851	−7.050489899i	3.7×10^{-12}
8	0				−33221096.96i	1.5×10^{-13}
8	4			21338984.36	−3037078.345i	1.4×10^{-13}
8	8			477641.3476	19002073.85i	2.2×10^{-13}
9	1			−3433917.370	−335677297.6i	3.2×10^{-13}
9	5			233343355.6	233273886.3i	7.2×10^{-14}
9	9			−315405665.6	267897011.8i	3.5×10^{-13}

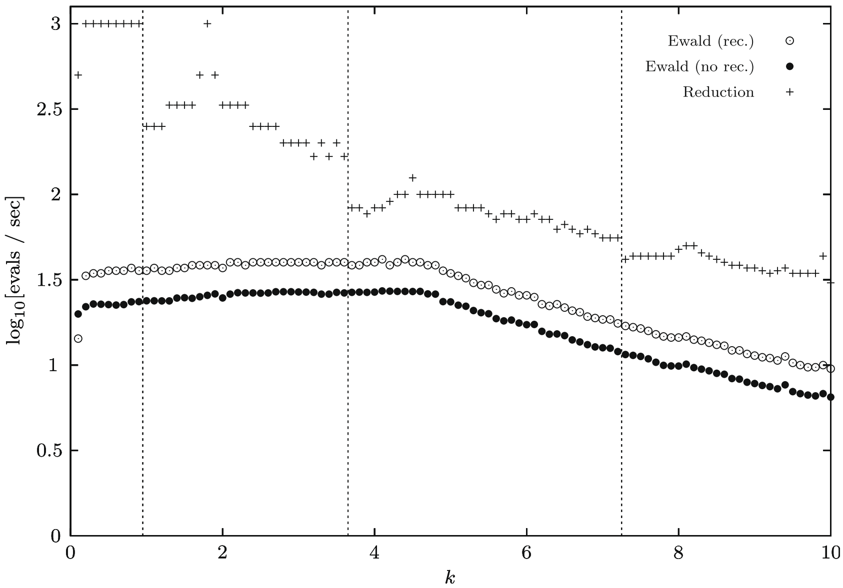

Fig. 1. Plots showing evaluations per second of σ_n^m for all $n \leqslant 5$ and $-m \leqslant n \leqslant m$ performed using the different methods. The parameter values used are $\mathbf{a}_1 = [1, 0]$, $\mathbf{a}_2 = [0.2, 1.2]$, and $\boldsymbol{\beta} = [1.8, 0.6]$. Note that the vertical axis is shown on a logarithmic scale. Unshaded circles denote results obtained using the Ewald method with recurrence relations for the integrals in $\sigma_n^{m(2)}$ and incomplete gamma functions in $\sigma_n^{m(1)}$. Shaded circles denote results obtained with the recurrence relations disabled.

servative; using a smaller value would significantly increase performance for $0.9 < k < 1.8 - \epsilon$ without adversely affecting precision.

The most complicated object in any of the summands is the Schlömilch series in (4.28). As noted in Appendix D there are several ways to compute these, though it should be noted that calculations at 'unusual' parameter values (eg. with k complex or equal to zero) are required. We calculate these series via the dual series/Twersky method with convergence acceleration using Kummer's transformation as described in [30].

6. Conclusion

We have developed accurate and efficient computational schemes for the calculation of lattice sums for the three-dimensional Helmholtz equation. For one-dimensional lattices we have used a representation in terms of a finite sum of Clausen functions and provided exponentially convergent series representations for these functions. For two-dimensional lattices we have compared two approaches: the well-known Ewald representation and the lattice reduction approach in which the two-dimensional sums are expressed as a sum of one-dimensional lattice sums.

The only disadvantage of the reduction method would appear to be the presence of removable singularities as described in Section 4.4, which complicates the program code. On the other hand lattice reduction has three significant advantages. First, it imposes a simple preferred ordering on the terms in the two-dimensional sums, expressing these as one-dimensional sums of one-dimensional sums. The second advantage is the relative simplicity of the objects to be summed, largely consisting of exponentials and standard special functions. Consequently, it is relatively easy to control the precision level of this method. Finally, and perhaps most importantly, the reduction method leads to an order-of-magnitude improvement in performance over the well-known Ewald method.

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Appendix A. Associated Legendre functions

The associated Legendre function is defined here, for non-negative order and $|x| \leqslant 1$, by

$$P_n^m(x) = (1-x^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}x^m}P_n(x) = \frac{(1-x^2)^{m/2}}{2^n n!}\frac{\mathrm{d}^{m+n}}{\mathrm{d}x^{m+n}}(x^2-1)^n, \quad n \geqslant m \geqslant 0 \tag{A.1}$$

$$= \frac{(1-x^2)^{m/2}}{2^n}\sum_{s=0}^{[(n-m)/2]} C_{ns}^m x^{n-m-2s}, \tag{A.2}$$

where

$$C_{ns}^m = \frac{(-1)^s(2n-2s)!}{s!(n-s)!(n-2s-m)!}. \tag{A.3}$$

This is the convention adopted in [20]. It differs by a factor of $(-1)^m$ (sometimes referred to as the Condon-Shortley phase) from the definition used in [22,24]. If $m > n$, $P_n^m(x) \equiv 0$. The extension to negative order is accomplished via

$$P_n^{-m}(x) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(x), \quad n \geqslant |m|, \tag{A.4}$$

and we note that

$$P_n^m(-x) = (-1)^{n+m} P_n^m(x), \tag{A.5}$$

$$P_n^m(\pm 1) = (\pm 1)^n \delta_{m0} \tag{A.6}$$

$$P_n^m(0) = \begin{cases} 0 & n+m \text{ odd} \\ \dfrac{(-1)^{(n-m)/2}(n+m)!}{2^n((n-m)/2)!((n+m)/2)!} & n+m \text{ even.} \end{cases} \tag{A.7}$$

Eq. (A.1) can easily be used to define a function of arbitrary complex argument by using the function $\gamma(z)$ defined via

$$\gamma(z) = (z-1)^{1/2}(z+1)^{1/2}, \quad -\frac{3\pi}{2} < \arg(z-1) < \frac{\pi}{2}, \quad -\frac{\pi}{2} < \arg(z+1) < \frac{3\pi}{2}, \tag{A.8}$$

which corresponds to taking branch cuts along $(1, 1+\mathrm{i}\infty)$ and $(-1, -1-\mathrm{i}\infty)$. In particular, for real argument we have

$$\gamma(t) = \begin{cases} \sqrt{t^2-1} & |t| \geqslant 1 \\ -\mathrm{i}\sqrt{1-t^2} & |t| < 1. \end{cases} \tag{A.9}$$

Thus we define

$$P_n^m(z) = [\mathrm{i}\gamma(z)]^m \frac{\mathrm{d}^m}{\mathrm{d}z^m} P_n(z), \quad n \geqslant m \geqslant 0, \tag{A.10}$$

with (A.4) serving to define the extension to negative m. Note that this function is not the usual associated Legendre function found in books since the branch cut is normally taken along the interval $(-1, 1)$ of the real axis.

For the purposes of numerical evaluation, we in fact work with the normalised associated Legendre function $\lambda_{nm} P_n^m(z)$ and the formula (A.2). Then, to calculate the first term in the series, we write

$$\sqrt{\frac{(n-m)!}{(n+m)!}} C_{n0}^m = \sqrt{\frac{(2n)!}{n!n!} \times \frac{(2n)!}{(n+m)!(n-m)!}}, \tag{A.11}$$

because both terms on the right-hand side can be written as a product of j consecutive integers divided by $j!$. This avoids the need to compute ratios of very large integers, which is attractive from a numerical point of view. Subsequent terms in the series are obtained using recurrence relations.

Appendix B. Clausen functions

We have the closed form sum [22, 1.441(2)]

$$Cl_1(x) \equiv \sum_{j=1}^{\infty} \frac{\cos jx}{j} = -\frac{1}{2}\log(2 - 2\cos x), \tag{B.1}$$

valid for all x except multiples of 2π, and the alternative representation [22, 1.518(1)]

$$Cl_1(x) = -\log x - \sum_{j=1}^{\infty} \frac{(-1)^j B_{2j} x^{2j}}{2j(2j)!}, \quad 0 < x < 2\pi, \tag{B.2}$$

as a rapidly converging series involving the Bernoulli numbers B_{2j}. This series representation allows us to derive series representations for all the Clausen functions by repeated integration. Thus we can show that, for $n \geqslant 2$, and $0 \leqslant x \leqslant 2\pi$,

$$Cl_n(x) = \Omega_n \left[\frac{x^{n-1}}{(n-1)!} \left(\log x - \sum_{s=1}^{n-1} \frac{1}{s} \right) + \sum_{j=1}^{\infty} \frac{(-1)^j B_{2j} x^{2j+n-1}}{2j(2j+n-1)!} - \sum_{j=1}^{[(n-1)/2]} \frac{(-1)^j \zeta(2j+1)}{(n-2j-1)!} x^{n-2j-1} \right], \tag{B.3}$$

where Ω_n is defined in (3.14). This formula is unsuitable for numerical computation when $\pi < x \leqslant 2\pi$; instead we use the fact that $Cl_n(x) = (-1)^{n+1} Cl_n(2\pi - x)$ when x is in this range.

The sums derived above can all be accelerated. The infinite sum over j in (B.3) is

$$\sum_{j=1}^{\infty}\frac{(-1)^j B_{2j}x^{2j+n-1}}{2j(2j+n-1)!} = -x^{n-1}\sum_{j=1}^{\infty}\frac{(2j)!\zeta(2j)}{j(2j+n-1)!}\left(\frac{x}{2\pi}\right)^{2j}$$
$$= -x^{n-1}\sum_{j=1}^{\infty}\frac{(2j)!(\zeta(2j)-1)}{j(2j+n-1)!}\left(\frac{x}{2\pi}\right)^{2j} - x^{n-1}\sum_{j=1}^{\infty}\frac{(2j)!}{j(2j+n-1)!}\left(\frac{x}{2\pi}\right)^{2j}. \tag{B.4}$$

The first sum now decays exponentially (since $\zeta(2j)-1=(1/2)^{2j}+(1/3)^{2j}+\cdots$) and the second can be evaluated in closed form (the case $n=2$ was considered in [31]. We define

$$g_m = \sum_{j=1}^{\infty}\frac{(2j)!\theta^{2j}}{j(2j+m)!} = 2\sum_{j=1}^{\infty}\frac{\theta^{2j}}{2j(2j+1)\ldots(2j+m)} = 2\sum_{j=1}^{\infty}\theta^{2j}\sum_{q=0}^{m}\frac{a_{qm}}{2j+q}, \tag{B.5}$$

where

$$a_{qm} = \frac{(-1)^q}{q!(m-q)!}. \tag{B.6}$$

We have the standard expansions

$$\log(1-x) = -\sum_{j=1}^{\infty}\frac{x^j}{j}, \quad \log\left(\frac{1+x}{1-x}\right) = 2\sum_{j=0}^{\infty}\frac{x^{2j+1}}{2j+1} \tag{B.7}$$

and so

$$g_m = \sum_{s=0}^{[m/2]} a_{2s,m}\sum_{j=1}^{\infty}\frac{\theta^{2j}}{j+s} + 2\sum_{s=0}^{[(m-1)/2]} a_{2s+1,m}\sum_{j=1}^{\infty}\frac{\theta^{2j}}{2j+2s+1} \tag{B.8}$$
$$= \sum_{s=0}^{[m/2]}\frac{a_{2s,m}}{\theta^{2s}}\sum_{j=s+1}^{\infty}\frac{\theta^{2j}}{j} + 2\sum_{s=0}^{[(m-1)/2]}\frac{a_{2s+1,m}}{\theta^{2s+1}}\sum_{j=s+1}^{\infty}\frac{\theta^{2j+1}}{2j+1} \tag{B.9}$$
$$= \sum_{s=0}^{[m/2]}\frac{a_{2s,m}}{\theta^{2s}}\left(-\log(1-\theta^2) - \sum_{j=1}^{s}\frac{\theta^{2j}}{j}\right) + \sum_{s=0}^{[(m-1)/2]}\frac{a_{2s+1,m}}{\theta^{2s+1}}\left(\log\left(\frac{1+\theta}{1-\theta}\right) - 2\sum_{j=0}^{s}\frac{\theta^{2j+1}}{2j+1}\right). \tag{B.10}$$

In particular

$$g_1 = 2 - \log(1-\theta^2) - \frac{1}{\theta}\log\left(\frac{1+\theta}{1-\theta}\right), \tag{B.11}$$
$$g_2 = \frac{3}{2} - \frac{1+\theta^2}{2\theta^2}\log(1-\theta^2) - \frac{1}{\theta}\log\left(\frac{1+\theta}{1-\theta}\right), \tag{B.12}$$
$$g_3 = \frac{6+11\theta^2}{18\theta^2} - \frac{3+\theta^2}{6\theta^2}\log(1-\theta^2) - \frac{1+3\theta^2}{6\theta^3}\log\left(\frac{1+\theta}{1-\theta}\right). \tag{B.13}$$

There is little to be gained in using this approach when calculating Clausen functions of order greater than four since the series in (3.15) are rapidly convergent already.

Appendix C. Rotation of lattice sums

From [20] Appendix C it follows that

$$\sigma_{n\uparrow}^{m} = \sum_{\ell=-n}^{n} d_n^{m\ell}\sigma_{n\rightarrow}^{\ell}, \tag{C.1}$$

where $\sigma_{n\uparrow}^{m}$ corresponds to the sums of Section 4.1 in which the polar coordinate axis is perpendicular to the lattice and $\sigma_{n\rightarrow}^{\ell}$ to those treated in Section 4.3 where the polar axis lies in the plane of the lattice and for which the coordinate system has been rotated through an angle $-\pi/2$ about the y-axis. The elements of the (real) rotation matrix $d_n^{m\ell}$ are given explicitly by

$$d_n^{m\ell} = \frac{1}{2^n}\sum_{j=0}^{n-\ell}\frac{(-1)^j\sqrt{(n+\ell)!(n-\ell)!(n+m)!(n-m)!}}{(n-\ell-j)!(\ell-m+j)!j!(n+m-j)!}, \quad \ell \pm m \geqslant 0, \tag{C.2}$$

with

$$d_n^{m\ell} = (-1)^{m+n}d_n^{\ell m}, \quad m \pm \ell \geqslant 0, \tag{C.3}$$
$$= (-1)^{m+n}d_n^{-m,-\ell}, \quad \ell \pm m \leqslant 0, \tag{C.4}$$
$$= d_n^{-\ell,-m}, \quad m \pm \ell \leqslant 0. \tag{C.5}$$

We evaluate $d_n^{m\ell}$ using recurrence relations as in [32] (note that the Euler angle β used in [32] is taken as positive clockwise).

Appendix D. Schlömilch series

In (4.28) we have a sum of the form

$$S_n(\lambda,\mu)=\sum_{j=1}^{\infty}[\mathrm{e}^{\mathrm{i}\lambda j}+(-1)^n\mathrm{e}^{-\mathrm{i}\lambda j}]H_n(\mu j). \tag{D.1}$$

This sum can be evaluated efficiently in many different ways. One can use integral representations [33,34] or Ewald representations [35,36], but perhaps the simplest method is to use the series representations derived in [17], accelerated if necessary [30]. One of the advantages of these series is that the singularities appear explicitly.

For the sum in (D.1) to exist, λ must be real and without loss of generality we can assume that $\lambda\in[0,2\pi)$. On the other hand μ can have a positive imaginary part (in which case the series converges exponentially; see [24, 9.2.3]. For simplicity we will assume that μ is either positive real or positive imaginary, since these are the only situations that arise here. Then

$$S_0(\lambda,\mu)=-1-\frac{2\mathrm{i}}{\pi}\left(C+\log\frac{\mu}{4\pi}\right)+\frac{2}{\Theta_0}+\sum_{q\in\mathbb{Z}}{}'\left(\frac{2}{\Theta_q}+\frac{\mathrm{i}}{\pi|q|}\right), \tag{D.2}$$

where $C\approx 0\cdot 5772$ is Euler's constant and

$$\Theta_q=(\mu^2-\lambda_q^2)^{1/2},\quad \lambda_q=\lambda+2q\pi, \tag{D.3}$$

with Θ_q being either positive real or positive imaginary. Note that $\log\mu$ has imaginary part 0 or $\pi/2$, and in the latter case (D.2) yields a purely imaginary result, which is consistent with (D.1). For $s\geqslant 1$, with the convention that $\mathrm{sgn}(0)=+1$,

$$S_{2s}(\lambda,\mu)=2(-1)^s\sum_{q\in\mathbb{Z}}\frac{1}{\Theta_q}[(\lambda_q+\mathrm{i}\Theta_q)/\mu]^{2s\,\mathrm{sgn}(q)}+\frac{\mathrm{i}}{\pi}\sum_{m=0}^{s}\frac{(-1)^m(s+m-1)!}{(2m)!(s-m)!}\left(\frac{4\pi}{\mu}\right)^{2m}B_{2m}\left(\frac{\lambda}{2\pi}\right), \tag{D.4}$$

$$S_{2s-1}(\lambda,\mu)=-2\mathrm{i}(-1)^s\sum_{q\in\mathbb{Z}}\frac{1}{\Theta_q}[(\lambda_q+\mathrm{i}\Theta_q)/\mu]^{(2s-1)\mathrm{sgn}(q)}-\frac{1}{\pi}\sum_{m=0}^{s-1}\frac{(-1)^m(s+m-1)!}{(2m+1)!(s-m-1)!}\left(\frac{4\pi}{\mu}\right)^{2m+1}B_{2m+1}\left(\frac{\lambda}{2\pi}\right), \tag{D.5}$$

where $B_m(\cdot)$ is a Bernoulli polynomial. It is clear that $S_n(\lambda,\mu)$ is singular if either $\mu=0$ or $\Theta_q=0$ for some integer q. Note that for $n>0$, $[(\lambda_q+\mathrm{i}\Theta_q)/\mu]^{n\,\mathrm{sgn}(q)}\sim(\mu/2\lambda_q)^n$ as $\mu\to 0$. The expressions (D.2,D.4) and (D.5) can be considered as the analytic continuation of (D.1) into a cut μ-plane.

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