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Short Communication

Electrostatic potential of a homogeneously charged square and cube in two and three dimensions

Gerhard Hummer*

Theoretical Biology and Biophysics Group (T-10) and Center for Nonlinear Studies (CNLS), MS K710, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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Abstract

A closed form of the electrostatic potential of a homogeneously charged cube is derived by integration. The exact result is compared with multipole expansions for the exterior and interior of the cube. The electrostatic potential of a homogeneously charged square in two-dimensional electrostatics is also determined.

Keywords: Electrostatic potential; Ionic systems; Wigner lattice; Homogeneously charged cube; "Kubic" harmonics

1. Introduction

The electrostatic potential of a homogeneously charged cube appears in theoretical studies of Wigner lattices [1]. In computer simulations of ionic systems using minimum-image electrostatics, it determines the electrostatic self-interaction of ions [2–6]. Hummer et al. [5] presented a simple calculation of the electrostatic potential at the center of a homogeneously charged cube. In this work, a closed form of the electrostatic potential will be determined for arbitrary positions. This analytic form can be used for the evaluation of lattice sums. It can also be applied as a correction when electrostatic potentials are calculated on a grid, assuming that the grid volumes are uniformly charged rather than carrying a point charge at the center. The analytic form of the potential will be compared with multipole expansions [1, 7].

* E-mail: hummer@t10.lanl.gov. Tel.: 1-505-665-1923; Fax: 1-505-665-3493

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2. Calculation of the electrostatic potential of a cube

The electrostatic potential ϕ_c of a cube $[-\frac{1}{2}, \frac{1}{2}]^3$ with charge density one will be calculated by integration. The potential at a point with Cartesian coordinates (u, v, w) can be written as

$$\phi_c(u,v,w) = \int_{-1/2}^{1/2} dx \int_{-1/2}^{1/2} dy \int_{-1/2}^{1/2} dz \left[(x-u)^2 + (y-v)^2 + (z-w)^2\right]^{-1/2} , \quad (1)$$

where Gaussian units are used. ϕ_c can be rewritten as

$$\int_{-1/2-u}^{1/2-u} dx \int_{-1/2-v}^{1/2-v} dy \int_{-1/2-w}^{1/2-w} dz \left(x^2 + y^2 + z^2\right)^{-1/2} . \quad (2)$$

Summation of the results of partial integration with respect to x, y, and z yields a reduction to three two-dimensional integrals,

$$\begin{aligned} 2\phi_c(u,v,w) = & \int_{-1/2-u}^{1/2-u} dx \int_{-1/2-v}^{1/2-v} dy \left[z\left(x^2 + y^2 + z^2\right)^{-1/2}\right]_{z=-1/2-w}^{z=1/2-w} \\ & + \text{cyclic permutations } (x,u;y,v;z,w) \to (y,v;z,w;x,u) \\ & \text{and } (z,w;x,u;y,v). \end{aligned} \quad (3)$$

The two-dimensional integrals can be further reduced using

$$\int_{x_0}^{x_1} dx \int_{y_0}^{y_1} dy \left(x^2 + y^2 + z^2\right)^{-1/2} = \int_{x_0}^{x_1} dx \frac{1}{2}\left[\ln \frac{(x^2 + y^2 + z^2)^{1/2} + y}{(x^2 + y^2 + z^2)^{1/2} - y}\right]_{y_0}^{y_1} , \quad (4)$$

where x_0, x_1, y_0, and y_1 are arbitrary integral boundaries. The remaining one-dimensional integrals can be calculated using partial integration and conventional substitution for algebraic integrands,

$$\begin{aligned} \int dx \ln[(x^2 + a^2)^{1/2} + b] = & x \ln[(x^2 + a^2)^{1/2} + b] - x \\ & + 2|a^2 - b^2|^{1/2} A\left[\frac{x + (x^2 + a^2)^{1/2} + b}{|a^2 - b^2|^{1/2}}\right] \\ & + b \ln[x + (x^2 + a^2)^{1/2}], \end{aligned} \quad (5)$$

where

$$A(x) = \begin{cases} \arctan(x) & \text{for } a^2 > b^2, \\ \operatorname{artanh}(x) & \text{for } a^2 < b^2 . \end{cases} \quad (6)$$

Combining the previous results yields a closed form for the electrostatic potential of a unit cube:

$$\phi_c(u,v,w) = \frac{1}{2}\left\{ \frac{1}{2} \sum_{i=0}^{1} \sum_{j=0}^{1} \sum_{l=0}^{2} (-1)^{i+j} c_{i,l} c_{j,l+1} \right.$$

$$\times \ln \frac{\left[\left(c_{i,l}^2 + c_{j,l+1}^2 + c_{1,l+2}^2\right)^{1/2} + c_{1,l+2}\right]^3 \left[\left(c_{i,l}^2 + c_{j,l+1}^2 + c_{0,l+2}^2\right)^{1/2} - c_{0,l+2}\right]}{\left[\left(c_{i,l}^2 + c_{j,l+1}^2 + c_{1,l+2}^2\right)^{1/2} - c_{1,l+2}\right] \left[\left(c_{i,l}^2 + c_{j,l+1}^2 + c_{0,l+2}^2\right)^{1/2} + c_{0,l+2}\right]^3}$$

$$+ \sum_{i=0}^{1} \sum_{j=0}^{1} \sum_{k=0}^{1} \sum_{l=0}^{2} (-1)^{i+j+k+1} c_{i,l}^2$$

$$\times \arctan \frac{c_{i,l}\, c_{k,l+2}}{c_{i,l}^2 + c_{j,l+1}^2 + c_{j,l+1}\left(c_{i,l}^2 + c_{j,l+1}^2 + c_{k,l+2}^2\right)^{1/2}} \Bigg\}. \tag{7}$$

The integration boundaries are defined as $c_{0,0} = -\frac{1}{2} - u$, $c_{1,0} = \frac{1}{2} - u$, $c_{0,1} = -\frac{1}{2} - v$, $c_{1,1} = \frac{1}{2} - v$, $c_{0,2} = -\frac{1}{2} - w$, and $c_{1,2} = \frac{1}{2} - w$. The values of $l+1$ and $l+2$ in Eq. (7) are defined modulo 3, i.e., $c_{0,3} \equiv c_{0,0}$, etc. The arctan function to be used in Eq. (7) takes into account the sign of numerator and denominator and yields results between $-\pi$ and π ("atan2" in FORTRAN and C).

An immediate consequence of Eq. (7) is the electrostatic potential at the center of a unit cube

$$\phi_c(0,0,0) = 3 \ln \left(3^{1/2} + 2\right) - \pi/2. \tag{8}$$

Previous calculations of $\phi_c(0,0,0)$ involved rather elaborate manipulations [1, 3].

3. Calculation of the electrostatic potential of a square

In two-dimensional electrostatics, the charge interaction (Green's function of the Laplacian) is given by $-\ln r$, where r is the distance. The electrostatic potential ϕ_s of a square $[-\frac{1}{2}, \frac{1}{2}]^2$ with unit charge density will again be calculated by integration. ϕ_s is also the electrostatic potential of a square cylinder that is infinitely extended in z direction. The potential at a point with Cartesian coordinates (u, v) is written as

$$\phi_s(u,v) = -\frac{1}{2} \int_{-1/2}^{1/2} \mathrm{d}x \int_{-1/2}^{1/2} \mathrm{d}y \ln\left[(x-u)^2 + (y-v)^2\right] . \tag{9}$$

Elementary integration yields

$$\phi_s(u,v) = -\frac{1}{2} \sum_{i=0}^{1} \sum_{j=0}^{1} \Bigg[x_i y_j \ln\left(x_i^2 + y_j^2\right) - 3 x_i y_j + y_j^2 \arctan \frac{x_i}{y_j} + x_i^2 \arctan \frac{y_j}{x_i} \Bigg], \tag{10}$$

where $x_0 = -\frac{1}{2} - u$, $x_1 = \frac{1}{2} - u$, $y_0 = -\frac{1}{2} - v$, and $y_1 = \frac{1}{2} - v$. The appropriate arctan function to be used in Eq. (10) yields values between $-\pi/2$ and $\pi/2$ ("atan" in FORTRAN and C).

4. Multipole expansion

The electrostatic potential of a cube can be expanded in "kubic" harmonics, i.e., harmonic functions with cubic symmetry [1, 4, 8–10]. For the exterior, one obtains

$$\phi_c(\boldsymbol{r}) = \frac{1}{r} + C_4 K_4(\boldsymbol{r}) r^{-9} + C_6 K_6(\boldsymbol{r}) r^{-13} + \cdots , \tag{11}$$

where $\boldsymbol{r}=(u,v,w)$, $r=|\boldsymbol{r}|$. With $T_n = u^n + v^n + w^n$, the kubic harmonics of order 4 and 6 can be written as [10]

$$K_4(\boldsymbol{r}) = T_4 - \frac{3}{5} r^4, \tag{12}$$

$$K_6(\boldsymbol{r}) = T_6 - \frac{15}{11} T_4 r^2 + \frac{30}{77} r^6. \tag{13}$$

For this form, the expansion coefficients are $C_4 = -7/192$ and $C_6 = 11/192$ [1, 7].

For the interior of the cube, we derive the multipole-expansion coefficients of order 2, 4, and 6 from a direct Taylor expansion in x direction. The angular dependence can then be inferred by cubic symmetry.[1] The electrostatic potential on the x axis can be expressed as

$$\phi_c(u,0,0) = \int_{-1/2-u}^{1/2-u} \mathrm{d}x\, f(x), \tag{14}$$

where

$$\begin{aligned} f(x) &= \int_{-1/2}^{1/2} \mathrm{d}y \int_{-1/2}^{1/2} \mathrm{d}z \left(x^2 + y^2 + z^2\right)^{-1/2} \\ &= 2 \ln \frac{(4x^2+2)^{1/2}+1}{(4x^2+2)^{1/2}-1} - 2x \arctan \frac{4x(4x^2+2)^{1/2}}{16x^4+8x^2-1}. \end{aligned} \tag{15}$$

Taylor expansion of $\phi_c(u,0,0)$ around $u=0$ yields the expansion

$$\phi_c(\boldsymbol{r}) = 3 \ln \left(3^{1/2}+2\right) - \frac{\pi}{2} - \frac{2\pi}{3} r^2 - \frac{40}{243^{1/2}} K_4(\boldsymbol{r}) - \frac{308}{19683^{1/2}} K_6(\boldsymbol{r}) + \cdots . \tag{16}$$

Fig. 1 shows the electrostatic potential ϕ_c along the directions $(u,0,0)$, $(u,u,0)$, and (u,u,u) calculated from the exact result Eq. (7) and the expansions (11) and (16), both including terms up to K_4. The expansions show the largest disagreement near the surface of the cube ($u = \frac{1}{2}$) where they start to diverge. Otherwise, they closely reproduce the exact potential [Eq. (11) for $r \to \infty$ and Eq. (16) for $r \to 0$].

The divergent behavior reflects an inherent problem of the near- and far-field expansions. By construction, the Laplacians of Eqs. (11) and (16) are a delta function at $r = 0$ and a constant -4π, respectively, independent of the order of the expansions.

[1] Some higher-order kubic harmonics are degenerate [9], requiring two independent expansion directions to get the correct angular dependence.

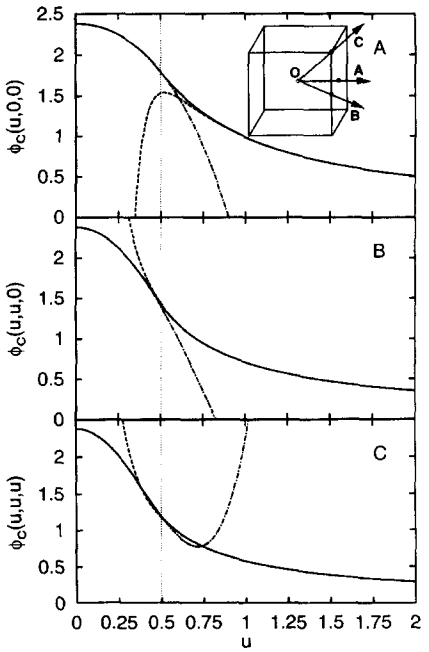

Fig. 1. Electrostatic potential $\phi_c(u,v,w)$ of a homogeneously charged cube. Panels A, B, and C show ϕ_c for directions $(u,0,0)$, $(u,u,0)$, and (u,u,u) as a function of u, respectively. The insert in panel A shows a unit cube illustrating the directions A, B, and C. The solid line is the exact result Eq. (7). The dashed and dot-dashed lines are the expansions Eq. (11) and (16) up to K_4 for the exterior and interior, respectively. The vertical dotted line at $u = 0.5$ indicates the boundary of the cube.

The former corresponds to a unit point charge and is correct only outside the cube; the latter corresponds to a homogeneous charge density and is correct only inside the cube.

5. Conclusion

Nijboer and Ruijgrok [1] analyzed the difference between the energy per particle in a Wigner lattice and the energy of a point charge in the field of the other charges. These authors studied an infinite replication of neutral cubes consisting of a unit point charge at the center and a compensating background. A reduction of the electrostatic potential ϕ_c of a homogeneously charged cube to a one-dimensional integral resulted in

$$\phi_c(u,v,w) = \frac{\pi}{8}\int_0^\infty \mathrm{d}t\; t^{-2}\,\frac{\partial}{\partial t}\,[h(u,t)h(v,t)h(w,t)]\,, \tag{17}$$

where

$$h(x,t) = \mathrm{erf}\big[\,(x+\tfrac{1}{2})t\big] - \mathrm{erf}\big[\,(x-\tfrac{1}{2})t\big] \tag{18}$$

and erf is the error function.[2] The solution of the one-dimensional integral in Eq. (17) would give the closed form Eq. (7) of this work. Eq. (7), numerical integration of Eq. (17), and direct Monte Carlo integration of Eq. (1) were compared for a few hundred points and gave identical results within the error margins of the numerical integration in Eq. (17) and the statistical errors of the Monte Carlo procedure. Eq. (7) has the advantage of being analytical. It can be evaluated fast and with arbitrary precision on the computer.

The electrostatic potential $\phi_c(0,0,0)$ at the center of the cube as listed in Eq. (8) can be used to correct effectively for finite-size effects in computer simulations of ionic systems under periodic boundary conditions, when minimum-image electrostatics is used [11]. An example is the calculation of single-ion chemical potentials [2–6], where the electrostatic energy of an excess ion has to be calculated. The system-size dependence is greatly reduced if the excess charge is compensated with a homogeneous background. The electrostatic energy u of the excess charge q at $\boldsymbol{r} = 0$ is then the sum of the interactions with the other charges q_i at $\boldsymbol{r}_i$ and with the background,

$$u = q\sum_{i=1}^{N} q_i/r_i + q^2\phi_c(0,0,0)/L, \tag{19}$$

where a cubical box of length L is used.

Another application is the calculation of electrostatic potentials when charges are given on a grid, for instance, when ionic density distributions are known [12]. Usually, the grid charges are assumed to be point charges. In an improved description, the charges are smeared out over the grid cells. The electrostatic potentials can then be calculated using Eq. (7) or the multipole expansions Eqs. (11) and (16). This eliminates the singularities in the electrostatic potential and gives a more accurate description near local charge concentrations.

Note added in proof

I am indebted to Dr. Michael Trott (Wolfram Research) who after reading a preprint pointed out several earlier calculations of the potential of a cube in the context of gravitational fields. Most notably, the problem was studied by MacMillan [13] and Waldvogel [14] (see also [15]).

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