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Extension and simple proof of Lekner's summation formula for Coulomb forces

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Research Report No. 93-06
October 1993

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Abstract

A summation formula is proven for a lattice sum occurring frequently in molecular dynamics calculations. It has a much faster convergence rate than the original sum. An important application is in the case of Coulomb forces.

Keywords: Coulomb forces, lattice sums, molecular dynamics

Subject Classification: 82 B80, 82 C22

1. Introduction

In [3] J. Lekner derived an elegant and very useful summation formula for Coulomb forces. In his derivation he used some powerful identities like the Poisson-Jacobi identity for example, the application of which was not straightforward at all. In this note it is shown that Lekner's result and an extension to more general potentials can be obtained in a rather simple and straightforward way.

2. A summation formula for forces derived from a power-law potential

We consider the same situation as Lekner: N particles in a central cell interacting with forces derived from a potential containing only powers of the distance: the force on particle $^{\#}i$ due to particle $^{\#}j$ and all periodic repetitions of $^{\#}j$ is assumed to be of the form

$$\mathbf{F}_i = q_i\, q_j \cdot p \sum_{\text{all cells}} \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^{p+2}} \,, \tag{1}$$

where $\mathbf{r}_i - \mathbf{r}_j$ are position vectors, q_i, q_j may be charges, and $p \geq 1$. The "cells" are periodic repetitions of a central cell. We proceed as in [3] and compute only one component of the force since the other components have completely analogous expressions. We set

$$x_i - x_j = \xi \cdot L, \quad y_i - y_j = \eta \cdot L, \quad z_i - z_j = \zeta \cdot L \,, \tag{2}$$

where L is the length of the side of the central cell parallel to the x-direction. Note that the cell may be any rectangular parallelepiped (not necessarily a cube). Then the x-component of the force is $p\, q_i\, q_j / L^{p+1}$ times $X(\xi, \eta, \zeta)$ where

$$X(\xi,\eta,\zeta) = \sum_{\ell,m,n=-\infty}^{\infty} \frac{\xi + \ell}{[(\xi+\ell)^2 + \alpha^2(\eta+m)^2 + \beta^2(\zeta+n)^2]^{\frac{p}{2}+1}} \,. \tag{3}$$

Here $0 \leq \xi \leq 1$ and $0 \leq \eta \leq \eta_1$, $0 \leq \zeta \leq \zeta_1$, and η_1, ζ_1 are arbitrary positive numbers, and $\alpha = \frac{L_y}{L}$, $\beta = \frac{L_z}{L}$, where L_y, L_z are the corresponding lengths. In order to derive a summation formula with fast convergence for $X(\xi,\eta,\zeta)$ we consider the function

$$g_p(r,\xi) := \sum_{\ell=-\infty}^{\infty} \frac{\xi+\ell}{[(\xi+\ell)^2 + r^2]^{\frac{p}{2}+1}} \,. \tag{4}$$

The function $g_p(r,\xi)$ has the properties

(a) $g_p(r, \xi + n) = g_p(r,\xi), \quad n \in \mathbb{Z}$,

(b) $g_p(r, -\xi) = -g_p(r,\xi)$,

which follows immediately by replacing the summation index ℓ in (4) by $\ell + n$ or $-\ell$ respectively. As a consequence it follows that

(c) $g_p(r,0) = 0$,

and from (a), (b) combined:

(d) $g_p(r,\, \frac{1}{2}) = -g_p(r, \frac{1}{2} - 1) = 0$.

Since $g_p(r,\xi)$ is defined for any $r > 0$ and vanishes for $\xi = 0$ and $\xi = \frac{1}{2}$ we can expand $g_p(r,\xi)$ in a Fourier series:

$$g_p(r,\xi) = 2 \sum_{k=1}^{\infty} C_k^p(r)\, \sin(2\,\pi\, k\, \xi)\ , \tag{5}$$

and

$$C_k^p(r) = 2 \int_0^{\frac{1}{2}} \sum_{\ell=-\infty}^{\infty} \frac{\xi + \ell}{[(\xi+\ell)^2 + r^2]^{\frac{p}{2}+1}}\ \sin(2\,\pi\, k\, \xi)\, d\xi\ . \tag{6}$$

We may interchange integration and summation. An integration by parts then gives

$$C_k^p(r) = \frac{2}{p} \sum_{\ell=-\infty}^{\infty} 2\,\pi\, k \int_0^{\frac{1}{2}} \frac{\cos(2\,\pi\, k\, \xi)}{[(\xi+\ell)^2 + r^2]^{\frac{p}{2}}}\ d\xi\ . \tag{7}$$

We choose a new integration variable $s = \xi + \ell$. This leads to

$$C_k^p(r) = \frac{4\,\pi\, k}{p} \sum_{\ell=-\infty}^{\infty} \int_{\ell}^{\ell+\frac{1}{2}} \frac{\cos(2\,\pi\, k\, s)}{[s^2 + r^2]^{\frac{p}{2}}}\ ds\ . \tag{8}$$

Since $\cos(2\,\pi\, k\, s)$ is symmetric in s with period 1 we arrive at

$$\begin{aligned} C_k^p(r) &= \frac{4\,\pi\, k}{p} \int_0^{\infty} \frac{\cos(2\,\pi\, k\, s)}{[s^2 + r^2]^{\frac{p}{2}}}\ ds \\ &= \frac{4\,\pi\, k}{p} \cdot \Big(\frac{\pi\, k}{r}\Big)^{\frac{p-1}{2}} \frac{\pi^{\frac{1}{2}}}{\Gamma(\frac{p}{2})}\ K_{\frac{p-1}{2}}(2\,\pi\, k\, r), \quad K = \text{modified Bessel function}\ , \end{aligned} \tag{9}$$

where the last integral can be looked up in any table on Fourier-transforms (see e.g. [1], p. 376). Inserting the last expression into (5) leads to

$$g_p(r,\xi) = \frac{8\,\pi^{\frac{p}{2}+1}}{p \cdot \Gamma(\frac{p}{2})} \sum_{k=1}^{\infty} k \Big(\frac{k}{r}\Big)^{\frac{p-1}{2}} \cdot K_{\frac{p-1}{2}}(2\,\pi\, k\, r)\ \sin(2\,\pi\, k\, \xi)\ . \tag{10}$$

Hence the extension of Lekner's formula (17) to arbitrary powers $p \geq 1$ reads

$$X(\xi,\eta,\zeta) = \frac{8\,\pi^{\frac{p}{2}+1}}{p \cdot \Gamma(\frac{p}{2})} \sum_{\ell=1}^{\infty} \ell \cdot \sin(2\,\pi\, \ell\, \xi) \cdot \sum_{n,m=-\infty}^{\infty} \Big(\frac{\ell}{r_{mn}}\Big)^{\frac{p-1}{2}} K_{\frac{p-1}{2}}(2\,\pi\, \ell \cdot r_{mn})\ , \tag{11}$$

where $r_{mn} = [\alpha^2(\eta + m)^2 + \beta^2(\xi + n)^2]^{\frac{1}{2}}$.

For the case of Coulomb forces ($p = 1$) (11) simplifies to Lekner's formula which is

$$X(\xi,\eta,\zeta) = 8\pi \sum_{\ell=1}^{\infty} \ell \cdot \sin(2\pi\ell\xi) \cdot \sum_{n,m=-\infty}^{\infty} K_0(2\pi\ell\, r_{mn}) \; . \tag{12}$$

For $K_0(s)$ approximation formulas can be found e.g. in [1], p. 379.

3. Discussion

(a) An important point is to realize that in fact the derivation of the summation formula given here can be extended to general potentials. Suppose that instead of a power law we have a potential $P(|\mathbf{r}_i - \mathbf{r}_j|)$, where the function $P(s)$ satisfies $\lim_{s\to\infty} P(s) = 0$ and $\frac{dP}{ds} = -F(s)$, where $F(s)$ is such that the infinite sum corresponding to (4), namely

$$g(r,\xi) := \sum_{\ell=-\infty}^{\infty} \frac{(\xi+\ell)}{((\xi+\ell)^2 + r^2)^{1/2}}\; F([(\xi+\ell)^2 + r^2]^{1/2}) \tag{13}$$

still converges.

One can check that all steps leading to the formulas (10) and (11) can be repeated similarly. One just has to replace the Fourier-coefficient in (9) by

$$C_k(r) = 4\pi k \int_0^{\infty} P([s^2 + r^2]^{1/2}) \cdot \cos(2\pi k s) ds \; . \tag{14}$$

In a number of examples the expression $C_k(r)$ can be given explicitly. As an example let us take

$$P(s) = e^{-\beta s} \text{ for some } \beta > 0 \; .$$

Then one has (see [2])

$$C_k(r) = 4\pi k r \beta (4\pi^2 k^2 + \beta^2)^{-1/2}\; K_1[r(4\pi^2 k^2 + \beta^2)^{1/2}] \tag{15}$$

and formula (11) has to be changed in an obvious way.

(b) The convergence in formula (10) is slow if r is less than 0.1. It suffices therefore to give an alternative to (11) only for $n = m = 0$. We go back to (4) which can be written as

$$g_p(r,\xi) = \frac{\xi}{(r^2+\xi^2)^{\frac{p+2}{2}}} + \sum_{\ell=1}^{\infty} \frac{\ell+\xi}{(r^2 + (\ell+\xi)^2)^{\frac{p+2}{2}}} - \sum_{\ell=1}^{\infty} \frac{\ell-\xi}{(r^2 + (\ell-\xi)^2)^{\frac{p+2}{2}}} \tag{16}$$

Furthermore we have

$$\begin{aligned}
\frac{\ell+\xi}{(r^2+(\ell+\xi)^2)^{\frac{p+2}{2}}} &= \frac{1}{(\ell+\xi)^{p+1}}\ \frac{1}{(1+(\frac{r}{\ell+\xi})^2)^{\frac{p+2}{2}}} \\
&= \frac{1}{(\ell+\xi)^{p+1}} \cdot \sum_{k=0}^{\infty} \binom{-\frac{p+2}{2}}{k} r^{2k}\ \frac{1}{(\ell+\xi)^{2k}} \\
&= \sum_{k=0}^{\infty} \binom{-\frac{p+2}{2}}{k} r^{2k}\ \frac{1}{(\ell+\xi)^{2k+p+1}}
\end{aligned}$$

We now use the Hurwitz Zeta function $\zeta(m,\xi)$ (see e.g. [1] Eq. 6.4.10, p.220), which is just a multiple of the Polygamma function ψ^{m-1} in our case:

$$\zeta(m,\xi) = \sum_{\ell=0}^{\infty} \frac{1}{(\ell+\xi)^m} = (-1)^m\ \frac{1}{(m-1)!} \cdot \psi^{m-1}(\xi) \tag{17}$$

It is easy to check that the expression for $g_p(r,\xi)$ becomes

$$g_p(r,\xi) = \frac{\xi}{(r^2+\xi^2)^{\frac{p+2}{2}}} + \sum_{k=0}^{\infty} \binom{-\frac{p+2}{2}}{k} r^{2k}\ \{\zeta(2k+1+p,\xi) - \zeta(2k+p+1,-\xi)\} \tag{18}$$

Numerical tests show that the sum in formula (18) converges very fast if $r < 0.2$.

(c) The function $g_1(r,\xi)$ is a radially symmetric (with respect to r) solution of

$\Delta u = 0$ for $r > 0$, $\xi \in \mathbb{R}$,
$u(r,0) = u(r,\frac{1}{2}) = 0$,
$\lim_{r\to\infty} u(r,\xi) = 0$.

Separation of variables then shows that any solution $u(r,\xi)$ can be written in the form

$$u(r,\xi) = \sum_{\ell=1}^{\infty} C_\ell\, K_0(2\,\pi\,\ell\, r)\ \sin(2\,\pi\,\ell\,\xi)\ ,$$

for any C_ℓ for which series converges.

For $C_\ell = 8\,\pi\cdot\ell$ one is led to Lekner's summation formula.

(d) For $p = 2, 4, 6, ...$ the Bessel functions appearing in (11) can be written in terms of elementary expressions. One has (see e.g. [1])

$$K_{n+\frac{1}{2}}(s) = \sqrt{\frac{\pi}{2s}}\ e^{-s}\ f_n(s)\ ,$$

with $f_0 \equiv 1$, $f_1 = 1 + \frac{1}{s}$ and

$$f_{n+1}(s) = \frac{2n+1}{s}\, f_n(s) + f_{n-1}(s)\ .$$

For example for $p = 6$ and $p = 12$ as is the case for the Lennard-Jones potential one would need in (11)

$$K_{\frac{5}{2}}(s) = \sqrt{\frac{\pi}{2s}}\, e^{-s}(1 + \frac{3}{s} + \frac{3}{s^2})$$

and

$$K_{\frac{11}{2}}(s) = \sqrt{\frac{\pi}{2s}}\, e^{-s} \cdot \left(1 + \frac{15}{s} + \frac{105}{s^2} + \frac{1120}{s^3} + \frac{945}{s^4} + \frac{945}{s^5}\right)\ .$$

(e) As a simple approximation for $g_p(r,\xi)$ one could replace the sum in (10) by an integral

$$(19) \qquad g_p(r,\xi) \cong \frac{8\,\pi^{\frac{p}{2}+1}}{p \cdot \Gamma(\frac{p}{2})} \int_0^\infty k(\frac{k}{r})^{\frac{p-1}{2}} \cdot K_{\frac{p-1}{2}}(2\,\pi\,k\,r)\ \sin(2\pi\,k\,\xi)\ dk\ .$$

After some simplification one gets (see [2])

$$g_p(r,\xi) \cong \frac{\xi}{(\xi^2 + r^2)^{\frac{p}{2}+1}}\ ,$$

that is, the approximation of the sum in (10) by an integral leads back to the term for $\ell = 0$ in (4)!

(f) In order to illustrate the speed-up of convergence given by formulas (10), (11) consider unit charges at points $0, \pm 1, \pm 2, \ldots$ on the ξ-axis. Then in order to calculate the Coulomb force, say at $\xi = 0.2$ and distance 1 from the ξ-axis, directly, one needs 3600 terms to get seven digits accuracy. Using formula (10) in this case we get the same accuracy with only two terms!

(g) It will be shown in a forthcoming paper how the energy can be calculated as well by our method (N charges in the central cell, assuming charge neutrality).

References

[1] M. Abramowitz & I. Stegun: Handbook of Mathematical functions, Dover, New York (1970).

[2] Tables of Integral Transforms, Vol, I, Bateman Manuscript Project, McGraw Hill (1954).

[3] J. Lekner: Summation of Coulomb Fields in Computer-Simulated Disordered Systems, Physica A 176 (1991), 485-498.

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