Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo
Swiss Federal Institute of Technology Zurich

An alternative to Ewald sums

R. Sperb

Research Report No. 94-01
June 1994

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

An alternative to Ewald sums

R. Sperb

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

Research Report No. 94-01 June 1994

Abstract

In this paper identities are derived which allow to compute the Coulomb energy associated with N charges in a central cell and all their periodic images. These identities are all consequences of one basic identity which is obtained in a simple and straightforward way. It is possible to extend the results to other types of potentials as well.

I. Introduction

In a recent paper [Sp] it was shown how an extension of an elegant summation formula for Coulomb forces of Lekner [Le] could be derived. In this paper expressions are given for the Coulomb energy for N charges in a central cell and their periodic images. The problem is therefore to calculate

$$E = \frac{1}{2} \sum_{\vec{n} \in \mathbf{Z}^3} \sum_{i \neq j = 1}^{N} q_i \, q_j \, \frac{1}{| \vec{r}_i - \vec{r}_j + \vec{n} |} \tag{1.1}$$

where $\vec{r}$ are positions of charges and $\vec{n}$ is a lattice vector. Of course for convergence one has to assume that

$$\sum_{i=1}^{N} q_i = 0 \; . \tag{1.2}$$

We first consider a potential of the form

$$U(\vec{r}) = \sum_{\vec{n} \in \mathbf{Z}^3} \sum_{i=1}^{N} \frac{q_i}{| \vec{r} - \vec{r}_i + \vec{n} |} \; . \tag{1.3}$$

We may assume that the central cell is the unit cube since it is not hard to extend our results to the case in which the central cell is an arbitrary rectangular block (see [Sp]). The formulae to be given for the Coulomb energy have two important features:

(a) The amount of work required is linear in N;

(b) The accuracy is proportional to the number of terms per charge that are used.

II. Basic Identities

All the summation formulae to follow are consequences of a basic identity for sums of the general form

$$S(x, r) = \sum_{k=-\infty}^{\infty} p(x + k, r) \; . \tag{2.1}$$

Here $x \in (0, 1)$, $r > 0$ and p is an arbitrary function such that the series converges for $x \in (0, 1)$ and $r > 0$.

It is easy to see that $S(x, r)$ is a periodic function in x (with period 1) for any $r > 0$. Therefore an obvious way to handle $S(x, r)$ is to expand it in a Fourier series with respect to x. This leads to

Lemma 1 *Suppose that $p(s,r)$ is such that*

$$\begin{aligned} a_0(r) &\equiv \int_{-\infty}^{\infty} p(s,r)ds \\ a_\ell(r) &\equiv \int_{-\infty}^{\infty} p(s,r)\cos(2\pi\ell s)ds \\ b_\ell(r) &\equiv \int_{-\infty}^{\infty} p(s,r)\sin(2\pi\ell s)ds \end{aligned} \left.\vphantom{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}}\right\} \ell+1,2,3,...$$

all exist .

Then the following identity holds

(2.2)
$$S(x,r) = a_0(r) + 2\sum_{\ell=1}^{\infty} [a_\ell(r)\cos(2\pi\ell x) + b_\ell(r)\sin(2\pi\ell x)] .$$

Proof: We use the complete orthonormal set of functions for the interval $(0,1)$, given by

$$\{1, \sqrt{2}\cos(2\pi\ell x),\ \sqrt{2}\sin(2\pi\ell x)\},\ \ell = 1,2,3,... .$$

The Fourier coefficients of $S(x,r)$ are

$$a_\ell = \sqrt{2}\int_0^1 \sum_{k=-\infty}^{\infty} p(s+k,r)\cos(2\pi\ell s)ds .$$

Interchanging summation and integration and choosing the new integration variable $t = s+k$ we have

$$a_\ell = \sqrt{2}\sum_{k=-\infty}^{\infty}\int_k^{k+1} p(t,r)\cos(2\pi\ell t)dt = \sqrt{2}\int_{-\infty}^{\infty} p(t,r)\cos(2\pi\ell t)dt ,$$

and the same reasoning holds for a_0 and b_ℓ. This leads to the identity (2.2).

Remarks: Two special cases are of importance.

(a) If $p = p(|x+k|,r)$ then p is symmetric in its first variable and all coefficients b_ℓ vanish. Then identity (2.2) reduces to

(2.3)
$$S(x,r) = 2\int_0^{\infty} p(s,r)ds + 4\sum_{\ell=1}^{\infty}\int_0^{\infty} p(s,r)\cos(2\pi\ell s)ds\cdot\cos(2\pi\ell x) .$$

(b) If $p(x+k,r) = -\frac{\partial P}{\partial x}$ and $P = P(|x+k|,r)$, then $p(-s,r) = -p(s,r)$ and all coefficients a_ℓ vanish. Furthermore

$$\begin{aligned} b_\ell = 2\sqrt{2}\int_0^{\infty} p(s,r)\sin(2\pi\ell s)ds &= -2\sqrt{2}\,P(s,r)\sin(2\pi\ell s)\Big|_0^{\infty} \\ &\quad + 2\sqrt{2}\cdot 2\pi\ell\int_0^{\infty} P(s,r)\cos(2\pi\ell s)ds . \end{aligned}$$

Assuming that $\lim_{s\to\infty} P(s,r) = 0$ we thus arrive at the identity

$$S(x,r) = 8\pi \sum_{\ell=1}^{\infty} \ell \cdot \int_0^{\infty} P(s,r)\, \cos(2\pi\ell s) ds \cdot \sin(2\pi\ell x)\ . \tag{2.4}$$

Examples:

(a) For Coulomb forces we can apply identity (2.4) with $P(s,r) = (s^2 + r^2)^{-\frac{1}{2}}$. Consider now a cube of side 1 and a unit charge at the origin. Then the x-component of the Coulomb force at the point (x,y,z), due to the charge and all its periodic images, is given by

$$F_x = \sum_{k,j,m=-\infty}^{\infty} \frac{x+k}{[(x+k)^2 + (y+j)^2 + (z+m)^2]^{\frac{3}{2}}}\ .$$

Setting $r_{jm} = ((y+j)^2 + (z+m)^2)^{\frac{1}{2}}$ and

$$S(x, r_{jm}) = \sum_{k=-\infty}^{\infty} \frac{x+k}{[(x+k)^2 + r_{jm}^2]^{\frac{3}{2}}}$$

we can apply identity (2.4) to obtain

$$S(x, r_{jm}) = 8\pi \sum_{\ell=1}^{\infty} \ell \cdot K_0(2\pi\ell r_{jm})\, \sin(2\pi\ell x), \tag{2.5}$$

where K_0 denotes a modified Bessel function. Since K_0 decays exponentially for large argument the sum over j and m converges fast and we arrive at

$$F_x = 8\pi \sum_{\ell=1}^{\infty} \ell \cdot \sin(2\pi\ell x) \sum_{j,m=-\infty}^{\infty} K_0(2\pi\ell r_{jm})\ . \tag{2.6}$$

Identity (2.6) was derived by Lekner in [Le] by different methods.

As an illustration of the improved convergence rate we give a few numerical examples for the sum $S(x,r)$:

Set $S_1(x,r,K) = \sum_{k=-K}^{K} \frac{x+k}{[(x+k)^2+r^2]^{\frac{3}{2}}}$ and $S_2(x,r,L) = 8\pi \sum_{\ell=1}^{L} \ell \cdot K_0(2\pi\ell r)\, \sin(2\pi\ell x)$. We choose $x = 0.3$, $r = 1$ and list the values of S_1, S_2 for different values of K, L:

S_1		S_2	
$K = 400$	0.02187	$L = 1$	0.0219
800	0.021873	2	0.0218727
1600	0.0218728	3	0.021872638
3200	0.02187269	4	0.0218726 384973

It is remarkable that (2.5) gives 13 correct digits with only 4 terms in the sum, while the direct summation needs 6401 terms for 7 correct digits.

(b) For $p(s,r) = \exp(-\beta(s^2+r^2)^{\frac{1}{2}}) \cdot (s^2+r^2)^{-\frac{1}{2}}$ we can apply identity (2.3). The corresponding Fourier-transform (see e.g. [EM1], p. 17, #27) then yields

$$\begin{aligned}(2.7)\qquad &\sum_{k=-\infty}^{\infty} \exp(-\beta[(x+k)^2+r^2]^{\frac{1}{2}}) \cdot [(x+k)^2+r^2]^{-\frac{1}{2}} = \\ &2K_0(\beta r) + 4\sum_{\ell=1}^{\infty} K_0[r(\beta^2+4\pi^2\ell^2)^{\frac{1}{2}}] \cdot \cos(2\pi\ell x)\ .\end{aligned}$$

(c) For $p(s,r) = (s^2+r^2)^{-\frac{1}{2}-\nu}$, $\nu > 0$, identity (2.3) and the table in [EM1], p. 11, #7, together with the asymptotic formula for K_ν ([AS], p. 375, #9.69) lead to

$$\begin{aligned}(2.8)\qquad \sum_{k=-\infty}^{\infty} \frac{1}{[(x+k)^2+r^2]^{\frac{1}{2}+\nu}} = \frac{\pi^{\frac{1}{2}}}{\Gamma(\nu+\frac{1}{2})} &\Big\{\frac{\Gamma(\nu)}{r^{2\nu}} + 4\Big(\frac{\pi}{r}\Big)^{\nu} \cdot \\ &\sum_{\ell=1}^{\infty} \ell^{\nu} \cdot K_\nu(2\pi\ell r) \cdot \cos(2\pi\ell x)\Big\}\ .\end{aligned}$$

The sum on the left in (2.8) diverges if $\nu \to 0$. However we may take a collection of charges q_i such that

$$\sum_{i=1}^{I} q_i = 0,$$

and consider instead the sum

$$S := \sum_{k=-\infty}^{\infty} \sum_{i=1}^{I} \frac{q_i}{[(x_i+k)^2+r_i^2]^{\frac{1}{2}}}\ .$$

We can use the asymptotic formulae

$$\Gamma(\nu) = \frac{1}{\nu} + o(\nu)$$

and

$$r_i^{-2\nu} = 1 - \ell n r_i \cdot 2\nu + o(\nu^2)$$

to conclude from (2.8) letting $\nu \to 0$ that

$$(2.9)\quad \sum_{k=-\infty}^{\infty} \sum_{i=1}^{I} \frac{q_i}{[(x_i+k)^2+r_i^2]^{\frac{1}{2}}} = \sum_{i=1}^{I} q_i \Big\{ -2\cdot \ell n r_i + 4 \sum_{\ell=1}^{\infty} K_0(2\pi\ell r_i)\,\cos(2\pi\ell x_i) \Big\} .$$

As an illustration for identity (2.9) we consider

$$S(x_1,x_2,r) := \sum_{k=-\infty}^{\infty} \left\{ \frac{1}{[(x_1+k)^2+r^2]^{\frac{1}{2}}} - \frac{1}{[(x_2+k)^2+r^2)^{\frac{1}{2}}]} \right\}$$

corresponding to the Coulomb potential due to a charge +1 at x_1, a charge −1 at x_2 and all periodic images on the x-axis. Then at a distance r on the y axis the Coulomb-potential is given by $S(x_1,x_2,r)$.

From (2.9) we get as a fast alternative

$$(2.10)\qquad S(x_1,x_2,r) = 4\sum_{\ell=1}^{\infty} K_0(2\pi\ell r)\{\cos(2\pi\ell x_1) - \cos(2\pi\ell x_2)\} .$$

We list a few numerical values choosing $x_1 = 0.2$, $x_2 = 0.44$, $r = 0.8$:

S :	direct sum		sum of (2.10)	
#of terms:	401	0.01767	1	0.01776
	801	0.0176631	2	0.01766238
	1601	0.0176624	3	0.01766214

The sum given by (2.10) yields 8 correct digits with only 3 terms!

III. Potentials

The main goal of this section is to derive an expression for the potential

$$(3.0)\qquad U(\vec{r}) = \sum_{\vec{n}\in\mathbb{Z}^3} \sum_{i=1}^{N} \frac{q_i}{|\vec{r} - \vec{r}_i + \vec{n}|} .$$

To this end we first consider

$$(3.1)\qquad S(x,y,z) := \sum_{k,\ell,m=-\infty}^{\infty} ((x+k)^2+(y+\ell)^2+(z+m)^2)^{-\frac{1}{2}} \cdot \exp(-\beta[(x+k)^2+(y+\ell)^2+(z+m)^2]^{\frac{1}{2}}) .$$

We set

$$r_{\ell m} = ((y+\ell)^2+(z+m)^2)^{\frac{1}{2}} .$$

and use identity (2.7) with r replaced by $r_{\ell m}$ to find

$$\begin{aligned}(3.2)\qquad &\sum_{k=-\infty}^{\infty} ((x+k)^2 + r_{\ell m}^2)^{-\frac{1}{2}} \cdot \exp(-\beta[(x+k)^2 + r_{\ell m}^2)] = \\ &2\,K_0(\beta\, r_{\ell m}) + 4\sum_{k=1}^{\infty} K_0[r_{\ell m}(\beta^2 + (2\pi k)^2)^{\frac{1}{2}}] \cdot \cos(2\pi k x)\ .\end{aligned}$$

In the sum (we denote it by $T^1_{\ell m}(x,\beta)$) on the right side of Eq. (3.2) the limit $\beta \to 0$ is well behaved, also when the summation over ℓ and m is performed. Thus we have to deal with the term $K_0(\beta\, r_{\ell m})$ in more detail.

We now write $r_{\ell m} = ((y+\ell)^2 + r_m^2)^{\frac{1}{2}}$, $r_m = |z+m|$, and use (2.7) again with $p(s,r) = 2K_0[\beta(s^2+r^2)^{-\frac{1}{2}}]$. From the table in [EM1], p. 56, #43, we get

$$\begin{aligned}(3.3)\qquad &\sum_{\ell=-\infty}^{\infty} K_0[\beta(((y+\ell)^2) + r_m^2)^{\frac{1}{2}}] = \frac{\pi}{\beta}\ \exp(-\beta r_m) + \\ &\underbrace{2\pi\sum_{\ell=1}^{\infty} \frac{1}{((2\pi\ell)^2+\beta^2)^{\frac{1}{2}}}\ \exp[-r_m((2\pi\ell)^2+\beta^2)] \cdot \cos(2\pi\ell y)}_{\frac{1}{2}T^2_m(y,\beta)}\ .\end{aligned}$$

Again, the term $T^2_m(y,\beta)$ makes no difficulties as $\beta \to 0$ and the summation over m is performed. It remains to analyse

$$T^3(\beta,z) = \frac{2\pi}{\beta}\sum_{m=-\infty}^{\infty} \exp(-\beta|z+m|)\ ,$$

which consists of two geometric series. A few routine steps yield

$$T^3(\beta,z) = \frac{2\pi}{\beta}\ \frac{\exp(-\beta z) + \exp(\beta(1-z))}{1-\exp(-\beta)}\ ,$$

and an expansion with respect to β gives

$$(3.4)\qquad T^3(\beta,z) = 2\pi\Big[\frac{1}{\beta^2} + \frac{1}{6} + z^2 - z + O(\beta^2)\Big]\ .$$

Hence, if we form

$$\sum_{i=1}^{N} q_i\ T^3(\beta, z_i)\ ,$$

and let $\beta \to 0$ we are left with the simple expression

$$(3.5)\qquad T^3(0) := 2\pi\ \sum_{i=1}^{N}(z_i^2 - z_i)\,q_i\ .$$

This holds for any set of N charges with charge neutrality. Next we analyze the term

$$V(y,z) := \sum_{m=-\infty}^{\infty} T_m^2(y,0) = 2 \sum_{m=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} \frac{1}{\ell} \cdot \exp[-2\pi\ell|z+m|] \; \cos(2\pi\ell y) \;, \tag{3.6}$$

stemming from the second term on the right of (3.3).

A first possibility is to sum over m first, which is a geometric series:

$$\sum_{m=-\infty}^{\infty} \exp[-2\pi\ell|z+m|] = \frac{\exp(-2\pi\ell z) + \exp(-2\pi\ell(1-z))}{1-\exp(-2\pi\ell)}, \; (0 \le z \le 1) \;.$$

Thus, a first way to write $V(y,z)$ is

$$V(y,z) = 2 \sum_{\ell=1}^{\infty} \frac{1}{\ell} \, \frac{\exp(-2\pi\ell z) + \exp(-2\pi\ell(1-z))}{1-\exp(-2\pi\ell)} \cdot \cos(2\pi\ell y)$$

that is,

$$V(y,z) = 2 \sum_{\ell=1}^{\infty} \frac{1}{\ell} \, \frac{Ch(2\pi\ell(z-\frac{1}{2}))}{Sh(\pi\ell)} \cdot \cos(2\pi\ell y) \;. \tag{3.7}$$

A second possibility is to sum over ℓ first. To do so we write the term as the real part of a complex function:

$$\frac{1}{\ell} \, \exp(-|z+m|2\pi\ell) \cos(2\pi\ell y) = \frac{1}{2} \, Re[\exp(-\zeta \cdot \ell)]$$

with $\zeta = |z+m| - i \cdot y$. Then, since $Re\,\zeta > 0$ we have

$$\begin{aligned} \sum_{\ell=1}^{\infty} \frac{1}{\ell} \, \exp(-\ell \cdot \zeta) = \int_{\zeta}^{\infty} \sum_{\ell=1}^{\infty} \exp(-\ell \cdot w) dw \; &= \; \int_{\zeta}^{\infty} \frac{\exp(-w)}{1-\exp(-w)} \, dw \\ &= \; -\log(1-\exp(-\zeta)) \;. \end{aligned}$$

Now

$$\begin{aligned} Re[\log(1-\exp(-\zeta))] \; &= \; \log\, |1-\exp(-(|z+m| - i \cdot y)2\pi)| \\ &= \; \tfrac{1}{2} \, \log\Big\{1 - 2\,\exp(-|z+m|2\pi)\,\cos(2\pi y) + \exp(-|z+m|4\pi)\Big\} \;, \end{aligned}$$

and therefore a second way to express $V(y,z)$ is

$$V(y,z) = -\sum_{m=-\infty}^{\infty} \log\Big\{1 - 2\,\exp(-|z+m|2\pi)\,\cos(2\pi y) + \exp(-|z+m|4\pi)\Big\} \;. \tag{3.8}$$

Remark: Numerical tests show that the sum in (3.8) converges very fast in the whole range $y, z \in (0,1)$, whereas the convergence becomes slow in (3.7) if z approaches 0 or 1.

For the calculation of the Coulomb energy later on it is useful to derive yet another expression for $V(y,z)$. We note that $V(y,z)$ is symmetric with respect to $y=\frac{1}{2}$, $z=\frac{1}{2}$. Hence we set

$$\hat{V}(y,z) = V(y+\tfrac{1}{2},\, z+\tfrac{1}{2})$$

and use (3.7) to find

$$\hat{V}(y,z) = 2\,Re\sum_{\ell=1}^{\infty}\frac{(-1)^{\ell}}{\ell}\,\frac{1}{Sh(\pi\ell)}\,Ch(2\pi\ell\zeta),\quad \zeta = z+iy\ , \tag{3.9}$$

where now $y,z\in(-\frac{1}{2},\frac{1}{2})$. Next we expand $Ch(2\pi\ell\zeta)$ in a power series and sum over ℓ. This leads to

$$\hat{V}(y,z) = Re\sum_{k=0}^{\infty} C_{2k}\cdot\zeta^{2k} = Re(\hat{V}(\zeta)) \tag{3.10}$$

with

$$C_k = 2\,\frac{(2\pi)^k}{k!}\cdot\sum_{\ell=1}^{\infty}\frac{(-1)^{\ell}\cdot\ell^{k-1}}{Sh(\pi\ell)}\ . \tag{3.11}$$

It is known (see [Ha], p. 283) that

$$\sum_{\ell=1}^{\infty}\frac{(-1)^{\ell-1}\cdot\ell^{m}}{Sh(\pi\ell)} = \begin{cases}\frac{1}{4\pi} & ,\quad m=1\\ 0 & ,\quad m=4n+1,\ n=1,2,3,\dots\end{cases}\ . \tag{3.12}$$

Hence $\hat{V}(\zeta)$ can be written in the form

$$\hat{V}(\zeta) = -c_0 - \pi\cdot\zeta^2 + \sum_{k=1}^{\infty} C_{4k}\cdot\zeta^{4k},\ c_0\cong 0.169548\ . \tag{3.13}$$

The expression for $U(\vec{r})$ defined by (1.3) can now be determined from (3.2), (3.5), (3.6). We set

$$\vec{r} = (x,y,z),\ \vec{r}_i = (x_i,\, y_i,\, z_i)$$

and

$$W(y,z) = \sum_{i=1}^{N} q_i\, V(y-y_i,\, z-z_i) \tag{3.14}$$

where for V any of the expressions (3.7), (3.8) or (3.13) may be used. Let us further define

$$B(x,y,z) = 4\sum_{i=1}^{N} q_i\sum_{k=1}^{\infty}\cos(2\pi k(x-x_i))\sum_{\ell,m=-\infty}^{\infty} K_0[2\pi k((y-y_i+\ell)^2 + (z-z_i+m)^2)^{\frac{1}{2}}]\ . \tag{3.15}$$

With these definitions the expression for the Coulomb potential becomes

$$U(x,y,z) = B(x,y,z) + W(y,z) + 2\pi \sum_{i=1}^{N} q_i (z - z_i)(z - z_i - 1) \,. \tag{3.16}$$

Remarks:

(a) Another expression for $U(x,y,z)$ (differing from (3.16) only by a constant) was derived by Lekner [Le]. There the second and third term in (3.16) are given in a different form. The derivation of the corresponding formulae in [Le] however is quite different.

(b) It is tempting to think that the double sum in (3.15) involving the Bessel function K_0 could be compressed further by again using Lemma 1. The calculation of the corresponding alternative sum and a numerical test however revealed that the convergence becomes slower again.

(c) The role in which x, y, z enter into (3.16) is quite unsymmetric in contrast to the original form (3.0) of the direct sum. This is due to the derivation which starts by first compressing the sum over the x-part. Of course, one could start with any of the three sums in the triple sum in (3.1). One can however derive a different expression as shown in the following.

Define

$$F(x,y,z,p) = \sum_{k,\ell,m=-\infty}^{\infty} [(x+k)^2 + (y+\ell)^2 + (z+m)^2]^{-\frac{1}{2}-p} \tag{3.17}$$

Then we have

$$U(x,y,z) = \lim_{p\to 0} \sum_{i=1}^{N} q_i \; F(x - x_i, y - y_i, z - z_i, p) \,. \tag{3.18}$$

Now we make use of the following algebraic identity:

$$\begin{aligned} \sum_{i=1}^{N} q_i \; F(\xi_i, \eta_i, \zeta_i, p) \;&=\; \sum_{i=1}^{N} q_i \; F(\xi_i, \eta_1, \zeta_1, p) + \\ &+\; \sum_{i=2}^{N} q_i \, [F(\xi_i, \eta_i, \zeta_1, p) - F(\xi_i, \eta_1, \zeta_1, p)] \\ &+\; \sum_{i=2}^{N} q_i \, [F(\xi_i, \eta_i, \zeta_i, p) - F(\xi_i, \eta_i, \zeta_1, p)] \,. \end{aligned} \tag{3.19}$$

For the sums appearing on the right side of (3.19) one can apply identity (2.8) and then let $p \to 0$. One has to set

$$\xi_i = x - x_i, \; \eta_i = y - y_i, \; \zeta_i = z - z_i$$

and

$$
\begin{aligned}
r_{1\ell m} &= [(\eta_1+\ell)^2+(\zeta_1+m)^2]^{\frac{1}{2}} \ ,\\
r_{ikm} &= [(\xi_i+k)^2+(\zeta_1+m)^2]^{\frac{1}{2}} \ ,\\
r_{ik\ell} &= [(\xi_i+k)^2+(\eta_i+\ell)^2]^{\frac{1}{2}} \ .
\end{aligned}
$$

Furthermore define

$$
S(r,s) = 4\sum_{j=1}^{\infty} K(2\pi jr)\,\cos(2\pi js)\ . \tag{3.20}
$$

Then identity (3.19) combined with (2.9) leads to an alternative expression for U:

$$
\begin{aligned}
U(x,y,z) &= \sum_{i=1}^{N} q_i \sum_{\ell,m=-\infty}^{\infty} S(r_{1\ell m},\xi_i) + \\
&+ \sum_{i=2}^{N} q_i \sum_{k,m=-\infty}^{\infty} [S(r_{ikm},\eta_i) - S(r_{ikm},\eta_1)] \\
&+ \sum_{i=2}^{N} q_i \sum_{k,\ell=-\infty}^{\infty} [S(r_{ik\ell},\zeta_i) - S(r_{ik\ell},\zeta_1)]\ .
\end{aligned} \tag{3.21}
$$

Note that e.g. the last term on the right side of (3.21) would become, when written explicitly,

$$
4\sum_{i=2}^{N} q_i \sum_{j=1}^{\infty}\{\cos(2\pi j\zeta_i)-\cos(2\pi j\zeta_1)\} \sum_{k,\ell=-\infty}^{\infty} K_0([2\pi j(\xi_i+k)^2+(\eta_i+\ell)^2]^{\frac{1}{2}})\ .
$$

(d) There is a situation in which many terms in (3.15) are needed. If $\ell = m = 0$ and $[(y-y_i)^2+(z-z_i)^2]^{\frac{1}{2}} = r_i =$ small, then the sum $\sum_{k=1}^{\infty} K_0(2\pi r_i)\,\cos(2\pi k(x-x_i))$ may require many terms for sufficient accuracy.

The number of terms required for six digits accuracy is about $\frac{20}{r}$ for $r << 1$.

It is crucial at this point that we have used identities for single sums, such as (2.9). In order to derive an alternative expression which converges fast for small r_i let us first consider

$$
F(x,r,p) = \sum_{k=-\infty}^{\infty} [(x+k)^2+r^2]^{-\frac{1}{2}-p}\ , \tag{3.22}
$$

where we assume $p > 0$ and $0 \le r < 1$, $0 < x < 1$.

Since

$$
[(x+k)^2+r^2]^{-\frac{1}{2}-p} = |x+k|^{-1-2p}\cdot\Big[1+\Big(\frac{r}{x+k}\Big)^2\Big]^{-\frac{1}{2}-p}
$$

we find by expansion that

$$[(x+k)^2+r^2]^{-\frac{1}{2}-p} = \sum_{\ell=0}^{\infty} \binom{-p-\frac{1}{2}}{\ell} r^{2\ell} \frac{1}{|x+k|^{2\ell+2p+1}} . \tag{3.23}$$

The generalized Zeta-function (Hurwitz Zeta-function) is defined for arbitrary $m \neq 0, -1, -2, ...$ and $x \in \mathbb{C}$ by

$$\zeta(m,x) = \sum_{k=0}^{\infty} \frac{1}{(k+x)^m} . \tag{3.24}$$

We may write $F(x,r,p)$ in the form

$$\begin{aligned} F(x,r,p) &= \sum_{k=0}^{\infty} [(1+x+k)^2+r^2]^{-\frac{1}{2}-p} + \\ & \sum_{k=0}^{\infty} [(1-x+k)^2+r^2]^{-\frac{1}{2}-p} + [x^2+r^2]^{-\frac{1}{2}-p} \end{aligned} \tag{3.25}$$

and then use the definition (3.24) to find

$$\begin{aligned} F(x,r,p) = \sum_{\ell=0}^{\infty} \binom{-p-\frac{1}{2}}{\ell} r^{2\ell} & \Big\{\zeta(2\ell+1+2p, 1+x) \\ & + \zeta(2\ell+1+2p, 1-x)\Big\} + [x^2+r^2]^{-\frac{1}{2}-p} . \end{aligned} \tag{3.26}$$

The only term in (3.26) which needs special attention when $p \to 0$ is the one with $\ell = 0$. The asymptotic behavior of $\zeta(m,x)$ is given by (see [EM2], p. 26)

$$\zeta(m,x) = \frac{1}{m-1} - \psi(x) + o(m-1) , \tag{3.27}$$

where $\psi(x)$ is the Digamma-function.

Hence for any collection of M charges q_i for which

$$\sum_{i=1}^{M} q_i = 0$$

we have

$$\sum_{i=1}^{M} q_i \, F(x_i, r_i, 0) = \sum_{i=1}^{M} q_i \, G(x_i, r_i) , \tag{3.28}$$

where $G(x,r)$ is defined by

$$\begin{aligned} G(x,r) &= \sum_{\ell=1}^{\infty} \binom{-\frac{1}{2}}{\ell} r^{2\ell} \Big\{\zeta(2\ell+1, 1+x) + \zeta(2\ell+1, 1-x)\Big\} \\ & -\psi(1+x) - \psi(1-x) + \frac{1}{\sqrt{x^2+r^2}} . \end{aligned} \tag{3.29}$$

Numerical example: As an illustration we consider two charges ±1 and compare

$$Sd\,[x_1, x_2, r] = \sum_{k=-\infty}^{\infty} \left\{ \frac{1}{\sqrt{(x_1+k)^2+r^2}} - \frac{1}{\sqrt{(x_2+k)^2+r^2}} \right\}$$

with the expression from (2.10), namely

$$S[x_1, x_2, r] = 4\sum_{\ell=1}^{\infty} K_0(2\pi\ell r)\{\cos(2\pi\ell x_1) - \cos(2\pi\ell x_2)\} ,$$

as well as the formula following from (3.29) which is

$$H[x_1, x_2, r] = G(x_1, r) - G(x_2, r) .$$

We choose $x_1 = 0.2$, $x_2 = 0.3$ and $r = 0.5$

$$\begin{array}{lclcrcl} Sd & = & 0.0727395 & k & = & -500 & \text{to } 500 \\ S & = & 0.0727393 & \ell & = & 1 & \text{to } 5 \\ H & = & 0.07274 & \ell & = & 1 & \text{to } 15 \quad . \end{array}$$

Now if r becomes smaller the sum in (3.29) converges much faster. With the same values of x_1, x_2 and $r = 0.01$:

$$\begin{array}{lclcrcl} Sd & = & 1.5271559 & k & = & -600 & \text{to } 600 \\ S & = & 1.5271557 & \ell & = & 1 & \text{to } 200 \\ H & = & 1.5271558 & \ell & = & 1 & \text{to } 2 \quad . \end{array}$$

4. Coulomb Energy

The main goal of this section is to show that the amount of work required to calculate the Coulomb energy of an N-particle system depends linearly on N, in contrast to the Ewald method where the dependence is $N^{\frac{3}{2}}$.

Let the particles in the unit cube have positions $\vec{r}_i$ and set $\vec{\rho}_{ij} = \vec{r}_i - \vec{r}_j$. Then our problem is to calculate

$$E = \frac{1}{2} \sum_{i \neq j = 1}^{N} q_i\, q_j\, U(\vec{\rho}_{ij}) , \tag{4.1}$$

where U is the potential given by (3.0). In the form (4.1) the number of terms required is $O(N^2)$. We will be able to reduce this to $O(N)$ by splitting $U(\rho_{ij})$ into a sum of products. Fortunately this can be carried out for all terms appearing in formula (3.16).

We now consider separately the terms B and W.

(a) $\mathbf{B(x,y,z)}$

The basis is in this case the Addition-Theorem of Gegenbauer which states that for any $0 \le s < S$

$$K_0(\sqrt{s^2 + S^2 - 2s \cdot S\cos\varphi}) = I_0(s)\,K_0(S) + 2\sum_{p=1}^{\infty} I_p(s)\,K_p(S)\,\cos(p\varphi)\,, \tag{4.2}$$

where $I_p(s)$ are modified Bessel functions. We set

$$\vec{\rho}_{ij} = (x_i - x_j, y_i - y_j, z_i - z_j)\,.$$

Then, according to (3.15) we need the term

$$\begin{aligned} E_B &= 2\sum_{i\neq j=1}^{N} q_i\,q_j \sum_{k=1}^{\infty}\cos(2\pi k(x_j - x_i))\,\cdot \\ &\quad \cdot \sum_{\ell,m=-\infty}^{\infty} K_0[2\pi k((y_j - y_i + \ell)^2 + (z_j - z_i + m)^2)^{\frac{1}{2}}]\,. \end{aligned} \tag{4.3}$$

We now express the argument of K_0 in polar coordinates as follows:

$$(y_j - y_i + \ell)^2 + (z_j - z_i + m)^2 = r_i^2 + r_{j\ell m}^2 - 2r_i\,r_{j\ell m}\cos(\varphi_{ij\ell m})$$

where

$$\begin{aligned} r_i^2 &= y_i^2 + z_i^2\,,\ \varphi_i = \text{arc tan}\left(\frac{y_i}{z_i}\right) \\ r_{j\ell m}^2 &= (y_j + \ell)^2 + (z_j + m)^2\,,\ \varphi_{j\ell m} = \text{arc tan}\left(\frac{y_j + \ell}{z_j + m}\right) \\ \varphi_{ij\ell m} &= \varphi_i - \varphi_{j\ell m}\,. \end{aligned}$$

In the addition theorem we then choose

$$s = 2\pi k r_i\,, \quad S = 2\pi k r_{j\ell m}$$

where we have assumed that $r_i < r_{j00}$. Terms where $r_i = r_{j00}$, i.e. $y_i = y_j$, $z_i = z_j$ have to be treated separately by means of the relation (3.29) with $r = 0$ there. Thus we have

$$\begin{aligned} K_0[2\pi k((y_j - y_i + \ell)^2 + (z_j - z_i + m)^2)^{\frac{1}{2}}] &= I_0(2\pi k r_i)K_0(2\pi k r_{j\ell m}) \\ &\quad + 2\sum_{p=1}^{\infty} I_p(2\pi k r_i)\,K_p(2\pi k r_{j\ell m})\cdot\cos[p(\varphi_i - \varphi_{j\ell m})]\,. \end{aligned} \tag{4.4}$$

We also apply the addition theorem for cosines to express the terms $\cos(2\pi k(x_j - x_i))$ and $\cos(p(\varphi_i - \varphi_{j\ell m}))$. In order to evaluate E_B we introduce the following terms:

$$
\begin{aligned}
\alpha_{\ell j} &= \sum_{i=1}^{N} q_i\, I_0(2\pi\ell r_i)\, \cos(2\pi\ell x_i)(1-2\delta_{ij}),\ \ \delta_{ij} = \mathrm{Kronecker-symbol} \\
\beta_{\ell j} &= \sum_{i=1}^{N} q_i\, I_0(2\pi\ell r_i)\, \sin(2\pi\ell x_i)(1-2\delta_{ij}) \\
\alpha_{\ell jp} &= 2\sum_{i=1}^{N} q_i\, I_p(2\pi\ell r_i)\, \cos(2\pi\ell x_i)\, \cos(p\varphi_i)(1-2\delta_{ij}) \\
\beta_{\ell jp} &= 2\sum_{i=1}^{N} q_i\, I_p(2\pi\ell r_i)\, \sin(2\pi\ell x_i)\, \cos(p\varphi_i)(1-2\delta_{ij}) \\
\gamma_{\ell jp} &= 2\sum_{i=1}^{N} q_i\, I_p(2\pi\ell r_i)\, \cos(2\pi\ell x_i)\, \sin(p\varphi_i)(1-2\delta_{ij}) \\
\delta_{\ell jp} &= 2\sum_{i=1}^{N} q_i\, I_p(2\pi\ell r_i)\, \sin(2\pi\ell x_i)\, \sin(p\varphi_i)(1-2\delta_{ij})\ .
\end{aligned} \tag{4.5}
$$

Then the contribution of the first term E_B to the total energy E is given by

$$
\begin{aligned}
E_B = {} & 2\sum_{i=1}^{N} q_j \sum_{\ell=1}^{\infty} \sum_{m,n=-\infty}^{\infty} \Big\{ [\alpha_{\ell j} \cos(2\pi\ell x_j) + \beta_{\ell j} \sin(2\pi\ell x_j)] K_0(2\pi\ell r_{jmn}) \\
& + \sum_{p=1}^{\infty} \Big[[\alpha_{\ell jp} \cos(2\pi\ell x_j)\, \cos(p\varphi_{jmn}) + \beta_{\ell jp} \sin(2\pi\ell x_j)\, \cos(p\varphi_{jmn})] \\
& \cdot K_p(2\pi\ell r_{jmn}) \\
& + [\gamma_{\ell jp} \cos(2\pi\ell x_j)\, \sin(p\varphi_{jmn}) + \delta_{\ell jp} \sin(2\pi\ell x_j)\, \sin(p\varphi_{jmn})] \\
& \cdot K_p(2\pi\ell r_{jmn}) \Big] \Big\}\ .
\end{aligned} \tag{4.6}
$$

Of course, formula (4.6) looks discouragingly involved at first sight. One has to realize however that in the summations over ℓ, m, n typically about 80 terms are needed totally to achieve about 6 digits accuracy. Similarly in the summation over p about 6-10 different values of p have to be evaluated. The main point however is that the amount of work required is $A \cdot N$, where N is the number of charges and A is a measure for the accuracy.

(b) $\mathbf{W}(\mathbf{x}, \mathbf{y}, \mathbf{z})$

We set

$$E_W = \frac{1}{2} \sum_{i \neq j = 1}^{N} q_i\, q_j\, V(y_i - y_j, z_i - z_j)\ . \tag{4.7}$$

First we use the form (3.9) in which the arguments of $\hat{V}$ are in the range $(-\frac{1}{2}, \frac{1}{2})$.

Setting $\zeta_k = z_k + iy_k$ we have

$$E_W = Re \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell \cdot Sh(\pi\ell)} \sum_{\substack{k,j=1 \\ k\neq j}}^{N} q_k\, q_j\, Ch(2\pi\ell(\zeta_k - \zeta_j)) \ . \tag{4.8}$$

Using the addition theorem for $Ch(2\pi\ell(\zeta_k - \zeta_j))$ and defining

$$\begin{cases} a_\ell &= \sum_{k=1}^{N} q_k\, Ch(2\pi\ell\zeta_k) \\ b_\ell &= \sum_{k=1}^{N} q_k\, Sh(2\pi\ell\zeta_k) \end{cases} \tag{4.9}$$

one has

$$E_W = Re\Big\{ \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell \cdot Sh(\pi\ell)} \Big[a_\ell^2 + b_\ell^2 - \sum_{k=1}^{N} q_k^2 (Ch^2(2\pi\ell\zeta_k) - Sh^2(2\pi\ell\zeta_k)) \Big] \Big\} \ . \tag{4.10}$$

We define

$$Q = \sum_{k=1}^{N} q_k^2, \ \ c_0 = \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell-1}}{\ell \cdot Sh(\pi\ell)} \cong 0.169548 \ , \tag{4.11}$$

and use that

$$Re\, Ch(2\pi\ell\zeta_k) = Ch(2\pi\ell z_k) \cos(2\pi\ell y_k), \ Re\, Sh(2\pi\ell\zeta_k) = Sh(2\pi\ell z_k) \cos(2\pi\ell y_k) \ .$$

Then in the next step we can put (4.10) into the form

$$E_W = c_0 \cdot Q + \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell \cdot Sh(\pi\ell)} \Big[(Re\, a_\ell)^2 + (Re\, b_\ell)^2 - (Im\, a_\ell)^2 - (Im\, b_\ell)^2 \Big] \ , \tag{4.12}$$

where

$$\begin{aligned} Re\, a_\ell &= \sum_{k=1}^{N} q_k\, Ch(2\pi\ell z_k)\, \cos(2\pi\ell y_k) =: \alpha_\ell \\ Im\, a_\ell &= \sum_{k=1}^{N} q_k\, Sh(2\pi\ell z_k)\, \sin(2\pi\ell y_k) =: \beta_\ell \\ Re\, b_\ell &= \sum_{k=1}^{N} q_k\, Sh(2\pi\ell z_k)\, \cos(2\pi\ell y_k) =: \gamma_\ell \\ Im\, b_\ell &= \sum_{k=1}^{N} q_k\, Ch(2\pi\ell z_k)\, \sin(2\pi\ell y_k) =: \delta_\ell \ . \end{aligned}$$

Thus

$$E_W = c_0 \cdot Q + \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell \cdot Sh(\pi\ell)} \left[\alpha_\ell^2 + \gamma_\ell^2 - \beta_\ell^2 - \delta_\ell^2 \right] \ . \tag{4.13}$$

Of course one could also use (3.8) to give an alternative expression for E_W. But this form seems to be much more involved so that it may be preferable to take E_W as given by (4.13). The last term in the energy stems from the third term in (3.16). An easy calculation shows that the contribution to the Coulomb energy is

$$E_z = -2\pi\Big(\sum_{i=1}^{N} q_i\, z_i\Big)^2 \,. \tag{4.14}$$

The main result thus is that the Coulomb energy E can be written as

$$E = E_B + E_W + E_z \tag{4.15}$$

where E_B is given by (4.6), E_W by (4.13) and E_z by (4.14).

5. Concluding Remarks

(a) In this paper the main concern was to derive identities which allow to calculate the Coulomb energy by quickly convergent series. For the actual procedure on a computer the CPU time will depend very much on the programming skill. Numerical tests comparing the method proposed here with the Ewald summation method are planned for a forthcoming paper.

(b) It is evident that the way the identities were derived can be adapted to other types of interactions, such as potentials of type $|\vec{r}_i - \vec{r}_j|^{-p}$, for any $p > 0$.

References

[Le] Lekner J., *Summation of Coulomb fields in computer simulated disordered systems*, Physica A 176 (1991), 485-498.

[Sp] Sperb R.P., *Extension and simple proof of Lekner's summation formula for Coulomb forces*, Molecular Simulation, Vol. (1994).

[EM1] Erdélyi A., Magnus W., Oberkettinger F., Tricomi F.G., *Tables of integral transforms*, Vol. I, McGraw-Hill, 1954.

[EM2] Erdélyi A., Magnus W., Oberkettinger F., Tricomi F.G., *Higher transcendental functions*, Vol. 1, McGrawHill, 1953.

[AS] Abramowitz, Stegun I., *Handbook of Mathematical Functions*, Dover, N.Y., 1970.

[HA] Hansen, *A table of series and products*, Prentice Hall, 1975.

Research Reports

No.	Authors	Title
94-01	R. Sperb	An alternative to Ewald sums
93-07	R. Sperb	Isoperimetric Inequalities in a Boundary Value Problem in an Unbounded Domain
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: RK-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