Extension and simple Proof of Lekner's Summation Formula for Coulomb Forces

Report**Author(s):**

Sperb, René

Publication date:

1993-10

Permanent link:

<https://doi.org/10.3929/ethz-a-004284027>

Rights / license:

In Copyright - Non-Commercial Use Permitted

Originally published in:

SAM Research Report 1993-06

Extension and simple Proof of Lekner's Summation Formula for Coulomb Forces

R. Sperb

Research Report No. 93-06
October 1993

Seminar für Angewandte Mathematik
und Institut für Polymere
Eidgenössische Technische Hochschule
CH-8092 Zürich
Switzerland

Extension and simple Proof of Lekner's Summation Formula for Coulomb Forces

R. Sperb

Seminar für Angewandte Mathematik
und Institut für Polymere
Eidgenössische Technische Hochschule
CH-8092 Zürich
Switzerland

Research Report No. 93-06

October 1993

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

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

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

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

$$(2) \quad x_i - x_j = \xi \cdot L, \quad y_i - y_j = \eta \cdot L, \quad z_i - z_j = \zeta \cdot L ,$$

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

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

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

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

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

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

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

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

and from (a), (b) combined:

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

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:

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

and

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $\lim_{s \rightarrow \infty} P(s) = 0$ and $\frac{dP}{ds} = -F(s)$, where $F(s)$ is such that the infinite sum corresponding to (4), namely

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

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

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

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

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

Then one has (see [2])

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

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

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

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

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:

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

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

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

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

$$\begin{aligned}
\Delta u &= 0 \text{ for } r > 0, \xi \in \mathbb{R}, \\
u(r, 0) &= u(r, \tfrac{1}{2}) = 0, \\
\lim_{r \rightarrow \infty} u(r, \xi) &= 0.
\end{aligned}$$

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

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

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

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

$$K_{\frac{6}{2}}(s) = \sqrt{\frac{\pi}{2s}} e^{-s} \left(1 + \frac{3}{s} + \frac{3}{s^2}\right)$$

and

$$K_{\frac{12}{2}}(s) = \sqrt{\frac{\pi}{2s}} e^{-s} \cdot \left(1 + \frac{15}{s} + \frac{105}{s^2} + \frac{1120}{s^3} + \frac{945}{s^4} + \frac{945}{s^5}\right) .$$

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

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

After some simplification one gets (see [2])

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

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 $0, \pm 1, \pm 2, \dots$ 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).

- [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.

NO.	Authors	Title
93-06	R. Sperb	Extension and simple Proof of Lekner's Summation Formula for Coulomb Forces
93-05	A. Frommer, B. Pohl	A Comparison Result for Multisplittings Based on Overlapping Blocks and its Application to Waveform Relaxation Methods
93-04	M. Pirovino	The Inverse Sturm-Liouville Problem and Finite Differences
93-03	R. Jeltsch, X. Wang	Uniqueness of Piecewise Lipschitz Continuous Solutions of the Cauchy-Problem for 2×2 Conservation Laws
93-02	W.-A. Yong	Difference approximations to the global $W^{1,\infty}$ solutions of the isentropic gas equations
93-01	Ch. Lubich, K. Nipp, D. Stoffer	Runge-Kutta solutions of stiff differential equations near stationary points
92-15	N. Botta	Is the transonic flow around a cylinder always periodic?
92-14	K. Nipp, D. Stoffer	Invariant manifolds of numerical integration schemes applied to stiff systems of singular perturbation type - Part I: <i>RK</i> -methods
92-13	K. Nipp	Smooth attractive invariant manifolds of singularly perturbed ODE's
92-12	D. Mao	A Shock Tracking Technique Based on Conservation in One Space Dimension
92-11	K. Nipp, D. Stoffer	Attractive invariant manifolds for maps: Existence, smoothness and continuous dependence on the map
92-10	M. Fey, R. Jeltsch	A Simple Multidimensional Euler Scheme
92-09	M. Fey, R. Jeltsch	A New Multidimensional Euler Scheme
92-08	M. Fey, R. Jeltsch, P. Karmann	Numerical solution of a nozzle flow
92-07	M. Fey, R. Jeltsch, P. Karmann	Special aspects of reacting inviscid blunt body flow
92-06	M. Fey, R. Jeltsch, S. Müller	The influence of a source term, an example: chemically reacting hypersonic flow
92-05	N. Botta, J. Sesterhenn	Deficiencies in the numerical computation of nozzle flow
92-04	Ch. Lubich	Integration of stiff mechanical systems by Runge-Kutta methods
92-03	M. Fey, R. Jeltsch, S. Müller	Stagnation point analysis