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Rapid evaluation of the periodic Green function in *d* dimensions

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Abstract

A method is given to obtain the Green function for the Poisson equation in any arbitrary integer dimension under periodic boundary conditions. We obtain recursion relations which relate the solution in d-dimensional space to that in $(d-1)$-dimensional space. Near the origin, the Green function is shown to split into two parts, one is the essential Coulomb singularity and the other is regular. We are thus able to give representations of the Coulomb sum in higher dimensions without recourse to any integral representations. The expressions converge exponentially fast in all parts of the simulation cell. Works of several authors are shown to be special cases of this more general method.

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1. Introduction

The Poisson equation is probably one of the most useful equations in physics. In a two-dimensional (2D) space, the periodic solution of this equation corresponds to the solution of particles interacting with the logarithmic interaction, and it has applications in simulations of 2D pancake vortices in high-temperature superconductors [1]. In 3D, periodic solutions to the Poisson equation are used in electromagnetism. Here, the solution of the Poisson equation corresponds to a number of charges interacting with the Coulomb potential. This 3D periodic solution is routinely used in most simulations involving charged particles. Recently, the periodic solution of the Poisson equation in higher dimensions has found use in the string theory.

In 1D and 2D, the Green function for the Poisson equation for a charge neutral box may be obtained in a closed form. In 3D, one can obtain rapidly converging series representations using the well-known method by Ewald [2]. Two other approaches for the 3D case were given by Lekner [3] and Sperb [4]. However, in higher dimensions, one can either use the Ewald method which has its drawbacks, or use the Jacobi theta function identities [5]. In general, there is no efficient way to calculate the Green function in a general d-dimensional space with $d > 3$.

In this paper, we give two exponentially fast converging series representations for the Green function of the Poisson equation in any positive integer dimension. This work will generalize the methods employed for 2D and 3D cases [7], and will tie together the different approaches taken by Lekner [3] and Sperb [4] for the special case of $d = 3$. The outline of the paper is as follows. In section 2 we derive expressions giving the Coulomb sum in the d-dimensional space. In section 3 we derive recursive relations using the result of section 2. In section 4 we discuss the results.

2. Green function in *d* dimensions

For simplicity, we consider the case of a unit charge situated within a cubic box in d dimensions. The sides of the box are all assumed to be of unit length. From here onwards, we will refer to the box as the simulation cell. The basic simulation cell repeats itself in all d dimensions. We also assume a charge neutral system. 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_1q_2) situated at the vertices of the periodic structure. The periodic Green function in d dimensions satisfies the Poisson equation,

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

where ∇_d^2 is the Laplacian operator in d dimensions, $\boldsymbol{l}$ denotes a d-dimensional vector, whose components are integers ranging over $-\infty$ to $+\infty$, and C_d is a dimension-dependent factor. The value of C_d for various dimensions is

$$C_d = \begin{cases} 2 & d = 1 \\ 2\pi & d = 2, \\ 4\pi^{\nu+1}/\Gamma(\nu) & d > 2. \end{cases}$$

Here, $\Gamma(\nu)$ stands for the Gamma function, and $\nu = (d-2)/2$. We note that with this choice of C_d in equation (2.1), the G stands for the Coulomb-type summation in d dimensions. Thus, G corresponds to a sum of the type $-|\boldsymbol{r}|$ in 1D, a logarithmic sum, $-\ln|\boldsymbol{r}|$, in 2D and a sum of the type $|\boldsymbol{r}|^{-(d-2)}$ for a d-dimensional space with $d > 2$. The solution of equation (2.1) diverges, which is a simple consequence of the fact that the interaction energy of a charge with another charge and all its periodic images is infinite. To obtain a meaningful value of G we will have to modify equation (2.1) as follows [6]:

$$\nabla^2 G_d(\boldsymbol{r}) = -C_d \sum_{\boldsymbol{l}} \delta(\boldsymbol{r}+\boldsymbol{l}) + C_d. \tag{2.2}$$

The second term in equation (2.2) amounts to the presence of a uniform background charge. Thus, for every charge, q, one may imagine a uniform distribution of charge, such that the total charge per basic simulation 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 basic simulation cell at position $\{x_i\}$ not only interacts with a second charge located at the origin and its periodic images, but also interacts with the neutralizing background charge accompanying the second particle. This particular way of introducing the artificial neutralizing background charge leads to only the intrinsic part [3] of the potential energy. We note that once the Green function is obtained, the solution of the equation

$$\nabla^2 V_d = -C_d \boldsymbol{\rho}(\boldsymbol{r})$$

under periodic boundary conditions could be simply obtained from

$$V_d = \int_{\text{cell}} G_d(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{\rho}(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}',$$

where $\boldsymbol{\rho}$ is periodic and the simulation cell is overall charge neutral. The rapid evaluation of the G_d is discussed in the next section.

The solution of equation (2.2) can be written easily in the Fourier space as [7]:

$$G_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \lim_{\beta\to 0} \left(\sum_{\{m\}_d} \frac{\mathrm{e}^{\mathrm{i}2\pi(m_1x_1+m_2x_2+\cdots+m_dx_d)}}{\{m_1^2+m_2^2+\cdots+m_d^2+\beta^2/4\pi^2\}} - \frac{4\pi^2}{\beta^2}\right), \tag{2.3}$$

where β is an infinitesimal parameter which tends to zero. Here, the set $\{m_{1,d}\}$ denotes a set of d integers $\{m_1, m_2, \ldots, m_d\}$. Each one of these integers m_i runs over $-\infty$ to $+\infty$. Also, $x_1, x_2, \ldots, x_d$ denote the components of vector $\boldsymbol{r}_d$ in d dimensions. Due to the periodic boundary conditions, it is sufficient to treat the case where each x_i satisfies $-0.5 < x \leqslant 0.5$. The complete expression for the potential has a term arising from the surface contribution. For the 2D case this term turns out to be zero, but for 3D one obtains a contribution from a dipole term [9]. At this point, we would recast equation (2.3) in an alternative form. For that, we use the fact that the solution of

$$(\nabla^2 - \beta^2)Q_0(\boldsymbol{r};\beta) = -\delta(\boldsymbol{r}) \tag{2.4}$$

in d-dimensional space is given by

$$Q_0(\boldsymbol{r};\beta) = \frac{1}{(2\pi)^{\nu+1}}\frac{\beta^\nu K_\nu(\beta|\boldsymbol{r}|)}{r^\nu}. \tag{2.5}$$

Thus, the solution of

$$(\nabla^2 - \beta^2)Q_d(\boldsymbol{r};\beta) = -C_d\sum_{\boldsymbol{l}}\delta(\boldsymbol{r}+\boldsymbol{l}) \tag{2.6}$$

in d-dimensional space will be given by

$$Q_d(\boldsymbol{r};\beta) = \frac{C_d}{(2\pi)^{\nu+1}}\sum_{\{m_{1,d}\}}\left[\beta^\nu\frac{K_\nu(\beta r_{1,d})}{r_{1,d}^\nu}\right], \tag{2.7}$$

where

$$r_{1,d} = \left[\sum_{i=1}^{d}(m_i-x_i)^2\right]^{1/2}. \tag{2.8}$$

On the other hand, the solution of equation (2.4) can be written down in the Fourier space easily as

$$Q_d(\boldsymbol{r};\beta) = \frac{C_d}{(2\pi)^2}\sum_{\{m\}_d}\frac{\mathrm{e}^{\mathrm{i}2\pi(m_1x_1+m_2x_2+\cdots+m_dx_d)}}{\{m_1^2+m_2^2+\cdots+m_d^2+\beta^2/4\pi^2\}}. \tag{2.9}$$

Using equations (2.3) and (2.7) we see that one can write

$$G_d(x_1, x_2, \ldots, x_d) = C_d\lim_{\beta\to 0}\left(\frac{1}{(2\pi)^{\nu+1}}\sum_{\{m_{1,d}\}}\left[\beta^\nu\frac{K_\nu(\beta r_{1,d})}{r_{1,d}^\nu}\right] - \frac{1}{\beta^2}\right). \tag{2.10}$$

Yet another alternative form of G_d can be obtained as follows. We can perform one of the d sums in equation (2.3) analytically using the formula [8]

$$\sum_{m=-\infty}^{\infty}\frac{\exp(2\pi\mathrm{i}mx)}{m^2+\gamma^2} = \frac{\pi}{\gamma}\frac{\cosh[\pi\gamma(1-2|x|)]}{\sinh(\pi\gamma)}. \tag{2.11}$$

Thus, we obtain

$$G_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \lim_{\beta \to 0} \left(\sum_{\{m_{2,d}\}} \frac{\pi}{\gamma_{\{m_{2,d}\}}} \frac{\cosh[\pi \gamma_{\{m_{2,d}\}}(1 - 2|x_1|)]}{\sinh(\pi \gamma_{\{m_{2,d}\}})} \right.$$
$$\left. \times \exp\left[2\pi \mathrm{i} \sum_{i=2}^{d} m_i x_i\right] - \frac{1}{\beta^2} \right), \tag{2.12}$$

where $\gamma_{\{m_{2,d}\}}$ is defined as

$$\gamma_{\{m_{2,d}\}} = \left(\sum_{i=2}^{d} m_i^2 + \beta^2 \right)^{1/2}. \tag{2.13}$$

For the purpose of taking the limit $\beta \to 0$, the sum in the first part of equation (2.12) is broken as

$$\sum_{\{m_{2,d}\}} = \sum_{\{m_{2,d}\}}{}' + (\text{Term with } m_2 = 0, m_3 = 0, \ldots, m_d = 0), \tag{2.14}$$

where a prime over the summation sign indicates that the term corresponding to all m_i being zero is to be excluded from the summation. This leads to the following representation for G_d:

$$G_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \sum_{\{m_{2,d}\}}{}' \frac{\pi}{\gamma_{\{m_{2,d}\}}} \frac{\cosh\left[\pi \gamma_{\{m_{2,d}\}}(1 - 2|x_1|)\right]}{\sinh\left(\pi \gamma_{\{m_{2,d}\}}\right)}$$
$$\times \exp\left(2\pi \mathrm{i} \sum_{i=2}^{d} m_i x_i\right) + H_d(x_1, x_2, \ldots, x_d), \tag{2.15}$$

where we have taken the limit $\beta \to 0$, i.e. we have substituted $\beta = 0$ in the first part, and H_d is given by

$$H_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \lim_{\beta \to 0} \left(\frac{2\pi^2}{\beta} \frac{\cosh\left[(1/2 - |x_1|)\beta\right]}{\sinh(\beta/2)} - \frac{4\pi^2}{\beta^2} \right)$$
$$= C_d \frac{1}{12}\left(1 - 6|x_1| + 6x_1^2\right). \tag{2.16}$$

To avoid the bad convergence towards $x_1 \to 0$, we further modify the summation in the first part of equation (2.15) by using the following trigonometric identity

$$\frac{\cosh(a - b)}{\sinh(b)} = \exp(-b)\frac{\cosh(a)}{\sinh(b)} + \exp(-a). \tag{2.17}$$

Thus, G_d can be written as

$$G_d = H_d + J_d + M_d, \tag{2.18}$$

where H_d is defined in equation (2.16), J_d is given by

$$J_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \sum_{\{m_{2,d}\}}{}' \frac{\pi}{\gamma_{\{m_{2,d}\}}} \exp\left(-\pi \gamma_{\{m_{2,d}\}}\right)$$
$$\times \frac{\cosh\left[\pi \gamma_{\{m_{2,d}\}}(1 - 2|x_1|)\right]}{\sinh\left(\pi \gamma_{\{m_{2,d}\}}\right)} \exp\left(2\pi \mathrm{i} \sum_{i=2}^{d} m_i x_i\right) \tag{2.19}$$

and

$$M_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{(2\pi)^2} \sum_{\{m_{2,d}\}}' \frac{\pi}{\gamma_{\{m_{2,d}\}}} \exp\left[-2|x_1|\pi\gamma_{\{m_{2,d}\}}\right] \exp\left(2\pi\mathrm{i}\sum_{i=2}^{d} m_i x_i\right). \qquad (2.20)$$

In equations (2.19) and (2.20) β is to be set equal to zero. It is easy to see that equation (2.19) does not have any convergence problem as x_1 tends to zero. Thus, the whole problem has reduced to evaluating the M_d term efficiently. This will be done in the next section.

3. Recursive formulae

In this section we obtain recursive formulae for G_d in two different ways, starting with the expressions in equations (2.10) and (2.18) respectively. The first method, with equation (2.10) as the starting point, will contain Lekner's results for $d = 3$ as a special case, while the second method will contain Sperb's result in 3D as a special case. With the help of equations (2.10) and (2.3) we can write

$$\begin{aligned} G_d(x_1, x_2, \ldots, x_d) &= \frac{C_d}{(2\pi)^2} \lim_{\beta\to 0}\left(Q_d(x_1, x_2, \ldots, x_d; \beta) - \frac{1}{\beta^2}\right) \\ &= \frac{C_d}{(2\pi)^2} \lim_{\beta\to 0}\left(\sum_{\{m_{1,d}\}} \exp(2\pi\mathrm{i}m_1 x) \times \frac{\exp\left(2\pi\mathrm{i}\sum_{i=2}^{d} m_i x_i\right)}{\sum_{i=2}^{d} m_i^2 + \left[\beta^2 + m_1^2\right]} - \frac{1}{\beta^2}\right). \end{aligned} \qquad (3.1)$$

Using the definition of G_d, equation (3.1) can be written as

$$\begin{aligned} G_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{C_{d-1}} \lim_{\beta\to 0}\Bigg[&\sum_{m_1} \exp(2\pi\mathrm{i}m_1 x_1) \\ &\times Q_{d-1}\left(x_2, \ldots, x_d; \sqrt{\beta^2 + (2\pi m_1)^2}\right) - \frac{C_{d-1}}{\beta^2}\Bigg]. \end{aligned} \qquad (3.2)$$

We separate out the term corresponding to $m_1 = 0$ in equation (3.2) so that the limit corresponding to β can be taken. Thus, we write equation (3.1) as

$$\begin{aligned} G_d(x_1, x_2, \ldots, x_d) &= 2\frac{C_d}{C_{d-1}} \sum_{m_1=1}^{\infty} \cos(2\pi m_1 x_1) Q_{d-1}(x_2, x_3, \ldots, x_d; 2\pi m_1) \\ &\quad + \frac{C_d}{C_{d-1}} \lim_{\beta\to 0}\left[Q_{d-1}(x_2, x_3, \ldots, x_d; \beta) - \frac{C_{d-1}}{\beta^2}\right] \\ &= 2\frac{C_d}{C_{d-1}} \sum_{m_1=1}^{\infty} \cos(2\pi m_1 x_1) Q_{d-1}(x_2, x_3, \ldots, x_d; 2\pi m_1) \\ &\quad + \frac{C_d}{C_{d-1}} G_{d-1}(x_2, x_3, \ldots, x_d), \end{aligned} \qquad (3.3)$$

where we have taken the limit $\beta \to 0$ in the first term. Equation (3.3) is one of the most important results of this paper. This relates a d-dimensional sum to a $(d-1)$-dimensional sum. This is a recursive relation. If one is able to obtain the Green function for the $(d-1)$-dimensional space, one can obtain the Green function for the d-dimensional space. The first term in equation (3.3) can be modified in the following way. We can use a form of G_{d-1}

similar to the one used in equation (2.7) to obtain

$$G_d(x_1, x_2, \ldots, x_d) = 2\frac{C_d}{(2\pi)^{\nu+1/2}} \sum_{m_1=1}^{\infty} \sum_{\{m_{2,d}\}} \cos(2\pi m_1 x_1) \times (2\pi m_1)^{\nu-1/2} \frac{K_{\nu-1/2}(2\pi m_1 r_{2,d})}{r_{2,d}^{\nu-1/2}} + \frac{C_d}{C_{d-1}} G_{d-1}(x_2, x_3, \ldots, x_d), \tag{3.4}$$

where $\{m_{2,d}\}$ denotes a sum over sets $\{m_2, m_3, \ldots, m_d\}$ and $r_{2,d}$ is defined like equation (2.8)

$$r_{2,d} = \left[\sum_{i=2}^{d} (m_i - x_i)^2\right]^{1/2}. \tag{3.5}$$

Let us now consider three different cases corresponding to $d = 1$, $d = 2$ and $d > 2$. For $d = 1$ we can evaluate $G_{d=1}$ in closed form:

$$\begin{aligned} G_1(x_1) &= \frac{C_1}{(2\pi)^2} \lim_{\beta\to 0} \left(\sum_{m_1} \frac{\exp(2\pi \mathrm{i} m_1 x_1)}{\beta^2 + m_1^2} - \frac{1}{\beta^2} \right) \\ &= \frac{C_1}{(2\pi)^2} \lim_{\beta\to 0} \left(\frac{\pi}{\beta} \frac{\cosh[\pi\beta(1 - 2|x_1|)]}{\sinh[\pi\beta]} - \frac{1}{\beta^2} \right) \\ &= C_1 \frac{1}{12}\left(1 - 6|x_1| + 6x_1^2\right). \end{aligned} \tag{3.6}$$

Also, the self-energy for this case may be obtained as

$$G_1^{\mathrm{self}} = \lim_{x_1\to 0} G_1 + |x_1| = \frac{C_1}{12}. \tag{3.7}$$

For $d = 2$, we obtain using equation (2.10):

$$G_2(x_1, x_2) = 2\frac{C_2}{(2\pi)^{1/2}} \sum_{m_1=1}^{\infty} \sum_{m_2=-\infty}^{\infty} \cos(2\pi m_1 x_1)(2\pi m_1)^{-1/2} \times \frac{K_{-1/2}\,(2\pi m_1 |x_2 + m_2|)}{|x_2 + m_2|^{-1/2}} + \frac{C_2}{C_1} G_1(x_2). \tag{3.8}$$

Now, using the relation [8]

$$K_{-1/2}(r) = \sqrt{\frac{\pi}{2r}} \exp(-r), \tag{3.9}$$

we can write

$$G_2(x_1, x_2) = \frac{C_2}{2\pi} \sum_{m_2=-\infty}^{\infty} \sum_{m_1=1}^{\infty} \frac{\cos(2\pi m_1 x_1)}{|m_1|} \exp(-2\pi m_1 |x_2 + m_2|) + \frac{C_2}{C_1} G_1(x_2). \tag{3.10}$$

The sum over m_1 can be easily carried out using the identity [7]

$$\begin{aligned} L(x_1, x_2) &= \sum_{m_1=1}^{\infty} \frac{\cos(2\pi m_1 x_1)}{m_1} \exp(-2\pi m_1 |x_2|) \\ &= -\frac{1}{2} \ln(1 - 2\,\exp[-2\pi x_2] \cos[2\pi x_1] + \exp[-4\pi x_2]). \end{aligned} \tag{3.11}$$

Thus, G_2 can be written as

$$G_2(x_1, x_2) = \frac{C_2}{2\pi} \sum_{m_2=1}^{\infty} L(x_1, |x_2 + m_2|) + L(x_1, |x_2 - m_2|) + L(x_1, x_2) + \frac{C_2}{C_1} G_1(x_2). \tag{3.12}$$

It is also trivial to derive

$$G_2^{\text{self}} = 2\frac{C_2}{2\pi}\sum_{m_2=1}^{\infty} L(0,|m_2|) - \ln 2\pi + \frac{C_2}{12}. \tag{3.13}$$

Now we consider the case for $d > 2$. We can obtain G_d from equation (3.4). It is seen that for large arguments the modified Bessel functions decay as

$$K_\nu(r) \sim \sqrt{\frac{\pi}{2r}}\exp(-r). \tag{3.14}$$

As a result, the first term in equation (3.4) decays exponentially. However, one may run into a problem if $r_{2,d}$ is very small. In such a case the terms corresponding to $\{m_{2,d}\}$ all being zero form a very slowly converging series over m_1. This problem of slow convergence when $r_{2,d}$ is small can be handled in the following recursive manner. We separate out the particular terms corresponding to $\{m_{2,d}\}$ all being zero, and define

$$\begin{aligned} E_d(x_1,x_2,\ldots,x_d) &= 2\frac{C_d}{(2\pi)^{\nu+1/2}}\sum_{m_1=1}^{\infty}\sum_{\{m_{2,d}\}}\cos(2\pi m_1x_1)(2\pi m_1)^{\nu-1/2}\frac{K_{\nu-1/2}(2\pi m_1 r_{2,d})}{r_{2,d}^{\nu-1/2}} \\ &= 2\frac{C_d}{(2\pi)^{\nu+1/2}}\sum_{m_1=1}^{\infty}\sum_{\{m_{2,d}\}}{}^{'}\cos(2\pi m_1x_1)(2\pi m_1)^{\nu-1/2}\frac{K_{\nu-1/2}(2\pi m_1 r_{2,d})}{r_{2,d}^{\nu-1/2}} \\ &\quad + 2\frac{C_d}{(2\pi)^{\nu+1/2}}\sum_{m_1=1}^{\infty}\cos(2\pi m_1x_1)(2\pi m_1)^{\nu-1/2}\frac{K_{\nu-1/2}(2\pi m_1 r)}{r_\perp^{\nu-1/2}}, \end{aligned} \tag{3.15}$$

where

$$r_\perp^2 = \sum_{i=2}^{d} x_i^2. \tag{3.16}$$

Now, we show how to handle the evaluation of E_d corresponding to $d > 3$. The case for $d = 3$ will be almost the same. Using the relation [8] (which by the way can be derived from equation (3.1))

$$\begin{aligned} \sum_{k=-\infty}^{\infty}\frac{1}{[(x+k)^2+r^2]^{\frac{1}{2}+\nu}} &= \frac{\sqrt{\pi}}{\Gamma\left(\nu+\frac{1}{2}\right)}\left\{\frac{\Gamma(\nu)}{r^{2\nu}} + 4\left(\frac{\pi}{r}\right)^{\nu}\right. \\ &\quad \times \left.\sum_{l=1}^{\infty} l^\nu K_\nu(2\pi l r)\cos(2\pi l x)\right\}, \qquad \nu > 0, \end{aligned} \tag{3.17}$$

we can write

$$\begin{aligned} E_d(x_1,x_2,\ldots,x_d) &= 2\frac{C_d}{(2\pi)^{\nu+1/2}}\sum_{m_1=1}^{\infty}\sum_{\{m_{2,d}\}}{}^{'}\cos(2\pi m_1x_1)\left[(2\pi m_1)^{\nu-1/2}\frac{K_{\nu-1/2}(2\pi m_1 r_{2,d})}{r_{2,d}^{\nu-1/2}}\right] \\ &\quad + \sum_{k=-\infty}^{\infty}\frac{1}{\left[(x_1+k)^2+r_\perp^2\right]^\nu} - \frac{\sqrt{\pi}}{\Gamma(\nu)}\frac{\Gamma(\nu-1/2)}{r_\perp^{2\nu-1}}. \end{aligned} \tag{3.18}$$

Also, the sum over k in equation (3.18) can be written as

$$\begin{aligned} \sum_{k=-\infty}^{\infty}\frac{1}{[(x+k)^2+r^2]^\nu} &= \frac{1}{(x^2+r^2)^\nu} + \sum_{k=1}^{N-1}\left(\frac{1}{[(x+k)^2+r^2]^\nu} + \frac{1}{[(x-k)^2+r^2]^\nu}\right) \\ &\quad + \sum_{l=1}^{\infty}\binom{-\nu}{l} r^{2l}[\zeta(2l+2\nu,N+x)+\zeta(2l+2\nu,N-x)], \end{aligned} \tag{3.19}$$

where N is an arbitrary integer [7] such that $N > r + |x|$. Using equations (3.4), (3.18) and (3.19) we can now write

$$
\begin{aligned}
G_d(x_1, x_2, \ldots, x_d) - \frac{1}{\left(x_1^2 + r_\perp^2\right)^{\nu+1/2}} &= 2\frac{C_d}{(2\pi)^{\nu+1/2}} \sum_{m_1=1}^{\infty} {\sum_{\{m_{2,d}\}}}' \cos(2\pi m_1 x_1) \\
&\quad \times (2\pi m_1)^{\nu-1/2} \frac{K_{\nu-1/2}(2\pi m_1 r_{2,d})}{r_{2,d}^{\nu-1/2}} \\
&\quad + \sum_{k=1}^{N-1} \left(\frac{1}{\left[(x_1+k)^2 + r_\perp^2\right]^\nu} + \frac{1}{\left[(x_1-k)^2 + r_\perp^2\right]^\nu} \right) \\
&\quad + \sum_{l=1}^{\infty} \binom{-\nu}{l} r_\perp^{2l} [\zeta(2l+2\nu, N+x_1) + \zeta(2l+2\nu, N-x_1)] \\
&\quad + \frac{C_d}{C_{d-1}} \left(G_d(x_2, \ldots, x_d) - \frac{1}{r_\perp^{2\nu}} \right).
\end{aligned}
\tag{3.20}
$$

Note that if $d = 3$ then instead of equation (3.19) we should use

$$
\begin{aligned}
4\sum_{m_1=1}^{\infty} K_0\left(2\pi m_1 \left(x_2^2 + x_3^2\right)^{1/2}\right) \cos(2\pi m_1 x_1) &= 2\left\{\gamma + \ln\left(\frac{\left(x_2^2 + x_3^2\right)^{1/2}}{2}\right)\right\} \\
&\quad + \frac{1}{\sqrt{x_1^2 + x_2^2 + x_3^2}} + S(x_1, x_2, x_3),
\end{aligned}
\tag{3.21}
$$

where

$$
\begin{aligned}
S(x_1, x_2, x_3) &= \sum_{n=1}^{N-1} \left(\frac{1}{\sqrt{x_2^2 + x_3^2 + (n+x_1)^2}} + \frac{1}{\sqrt{x_2^2 + x_3^2 + (n-x_1)^2}} \right) \\
&\quad + \frac{1}{\sqrt{x_1^2 + x_2^2 + x_3^2}} - 2\gamma - [\psi(N+x_1) + \psi(N-x_1)] \\
&\quad + \sum_{l=1}^{\infty} \binom{-1/2}{l} \left(x_2^2 + x_3^2\right)^l [\zeta(2l+1, N+x) + \zeta(2l+1, N-x)].
\end{aligned}
\tag{3.22}
$$

Thus, for the 3D case one would make the following two changes in the expression given in equation (3.20). First, there would be an extra term containing $-2\gamma - [\psi(N + x_1) + \psi(N - x_1)]$ on the right-hand side, and second the last term in equation (3.20) would be changed to

$$
\frac{C_d}{C_{d-1}}[G_{d-1}(x_2, x_3) + \ln r_\perp]. \tag{3.23}
$$

Equation (3.20) provides us with a general algorithm to calculate G_d efficiently in any dimensions. For example, if we had started out with $d = 10$, we can obtain $G_{10} - r_8^{-8}$ by calculating $G_9 - r_7^{-7}$. Continuing in this fashion we will come down to calculating $G_2 + \ln r_2$. Now, this last part $G_2 + \ln r_2$ has been obtained by several authors. In fact, it can be obtained in a closed form [5]. Thus, we have been able to calculate $G_{10} - r_8^{-8}$ from which we can obtain G_{10} by taking the radial part r_8^{-8} on the other side. Other forms of G_2 are given by Gronbech-Jensen [11] and Tyagi [7]. For the sake of completeness we write down the result for G_2:

$$G_2(x_1, x_2) = \frac{1}{2\pi} \sum_m{}' \frac{\pi}{|m|} \frac{\exp(-\pi|m|)\cosh[2\pi m x_1]}{\sinh(\pi|m|)} \cos(2\pi m x_2) - \frac{1}{2} \ln[\cosh(2\pi x_1) \\ - \cos(2\pi x_2)] + \frac{\pi}{6}\left(1 + 6x_2^2\right) - \frac{\ln(2)}{2}. \tag{3.24}$$

In closed form G_2 is written as [10]

$$G_2(x_1, x_2) = 2\pi \left(\frac{x_2^2}{2} - \frac{\ln 2}{6\pi} + \frac{1}{2\pi} \ln \left| \frac{\vartheta_1[\pi(x_1 + \mathrm{i}x_2), \exp(-\pi)]}{\vartheta_1'[0, \exp(-\pi)]^{1/3}} \right| \right), \tag{3.25}$$

where ϑ_1 represents the Jacobi theta function of the first kind. Also, the self-energy for the 2D case can be obtained from equation (3.24)

$$G_2^{\text{self}} = \frac{1}{\pi} \sum_{m=1}^{\infty} \frac{\pi}{|m|} \frac{\exp(-\pi|m|)}{\sinh(\pi|m|)} - \ln(2\pi) + \frac{\pi}{6}, \tag{3.26}$$

or it can be obtained from equation (3.25):

$$G_2^{\text{self}} = -\frac{\ln 2}{3} - \ln\pi - \frac{2}{3}\ln|[\vartheta_1'(0, q)]|. \tag{3.27}$$

All three forms equations (3.13), (3.26) and (3.27) are equivalent and give numerically the same value for the self-energy. Similarly equations (3.12), (3.24) and (3.25) show perfect agreement.

Now, we give another alternative approach for the evaluation of G_d. This time we start with equation (2.18), where H_d, J_d and M_d are defined in equations (2.16), (2.19) and (2.20). H_d and J_d do not have any convergence problem in the region of interest. We show how to handle M_d. A recursion formula similar to equation (3.4) can be established for M_d. It is easy to see just by inspection that M_d obeys the following recursion formula:

$$M_d(x_1, x_2, \ldots, x_d) = \frac{C_d}{C_{d-1}} M_{d-1}(x_1, x_3, \ldots, x_d) \\ + 2\frac{C_d}{(2\pi)^{\nu+1/2}} \sum_{m_2=1}^{\infty} \cos(2\pi m_2 x_2)(2\pi m_2)^{\nu-1/2} \\ \times \sum_{\{m_{3,d}\}} \frac{K_{\nu-1/2}\left(2\pi m_2 \sqrt{x_1^2 + (m_3 - x_3)^2 + \cdots + (m_d - x_d)^2}\right)}{\left[\sqrt{x_1^2 + (m_3 - x_3)^2 + \cdots + (m_d - x_d)^2}\right]^{\nu-1/2}}, \tag{3.28}$$

where M_{d-1}, analogous to equation (2.20), stands for

$$M_{d-1}(x_1, x_3, \ldots, x_d) = \frac{C_{d-1}}{(2\pi)^2} \sum_{\{m_{3,d}\}}{}' \frac{\pi}{\gamma_{\{m_{3,d}\}}} \exp[-2|x_1|\pi\gamma_{\{m_{3,d}\}}] \exp\left(2\pi\mathrm{i}\sum_{i=3}^{d} m_i x_i\right). \tag{3.29}$$

In the final step, we break the sum in the second part of equation (3.28) as follows

$$\sum_{\{m_{3,d}\}} = \sum_{\{m_{3,d}\}}{}' + \sum_{m_3=0, m_4=0, \ldots,}, \tag{3.30}$$

The term corresponding to $m_3 = 0, m_4 = 0\ldots$ gives rise to a term F_d in equation (3.28):

$$
\begin{aligned}
F_d(x_1, x_2, \ldots, x_d) &= 2\frac{C_d}{(2\pi)^{\nu+1/2}} \sum_{m_2=1}^{\infty} \cos(2\pi m_2 x_2)(2\pi m_2)^{\nu-1/2} \\
&\quad \times \frac{K_{\nu-1/2}\left(2\pi m_2\sqrt{x_1^2 + x_3^2 + \cdots + x_d^2}\right)}{\left[\sqrt{x_1^2 + x_3^2 + \cdots + x_d^2}\right]^{\nu-1/2}} \\
&= \frac{1}{\sqrt{x_1^2 + x_2^2 + \cdots + x_d^2}} - \frac{C_d}{C_{d-1}} \frac{1}{\sqrt{x_1^2 + x_3^2 + \cdots + x_d^2}} \\
&\quad + \sum_{k=1}^{N-1} \left(\frac{1}{\left[(x_2+k)^2 + r_2^2\right]^{\nu}} + \frac{1}{\left[(x_2-k)^2 + r_2^2\right]^{\nu}} \right) \\
&\quad + \sum_{l=1}^{\infty} \binom{-\nu}{l} r_2^{2l} [\zeta(2l + 2\nu, N + x_2) + \zeta(2l + 2\nu, N - x_2)],
\end{aligned}
\tag{3.31}
$$

where

$$
r_2^2 = x_1^2 + x_3^2 + \cdots + x_d^2. \tag{3.32}
$$

Thus, we finally obtain the following recursion relationship for M_d:

$$
\begin{aligned}
\left(M_d - \frac{1}{\left(x_1^2 + x_2^2 + \cdots + x_d^2\right)^{\nu+1/2}} \right) &= \frac{C_d}{C_{d-1}} \left(M_{d-1} - \frac{1}{\left(x_1^2 + x_3^2 + \cdots + x_d^2\right)^{\nu}} \right) \\
&\quad + 2\frac{C_d}{(2\pi)^{\nu+1/2}} \sum_{m_2=1}^{\infty} \cos(2\pi m_2 x_2)(2\pi m_2)^{\nu-1/2} \\
&\quad \times \sum_{\{m_{3,d}\}}{}' \frac{K_{\nu-1/2}\left(2\pi m_2\sqrt{x_1^2 + (m_3 - x_3)^2 + \cdots + (m_d - x_d)^2}\right)}{\left[\sqrt{x_1^2 + (m_3 - x_3)^2 + \cdots + (m_d - x_d)^2}\right]^{\nu-1/2}} \\
&\quad + \sum_{k=1}^{N-1} \left(\frac{1}{\left[(x_2+k)^2 + r_2^2\right]^{\nu}} + \frac{1}{\left[(x_2-k)^2 + r_2^2\right]^{\nu}} \right) \\
&\quad + \sum_{l=1}^{\infty} \binom{-\nu}{l} r_2^{2l} [\zeta(2l + 2\nu, N + x_2) + \zeta(2l + 2\nu, N - x_2)].
\end{aligned}
\tag{3.33}
$$

For $d = 3$, once again, we will have to make two modifications in equation (3.33). With this approach we have obtained equation (3.33), which is analogous to equation (3.20). However, the analysis has become a little bit tedious. The advantage of the second method is that it reduces the computation time, as there is one less summation. The second advantage is that it can be written down in a product decomposition form. For an example how such a product decomposition form may be written, one may consult Sperb [4], where a special case corresponding to $d = 3$ is considered. In general, the procedure of dimensional reduction is to be continued until we have M_1 on the left-hand side. It is clear that $M_1 = 0$. Let us again consider three special cases. For $d = 1$ one only has $H_{d=1}$ and thus $G_1 = H_1$. For $d = 2$ one obtains

$$
J_2(x_1, x_2) = \frac{C_2}{(2\pi)^2} \sum_{m_2}{}' \frac{\pi}{\gamma_{m_2}} \exp\left(-\pi\gamma_{m_2}\right) \frac{\cosh\left[\pi\gamma_{m_2}(1 - 2|x_1|)\right]}{\sinh\left(\pi\gamma_{m_2}\right)} \exp(2\pi \mathrm{i} m_2 x_2), \tag{3.34}
$$

and M_2 from equations (2.20) and (3.11) turns out to be related to L:

$$M_2(x_1, x_2) = L(x_2, x_1). \tag{3.35}$$

Combining H_2, J_2 and M_2 we obtain the form of G_2 given in equation (3.24). Considering finally the case for $d > 2$, we can obtain G_d again from equation (2.18). Now K_d and H_d are convergent and M_d can be obtained using the recursive relation (3.33). For example:

$$\begin{aligned}
\left(M_3 - \frac{1}{\left(x_1^2+x_2^2+x_3^2\right)^{1/2}}\right) &= \frac{C_2}{C_1}\left[M_2(x_1,x_3) + \ln\left(\sqrt{x_1^2+x_3^2}\right)\right] \\
&\quad + 2\frac{C_2}{(2\pi)^{1/2}}\sum_{m_2=1}^{\infty}\cos(2\pi m_2 x_2)\sum_{m_3}{}' K_0\left(2\pi m_2\sqrt{x_1^2+(m_3-x_3)^2}\right) \\
&\quad + \sum_{k=1}^{N-1}\left(\frac{1}{\left[(x_2+k)^2+x_1^2+x_3^2\right]^{1/2}} + \frac{1}{\left[(x_2-k)^2+x_1^2+x_3^2\right]^{1/2}}\right) \\
&\quad - 2\gamma - \left[\psi(N+x_2)+\psi(N-x_2)\right] + \sum_{l=1}^{\infty}\binom{-\nu}{l}\left(x_1^2+x_3^2\right)^l \\
&\quad \times \left[\zeta(2l+2\nu, N+x_2) + \zeta(2l+2\nu, N-x_2)\right],
\end{aligned} \tag{3.36}$$

where M_2 has already been evaluated in equations (3.11) and (3.35) in terms of L_2. We see that in all cases, the expression could be written in a form such that the essential Coulomb singularity as the two charges approach each other has been isolated.

4. Conclusions

Using the limiting behaviour of the modified Bessel functions, we showed how conditionally convergent Coulomb sums may be handled in an elegant way. We gave two representations of the Green function for the Poisson equation in any integer-dimensional space. A recursive method was derived that can be applied for wholly periodic cases, as well as for those cases where one may have open boundary conditions along one of the directions. The method may be extended to cover the case where any number of directions may be open. The formulae obtained show rapid convergence in all parts of the simulation cell. This method is general enough that it can be easily generalized for a higher-dimensional 'triclinic' cell. A particular case of the application of this method for a triclinic cell can be seen in a recent paper [12]. We have shown that the present work generalizes the work of several authors on periodic and partial periodic systems [3, 4, 13]. To our knowledge, this treatment is the first of its kind ever taken in a dimension higher than $d = 3$.

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References

[1] Tyagi S and Goldschmidt Y Y 2004 *Phys. Rev.* B **70** 024501
[2] Ewald P P 1920 Die Berechnung optischer und elektrostatischer Gitterpotentiale *Ann. Phys., Lpz.* **64** 253–87
[3] Lekner J 1989 *Physica* A **157** 826
Lekner J 1991 *Physica* A **176** 485

[4] Sperb R 1994 *Mol. Simul.* **13** 189
Sperb R 1998 *Mol. Simul.* **20** 179
[5] Glasser M L and Zucker I J 1980 *Theoretical Chemistry, Advances and Perspectives* vol 5 (New York: Academic) pp 67–139
[6] Marshall S L 2000 *J. Phys.: Condens. Matter* **12** 4575
[7] Tyagi S 2004 *Phys. Rev.* E **70** 066703
[8] Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series and Products* (New York: Academic)
[9] De Leeuw S W, Perram J W and Smith E R 1980 *Proc. R. Soc.* A **373** 27–56
[10] Glasser M L 1974 *J. Math. Phys.* **15** 188
[11] Gronbech-Jensen N 1999 *Comput. Phys. Commun.* **119** 115
[12] Tyagi S 2005 *J. Chem. Phys.* **122** 014101
[13] Mazars M 2005 *Mol. Phys.* **103** 675