Effective way to sum over long-range Coulomb potentials in two and three dimensions

Sandeep Tyagi*
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA
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I propose a method to calculate the logarithmic interaction in two dimensions and the Coulomb interaction in three dimensions under periodic boundary conditions. This paper considers the case of a rectangular cell in two dimensions and an orthorhombic cell in three dimensions. Unlike the Ewald method, there is no parameter to be optimized, nor does the method involve error functions, thus leading to the accuracy obtained. This method is similar in approach to that of Sperb [Mol. Simul. **22**, 199 (1999)], but the derivation is considerably simpler and physically appealing. An important aspect of the proposed method is the faster convergence of the Green's function for a particular case as compared to Sperb's work. The convergence of the sums for most parts of the unit cell is exponential, and hence requires the calculation of only a few dozen terms. In a very simple way, we also obtain expressions for the interaction for systems with slab geometries. Expressions for the Madelung constants of CsCl and NaCl are also obtained.

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I. INTRODUCTION

In molecular dynamics (MD) and Monte Carlo (MC) simulations one is required to calculate the potential energy and forces acting on a particle due to other particles. Sometimes such forces have a long-range interaction. In such situations, periodic boundary conditions are usually imposed in order to avoid the boundary effects, which might be especially prominent for small systems that are usually employed in MD simulations. Under periodic boundary conditions interaction of a particle with another particle includes the direct interaction plus an interaction of the first particle with all replicas of itself as well as all replicas of the second particle. These replicas come into the picture due to the periodic repetitions of a charge under the periodic boundary conditions. The energy contribution arising from the interaction of a particle with its own replicas is termed the self-energy. The calculation of self-energy is important in a MC simulation, where the size of the box might change during simulation, such as in isobaric MC calculations. The natural question that arises is how one may compute the long-range interaction of a particle with a second particle along with all the replicas of the second particle. The self-energy part may then be obtained trivially as well. For 80 years, researchers have employed the Ewald sum technique [1] to perform such summations. However, the Ewald sum technique has certain drawbacks. The primary drawback is the optimization of a parameter that renders breakup of the original algebraic sum into two parts, one in real space and the other one in Fourier space. Only when this parameter is chosen properly do the sums in the real and Fourier spaces converge fast. A second problem with the Ewald sum is that even if one achieves optimal choice of the parameter for breaking up the sum, one might lose numerical accuracy as the terms in these sums involve error functions, whose evaluation to a high degree of accuracy is difficult. In this paper we will consider the logarithmic interaction in two dimensions (2D) and Coulomb interaction in three dimensions. The 2D case has been satisfactorily dealt with in Ref. [2]. Thus mainly we will concentrate on 3D results. The Ewald method is the most widely used technique for system in 3D. An alternative technique for summation over long-range forces in 3D for a cubic unit cell was given by Lekner [3]. A tedious method was employed to obtained the self-energy part of the interaction. However, Lekner generalized his work to an orthorhombic cell [4] and obtained self-energies in a much simpler manner. These recent methods by Lekner [3] and Sperb [5] are similar in spirit but their derivation involves complicated algebra. One problem with Lekner's expressions is that they involve a triple sum. Sperb's [5] results are better in that part of the interaction has only a double sum. Nevertheless a triple sum [Eqs. (2.4) and (2.7) in Ref. [5]] is still employed for the case when both particles are very close to each other.

The technique that we propose is based on a series summation in Fourier space. Work along these lines has been previously reported in recent papers [6,7], as well as by Harris *et al.* [8], Sperb [5], Crandall *et al.* [9], and Marshall [10]. The outline of this paper follows. In Sec. II, we derive a general formula for dimension $d \geqslant 2$. In Sec. III the formula is applied to get the logarithmic sum in 2D. Section IV describes application of the general formula to get the Coulomb summation $1/r$ for the slab geometry case as well as for 3D case. Section V considers evaluation of Madelung constants for CsCl and NaCl. Finally, we discuss our results in Sec. VI.

II. COULOMB SUM IN *d* DIMENSION

An interaction that satisfies the Poisson equation in d dimensions will be termed a Coulomb type potential for that particular dimension. For example, the logarithmic interaction is a Coulomb type interaction in 2D. In this section we discuss how one can calculate a pairwise Coulomb interaction between two particles, separated by a displacement $\mathbf{r}$. For simplicity, we consider the case of a unit charge situated within an orthorhombic cell in d dimensions. Let the d sides

*Electronic address: satst27@pitt.edu

of the unit cell be labeled by $l_1, l_2, \ldots, l_d$. The basic unit cell repeats itself in all d dimensions. The unit charge interacts with other identical unit charges (for the case of different charges q_1 and q_2 one just gets an extra factor of $q_1 q_2$) situated at the vertices of the periodic structure. The interaction between two particles is given by the Green's function in d dimension, $G(\mathbf{r})$, which satisfies the Poisson equation

$$\nabla^2 G(\mathbf{r}) = -C_d \sum_{\boldsymbol{l}} \delta(\mathbf{r}+\boldsymbol{l}). \tag{2.1}$$

where ∇^2 is the Laplacian operator in d dimensions, $\boldsymbol{l}$ denotes a d-dimensional vector, whose components are integer multiples of l_i's, and C_d is specified by

$$C_d = \begin{cases} B_2 & \text{for } d=2, \\ (d-2)B_d & \text{for } d>2, \end{cases}$$

where B_d stands for the coefficient of the $(d-1)$-dimensional surface element in d dimensions,

$$B_d = \frac{d(\pi)^{d/2}}{\Gamma(d/2+1)}. \tag{2.2}$$

Here $\Gamma(x)$ stands for the gamma function. Thus $B_2 = 2\pi$, $B_3 = 4\pi$, etc. We note that the coefficients in Eq. (2.1) have been chosen such that $G(\mathbf{r})$ stands for a Coulomb type summation in d dimensions. For example, if we consider N charges $q_i, q_2, \ldots, q_N$ in a neutral unit cell then for $d>2$, we will have a total energy of the system E given by

$$E = {\sum_{\{m\}_d}}' \sum_{i,j=1}^{N} \times \frac{q_i q_j}{\{(m_1 l_1 - r_{ij,1})^2 + (m_2 l_2 - r_{ij,2})^2 + \cdots + (m_d l_d - r_{ij,d})^2\}^{(d-2)/2}} \tag{2.3}$$

where $r_{ij,k}$ stands for the the kth component of vector $\mathbf{r}_{ij}$ and $\{m\}_d$ stands for a set of d numbers $m_1, m_2, \ldots, m_d$. The summation over each m_i runs from $-\infty$ to $+\infty$. The prime on the summation sign indicates that when all m_i are zero, the term corresponding to $i=j$ is not to be included.

The solution to Eq. (2.1) can be formally expressed in Fourier space,

$$G(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \frac{1}{l_1 l_2 \cdots l_d} \times \sum_{\{m\}_d} \frac{e^{i2\pi(m_1 x_1/l_1 + m_2 x_2/l_2 + \cdots + m_d x_d/l_d)}}{\{(m_1/l_1)^2 + (m_2/l_2)^2 + \cdots + (m_d/l_d)^2\}}, \tag{2.4}$$

where $0 \leqslant x_i/l_i < 1$. The function $G(x_1, x_2, \ldots, x_d)$, as defined above, diverges since the term corresponding to all m's being equal to zero blows up. This is expected since the sum defined in Eq. (2.4) has a contribution coming from an infinite set of identical charges, i.e., the unit cell is not charge neutral. For the sum in Eq. (2.4) to make sense we add an infinitesimal term to the denominator and subtract off a counterterm from the whole sum as follows:

$$G(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \frac{1}{l_1 l_2 \cdots l_d} \lim_{\xi \to 0} \left(\sum_{\{m\}_d} \frac{e^{i2\pi(m_1 x_1/l_1 + m_2 x_2/l_2 + \cdots + m_d x_d/l_d)}}{\{(m_1/l_1)^2 + (m_2/l_2)^2 + \cdots + (m_d/l_d)^2 + (\xi/l_d)^2\}} - \frac{1}{(\xi/l_d)^2} \right), \tag{2.5}$$

where ξ is an infinitesimal parameter which tends to zero. The prescription employed above amounts to assumption of the presence of a uniform background charge. For example, let us consider the case of 3D. For every charge q, one may imagine a uniform distribution of charge, such that the total charge per unit cell adds up to $-q$. For a charge neutral periodic system, imposing these kinds of background uniform charge distributions does not matter since the total uniform background charge adds up to zero. However, now a unit charge located within the unit cell at position (x_1, x_2, x_3) not only interacts with a second charge located at the origin and its periodic images, but also interacts with the neutralizing background charge, compensating the charge of the second particle. This particular way of introducing the neutralizing background charge leads to only the intrinsic part [3] of the potential energy. Now, it can be easily verified that Eq. (2.5) satisfies the following equation:

$$\nabla^2 G(\mathbf{r}) = -C_d \sum_{\boldsymbol{l}} \delta(\mathbf{r}+\boldsymbol{l}) + \frac{C_d}{l_1 l_2 \cdots l_d}, \tag{2.6}$$

where the last term in Eq. (2.6) represents the uniform background charge. The complete expression for the potential has a term arising from surface contribution. For the 2D case this turns out to be zero, but for 3D one obtains a contribution from a dipole term [11].

Moving further, we can perform one of the d sums in Eq. (2.5) analytically [12],

$$\begin{aligned} g(x_d, \{m\}, \xi) &= \sum_{m_d=-\infty}^{\infty} \frac{e^{i2\pi m_d x_d/l_d}}{(m_d)^2 + (m_1 l_{d,1})^2 + \cdots + (m_{d-1} l_{d,d-1})^2 + \xi^2} \\ &= \frac{\pi}{\gamma_d(\{m\}, \xi)} \frac{\cosh[\pi \gamma_d(\{m\}, \xi)(1 - 2|x_d|/l_d)]}{\sinh[\pi \gamma_d(\{m\}, \xi)]}, \end{aligned} \tag{2.7}$$

where $l_{i,j}$ stands for l_i/l_j and $\gamma_d(\{m\},\xi)$ is defined as

$$\gamma_d(\{m\},\xi) = \sqrt{(m_1 l_{d,1})^2 + \cdots + (m_{d-1} l_{d,d-1})^2 + \xi^2}. \quad (2.8)$$

For convenience we also define

$$\gamma_{d0}(\{m\},\xi) = \sqrt{(m_1 l_{d,1})^2 + \cdots + (m_{d-1} l_{d,d-1})^2}. \quad (2.9)$$

Using Eqs. (2.5) and (2.7) one obtains

$$G(x_1,x_2,\ldots,x_d) = \frac{C_d}{(2\pi)^2}\frac{l_d}{l_1 l_2 \cdots l_{d-1}} \times \lim_{\xi\to 0}\left(\sum_{\{m\}_{d-1}} g(x_d,\{m\},\xi) \times \prod_{i=1}^{(d-1)} \cos\left(2\pi m_i \frac{x_i}{l_i}\right) - \frac{1}{\xi^2}\right). \quad (2.10)$$

In the limit $\xi\to 0$, the term corresponding to all m_i being set to zero in Eq. (2.10) must be separated out as follows:

$$G(x_1,x_2,\ldots,x_d) = \frac{C_d}{(2\pi)^2}\frac{l_d}{l_1 l_2 \cdots l_{d-1}} \times \left[\sum_{\{m\}_{d-1}}{}' g(x_d,\{m\},\xi) \prod_{i=1}^{(d-1)} \cos\left(2\pi m_i \frac{x_i}{l_i}\right)\right]\Bigg|_{\xi=0} + \frac{C_d}{(2\pi)^2}\frac{l_d}{l_1 l_2 \cdots l_{d-1}}\frac{\pi^2}{3}\left\{1 - 6\left(\frac{|x_d|}{l_d}\right) + 6\left(\frac{x_d}{l_d}\right)^2\right\}, \quad (2.11)$$

where the prime on the summation sign implies that the term corresponding to all m_i being zero is not to be included. In Eq. (2.11), we separated out the term corresponding to all m_i being set to zero and took the limit $\xi\to 0$ as follows:

$$\lim_{\xi\to 0}\left(\frac{\pi}{\xi}\frac{\cosh[\pi\xi(1-2|x_d|/l_d)]}{\sinh[\pi\xi]} - \frac{1}{\xi^2}\right) = \frac{\pi^2}{3}\left\{1 - 6\left(\frac{|x_d|}{l_d}\right) + 6\left(\frac{x_d}{l_d}\right)^2\right\}. \quad (2.12)$$

Equation (2.11) forms the main result derived in this section. It is important to note that as a result of the symmetry present in the problem, it suffices to look at only that part of the unit cell which corresponds to $0 \leqslant x_i/l_i \leqslant 0.5$ for all i's. Hence, from here on we will assume $0 \leqslant x_i/l_i \leqslant 0.5$. In the next two sections, we investigate two important cases corresponding to $d=2$ and $d=3$.

III. LOGARITHMIC SUM IN TWO DIMENSIONS

The energy of N particles contained in a rectangular unit cell with periodic boundaries and interacting through a logarithmic potential in 2D can be expressed as [5]

$$E^{2D}_{\text{total}} = \frac{1}{2}\sum_{i,j;i\neq j} q_i q_j G_{2D}(\mathbf{r}_i - \mathbf{r}_j) + \sum_i q_i^2 G^{2D}_{\text{self}}, \quad (3.1)$$

where the charges are denoted by q_i and the position of the charges in the unit cell by $\mathbf{r}_i$ where $1 \leqslant i \leqslant N$. We will obtain expressions for $G_{2D}(\mathbf{r})$ and G^{2D}_{self} in this section. The pairwise interaction is given by the Green's function $G_{2D}(\mathbf{r})$ which satisfies the Poisson equation in 2D,

$$\nabla^2 G_{2D}(\mathbf{r}) = -2\pi\sum_{\boldsymbol{l}} \delta(\mathbf{r}+\boldsymbol{l}) + \frac{2\pi}{l_1 l_2}, \quad (3.2)$$

where the last term on the right-hand side (RHS) of Eq. (3.2) stands for the neutralizing background charge. Equation (3.2) is a special case of Eq. (2.1). We look for a solution of Eq. (3.2) with periodic boundary conditions along the x_1 and x_2 directions. This solution can be easily obtained from the general formula Eq. (2.11) derived in the previous section,

$$G_{2D}(x_1,x_2) = \frac{1}{2\pi}\frac{l_2}{l_1}\sum_{m'}\frac{\pi}{\gamma_{20}(m)} \times \frac{\cosh[\pi\gamma_{20}(m)(1-2|x_2|/l_2)]}{\sinh[\pi\gamma_{20}(m)]}\cos\left(2\pi m\frac{x_1}{l_1}\right) + \frac{1}{2\pi}\frac{l_2}{l_1}\frac{\pi^2}{3}\left\{1 - 6\left(\frac{|x_2|}{l_2}\right) + 6\left(\frac{x_2}{l_2}\right)^2\right\}, \quad (3.3)$$

where the prime on m implies that the term corresponding to $m=0$ is to be excluded. Without any loss of generality we may assume that sides of the rhombic cells have been labeled so that $l_1 \leqslant l_2$. This condition will make sure that $\gamma_{20}(m) > 1$ for all integer values of m. Let us now consider the convergence of the sum in Eq. (3.3). The first part of Eq. (3.3) converges exponentially, but in some cases the convergence may be very slow. Specifically, the leading term in Eq. (3.3) decays as $\exp(-2\pi|m||x_2|/l_1)$. Thus the convergence depends on the ratio x_2/l_1. We see that one obtains a slow exponential convergence when $0 \leqslant x_2/l_1 < 0.1$. To handle this case properly, we break the first sum in Eq. (3.3) into two parts by application of a trigonometric identity,

$$\frac{\cosh(a-b)}{\sinh(b)} = \frac{\cosh(a)\exp(-b)}{\sinh(b)} + \exp(-a). \quad (3.4)$$

This leads to the expression

$$\frac{1}{2\pi}\sum_{m'}\frac{\pi}{|m|}\frac{\cosh[\pi m l_{2,1}(1-2|x_2|/l_2)]}{\sinh(\pi|m|l_{2,1})}\cos\left(2\pi m\frac{x_1}{l_1}\right) = \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\pi}{m}\frac{\exp(-\pi|m|l_{2,1})\cosh[\pi m l_{2,1}(2x_2/l_2)]}{\sinh(\pi m l_{2,1})} \times\cos\left(2\pi m\frac{x_1}{l_1}\right) + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\pi}{m} \times\exp\left(-2\pi m\frac{|x_2|}{l_1}\right)\cos\left(2\pi m\frac{x_1}{l_1}\right). \quad (3.5)$$

We notice that the first part of Eq. (3.5) converges even for the case when $0 \leqslant x_2/l_1 < 0.1$. In fact the slowest convergence for the first part will now occur for the case when $2x_2 = l_2$. But even this "slowest" convergence amounts to a very rapid exponential convergence of $\exp(-\pi|m|l_2/l_1)$. We have yet to account for the last sum in Eq. (3.5). Using the identity

$$\sum_{n=1}^{\infty}\frac{1}{n}\exp(-2n\pi x)\cos(2\pi ny) = -\frac{1}{2}\ln[\cosh(2\pi x)-\cos(2\pi y)] + \pi x - \frac{\ln(2)}{2}, \quad x>0, \tag{3.6}$$

the last part of the sum in Eq. (3.5) may be explicitly evaluated to

$$-\frac{1}{2}\ln\left\{\cosh\left(2\pi\frac{x_2}{l_1}\right)-\cos\left(2\pi\frac{x_1}{l_1}\right)\right\}+\pi\frac{|x_2|}{l_1}-\frac{\ln(2)}{2}. \tag{3.7}$$

Assembling the terms together, we finally obtain the following expression for the 2D Green's function:

$$\begin{aligned}G_{2D}(x_1,x_2) = {} & \frac{1}{2\pi}\sum_{m'}\frac{\pi}{|m|} \\ & \times\frac{\exp(-\pi|m|l_2/l_1)\cosh[2\pi m x_2/l_1]}{\sinh(\pi|m|l_2/l_1)}\cos\left(2\pi m\frac{x_1}{l_1}\right) \\ & -\frac{1}{2}\ln\left\{\cosh\left(2\pi\frac{x_2}{l_1}\right)-\cos\left(2\pi\frac{x_1}{l_1}\right)\right\} \\ & +\frac{\pi l_2}{6l_1}\left\{1+6\left(\frac{x_2}{l_2}\right)^2\right\}-\frac{\ln(2)}{2}.\end{aligned} \tag{3.8}$$

The self-energy may be easily obtained as

$$\begin{aligned}G_{\text{self}}^{2D} = {} & \lim_{(x_1,x_2)\to(0,0)}\{G_{2D}(x_1,x_2)+\ln(\sqrt{x_1^2+x_2^2})\} \\ = {} & \frac{1}{2\pi}\sum_{m'}\frac{\pi}{|m|}\frac{\exp(-\pi|m|l_2/l_1)}{\sinh(\pi|m|l_2/l_1)}-\ln\left(\frac{2\pi}{l_1}\right)+\frac{\pi}{6}\frac{l_2}{l_1}.\end{aligned} \tag{3.9}$$

The results derived here may be trivially generalized to the case of a rhombic cell, but our concern in this paper has only been with orthorhombic cases. The results obtained here were numerically checked and found to be in agreement with those of Grønbech-Jensen [2].

IV. COULOMB SUM IN 3D

The energy of N particles contained in an orthorhombic unit cell with periodic boundaries and interacting through a Coulomb type potential in 3D can be expressed as

$$E_{\text{total}}^{3D} = \frac{1}{2}\sum_{i,j;i\neq j} q_i q_j G_{3D}(\mathbf{r}_i-\mathbf{r}_j)+\sum_i q_i^2 G_{\text{self}}^{3D}+\frac{2\pi}{3}\left(\sum_i q_i\mathbf{r}_i\right)^2, \tag{4.1}$$

where the charges are denoted by q_i and the positions of the charges in the unit cell by $\mathbf{r}_i$ and $1\leqslant i\leqslant N$. We will obtain expressions for $G_{3D}(\mathbf{r})$ and G_{self}^{3D} in this section. The application of Eq. (2.11) for an orthorhombic cell in 3D leads to

$$\begin{aligned}G_{3D}(x_1,x_2,x_3) = {} & \frac{1}{\pi}\frac{l_3}{l_1 l_2}{\sum_{m_1,m_2}}'\frac{\pi}{\gamma_{30}(\{m\})}\frac{\cosh[\pi\gamma_{30}(\{m\})(1-2|x_3|/l_3)]}{\sinh[\pi\gamma_{30}(\{m\})]} \\ & \times\prod_{i=1}^{2}\cos\left(2\pi m_i\frac{x_i}{l_i}\right)+\frac{l_3}{l_1 l_2}\frac{\pi}{3}\left\{1-6\left(\frac{|x_3|}{l_3}\right)+6\left(\frac{x_3}{l_3}\right)^2\right\},\end{aligned} \tag{4.2}$$

where

$$\gamma_{30}(\{m\},\xi) = \sqrt{(m_1 l_{3,1})^2+(m_2 l_{3,2})^2}. \tag{4.3}$$

Without any loss of generality we assume that the axes have been labeled such that

$$l_3 \geqslant l_2 \geqslant l_1. \tag{4.4}$$

The condition in Eq. (4.4) makes sure that $\gamma_{30}(\{m\})>1$ for all sets $\{m\}$. Equation (4.2) is one of our main results for the 3D case. We note that the potential energy obtained consists of only the intrinsic part [3]. A dipole contribution will have to be included in Eq. (4.2) to obtain the real potential energy [3,11]. This dipole contribution is represented by the last term on the RHS in Eq. (4.1). We notice that the sum in Eq. (4.2) converges exponentially. In fact the terms corresponding to large $|m_1|$ and $|m_2|$ decay as exp $\times[-2\pi x_3\sqrt{(m_1/l_1)^2+(m_2/l_2)^2}]$, which with the assumption in Eq. (4.4) means that terms decay faster than exp $\times[-2\pi x_3\sqrt{(m_1/l_2)^2+(m_2/l_2)^2}]$. Thus the convergence depends upon the ratio $r_{32}=x_3/l_2$. For $r_{32}>0.1$, the convergence of the series in Eq. (4.2) is extremely good. However, the convergence slows down for the case when $r_{32}<0.1$. This problem may be solved as follows. Applying the identity from Eq. (3.4) again, we break the first sum in Eq. (4.2) into three parts:

$$\begin{aligned}G_{3D}(x_1,x_2,x_3) = {} & G_{\text{ELC}}(x_1,x_2,x_3)+G_{\text{slab}}(x_1,x_2,x_3) \\ & +\frac{l_3}{l_1 l_2}\frac{\pi}{3}\left\{1+6\left(\frac{x_3}{l_3}\right)^2\right\},\end{aligned} \tag{4.5}$$

where

$$\begin{aligned}G_{\text{ELC}}(x_1,x_2,x_3) = {} & \frac{1}{\pi}\frac{l_3}{l_1 l_2}{\sum_{m_1,m_2}}'\frac{\pi}{\gamma_{30}(\{m\})} \\ & \times\frac{\exp[-\pi\gamma_{30}(\{m\})]\cosh[\pi\gamma_{30}(\{m\})(2x_3/l_3)]}{\sinh[\pi\gamma_{30}(\{m\})]} \\ & \times\prod_{i=1}^{2}\cos\left(2\pi m_i\frac{x_i}{l_i}\right)\end{aligned} \tag{4.6}$$

and

$$G_{\rm slab}(x_1,x_2,x_3)=\frac{1}{\pi}\frac{l_3}{l_1l_2}\sum_{m_1,m_2}{}'\frac{\pi}{\gamma_{30}(\{m\})}\exp\left(-2\pi\gamma_{30}(\{m\})\frac{|x_3|}{l_3}\right)\times\prod_{i=1}^{2}\cos\left(2\pi m_i\frac{x_i}{l_i}\right)-\frac{2\pi}{l_1l_2}|x_3|. \quad (4.7)$$

We note an important aspect of this breakup of the sum in Eq. (4.2) into three parts. Equation (4.7) is independent of l_3 as $l_3/\gamma_{30}(\{m\})$ does not depend on l_3. In fact the expression in Eq. (4.7) is a three-dimensional Coulomb sum for a cell that is open along the x_3 direction and periodic along x_1 and x_2. Thus the sum in Eq. (4.7) corresponds to the slab geometry. Note that the subscript ELC stands for the so called electrostatic correction term, a phrase borrowed from Ref. [13]. At this point it is worthwhile to recast the last term in Eq. (4.5) in a different form, which will prove to be useful later in the discussion. Suppose we have n charges in a charge neutral unit cell $\Sigma_i q_i=0$. Let us assume that the position of the q_i is denoted by (x_{1i},x_{2i},x_{3i}). Then the third term in Eq. (4.5) will give rise to a term in the total energy. This term will be given by

$$E_z=\frac{2\pi}{l_1l_2l_3}\left(\frac{1}{2}\sum_{i,j}q_iq_j|x_{3i}-x_{3j}|^2\right), \quad (4.8)$$

which after expanding the argument and using the charge neutrality condition gives

$$E_z=-\frac{2\pi}{V}M_3^2, \quad (4.9)$$

where $M_3=\Sigma_i q_i x_{3i}$ stands for the total dipole moment along the x_3 direction.

Let us now consider the convergence of $G_{\rm ELC}$ and $G_{\rm slab}$. The function $G_{\rm ELC}$ decays as $\exp(-2\pi\gamma_{30}(\{m\})[1-|x_3|/l_3])$. Thus we see that $G_{\rm ELC}$ converges exponentially fast for $0\leqslant r_3\leqslant 0.5$. In fact the slowest convergence of $G_{\rm ELC}$ occurs for the case $r_3=0.5$, but even this slowest convergence varies as $\exp[-\pi\gamma_{30}(\{m\})]$, which is extremely fast, keeping in mind the inequality of Eq. (4.4).

Now we consider the convergence of $G_{\rm slab}$. The previously mentioned problem of convergence still persists and $G_{\rm slab}$ fails to converge fast when $0\leqslant r_{32}<0.1$. So the next step is to separate out this diverging behavior toward small value of r_{32}. For that purpose we break the sum over m_i's in Eq. (4.7) as follows:

$$\sum_{m_1,m_2}{}' = \sum_{m_1=0,m_2'} + \sum_{m_1',m_2},$$

where m_1' implies that the term corresponding to $m_1=0$ is not to be included. Thus we break up $G_{\rm slab}$ as

$$G_{\rm slab}(x_1,x_2,x_3)=G_1(x_2,x_3)+G_2(x_1,x_2,x_3), \quad (4.10)$$

where

$$G_1(x_2,x_3)=\frac{1}{\pi}\frac{l_3}{l_1l_2}\left\{\frac{2}{l_{3,2}}\sum_{m_2=1}^{\infty}\frac{\pi}{m_2}\exp\left(-2\pi m_2\frac{|x_3|}{l_2}\right)\times\cos\left(2\pi m_2\frac{x_2}{l_2}\right)\right\} \quad (4.11)$$

and

$$G_2(x_1,x_2,x_3)=-\frac{2\pi}{l_1l_2}x_3+\frac{1}{\pi}\frac{1}{l_1l_2}\sum_{m_1',m_2}\frac{\pi}{\sqrt{(m_1/l_1)^2+(m_2/l_2)^2}}\times\exp\left[-2\pi\sqrt{\left(\frac{m_1}{l_1}\right)^2+\left(\frac{m_2}{l_2}\right)^2}|x_3|\right]\times\prod_{i=1}^{2}\cos\left(2\pi m_i\frac{x_i}{l_i}\right). \quad (4.12)$$

First we obtain G_1 in a closed form as follows. We may employ the identity from Eq. (3.6) to obtain

$$G_1(x_2,x_3)=-\frac{1}{l_1}\ln\left[\cosh\left(2\pi\frac{x_3}{l_2}\right)-\cos\left(2\pi\frac{x_2}{l_2}\right)\right]-\frac{\ln(2)}{l_1}+2\pi\frac{|x_3|}{l_1l_2}. \quad (4.13)$$

As discussed in Appendix A, G_1 has a logarithmic divergence when x_2/l_2 and x_3/l_2 tend to zero. As we will see soon, a similar logarithmic divergence with opposite sign arises from the term G_2. These two divergences cancel each other to give a finite contribution to $G_{\rm slab}$ toward small values of x_2 and x_3.

We consider the case of G_2 from Eq. (4.12). Applying the Poisson summation rule [14], the sum over m_2 in Eq. (4.12) may be transformed to a sum involving Bessel functions of the second kind [14]:

$$\frac{1}{|\delta|}\sum_m\pi\frac{\exp\left[-|z|\sqrt{\alpha^2+(2\pi m/\delta)^2}\right]}{\sqrt{\alpha^2+(2\pi m/\delta)^2}}\exp\left(2\pi i m\frac{x}{\delta}\right)=\sum_m K_0\left(\alpha\sqrt{z^2+(x+\delta m)^2}\right). \quad (4.14)$$

Identifying

$$\delta=l_2,\quad z=x_3,\quad \alpha=2\pi\frac{|m_1|}{l_1},\quad \text{and } x=x_2, \quad (4.15)$$

we can write

$$G_2(x_1,x_2,x_3)=\frac{2}{l_1}\sum_{m_1',m_2}K_0\left(2\pi\frac{|m_1|}{l_1}\sqrt{(x_2+m_2l_2)^2+x_3^2}\right)\times\cos\left(2\pi m_1\frac{x_1}{l_1}\right)-\frac{2\pi}{l_1l_2}|x_3|. \quad (4.16)$$

The sum in Eq. (4.16) may be expressed in two parts as

$$G_2(x_1,x_2,x_3)=\frac{2}{l_1}\sum_{m_1',m_2'}K_0\left(2\pi\frac{|m_1|}{l_1}\sqrt{(x_2+m_2l_2)^2+x_3^2}\right)\times\cos\left(2\pi m_1\frac{x_1}{l_1}\right)+\frac{2}{l_1}\sum_{m_1'}K_0\left(2\pi\frac{|m_1|}{l_1}\sqrt{x_2^2+x_3^2}\right)\times\cos\left(2\pi m_1\frac{x_1}{l_1}\right)-\frac{2\pi}{l_1l_2}|x_3|. \quad (4.17)$$

We note that the first term in Eq. (4.17) has no convergence problem as x_2 and x_3 are positive numbers and $l_2\geqslant l_1$. This term will converge even for the case when $0\leqslant x_2$ and x_3 is zero. The convergence of G_2, and thus that of G_{slab} and G_{3D}, depends upon the ratio

$$\rho=\frac{(x_2^2+x_3^2)^{1/2}}{l_1}, \quad (4.18)$$

which appears in the second term on the RHS of Eq. (4.17). For $\rho>0.1$, Eq. (4.17) will have a very good convergence. However, if x_2 and x_3 are such that the condition $\rho>0.1$ is not satisfied then we should transform Eq. (4.17) further. This can be done by using the results derived in Appendix B where it is shown that

$$\begin{aligned}f(x_1,x_2,x_3)&=\frac{4}{l_1}\sum_{m_1=1}^{\infty}K_0\left(\frac{2\pi m_1}{l_1}(x_2^2+x_3^2)^{1/2}\right)\cos\left(\frac{2\pi m_1}{l_1}x_1\right)\\&=\frac{2}{l_1}\ln\left(\frac{(x_2^2+x_3^2)^{1/2}}{2l_1}\right)+\frac{1}{\sqrt{x_1^2+x_2^2+x_3^2}}\\&\quad+\frac{1}{l_1}\sum_{n_1=1}^{N-1}\left(\frac{1}{\sqrt{\rho^2+(n_1+x)^2}}+\frac{1}{\sqrt{\rho^2+(n_1-x)^2}}\right)\\&\quad-\frac{\{\psi(N+x)+\psi(N-x)\}}{l_1}+\frac{1}{l_1}\sum_{l=1}^{\infty}\binom{-1/2}{l}\\&\quad\times\rho^{2l}[\zeta(2l+1,N+x)+\zeta(2l+1,N-x)],\end{aligned} \quad (4.19)$$

where $x=x_1/l_1$ and ψ and ζ stand for the digamma and Hurwitz zeta functions, respectively. $N\geqslant 1$ is the smallest integer satisfying the condition $N>\rho+x$. Thus we can choose $N=1$, as even for the worst case one has $\rho=0.1$ and $x=0.5$. However, for better convergence it is desirable that one chooses N such that $N>\rho+1$.

We can now write the following short algorithm to calculate G_{slab}. First we set our axis such that $l_3\geqslant l_2\geqslant l_1$. Next, using the periodic boundary conditions, the separation between two particles can always be reduced in such a way that the individual components satisfy $0\leqslant x_i<l_i$. Thus, the values of $r_i=x_i/l_i$ lie between 0 and 1. From the inherent symmetry of the problem, the energy corresponding to eight different separations of $\mathbf{((}(1\pm r_1)/2,(1\pm r_2)/2,(1\pm r_3)/2\mathbf{)}$ is the same. This essentially means that we can concentrate our attention on only those separations between the particles that correspond to $0\leqslant r_i\leqslant 0.5$. If some $r_i>0.5$, we can replace it with $1-r_i$. Next, we look at the value of $r_{32}=r_3/l_2$. If $r_{32}>0.1$, we can combine Eq. (4.13) with Eq. (4.12) to obtain the following form for G_{slab}:

$$\begin{aligned}G_{\text{slab}}(x_1,x_2,x_3)&=-\frac{1}{l_1}\ln\left[\cosh\left(2\pi\frac{x_3}{l_2}\right)-\cos\left(2\pi\frac{x_2}{l_2}\right)\right]-\frac{\ln(2)}{l_1}\\&\quad+\frac{1}{\pi}\frac{1}{l_1l_2}\sum_{m_1',m_2}\frac{\pi}{\sqrt{(m_1/l_1)^2+(m_2/l_2)^2}}\\&\quad\times\exp\left(-2\pi\sqrt{\left(\frac{m_1}{l_1}\right)^2+\left(\frac{m_2}{l_2}\right)^2}|x_3|\right)\\&\quad\times\prod_{i=1}^{2}\cos\left(2\pi m_i\frac{x_i}{l_i}\right).\end{aligned} \quad (4.20)$$

However, if $0\leqslant r_{32}<0.1$, then we look at the value of ρ, which is defined in Eq. (4.18). If $\rho>0.1$, we should use the following form of G_{slab} which is obtained after combining Eqs. (4.13) and (4.17):

$$\begin{aligned}G_{\text{slab}}(x_1,x_2,x_3)&=-\frac{1}{l_1}\ln\left[\cosh\left(2\pi\frac{x_3}{l_2}\right)-\cos\left(2\pi\frac{x_2}{l_2}\right)\right]-\frac{\ln(2)}{l_1}+\frac{2}{l_1}\sum_{m_1',m_2'}K_0\left(2\pi\frac{|m_1|}{l_1}\sqrt{(x_2+m_2l_2)^2+x_3^2}\right)\cos\left(2\pi m_1\frac{x_1}{l_1}\right)\\&\quad+\frac{4}{l_1}\sum_{m_1=1}^{\infty}K_0\left(\frac{2\pi m_1}{l_1}(x_2^2+x_3^2)^{1/2}\right)\cos\left(\frac{2\pi m_1}{l_1}x_1\right).\end{aligned} \quad (4.21)$$

If $\rho<0.1$ then we use the identity in Eq. (4.19) to write G_{slab} as

$$\begin{aligned}G_{\text{slab}}(x_1,x_2,x_3)&=-\frac{1}{l_1}\ln\left[\cosh\left(2\pi\frac{x_3}{l_2}\right)-\cos\left(2\pi\frac{x_2}{l_2}\right)\right]-\frac{\ln(2)}{l_1}+\frac{2}{l_1}\sum_{m_1',m_2'}K_0\left(2\pi\frac{|m_1|}{l_1}\sqrt{(x_2+m_2l_2)^2+x_3^2}\right)\cos\left(2\pi m_1\frac{x_1}{l_1}\right)\\&\quad+\frac{2}{l_1}\ln\left(\frac{(x_2^2+x_3^2)^{1/2}}{2l_1}\right)+\frac{1}{\sqrt{x_1^2+x_2^2+x_3^2}}+\frac{1}{l_1}\sum_{n_1=1}^{N-1}\left(\frac{1}{\sqrt{\rho^2+(n_1+x)^2}}+\frac{1}{\sqrt{\rho^2+(n_1-x)^2}}\right)-\frac{\{\psi(N+x)+\psi(N-x)\}}{l_1}\\&\quad+\frac{1}{l_1}\sum_{l=1}^{\infty}\binom{-1/2}{l}\rho^{2l}[\zeta(2l+1,N+x)+\zeta(2l+1,N-x)].\end{aligned} \quad (4.22)$$

Although Eq. (4.22) is meant to be used only when $\rho<0.1$, the equation is defined for all values of ρ as long as N is chosen such that $N>\rho+1$. The series given in Eq. (4.22) is valid when both x_2 and x_3 are nonzero. In this case, the argument of the first logarithmic term on the RHS of Eq. (4.22) is always greater than zero. However, for very small values of x_2 and x_3 (say both less than $\varepsilon=10^{-3}$) the first and the fourth terms diverge. In this situation one should combine the diverging terms together using the function L defined in Appendix B.

We have thus shown how to compute $G_{\rm slab}$ for all regions of the unit cell. Similar results for the slab geometry have previously been obtained in Refs. [14,15,16]. The results in Eqs. (4.20) and (4.22) correspond, respectively, to the "near" and "far" formulas derived by Arnold and Holm [14]. Also, it is an easy matter now to obtain expressions for $G_{\rm 3D}$ from Eq. (4.5). One can obtain the self-energy for a 3D system as

$$G^{\rm 3D}_{\rm self}=\lim_{(x_1,x_2,x_3)\to(0,0,0)}\left(G_{\rm 3D}(x_1,x_2,x_3)-\frac{1}{\sqrt{x_1^2+x_2^2+x_3^2}}\right)$$
$$=\frac{1}{\pi}\frac{l_3}{l_1l_2}{\sum_{m_1,m_2}}'\frac{\pi}{\gamma_{30}(\{m\})}\frac{\exp[-\pi\gamma_{30}(\{m\})]}{\sinh[\pi\gamma_{30}(\{m\})]}+\frac{2}{l_1}$$
$$\times\sum_{m_1',m_2'}K_0\left(2\pi|m_1m_2|\frac{l_2}{l_1}\right)+\frac{l_3}{l_1l_2}\frac{\pi}{3}-\frac{2}{l_1}\ln\left(\frac{4\pi l_1}{l_2}\right)+\frac{2\gamma}{l_1}, \tag{4.23}$$

where for $G_{\rm 3D}$ we use Eqs. (4.5) and (4.22).

V. MADELUNG CONSTANTS

Using the formulas developed above, it is an easy matter to obtain expressions for the Madelung constants of NaCl and CsCl. A simple structural analysis of CsCl easily leads to the expression

$$M_{\rm CsCl}=G_{\rm 3D}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)-G^{\rm 3D}_{\rm self}, \tag{5.1}$$

and similarly for NaCl we see that

$$M_{\rm NaCl}=\frac{1}{2}\left[G_{\rm 3D}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)+3G_{\rm 3D}\left(0,0,\frac{1}{2}\right)\right.$$
$$\left.-3G_{\rm 3D}\left(\frac{1}{2},0,\frac{1}{2}\right)-G^{\rm 3D}_{\rm self}\right], \tag{5.2}$$

where Eq. (4.5) can be used for $G_{\rm 3D}(x_1,x_2,x_3)$ with all l_i's set equal to 1. From the above equations we obtain the following expressions for the Madelung constants of CsCl and NaCl:

$$M_{\rm CsCl}=-\frac{1}{\pi}{\sum_{m_1,m_2}}'\frac{\pi}{\sqrt{m_1^2+m_2^2}}\frac{[\exp(-\pi\sqrt{m_1^2+m_2^2})-(-1)^{m_1+m_2}]}{\sinh(\pi\sqrt{m_1^2+m_2^2})}$$
$$-2\left(\sum_{m_1',m_2'}K_0(2\pi|m_1m_2|)-\ln(4\pi)+\gamma-\pi\right) \tag{5.3}$$

and

$$2M_{\rm NaCl}=-\frac{1}{\pi}{\sum_{m_1,m_2}}'\frac{\pi}{\sqrt{m_1^2+m_2^2}}$$
$$\times\frac{\{\exp[-\pi\sqrt{m_1^2+m_2^2}]-(-1)^{m_1+m_2}-3+3(-1)^{m_1}\}}{\sinh(\pi\sqrt{m_1^2+m_2^2})}$$
$$-2\left(\sum_{m_1',m_2'}K_0(2\pi|m_1m_2|)-\ln(4\pi)+\gamma-\pi\right). \tag{5.4}$$

Restricting the sum over m_1 and m_2 between -4 and $+4$, a simple calculation on MATHEMATICA gives an $M_{\rm CsCl}$ value correct up to 10^{-8} and an $M_{\rm NaCl}$ value correct up to 10^{-6}. In addition we also obtain a simple relationship between the two Madelung constants:

$$2M_{\rm NaCl}=M_{\rm CsCl}+6\sum_{m_1,m_2}\frac{\csc[\pi\sqrt{(2m_1+1)^2+m_2^2}]}{\sqrt{(2m_1+1)^2+m_2^2}}. \tag{5.5}$$

This interesting relationship was first established by Hautot [17] in the 1970s using Hankel integrals and Schloimilch series.

VI. CONCLUSION

Complete expressions for the Coulomb sum for a rectangular cell in 2D and an orthorhombic cell in 3D were derived. We also obtained expressions for the self-energies. The expressions obtained provide convergence in all parts of the unit cell. Considerable simplification has been achieved over Sperb's work [5] in terms of deriving the equations. The proposed formula for the potential energy when the two charges are very close differs from that of Sperb. In particular, when the charges are close together, Sperb's [5] formula has a triple sum [Eqs. (2.4) and (2.7)]. In our expression, we have at most a double sum. Similar results for the 3D case have previously been obtained by Strebel using a rather involved procedure [18]. Our results do not require any convergence parameter like that used in Ewald sums, neither do our formulas involve any complementary error functions. These error functions in an Ewald sum are a source of loss of precision when calculating Madelung constants to higher accuracies.

In retrospect, we see that these results could be derived in another way by starting off with the Green's function expression for the $2D+h$ slab geometry system and then adding the ELC term which takes into account the rest of the layers. In this way we will get only the first two terms of Eq. (4.5). The third term is then obtained by adding a term proportional to M_3^2 from outside, where M_3 stands for the component of the total dipole moment along the x_3 direction. In the present work this dipole term arises naturally, as shown in Eq. (4.9). This dipole term has been discussed by Smith [19]. Thus this slabwise summation plus a dipole term added from outside, apart from an unimportant constant, leads to the same expression as in Eq. (4.5). Thus, our Eqs. (4.5) and (4.9) can be viewed as an alternative derivation of Eq. (4) in Ref. [13].

An advantage of the method developed here is that one can achieve better time scaling in a simulation. Using the

expressions presented in this paper, the time to calculate the forces and energy for a 3D system in a computer simulation scales as N^2, where N is the number of charges present in the unit cell. However, one can achieve $N^{5/3}\ln(N)^2$ scaling after a little modification in the expressions presented here. This is the same scaling as achieved by Arnold and Holm [14] for a $2D+h$ system. The scaling remains the same for the two cases because the electrostatic correction term can be computed linearly if we remove the contribution of the first two closest layers enclosing the unit cell in a given direction as opposed to removing the contribution of just one layer as done by Arnold *et al.* [13] and in this paper. Also the results presented here can be generalized to a rhombic cell in 2D and a triclinic cell in 3D [20].

Our proposed expressions can be applied to calculation of Madelung constants in 3D. Results obtained for the Madelung constants of CsCl and NaCl match those in the literature.

In conclusion we have provided a very simple derivation of complicated results previously obtained by many authors using different, sometimes complicated, techniques [3,5,14–16].

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APPENDIX A: LOGARITHMIC DIVERGENCE

Consider the function

$$L(x,y) = \ln[\cosh y - \cos x] - \ln\left[\frac{y^2+x^2}{2}\right]. \tag{A1}$$

We want to examine the limiting value of L as x and y tend to zero. For this reason we expand the argument of the first logarithmic term in Eq. (A1),

$$\cosh y - \cos x = \left(\frac{y^2+x^2}{2!}\right) + \left(\frac{y^4-x^4}{4!}\right) + \left(\frac{y^6+x^6}{6!}\right) + \left(\frac{y^8-x^8}{8!}\right) + O(x^{10},y^{10}). \tag{A2}$$

Factoring out the first term on the right-hand side, Eq. (A2) can be written as

$$\cosh y - \cos x = \left(\frac{y^2+x^2}{2!}\right) \times \left\{1 + \frac{2!}{4!}(y^2-x^2) + \frac{2!}{6!}(y^4-x^2y^2+x^4) + \frac{2!}{8!}(y^4+x^4)(y^2-x^2) + O(x^8,y^8)\right\}. \tag{A3}$$

Thus L can be written as

$$L(x,y) = \ln\left\{1 + \frac{2!}{4!}(y^2-x^2) + \frac{2!}{6!}(y^4-x^2y^2+x^4) + \frac{2!}{8!}(y^4+x^4)(y^2-x^2) + O(x^8,y^8)\right\}. \tag{A4}$$

Using the results from Eqs. (A1) and (A4) in Eq. (4.13), we see that for small values of x_2/l_2 and x_3/l_2, G_1 can be written as

$$G_1(x_2,x_3) = -\frac{1}{l_1}\ln\left[2\pi^2\frac{(x_2^2+x_3^2)}{l_2^2}\right] - \frac{\ln(2)}{l_1} + 2\pi\frac{|x_3|}{l_1 l_2} - \frac{1}{l_1}L\left(\frac{x_2}{l_2},\frac{x_3}{l_2}\right), \tag{A5}$$

which clearly shows a logarithmic divergence as x_2/l_2 and x_3/l_2 tend to zero.

APPENDIX B: LINE CHARGE

We commence with the identity [12],

$$f(x_1,x_2,x_3) = \frac{4}{l_1}\sum_{m_1=1}^{\infty} K_0\left(\frac{2\pi m_1}{l_1}(x_2^2+x_3^2)^{1/2}\right)\cos\left(\frac{2\pi m_1}{l_1}x_1\right) = \frac{2}{l_1}\left\{\gamma + \ln\left(\frac{(x_2^2+x_3^2)^{1/2}}{2l_1}\right)\right\} + \frac{1}{\sqrt{x_1^2+x_2^2+x_3^2}} + S(x_1,x_2,x_3), \tag{B1}$$

where

$$S(x_1,x_2,x_3) = \sum_{n=1}^{\infty}\left(\frac{1}{\sqrt{x_2^2+x_3^2+(nl_1-x_1)^2}} + \frac{1}{\sqrt{x_2^2+x_3^2+(nl_1+x_1)^2}} - \frac{2}{n}\right). \tag{B2}$$

We can further transform the identity in Eq. (B1) along the lines worked out by Strebel [18] and Arnold and Holm [14]. Let us look at

$$h(\rho,x_1) = \frac{1}{l_1}\sum_{n=N}^{\infty}\left(\frac{1}{\sqrt{\rho^2+(n+x_1/l_1)^2}} - \frac{1}{n}\right) = \frac{1}{l_1}\sum_{n=1}^{\infty}\left(\frac{1}{\sqrt{\rho^2+(n+N-1+x_1/l_1)^2}} - \frac{1}{n+N-1}\right) = \frac{1}{l_1}\sum_{n=1}^{\infty}\left(\frac{1}{\sqrt{\rho^2+(n+y)^2}} - \frac{1}{n}\right) + \frac{1}{l_1}\sum_{n=1}^{N}\frac{1}{n}, \tag{B3}$$

where $N \geqslant 1$, $y = N-1+x_1/l_1$, and

$$\rho = \frac{(x_2^2+x_3^2)^{1/2}}{l_1}, \quad x = \frac{x_1}{l_1}. \tag{B4}$$

Assuming $\rho < |1+y|$, the binomial expansion of the first term in the above equation gives

$$\frac{1}{\sqrt{\rho^2+(n+y)^2}} = \sum_{p=0}^{\infty} \binom{-1/2}{p} \rho^{2p} \frac{1}{|n+y|^{2p+1}} = \sum_{p=1}^{\infty} \binom{-1/2}{p} \rho^{2p} \frac{1}{|n+y|^{2p+1}} + \frac{1}{|n+y|}, \tag{B5}$$

where $\binom{-1/2}{p}$ stands for the binomial coefficient. We can take the sum over n inside and obtain

$$h(\rho,x_1) = \frac{1}{l_1} \sum_{p=1}^{\infty} \binom{-1/2}{p} \rho^{2p} \sum_{n=1}^{\infty} \frac{1}{|n+y|^{2p+1}} + \frac{1}{l_1} \sum_{n=1}^{\infty} \left(\frac{1}{|n+y|} - \frac{1}{n} \right) + \frac{1}{l_1} \sum_{n=1}^{N} \frac{1}{n}. \tag{B6}$$

Now, using the definition of the Hurwitz zeta function,

$$\zeta(l,y) = \sum_{k=0}^{\infty} \frac{1}{(k+y)^l}, \tag{B7}$$

we obtain

$$\sum_{n=1}^{\infty} \frac{1}{|n+y|^{2p+1}} = \zeta(2p+1,1+y). \tag{B8}$$

Also the second sum in Eq. (B6) is easy to obtain. By the definition of the digamma function ψ we have

$$\sum_{n=1}^{\infty} \left(\frac{1}{|n+y|} - \frac{1}{n} \right) = -\gamma - \psi(1+y). \tag{B9}$$

Thus $h(\rho,x_1)$ can be written as

$$h(\rho,x_1) = -\frac{\gamma}{l_1} - \frac{\psi(1+y)}{l_1} + \frac{1}{l_1} \sum_{l=1}^{\infty} \binom{-1/2}{l} \rho^{2l} \zeta(2l+1,1+y) + \frac{1}{l_1} \sum_{n=1}^{N} \frac{1}{n}. \tag{B10}$$

Using Eqs. (B2) and (B10) we obtain

$$S(x_1,x_2,x_3) = \frac{1}{l_1} \sum_{n=1}^{N-1} \left(\frac{1}{\sqrt{\rho^2+(n+x)^2}} + \frac{1}{\sqrt{\rho^2+(n-x)^2}} - \frac{2}{n} \right) + \frac{1}{l_1} \sum_{n=N}^{\infty} \left(\frac{1}{\sqrt{\rho^2+(n+x)^2}} + \frac{1}{\sqrt{\rho^2+(n-x)^2}} - \frac{2}{n} \right) \tag{B11}$$

$$= \frac{1}{l_1} \sum_{n=1}^{N-1} \left(\frac{1}{\sqrt{\rho^2+(n+x)^2}} + \frac{1}{\sqrt{\rho^2+(n-x)^2}} \right) - \frac{2\gamma}{l_1} - \frac{\psi(N+x)+\psi(N-x)}{l_1} + \frac{1}{l_1} \sum_{l=1}^{\infty} \binom{-1/2}{l} \times \rho^{2l} [\zeta(2l+1,N+x) + \zeta(2l+1,N-x)]. \tag{B12}$$

Note that for Eq. (B12) to be valid, the condition is that $\rho < |1+y|$, where $y = N-1 \pm x_1/l_1$. Keeping in mind that $x_1 \geqslant 0$ we get $\rho < |N \pm x_1/l_1|$, which will be satisfied if $N > \rho + x$. Combining Eq. (B1) and Eq. (B12) gives us the result that we set out to prove.

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