Electrostatic potentials in systems periodic in one, two, and three dimensions

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We consider the electrostatic potential in a unit cell containing \( N \) point charges \( Q_j \) with positions \( \mathbf{r}_j \) inside the cell. The cell is replicated periodically in one, two, and three dimensions. The purpose is to give representations for the potential which contain only lattice sums which are absolutely convergent and uniformly convergent in the sampling position \( \mathbf{r} \). These representations are derived using variants of the Ewald method and are primarily intended for use in evaluating the accuracy of any algorithm to evaluate electrostatic energies and forces in simulations of dense matter, rather than necessarily for use of themselves in simulations. In reduced dimensionality the Ewald representations can be numerically inefficient and other representations are also provided with careful specification which allows two forms to be used for the potential functions in order to improve numerical performance. These mixed representations may be satisfactory in simulations.


I. INTRODUCTION

Condensed matter simulations are necessarily simulations of finite samples of particles and thus would, under normal circumstances, display important surface effects which distort the bulk properties of the sample. Accordingly, most practitioners use periodic boundary conditions to suppress surface effects in the sample. When the particles are charged, or carry dipole moments, a variety of problems arise. If one uses simple periodic boundary conditions, with a periodic solution of the Poisson equation to give the electrostatic potential, the model system may have no proper “exterior.” In that case, modeling the response of the system to external stresses becomes problematic. Usually, “periodic boundary conditions” are implemented by considering an infinite array of periodic copies of the system, so that one particle, \( j \), interacts not only with another particle, \( k \), but also with every periodic copy of itself and of the particle \( k \). The energy of the simulation cell and the electrostatic potential in the cell may then be written in terms of lattice sums, and the forces on the sample’s particles evaluated from the gradient of the potential.

The simplest problem to formulate is that of the potential, which can be written for a system of \( N \) particles \( j \), with charge \( Q_j \) and position \( \mathbf{r}_j \) in the sample cell as

\[
\Phi(\mathbf{r}) = \sum_{m} \sum_{j=1}^{N} \frac{Q_j}{|\mathbf{m} + \mathbf{r}_j - \mathbf{r}|},
\]

where the vectors \( \mathbf{m} \) represent the centres of the periodic copies of the simulation cell. As we shall see below, this definition is not particularly useful. If we invert the order of summation over lattice vectors \( \mathbf{m} \) and particle label \( j \), then the result does not exist, so that we expect that lattice sums of electrostatic potentials are in fact only conditionally convergent. That means that we must be rather careful about defining the summation order over \( \mathbf{m} \) as well as ordering the sums as in Eq. (1). This paper gives a unified approach via the Ewald method to give representations of the potential for a wide range of summation orders. The purpose is not necessary to provide new or more quickly implementable forms for the potential, but to provide exact implementable representations for the potential that can be used to test any algorithm for the potential. The paper also gives alternative representations for the potential which can reduce computational load significantly. The results give absolutely convergent lattice sums for the potential which are also uniformly convergent in the sampling position \( \mathbf{r} \) for physically relevant values, that is, for \(|\mathbf{r}_j - \mathbf{r}| \geq \varepsilon \), with \( \varepsilon > 0 \) for \( 1 \leq j \leq N \). We can then use the potential to find the sample cell electrostatic energy, and also the electrostatic forces by term differentiation of the lattice sum representations of the potential.

While the details of the case of three dimensional periodicity and its implementation via Ewald methods are now reasonably well understood,\(^1\) the situation with two dimensional periodicity\(^6-10\) is not so well understood in the literature and the one dimensionally periodic case seems even less clear. At the same time, a great deal of work is now appearing on charged systems of reduced dimensionality, such as systems to simulate ionic system surfaces, films of charged particles, and nanopores containing charged species.\(^11-18\) A problem that arises in these simulations is that the representations of the potential that are used in reduced periodic dimensionality can be much more inefficient computationally than in the three dimensional case.

Of course, one does not have to be restricted to Ewald methods, one not only thinks particularly of fast multipole methods,\(^9\) other new methods,\(^20,21\) but also methods due to Nijboer and de Wette\(^8,9\) and Lekner.\(^10\) However, any method must address the problem of summation order and the proper definition of the electrostatic potential in the system. With all
of these methods, it is not necessarily simple to be sure that a
given representation of the potential function set up by one
particle and its periodic images is the same as another rep-
resentation: The two representations may differ by a con-
stant. This constant then vanishes from the cell energy by
charge neutrality and from the forces. Testing approxima-
tions to the electrostatic interactions by comparing the result-
ing total potentials may not be entirely reliable. By providing
reliable computable representations for the potential, we give
a way around these difficulties.

II. THE LATTICES AND THE REPRESENTATION OF 1/R

A. Three dimensional periodicity

In three dimensions we consider a simulation cell \( \Gamma(0) \)
defined by three basis vectors \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \). The basic simula-
tion cell is

\[
\Gamma(0) = \{ \mathbf{r} = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_3 \mathbf{a}_3 : -1/2 \leq x_\alpha \leq 1/2, \text{ for } \alpha = 1, 2, 3 \}. \tag{2}
\]

The vectors \( \mathbf{a}_\alpha \) are chosen so that \( V_\Lambda = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) > 0 \) is the
volume of the simulation cell.

Usually, of course, a simulation cell has the vectors \( \mathbf{a}_\alpha \)
all perpendicular to one another, but the problem is no more
difficult with general basis vectors, and these may be useful
for considering solid ordered systems when the structure of
the solid system has complicated basis vectors. It should be
remembered that we assume that the unit cells we use are
only translationally symmetric: “higher” symmetries of the
expected crystal structure (such as reflection and rotation
symmetries) turn out not to be useful in defining general
methods for computing potentials in a unified Ewald method.

We construct a lattice \( \Lambda \) of copies \( \Gamma(\mathbf{m}) \) of the cell \( \Gamma(0) \),
defined with \( \mathbf{m} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3 \) by

\[
\Gamma(\mathbf{m}) = \{ \mathbf{r} - \mathbf{m} \in \Gamma(0) \}. \tag{3}
\]

If the basic simulation cell \( \Gamma(0) \) contains \( N \) point charges \( Q_j \)
at \( \mathbf{r}_j \in \Gamma(0) \), then the copy cell \( \Gamma(\mathbf{m}) \) contains \( N \) point
charges \( Q_j \) at \( \mathbf{r}_j + \mathbf{m} \). Extending to dipoles causes little diffi-
culty, but extending to higher order point multipole induces
almost no convergence problems.

Next, we define a shape \( P \) in three dimensions. The
shape \( P \) contains the origin \( \mathbf{r} = \mathbf{0} \) and has surface \( s_P = 0 \).
(Think of a sphere \( S \) of radius 1, where \( f_P = r^2 - 1 \). Other
shapes merely have more complicated functions \( f_P \).) Im-
portantly, we assume that the shape \( P \) is even, in the sense that
if \( \mathbf{r} \in P \) then \( -\mathbf{r} \in P \). With \( P \) large, we consider a large finite
array \( \Lambda(3, P, R) \), which is the set of all lattice cells \( \Gamma(\mathbf{m}) \) for
which \( \mathbf{m}/R \in P \). This assumption seems quite appropriate for
potentials in simulation samples, but we should be aware that
in analyzing the energy of physical systems, such as bulk
crystals, crystalline layers, and one dimensional arrays, the
evenness of \( P \) may not be appropriate.

We can then define potentials

\[
\Phi(\mathbf{r}; P, R) = \sum_{\mathbf{m} \in \Lambda(3, P, R)} \sum_{j=1}^N \frac{Q_j}{| \mathbf{m} + \mathbf{r}_j - \mathbf{r} |},
\]

and

\[
\Psi(\mathbf{r}, P) = \lim_{R \to \infty} \Phi(\mathbf{r}; P, R). \tag{4}
\]

As we shall see in Sec. III, this defines a “P shaped” sum
for \( \Psi(\mathbf{r}, P) \).

Finally, we define the reciprocal lattice \( R \), which has
basis vectors \( \mathbf{b}_1, \mathbf{b}_2, \) and \( \mathbf{b}_3 \), where

\[
\mathbf{b}_1 = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_\Lambda}, \quad \mathbf{b}_2 = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_\Lambda}, \quad \mathbf{b}_3 = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_\Lambda}. \tag{5}
\]

A basic cell of the reciprocal lattice is

\[
\gamma(0) = \{ \mathbf{u} = u_1 \mathbf{b}_1 + u_2 \mathbf{b}_2 + u_3 \mathbf{b}_3 : -1/2 \leq u_\alpha \leq 1/2; \alpha = 1, 2, 3 \}, \tag{6}
\]

and the other cells of the reciprocal lattice are \( \gamma(\mathbf{k}) \), where

\[
\gamma(\mathbf{k}) = \{ \mathbf{u} : \mathbf{u} - \mathbf{k} \in \gamma(0) \}. \tag{7}
\]

B. Two dimensional periodicity

In two dimensions, we repeat the themes of the three
dimensional case. We assume the periodicity is in the \( x-y \)
plane and that the simulation cell \( \Gamma(0) \) is

\[
\Gamma(0) = \{ \mathbf{r} = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_3 (0, 0, 1) : -1/2 \leq x_1, x_2 \leq 1/2,
\]

\[
-\frac{1}{2} \leq x_3 \leq \frac{1}{2} \},
\]

where \( \mathbf{a}_1 = (a_{11}, a_{12}, 0) \), \( \mathbf{a}_2 = (a_{21}, a_{22}, 0) \) are chosen so that
\( A_\Lambda = a_{11}a_{22} - a_{12}a_{21} > 0 \). The volume of the unit cell is then

\[
V_\Lambda = L_z A_\Lambda.
\]

The lattice vectors of the two dimensional lattice are \( \mathbf{m} = m_1 \mathbf{a}_1 + m_3 \mathbf{a}_3 \), with \( m_1 \) and \( m_2 \) integers. The cells of
the periodic array are then \( \Gamma(\mathbf{m}) \), where \( \mathbf{r} \in \Gamma(\mathbf{m}) \) if \( \mathbf{r} - \mathbf{m} \in \Gamma(0) \). The reciprocal lattice is generated by vectors

\[
\mathbf{b}_1 = (a_{22}, -a_{21})/A_\Lambda; \quad \mathbf{b}_2 = (-a_{12}, a_{11})/A_\Lambda;
\]

\[
\mathbf{b}_3 = (0, 0, 1)/L_z,
\]

and this has cells \( \gamma(\mathbf{k}) \) which are translations of \( \gamma(0) \)
through \( \mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2 \) with \( k_1 \) and \( k_2 \) integers. The cell \( \gamma(0) \) is de-
fined in a method analogous to Eq. (6). We define a two
dimensional shape \( P \) which contains the origin and is even so
that if \( \mathbf{r} \in P \) then \( -\mathbf{r} \in P \). Then we define the finite array of
cells \( \Lambda(2, P, R) \) which is those cells \( \Gamma(\mathbf{m}) \) for which \( \mathbf{m}/R \in P \). We then define the potentials

\[
\Phi(\mathbf{r}; 2, P, R) = \sum_{\mathbf{m} \in \Lambda(2, P, R)} \sum_{j=1}^N \frac{Q_j}{| \mathbf{m} + \mathbf{r}_j - \mathbf{r} |},
\]

and

\[
\Psi(\mathbf{r}, 2, P) = \lim_{R \to \infty} \Phi(\mathbf{r}; 2, P, R). \tag{10}
\]

Notice immediately that, for large \( |\mathbf{m}| \), we have \( |\mathbf{m} + \mathbf{R}|^{-1} = |\mathbf{m}|^{-1} - |\mathbf{m} \cdot \mathbf{R}|/|\mathbf{m}|^3 + O(|\mathbf{m}|^{-3}) \). The \( O(|\mathbf{m}|^{-3}) \) terms here are
absolutely summable as \( R \to \infty \). The \( O(|\mathbf{m}|^{-2}) \) terms are odd
in \( m \) and so sum to zero by the evenness of \( P \). Those results lead us to consider
\[
J = \sum_{m \in \Lambda(2,P,R)} \frac{1}{|m|} \sum_{j=1}^{N_u} Q_j.
\] (11)

If we replace the sum on \( m \) for \( |m| = m_0 \) by an integral, then we have an integral \( J_\infty \), contributing to \( J \) which is approximately
\[
J_\infty = 2\pi |\Gamma(0)| \sum_{i=1}^{N} Q_j (R - m_0).
\] (12)
and this diverges as \( R \to \infty \) unless we have charge neutrality on the simulation cell. Thus, charge neutrality is again a necessary condition for the potential \( \Psi(r,2,P) \) in Eq. (10) to exist.

C. One dimensional periodicity

In one dimension, we also repeat the themes of the three dimensional case. We assume the periodicity is in the \( x \) axis, and that the simulation cell \( \Gamma(0) \) is
\[
\Gamma(0) = \{ r = (Lx_1, Lx_2, Lx_3) : -1/2 \leq x_1, x_2, x_3 \leq 1/2 \}.
\] (13)
The volume of the unit cell is then \( V_\Lambda = L_x L_y L_z \). The cells of the periodic array are those \( r \in \Gamma(m) \) if \( r - m(1,0,0) \in \Gamma(0) \). Then we define the finite array of cells \( \Lambda(1, L, M) \) which is those cells \( \Gamma(m) \) for which \( -M \leq m \leq M \). We then define the potentials
\[
\Phi(r;1,L,M) = \sum_{m=-M}^{M} \sum_{j=1}^{N} Q_j \frac{1}{|mL(0,0) + r_j - r|}
\]
and
\[
\Psi(r,1,L) = \lim_{M \to \infty} \Phi(r;1,L,M).
\] (14)
Notice again that for large \( |m| \), we still have \( |m + R| = |m| - m \cdot R / |m| + O(|m|^{-2}) \). The \( O(|m|^{-3}) \) and \( O(|m|^{-2}) \) terms here are absolutely summable as \( R \to \infty \). Using an integral estimate again we see that the potential diverges as \( \log(M) \) as \( M \to \infty \), unless the cell is charge neutral. Again, charge neutrality is necessary to obtain a finite potential.

To develop expressions for the potentials, we use
\[
\frac{1}{|r|} = \frac{1}{\sqrt{\pi}} \int_0^\infty t^{-1/2} \exp(-t r^2) dt
\]
\[
= \frac{\text{erfc}(\alpha |r|)}{|r|} + \frac{1}{\sqrt{\pi}} \int_0^\infty t^{-1/2} \exp(-t r^2) dt.
\] (15)
We then write \( \exp(-t r^2) \) in the integrand of the second integral as an inverse three dimensional Fourier transform to find
\[
\frac{1}{|r|} = \frac{\text{erfc}(\alpha |r|)}{|r|} + \frac{1}{\sqrt{\pi}} \int_{R^3} d^3 u \frac{1}{u^2} \exp(-\frac{\pi^2 u^2}{\alpha^2}) \Delta(u', 3, P, R).
\] (16)
Here, the number \( \alpha \) is real and positive, but otherwise arbitrary. It may be chosen to optimize numerical efficiency.

In summing such expressions over a lattice to find expressions for the potential, we use the result
\[
\Delta(u; d, P, R) = \sum_{m \in \Lambda(d,P,R)} \exp(2\pi i m \cdot u) = \frac{1}{V(\Lambda(d))} \sum_{k \in \Lambda(d)} \delta(u - k) + O(R^{-2}).
\] (17)
Here, \( u \) is \( d \) dimensional, \( V(d) \) is the \( d \) dimensional reciprocal lattice, \( V(\Lambda(d)) \) is the volume, area, or length of a cell of the \( d \) dimensional lattice \( \Lambda(d) \), and \( \delta(u) \) is a \( d \) dimensional Dirac delta function. This representation may only be used in integrals where the rest of the integrand has at least two continuous derivatives on the range of integration. We may prove this result first in one dimension, where the sum reduces to \( \sin((2M+1)u)/\sin(u) \). The status of the sum as an approximate delta function is then established by integrating by parts twice. In higher dimensions, we separate the sum into a sum of terms over the \( m \), which have the same range, which is taken as maximal. This contribution separates into one dimensional sums and acts as a delta function, with the \( 1/V \) weights deriving from the Jacobian for the integration over \( u \) when written in components using the basis vectors of the reciprocal lattice. The remainder of the sum may then be shown to be \( O(R^{-2}) \) by integrating by parts twice.

We now turn to developing results in each of 1, 2, and 3 dimensions from Eqs. (16) and (17).

III. SUMMARY OF THREE DIMENSIONAL CASE

In three dimensions the results are fairly well known, but it is useful to reiterate some of the details in such a well known situation because they inform the derivation in lower dimensions. We decompose the integral over \( u \) in Eq. (16) into a sum of integrals over the cells \( \gamma(k) \) of the reciprocal lattice. We can use the delta function representation of Eq. (17) in all the cells except \( \gamma(0) \). We then have
\[
\Phi(r; 3, P, R)
\]
\[
= \sum_{j=1}^{N} Q_j \left\{ \sum_{m \in \Lambda(3, P, R)} \frac{\text{erfc}(\alpha |m + r_j - r|)}{|m + r_j - r|} + \frac{1}{\pi V_\Lambda} \right. 
\]
\[
\times \sum_{k \in R^3} \frac{1}{k^2} \exp \left( -\frac{\pi k^2}{\alpha^2} + 2\pi i k \cdot (r_j + r) \right) + O(R^{-2}) \right\}
\]
\[
+ \frac{1}{\pi} \int_{\gamma(0)} d^3 u \frac{1}{u^2} \exp \left( -\frac{\pi^2 u^2}{\alpha^2} \right) \sum_{j=1}^{N} Q_j 
\]
\[
\times \exp(2\pi i u \cdot (r_j - r)) \Delta(u', 3, P, R).
\] (18)
We expand the exponentials in the integral in Eq. (18) in
powers of \( u' \), keeping only terms up to quadratic in \( u' \).

Higher order terms give zero in the limit as \( R \to \infty \), from using the delta function representation for the sum on \( m \). The term independent of \( u' \) then gives zero by charge neutrality while the term linear in \( u' \) is zero because the integrand is odd over the range.

In the remaining term, we substitute \( u' = u/2\pi R \) and introduce \( \rho(m) = m/R \) and factors \( V_A/R^3 \) and \( R^3/V_A \). The sum on \( m \) may then be recognized as a Riemann sum approximation to an integral over \( \rho \in P \). The range of integration over \( u \) may then be relaxed to \( R^3 \) and the integral over \( u \) recognized (up to factors of \( 2\pi \)) as an inverse Fourier transform with value \( 1/|\rho| \). We may then write the integral over \( \rho \) as a surface integral over \( \partial P \), the surface of \( P \). This process then gives

\[
\Psi(r, 3, P) = \sum_{j=1}^{N} Q_j \Psi_{EW}(r_j - r) + \frac{1}{V_A} \mathbf{M} \cdot \mathbf{J}(P) \cdot r
- \frac{1}{2V_A} \sum_{j=1}^{N} Q_j r_j \cdot \mathbf{J}(P) \cdot r_j,
\]

where

\[
\Psi_{EW}(r) = \sum_{m = \text{A}(3)} \frac{\text{erfc}(\alpha|m + r|)}{|m + r|} + \sum_{k \in \mathbb{Z}} \frac{1}{\pi V_A |k|^2} \exp\left(-\frac{\pi^2 k^2}{\alpha^2} + 2\pi i k \cdot r\right)
\]

is the Ewald potential.

\[
\Phi(r, 2, P, R) = \sum_{j=1}^{N} Q_j \left\{ \sum_{m \in \text{A}(2), P, R} \frac{\text{erfc}(\alpha|m + r_j - r|)}{|m + r_j - r|} + \frac{1}{\pi A} \sum_{k \neq 0} \exp\left(-\frac{\pi^2 k^2}{\alpha^2} + 2\pi i k \cdot (\rho_j - \rho)\right) F(\alpha, z_j - k, \zeta) + O(R^2) \right\}
+ \sum_{j=1}^{N} Q_j \int_{-\infty}^{\infty} dV \int_{\gamma(0)} d^2 u' \frac{1}{u'^2 + v^2} \exp\left(-\frac{\pi^2 (u'^2 + v^2)}{\alpha^2}\right) \exp(2\pi i u' \cdot (\rho_j - \rho) + 2\pi i v(z_j - \zeta) \Delta(u', 2, P, R),
\]

where

\[
F(\alpha, \zeta, k) = \int_{-\infty}^{\infty} d\nu \frac{\exp(-\pi^2 \nu^2 \alpha^2 / \nu^2 + k^2)}{v^2 + k^2} \exp(2\pi i \nu \zeta).
\]

We may evaluate the integral \( F(\alpha, \zeta, k) \) by replacing the factor \( 1/(\nu^2 + k^2) \) with an inverse Fourier transform \( (\pi/|k|) \text{exp}(-|\alpha|/|k|) \). We can then perform the integration over \( \nu \) as a standard Gaussian integral. The resulting inverse transform must be split into two parts to accommodate the factor \( \exp(-|\alpha|/|k|) \). Each part may be evaluated in terms of complementary error functions. We obtain

\[
M = \sum_{j=1}^{N} Q_j r_j
\]

is the total dipole moment of the unit cell and, with \( n(\rho) \) representing the unit outward normal to the surface \( \partial P \) of \( P \), and

\[
J(P) = \frac{\partial P}{\partial \rho} \frac{n(\rho)}{\rho^2}
\]

is an integral which depends on the shape of \( P \). It is easy to show then that if \( P \) is a sphere \( S \), then \( J(S) = 4\pi I/3 \), where \( I \) is the \( 3 \times 3 \) identity matrix.

We may construct the energy of the unit cell in the usual way, but should remember that when we calculate the energy of a charge interacting with its own images, we should replace the \( m=0 \) error function term in Eq. (20) by \(-2\alpha/\pi \). The two lattice sums in Eq. (20) are absolutely convergent and uniformly convergent for \( |r_j - r| \geq \varepsilon > 0 \), so that we may evaluate the electric field, and so the electrostatic forces on the charges by term by term differentiation of the lattice sums.

**IV. THE TWO DIMENSIONAL CASE**

In two dimensions we use the same representation of \( 1/|r| \) and obtain

\[
F(\alpha, \zeta, k) = \frac{\pi}{2|k|} \exp(\pi^2 k^2 / \alpha^2) \left\{ \exp(-2\pi |k| \zeta) \text{erfc}\left(\frac{|k|}{\alpha} - \frac{\alpha}{\alpha} \zeta\right) + \exp(2\pi |k| \zeta) \text{erfc}\left(\frac{|k|}{\alpha} + \frac{\alpha}{\alpha} \zeta\right) \right\}.
\]

In the remaining term in Eq. (23), we replace \( \exp(2\pi i v (z_j - \zeta)) \) by \( 1 - 2 \sin^2 ((\pi v (z_j - \zeta)) \), which we can do because the rest of the integrand is even in \( v \). Using charge neutrality, after expanding the integrand in powers of \( u \) up to second order, we find
\[ \sum_{j=1}^{N} \frac{Q_j}{\pi} \int_{-\infty}^{\infty} \int_{(0)} d^2u \frac{1}{u^2 + v^2} \exp\left(-\frac{\pi^2 (u^2 + v^2)}{\alpha^2}\right) \exp(2\pi i u \cdot (\mathbf{p}_j - \mathbf{p}) + 2\pi i v (z_j - z)) \Delta(u', 2, P, R) \]

\[ = -\sum_{j=1}^{N} \frac{2Q_j}{\pi} \int_{-\infty}^{\infty} \int_{(0)} d^2u \left( \frac{\pi u (\mathbf{p}_j - \mathbf{p})^2 + \sin^2(\pi v (z_j - z))}{u^2 + v^2} \right) \exp\left(-\frac{\pi^2 v^2}{\alpha^2}\right) \Delta(u, 2, P, R) \]

\[ = -\sum_{j=1}^{N} \frac{2Q_j}{\pi} \int_{-\infty}^{\infty} \int_{(0)} d^2u \sin^2(\pi v (z_j - z)) \exp\left(-\frac{\pi^2 v^2}{\alpha^2}\right) = -\sum_{j=1}^{N} \frac{2Q_j}{\pi} h(z_j - z), \quad \text{(26)} \]

where

\[ h(\zeta) = \frac{1}{A} \int_{-\infty}^{\infty} \frac{\sin^2(\pi v \zeta)}{v^2} \exp\left(-\frac{\pi^2 v^2}{\alpha^2}\right). \quad \text{(27)} \]

Notice that \( h(0) = 0 \) and \( h'(0) = 0 \). We can evaluate the second derivative as

\[ h''(\zeta) = \frac{2\alpha \pi^{3/2}}{\lambda} \exp(-\alpha^2 \zeta^2). \quad \text{(28)} \]

Integrating twice, we obtain

\[ h(\zeta) = \frac{1}{\lambda} \left( \frac{\pi^2 \zeta + \pi^{3/2}}{\alpha} \right)^2 - \pi^2 \left( \frac{\zeta \text{erfc}(\alpha \zeta) + \exp(-\alpha^2 \zeta^2)}{\alpha \lambda} \right). \quad \text{(29)} \]

These results then give

\[ \Psi(\mathbf{r}; 2) = \sum_{j=1}^{N} Q_j \Psi_{\text{EW}}(\mathbf{r}_j - \mathbf{r}; 2), \quad \text{(30)} \]

where

\[ \Psi_{\text{EW}}(\mathbf{r}; 2) = \sum_{\mathbf{m} \in \Lambda(2)} \frac{\text{erfc}(\alpha |\mathbf{m} + \mathbf{r}|)}{|\mathbf{m} + \mathbf{r}|} + \sum_{\mathbf{k} \in \Lambda(2) \setminus 0} \frac{1}{2|\mathbf{k}|} \exp(2\pi i \mathbf{k} \cdot \mathbf{r}) \]

\[ \times \left\{ \exp(-2\pi |\mathbf{k}| |z_j - z|) \text{erfc} \left( \frac{\pi |\mathbf{k}|}{\alpha} - \alpha |z_j - z| \right) \right. \]

\[ + \exp(2\pi |\mathbf{k}| |z_j - z|) \text{erfc} \left( \frac{\pi |\mathbf{k}|}{\alpha} + \alpha |z_j - z| \right) \right\} + \frac{2\pi}{\lambda} \left. \text{erfc}(\alpha z) + \exp(\alpha^2 z^2) \right] \frac{\alpha}{\alpha \lambda} - z). \quad \text{(31)} \]

Notice that the lattice sums in Eq. (31) are absolutely convergent and may be differentiated term by term. When \( z \to \infty \), the last terms in Eq. (31) tend to zero. When \( z \to -\infty \), the last terms in Eq. (31) tend to \(-2\pi \zeta /A \), and then the dipole term in Eq. (30) becomes \(-\pi M_z /A \). This term can be viewed as the result of sheets of averaged charges in two dimensions. If we adapt the definition of \( \Psi_{\text{EW}}(\mathbf{r}; 2) \) when \( \mathbf{r} = 0 \), the same way as in three dimensions, we can write out the unit cell energy without difficulty. Notice that there are \( M_z \) terms in the potential \( \Psi_{\text{EW}} \), but these vanish from the total potential and unit cell energy by charge neutrality.

An interesting feature of this two-dimensional result is that it does not depend on the shape of the summation region \( P \).

An unattractive feature of this representation is that not only are the numerical procedures available for the reciprocal lattice sum in three dimensions not available, both the real space lattice sum and the reciprocal space lattice sum involve complementary error functions. This makes the use of this representation expensive in a simulation. Accordingly, we seek another representation, using a method originally due to Nijboer and de Wette.8,9

We use

\[ \frac{1}{|\mathbf{r}|} = \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} \frac{dt}{t^{1/2}} \exp(-t z^2 - i \mathbf{p} \cdot \mathbf{r}) \]

\[ = \sqrt{\pi} \int_{0}^{\infty} \frac{dt}{t^{1/2}} \exp(-t z^2) \int_{\mathbb{R}^2} d^2 u \exp(-\pi^2 u^2 /t + 2\pi i u \cdot \mathbf{p}). \quad \text{(32)} \]

We can then perform the lattice sum using the delta function representation. The \( \mathbf{k} \neq 0 \) and \( \mathbf{k} = 0 \) terms must be treated separately. For the \( \mathbf{k} \neq 0 \) terms we integrate over \( \mathbf{u} \) first using the delta function representation, and then integrate over \( t \). For the \( \mathbf{k} = 0 \) term, we integrate over \( t \) first and then expand the integrand in \( \mathbf{u} \) and find a simple result. We obtain

\[ \Psi(\mathbf{r}; 2) = \sum_{j=1}^{N} Q_j \Psi_{\text{Ndw}}(\mathbf{r}_j - \mathbf{r}; 2), \quad \text{(33)} \]

where

\[ \Psi_{\text{Ndw}}(\mathbf{r}; 2) = \sum_{\mathbf{k} \in \Lambda(2) \setminus 0} \frac{1}{A^2|\mathbf{k}|} \exp(2\pi i \mathbf{k} \cdot (\mathbf{p}_j - \mathbf{p}) - 2\pi |\mathbf{k}| |z_j| - \frac{2\pi}{\lambda} |z|). \quad \text{(34)} \]

This has only one reciprocal lattice sum and is absolutely convergent, and uniformly convergent in \( \mathbf{r} \) provided that \( |z| \geq \varepsilon > 0 \). It has the awkward feature that the lattice sum does not converge when \( z = 0 \), and indeed converges only slowly when \( |z| \) is small.
From Eqs. (30) and (33), we have two representations for the potential, which are
\[
\Psi(r; 2) = \sum_{j=1}^{N} Q_j \Psi_{EW}(r_j - r; 2) = \sum_{j=1}^{N} Q_j \Psi_{Naw}(r_j - r; 2).
\]

We may rearrange this as
\[
\Psi_{EW}(r_N - r; 2) - \Psi_{Naw}(r_N - r; 2)
= \frac{1}{Q_n} \left\{ \sum_{j=1}^{N-1} Q_j \Psi_{EW}(r_j - r; 2) - \sum_{j=1}^{N-1} Q_j \Psi_{Naw}(r_j - r; 2) \right\}.
\]

(36)

If we vary \( r_N \), the right hand side of Eq. (36) remains constant, so the Ewald and Nijboer–de Wette potentials differ by a constant. If we examine the large positive \( z \) expansions of the two potentials, we see that they are, in fact, equal. In evaluating the potential in the system, we can use either potential [as defined here in Eqs. (31) and (34)] as is appropriate; \( \Psi_{EW} \) when \( |z_j - z| \) is small and \( \Psi_{Naw} \) when \( |z_j - z| \) is not small. Not only does this reduce the number of error function evaluations which must be performed when using the Ewald form, but the reciprocal space error functions may be evaluated by Taylor series.

V. THE ONE DIMENSIONAL CASE

In the one dimensional case we proceed as in higher dimensions and obtain, first, for the potential in a finite one dimensional array of cell copies,

\[
\Phi(r; 1, L, M) = \sum_{j=1}^{N} Q_j \left\{ \sum_{m \in M(1, L, M)} \exp(\alpha m L(1, 0, 0) + r_j - r) \right\} + \frac{1}{\pi L \lambda_{1,0,0}} \sum_{k \neq 0} \exp \left( -\frac{\pi^2 k^2}{\alpha^2 L^2} + 2\pi i k (x_j - x) / L \right) G(\alpha, \rho_j - \rho, k)
+ \frac{1}{\pi} \int_{-1/2}^{1/2} du \int_{\mathbb{R}^2} d^2 u \frac{1}{u^2 + v^2 / L^2} \exp \left( -\frac{\pi^2 (u^2 + v^2 / L^2)}{\alpha^2} \right) \left( 2\pi i u \cdot (\rho_j - \rho) + 2\pi i u (z_j - z) / L \right) \Delta(v, 1, L, M),
\]

(37)

where
\[
G(\alpha, \rho, k) = \int_{\mathbb{R}^2} d^2 u \frac{1}{u^2 + k^2 / L^2} \exp \left( -\frac{\pi^2 u^2}{\alpha^2} + 2\pi i u \cdot \rho \right).
\]

(38)

This is not entirely satisfactory, because while a simple representation for the last term in Eq. (37) in terms of the exponential integral \( E_1(z) \) (Ref. 22) may be found (see below), considerable effort has not been successful in deriving a representation of the integrals \( G(\alpha, \rho, k) \) in terms of known special functions for which algorithms are available. However, the object of this paper is to find convergent expressions for the potentials, forces, and cell energies, so all is not lost. The absolute value of \( G(\alpha, \rho, k) \) may be bounded by replacing the factor \( \exp(2\pi i u \cdot \rho) \) by 1 and neglecting the term \( u^2 \) in the denominator of the integrand. This gives the bound
\[
|G(\alpha, \rho, k)| \leq \frac{L^2}{k^2} \int_{\mathbb{R}^2} d^2 u \exp \left( -\frac{\pi^2 u^2}{\alpha} \right) = \frac{L^2 \alpha^2}{\pi k^2},
\]

(39)

so that the sum over \( k \neq 0 \) involving the \( G \) functions is indeed absolutely convergent. We give some more details of these functions in the Appendix.

In the last term of Eq. (37), we replace \( \exp(2\pi i u \cdot (\rho_j - \rho)) \) by \( 1 - 2 \sin^2(\pi u \cdot (\rho_j - \rho)) \) and expand \( \exp(-\pi^2 v^2 / \alpha^2 + 2\pi i u (z_j - z) / L) \) to second order in \( u \). We may then use the delta function and charge neutrality to obtain

\[
\sum_{j=1}^{N} \frac{Q_j}{\pi} \int_{-1/2}^{1/2} du \int_{\mathbb{R}^2} d^2 u \frac{1}{u^2 + v^2 / L^2} \exp \left( -\frac{\pi^2 (u^2 + v^2 / L^2)}{\alpha^2} \right) \exp(2\pi i u \cdot (\rho_j - \rho) + 2\pi i u (z_j - z) / L) \Delta(v, 1, L, M)
= \sum_{j=1}^{N} \frac{Q_j}{\pi} \int_{\mathbb{R}^2} d^2 u \cos(2\pi u \cdot (\rho_j - \rho)) \exp \left( -\frac{\pi^2 u^2}{\alpha^2} \right).
\]

(40)
If we replace the factor $1/\mathbf{u}^2$ by an integral of $\exp(-\mathbf{u}^2)$ with respect to $t$ on $[0,\infty)$, we can then perform the integration over $\mathbf{u}$ and then find

$$K(\mathbf{p}_j - \mathbf{p}) = \int_{\mathbb{R}^d} d^2\mathbf{u} \frac{\cos(2\pi \mathbf{u} \cdot (\mathbf{p}_j - \mathbf{p}))}{\mathbf{u}^2} \exp\left(-\frac{\pi^2 \mathbf{u}^2}{\alpha^2}\right) = \pi \sum_{m=0}^{\infty} \frac{(-\alpha^2(\mathbf{p}_j - \mathbf{p})^2)^m}{mn!} = -\pi(\gamma + \log(\alpha^2(\mathbf{p}_j - \mathbf{p})^2) + E_1(\alpha^2(\mathbf{p}_j - \mathbf{p})^2)),\tag{41}$$

where $\gamma$ is Euler’s constant and $E_1(z)$ is a exponential integral. The identification of the series in this integral in terms of the exponential integral is computationally useful, but it should be remembered that the series (and so the integral) contains no logarithmic singularities due to zero values of the argument of a logarithm.

We thus have the one dimensional potential in the form

$$\Psi(\mathbf{r},1) = \sum_{j=1}^{N} Q_j \Psi_{EW}(\mathbf{r}_j - \mathbf{r};1),\tag{42}$$

where

$$\Psi_{EW}(\mathbf{r};1) = \sum_{m=-\infty}^{\infty} \frac{\text{erfc}(\alpha |mL(1,0,0) + \mathbf{r}|)}{|mL(1,0,0) + \mathbf{r}|} + \frac{1}{\pi L} \sum_{k=0}^{\infty} \exp\left(-\frac{\pi^2 k^2}{\alpha^2 L^2} + 2\pi ikxL\right) G(\alpha,\mathbf{p},k) + \frac{1}{\pi L} K(\mathbf{p}).\tag{43}$$

This one dimensional Ewald potential contains two absolutely convergent lattice sums. The convergence is uniform in $\mathbf{r}$ for $|\mathbf{r}| \geq e > 0$ so that the electric field and, thus, the forces on charges may be found by differentiation term by term. Note that the potential function is periodic in $x$ with period $L$.

It is possible to seek other ways to perform this potential sum. We can follow the work of Nijboer and de Wette\textsuperscript{8,9} in the three dimensional case and start with the first step of Eq. (15), not split the integral over $t$ and only transform the factor $\exp(-t(mL+x_j+y_j)^2)$. This allows us to use the delta function representation of the sum over periodic copies. We can then perform the $u$ integration using the delta functions and then perform the $t$ integration. With some attention to the integral around $u=0$ using charge neutrality, this gives the potential as

$$\Psi(\mathbf{r};1) = \sum_{j=1}^{N} Q_j \hat{\Psi}(\mathbf{r}_j - \mathbf{r}),\tag{44}$$

where

$$\hat{\Psi}(\mathbf{r}) = \frac{2}{L} \left\{ -\log \left(\frac{\rho}{L}\right) + \sum_{k=-\infty}^{\infty} \exp(2\pi kxL) K_0(2\pi |\rho|/L) \right\}.\tag{45}$$

Here, $K_0$ is a modified Bessel function of the second kind of order zero. There are several comments that should be made about this representation of the potential. First, the logarithmic terms reflect the potential due to smeared out lines of charge. Second, the potential is periodic in $x$, with period $L$, as we would expect. Third, the series representation is absolutely convergent when $|\mathbf{p}_j - \mathbf{p}| > 0$ and uniformly convergent in $\mathbf{p}$ when $|\mathbf{p}_j - \mathbf{p}| \geq e > 0$. In that situation, the field may be evaluated by term by term differentiation. Fourth, the convergence collapses when $|\mathbf{p}_j - \mathbf{p}| = 0$. Finally, Eqs. (42) and (44) calculate the same potential in the system, but the functions of $(\mathbf{r}_j - \mathbf{r})$ [see Eqs. (43) and (45)] may differ by a constant. If we examine the asymptotic behaviour of these two functions at large $|\rho|$, then in Eq. (45) only the logarithmic term survives. From the asymptotics of the complementary error function, $E_i(z)$ and the functions $G(\alpha,\mathbf{p},k)$, we see that in this limit, only the same logarithmic term survives. Thus the functions of Eqs. (43) and (45) are equal.

Hence, for the purposes of finding an accurate result, the numerical evaluation of the one dimensional potential might best be effected by using Eqs. (44) and (45) when $|\mathbf{p}_j - \mathbf{p}|$ is large and Eqs. (42) and (43) when $|\mathbf{p}_j - \mathbf{p}|$ is small. If we were to take that approach, that would mean that we only need the integrals $G(\alpha,\mathbf{p},k)$ for small $|\rho|$. We analyze the Taylor series for the $G$ functions in the Appendix.

**VI. EFFECTS OF EXTERNAL ENVIRONMENTS**

The systems we have described have, to begin with, finite. Thus, in three dimensions, we can consider the region outside the $P$ shaped finite array to be a dielectric continuum with dielectric constant $\varepsilon$. It is known\textsuperscript{7} that if $P$ be a sphere, the effect of this construction, ignoring the quadrupole term as irrelevant to either energy or forces, is to replace the dipole term $4\pi \mathbf{M} \cdot \mathbf{r}/3$ in the potential by $4\pi \mathbf{M} \cdot \mathbf{r}^2/(2e+1)$. If the external environment is conducting so that $\varepsilon \to \infty$, then the dipole term vanishes, and the system becomes properly periodic in the limit of a large array.

In two dimensions, with periodicity in the $x$ and $y$ directions, and the $z$ component of the positions of the particles confined by $-L/2 < z < L/2$, we can consider the regions $z > L/2$ and $z < -L/2$ to be filled with a continuum dielectric of dielectric constant $\varepsilon$. In that case, lattices of images are established. Suppose we have a particle of charge $Q_j$ at $\mathbf{r}_j = (x_j, y_j, z_j)$. There are periodic copies of such charges at $\mathbf{r}_j + \mathbf{m}$ for $\mathbf{m}$ in the array. We define the parameter $\Delta(\varepsilon - 1)/(\varepsilon + 1)$. Then for $\varepsilon < n < \infty$, there are image charges $Q_j(n)$ at $\mathbf{r}_j(n) + \mathbf{m}$ where

$$Q_j(n) = (-\Delta)^{|n|} Q_j,$$

and $\mathbf{r}_j(n) = (x_j, y_j, z_j(n))$ where

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$$Q_j(n) = (-\Delta)^{|n|} Q_j,$$

and $\mathbf{r}_j(n) = (x_j, y_j, z_j(n))$ where
For finite $m$ and $n$, we then have the potential from Eq. (30),

$$
\Psi(r;2;\Delta) = \sum_{r=1}^{N} Q_j \sum_{n=-\infty}^{\infty} (-\Delta)^{|n|} \Psi_{\text{NEW}}(r_j - r - 2) \cdot (\Delta) \cdot |n| \cdot \exp(-2\pi|k|L) \cdot \exp(2\pi|k|L) \cdot \exp(-2\pi|k|L).
$$

We separate out the $n=0$ term in this expression. Below, we shall write this term using $\Psi_{\text{NEW}}$, but understand that if appropriate, we may use $\Psi_{\text{EW}}$ instead. We use $\Psi_{\text{NEW}}$ for all the other values of $n$, which give infinite geometric series. We obtain

$$
\Psi(r;2;\Delta) = \sum_{r=1}^{N} Q_j \left\{ \Psi_{\text{NEW}}(r_j - r;2) + \Psi_{\Delta}(r_j,r;2) \right\}.
$$

We may then evaluate the potential using Eq. (19). There is no dipole term. We need to be careful to evaluate the Ewald potential involved for the new three dimensional lattice described in Eq. (45). In evaluating the cell energy, we should only use the energy of charges in the original cell interacting with the potential.

One last system description should be mentioned in this section. When one wants to simulate surfaces of ionic systems, one can use the two dimensional systems just described. Another way is to set up a system in three dimensions in which a thick layer of sample is replicated periodically in two dimensions and in the third dimension the spacing $L_z$ between copies is considerably larger than the thickness of the layer. The thick layer must be thick enough to ensure that surface effects are not distorted by a lack of bulk system to support them. If the layer to be simulated is in the $x,y$ plane has thickness $L$ then we choose some $L_z \gg L$ and construct a three dimensional system of copies where the two dimensional lattice in the $x,y$ plane is augmented by $z$ direction lattice vectors $m_{z} = L_z(0,0,1)$ to give a three dimensional lattice of copies. We may then use the three dimensional Ewald potential for this lattice. The choice of $L_z$ is a matter for experiment to see how large the values of $L$ and $L_z$ need to be to give convincing results.

We must also define the shape $P$ that we use to represent the model system. One approach is to let $P$ be a sphere, in which case $J = 4\pi I/3$, and we can remove this by surrounding the sphere with a conductor. Another approach is to use a cylinder with axis along the $z$ axis. This might be thought preferable because it maintains the symmetry of the layers. If the cylinder has radius $a$ and length $W$, then
If the region outside the cylinder is a conductor, then the dipole term vanishes from the total potential.

VII. DISCUSSION

The results derived in this paper are not always sensible representations to use in a simulation, but there are alternatives which have been displayed. The three dimensional results may be used effectively unless the number of particles is large enough to make the fast multipole method useful. The rough scale for the changeover is $10^5$ particles if the $N^{3/2}$ method is used, and presumably rather more if a particle mesh method is used so that fast Fourier series methods can be used on the lattice sum over the reciprocal lattice.

These fast Ewald methods rely first on using a large value of the parameter $\alpha$ so that the complementary error function has an effective finite range $R_0$. A single particle will then interact via this part of the potential with approximately $4\pi\rho R_0^3/3$ other particles, where $\rho$ is the average particle density. Thus, this part of the potential function takes a computation time which is $O(N)$ or $O(N^{3/2})$ per time step.

Fast multipole methods rely on multipole expansions of the potential due to the particles in subregions of the whole simulation sample. They then use a tree algorithm to develop the potential. It seems clear that the computation time for a system of $N$ particles will not vary significantly with the dimensionality of the periodic lattice of copies used. All you need is to be able to understand the potential being used. The same cannot be said for the potential algorithms presented in this paper. This is perhaps clearest in the two dimensional case. The Ewald form of the potential is given in Eqs. (30) and (31). Both the real space lattice sum and the Fourier space lattice sum contain complementary error function terms.

Suppose we need the potential with an absolute error less than $\epsilon$. One way to arrange a potential calculation is to require that the error in both the real space lattice sum and the reciprocal lattice sum are both less than $\epsilon/2$.

Consider a simulation sample, periodic in the $x$-$y$ plane with period $L$ in each variable. We may then choose a simple simulation sample to be $-L/2 \leq x \leq L/2$, $-L/2 \leq y \leq L/2$, and $-L/2 \leq z \leq L/2$. We assume that the rate determining step in the potential evaluation is the computation of the complementary error functions, and assume further that each error function evaluation takes a time $T_0$. The lattice vectors are $m = (m_1, m_2, 0)L$ and the reciprocal lattice vectors are $k = (k_1, k_2, 0)$. Then in a rough estimate, we should use all lattice vectors $m$ such that $\exp(-\alpha^2L^2(m_1^2 + m_2^2)) \geq \epsilon/2$ in the real space lattice sum. Equally, we should use all reciprocal lattice vectors $k$ with $\exp(-\pi^2(k_1^2 + k_2^2)/\alpha^2L^2) \geq \epsilon/2$. These estimates come from approximating $\text{erfc}(z)$ by $\exp(-z^2)$. For each set of coordinates we then need $2\pi \log(2/\epsilon)/\alpha^2L^2$ complementary error function evaluations for the real space lattice sum and $4\pi \log(2/\epsilon)\alpha^2L^2/\pi^2$ complementary error function evaluations for the Fourier space lattice sum. We can then minimize the number of complementary error function evaluations by choosing $\alpha L = 2^{-1/4}\sqrt{\pi} = 1.49$, much less than values in the range of 5–7 which are commonly used. This may well mean that unlike the usual procedure in three dimensions, where only the minimum image term in the real space lattice sum is taken, we might use several lattice images in the real space lattice sum.

Of course, we may also use the Nijboer–de Wette representation [Eqs. (33) and (34)]. In that case there is no adjustable parameter to use to minimize the computational load for a single potential function. Numerical experiment would be necessary to optimize the critical value of $|z_j - z|$, where we change from a Taylor series technique for the Ewald potential to the Nijboer–de Wette potential. It should be noted that the Taylor series coefficients may be precomputed and tabulated to speed up their evaluations.

The idea of optimizing numerical performance of a potential calculation which is arbitrarily divided into two parts by demanding that both parts be calculated to an accuracy of one-half the accuracy for the whole potential evaluation, and optimizing the way the division is done is quite common. It is central to the $O(N^{3/2})$ methods for three dimensionally periodic potentials, the $O(N \log(N))$ smooth particle mesh Ewald methods, and the "very fast multipole method." The time estimate here may, of course, not be very accurate, because while it seems best to use a direct algorithm for the complementary error functions in the real lattice sum, those in the reciprocal lattice sum may only be evaluated by Taylor series. With precomputation of the expansion coefficients for these complementary error functions, it may be that roughly equating the computation time for the real lattice sum functions and for the reciprocal lattice functions is not an accurate representation of the situation. Numerical experiment would resolve this issue, but an extensive numerical experiment on this issue (and other similar issues in this paper) would take us far away from the simple objectives of properly defining the potentials, giving computable representations for the potentials for testing approximate algorithms to evaluate them and providing useable representations (rather than optimal representations) for use in simulations whose scale is insufficient to justify the use of fast multipole methods.

In the one dimensional case, the situation is not so clear, numerical experiment would be necessary to find how to choose $\alpha$ to minimize computation time by adjusting the load...
between real space and Fourier space lattice sums. The apparently necessary twofold representation of the potential function via $K_0$ Bessel functions or the Taylor series for $G(\alpha, \rho, k)$ makes simple accuracy and timing analysis complicated.

However, we choose to represent the potential, and thus the sample energy and the interparticle forces: The potentials have been explicitly defined. The representations may be used in simulations, but if they are used, then some attention to optimizing numerical efficiency is necessary. Perhaps most importantly, we have provided representations against which any formulation of the interaction energies and forces may be tested.

**APPENDIX: THE FUNCTION $G(\alpha, \rho, k)$**

This function, defined in Eq. (38) is

$$G(\alpha, \rho, k) = \int_{\mathbb{R}^2} \frac{1}{u^2 + k^2 L^2} \exp\left(-\frac{\pi^2 u^2}{\alpha^2} + 2\pi i u \cdot \rho\right),$$

(A1)

We may view it as a special function. We need simpler forms for its computation, a Taylor series and an asymptotic expansion for large $|\rho|$. One way to compute it is via a two dimensional numerical integration procedure, which will be computationally expensive. Another way which might be useful is to define

$$\Theta_k(\beta, \rho) = \int_{\mathbb{R}^2} \frac{1}{u^2 + k^2 L^2} \exp(-\beta u^2 + 2\pi i u \cdot \rho),$$

(A2)

and note that

$$\nabla^2 \Theta_k(\beta - \rho) = 4\pi^2 \frac{\partial}{\partial \beta} \Theta_k(\beta, \rho),$$

(A3)

with the conditions that $\Theta \rightarrow 0$ as $|\rho| \rightarrow \infty$, and the initial condition

$$\Theta_k(0, \rho) = 2\pi K_0(2\pi |k| |\rho|/L).$$

(A4)

To obtain a Taylor series for $G$, we expand the factor $\exp(2\pi i \rho \cdot u)$ in the integrand in powers of $u$, then integrate over the angular variable and then, with a little work, integrate over $|u|$. This process gives

$$G(\alpha, \rho, k) = \sum_{n=0}^{\infty} A_n(\alpha^2 \rho^2)^n,$$

(A5)

with

$$A_n = \frac{\pi}{(n!)^2} \left(\frac{\pi |k|}{\alpha L}\right)^{2n} E_1\left(\frac{\pi^2 k^2}{\alpha^2 L^2}\right) + \sum_{m=1}^{n} \frac{n!}{m!(n-m)!} \left(-\frac{\alpha^2 L^2}{\pi^2 k^2}\right)^m \Gamma(m, \frac{\pi^2 k^2}{\alpha^2 L^2}),$$

(A6)

where the sum on $m$ is absent if $n=0$ and $\Gamma(m, z)$ is an incomplete gamma function.

To find an expression for $G$ which contains only one dimensional integrals over finite range, we write $1/(u^2 + k^2/L^2)$ as an integral on $[0, \infty)$ of $\exp(-t(u^2 + k^2/L^2))$. We can then integrate over $u$ and find

$$G(\alpha, \rho, k) = \pi \exp\left(\frac{\pi^2 k^2}{\alpha^2 L^2} \right) \int_0^{\infty} \frac{dt}{t} \exp(-t(k^2/L^2 + \pi^2 \rho^2/t)).$$

(A7)

We use the substitution $y(t) = tk^2/L^2 + \pi^2 \rho^2/t$. Notice that $y(t)$ has a single simple minimum of $y_c = 2\pi |k| |\rho|/L$ at $t = t_c = \pi |k| L/|\rho|$ and that $y \rightarrow \infty$ as $t \rightarrow 0$ and as $t \rightarrow \infty$. Thus, there are two inverse functions $t_c(y) = (L^2/2k^2)(y + \sqrt{(y^2 - (2\pi |k| |\rho|/L)^2)})$ and we must be careful which branch we use in the substitution. We define $\rho_\epsilon = \pi |k|/L \rho^2$. If $|\rho| < \rho_\epsilon$, $\pi^2/\alpha^2 > t_c$ and we only need the branch $t_c(y)$. On the other hand, if $|\rho| > \rho_\epsilon$, $\pi^2/\alpha^2 < t_c$ and we need to use both branches. We then use $dt_c(y)/dy = \pm t_c'(y)/\sqrt{(y^2 - (2\pi |k| |\rho|/L)^2)}$. Finally, we use the substitution $y = (2\pi |k| |\rho|/L) \cosh(\varphi)$ with $\varphi = 0$ at $y = y_c$ and at $t = \pi^2/\alpha^2$, $\varphi(\pm) = \log(|\rho|/|\rho|)$ for $|\rho| < \rho_\epsilon$ while $\varphi(\pm) = -\log(|\rho|/|\rho|)$ for $|\rho| > \rho_\epsilon$. We then find

$$G(\alpha, \rho, k) = \pi \exp\left(\frac{\pi^2 k^2}{\alpha^2 L^2} \right) \left\{ K_0(2\pi |k| |\rho|/L) \right.$$

$$- \int_{0}^{\varphi(\pm)} \! d\varphi \exp\left(-2\pi |k| |\rho|/L \cosh(\varphi)\right) \right\},$$

(A8)

for $|\rho| < \rho_\epsilon$ and

$$G(\alpha, \rho, k) = \pi \exp\left(\frac{\pi^2 k^2}{\alpha^2 L^2} \right) \left\{ K_0(2\pi |k| |\rho|/L) \right.$$

$$- \int_{0}^{\varphi(-)} \! d\varphi \exp\left(-2\pi |k| |\rho|/L \cosh(\varphi)\right) \right\},$$

(A9)

for $|\rho| > \rho_\epsilon$. These two equations represent $G$ in terms of standard functions and finite range one dimensional integrals.

We may then develop an expansion at large $|\rho|$ of the integral in Eq. (A9) to give

$$G(\alpha, \rho, k) = \pi \exp\left(\frac{\pi^2 k^2}{\alpha^2 L^2} \right) \left\{ 2K_0(2\pi |k| |\rho|/L) \right.$$

$$- \frac{\exp\left(-\alpha^2 \rho^2 + \pi^2 k^2 / \alpha^2 L^2\right)}{(\alpha^2 \rho^2 - \pi^2 k^2 / \alpha^2 L^2)} \left(1 + O\left(\frac{1}{|\rho|}\right)\right) \right\},$$

(A10)

Thus, we see that $G$ tends to zero rather rapidly at large $|\rho|$.

22 M. Abramowitz and I. A. Stegun, Handbook of Mathematical functions (Dover, New York, 1965), Chap. 5.