

The Coulomb energy for dense periodic systems

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Abstract

A method for calculating the Coulomb energy in a periodic system is discussed for the case that the number N of charges is large, so that it would be too time consuming to calculate $1/2N(N-1)$ pairs.

1. Introduction

In the first part [5] identities for sums were derived which allow a rapid calculation of the Coulomb energy of an infinite periodic system. This system consists of a basic cell containing N charges (with charge neutrality) and all their periodic images. These periodic images can fill the whole space or, as is required in some applications, only a two-dimensional layer of finite height. The latter case was not treated by Ewald [2], but in the present treatment it is just a special case.

An important feature of the formulae derived in [5] is the application to dense systems, i.e. when N gets large, 10^3 or more. For the Coulomb energy and the Coulomb forces one has to calculate $\frac{1}{2} N(N-1)$ pairs and therefore the CPU time will increase drastically with N . It is desirable to have a method for which the number of terms required is not proportional to N^2 .

It will be shown that one can proceed in such a way that the CPU time is at most proportional to $N \cdot (\log N)^2$.

The basic idea is simple: one needs a complete product decomposition of the terms required for the computation of the energy. It turns out that the formulae derived in [4] and [5] are best suited for this procedure.

2. Product decomposition

In order to illustrate the basic idea we start with a somewhat simplified example. Suppose we have to calculate an expression of the form

$$(2.1) \quad S = \sum_{i,j=1}^N f(x^i, x^j)$$

and N may be large. For practical applications this means that we need an approximation for S with a given accuracy.

Assume now that a product decomposition formula for f is known of the form:

$$(2.2) \quad f(x^i, x^j) = \sum_{\ell=1}^{\infty} p_{\ell}(x^i) \cdot q_{\ell}(x^j) .$$

More precisely, assume that we know that

$$(2.3) \quad \left| f(x^i, x^j) - \sum_{\ell=1}^L p_{\ell}(x^i) q_{\ell}(x^j) \right| \leq \epsilon \quad \text{for } 1 \leq i, j \leq N .$$

If we now replace f in (2.1) by the product approximation and rearrange the sums we find

$$(2.4) \quad S \cong \sum_{\ell=1}^L \sum_{i=1}^N p_{\ell}(x^i) \sum_{j=1}^N q_{\ell}(x^j) = \sum_{\ell=1}^L P_{\ell} \cdot Q_{\ell} .$$

The important feature of the approximation (2.4) is now that we have to calculate $2L \cdot N$ terms instead of N^2 terms.

This procedure can be applied to both the Coulomb energy and the Coulomb forces, but it is somewhat delicate since the associated formula (2.2) puts a condition on the x^i and x^j .

3. Application of the product decomposition method to the calculation of the Coulomb energy

We first reproduce the formula for the Coulomb energy (Eq. (3.30) in [5]). The basic cell is assumed to be the unit cube

$$C : \left\{ (x, y, z) \mid |x| \leq \frac{1}{2}, |y| \leq \frac{1}{2}, |z| \leq \frac{1}{2} \right\}$$

and the N charges $q_i \in C$ have coordinates (x_i, y_i, z_i) . We then introduce the following notations

$$(3.1) \quad \left\{ \begin{array}{ll} \rho_{ij}(\ell, m) &= [(y_i - y_j + \ell)^2 + (z_i - z_j + m^2)^{\frac{1}{2}}], & \ell, m \in \mathbb{Z} \\ Be[\rho, x] &= 4 \sum_{p=1}^{\infty} K_0(2\pi p \cdot \rho) \cos(2\pi p x), & \rho > 0 \\ L[y, z] &= \log\{1 - 2 \cos(2\pi y) e^{-2\pi|z|} + e^{-4\pi|z|}\} \\ Q_0 &= -1.942248 \dots \end{array} \right. \quad K_0 = \text{Bessel function}$$

Then the Coulomb energy contained in C due to the N charges and all their periodic images is given by

$$(3.2) \quad \begin{aligned} E &= \frac{1}{2} \sum_{i \neq j=1}^N q_i q_j \left\{ \sum_{m, \ell=-\infty}^{\infty} Be[\rho_{ij}(\ell, m), x_i - x_j] \right. \\ &\quad \left. - \sum_{n=-\infty}^{\infty} L[y_i - y_j, z_i - z_j + n] \right. \\ &\quad \left. + \frac{2\pi}{3} \left(\sum_{i=1}^N q_i \vec{x}_i \right)^2 + 2\pi((z_i - z_j)^2 - |z_i - z_j|) \right\} + Q_0 \cdot \sum_{i=1}^N q_i^2 \\ &=: E_B + E_L + \frac{2\pi}{3} D^2 + E_z + Q_0 \cdot \sum_{i=1}^N q_i^2, \end{aligned}$$

with the obvious definitions of the five energy contributions, and $\vec{x} = (x, y, z)$.

Remarks:

- a) If the periodic system is only in x, y -direction and z ranges in a finite height then the corresponding expression is (see [5], formula (3.31))

$$(3.3) \quad E = \frac{1}{2} \sum_{i \neq j=1}^N q_i q_j \left\{ \sum_{\ell=-\infty}^{\infty} Be[\rho_{ij}(\ell, 0), x_i - x_j] - L[y_i - y_j, z_i - z_j] \right. \\ \left. - 2\pi |z_i - z_j| \right\} + \hat{Q}_0 \cdot \sum_{i=1}^N q_i^2$$

with $\hat{Q}_0 = -1.955013 \dots$

- b) If the basic cell is not a cube, but still orthorhombic, the expressions are just slightly changed (see [4]): putting $x = a \cdot \xi$, $y = b \cdot \eta$, $z = c \cdot \zeta$

$$\tilde{\rho}_{ij}(\ell, m) = \left(\frac{b}{a}\right)^2 (\eta_i - \eta_j + \ell)^2 + \left(\frac{c}{a}\right)^2 (\zeta_i - \zeta_j + m)^2 ,$$

$$\tilde{L}[\eta, \zeta] = \log[1 - 2 \cos(2\pi\eta) e^{-2\pi|\zeta|\cdot\frac{c}{b}} + e^{-4\pi|\zeta|\cdot\frac{c}{b}}]$$

one now has in the place of (3.2)

$$(3.4) \quad E = \frac{1}{2a} \sum_{i \neq j=1}^N q_i q_j \left\{ \sum_{m, \ell=-\infty}^{\infty} Be[\tilde{\rho}_{ij}(\ell, m), \xi_i - \xi_j] \right. \\ \left. - \sum_{n=-\infty}^{\infty} \tilde{L}[\eta_i - \eta_j, \zeta_i - \zeta_j + n] + 2\pi \frac{c}{b} ((\zeta_i - \zeta_j)^2 - |\zeta_i - \zeta_j|) \right\} \\ + Q_0(a, b, c) \cdot \sum_{i=1}^N q_i^2$$

with

$$(3.5) \quad Q_0(a, b, c) = 2 \sum_{\ell=1}^{\infty} \sum_{m, n=-\infty}^{\infty} ' K_0\left(\frac{2\pi\ell}{a} \sqrt{(b \cdot m)^2 + (c \cdot n)^2}\right) \\ - 2 \sum_{n=1}^{\infty} \log(1 - e^{-2\pi n \frac{c}{b}}) + \gamma - \log\left(4\pi \frac{a}{b}\right) ,$$

where $\gamma \cong 0.577216 \dots$ is Euler's constant and the prime on the summation sign indicates that the term with $(m, n) = (0, 0)$ is to be omitted. The alterations for the analog of (3.3) are obvious except for \hat{Q} which now becomes

$$(3.6) \quad \hat{Q}(a, b) = 4 \sum_{\ell, m=1}^{\infty} K_0\left(2\pi\ell \cdot m \cdot \frac{b}{a}\right) + \gamma - \log\left(4\pi \frac{a}{b}\right) .$$

- c) If $\rho_{ij}(\ell, m) \rightarrow 0$, which is possible for $-1 \leq \ell, m \leq 1$, then the two terms $Be[,]$ and $L[,]$ in (3.2) or (3.3) that become singular have to be combined and yield a regular

term. One is led to the following result: Set

$$(3.7) \quad G[\rho, x] := \frac{1}{\sqrt{x^2 + \rho^2}} + \sum_{\ell=1}^{\infty} \left(-\frac{1}{\ell^2} \right) \rho^{2\ell} \left\{ \zeta(2\ell + 1, 1 + x) + \zeta(2\ell + 1, 1 - x) \right\} \\ - \psi(1 + x) - \psi(1 - x) ,$$

where ψ is the Digamma function and

$$\zeta(n, s) = \sum_{k=0}^{\infty} \frac{1}{(s + k)^n} , \quad n \neq 0, -1, -2$$

is the Hurwitz Zeta-function (a multiple of the polygamma function). Further, define

$$(3.8) \quad \begin{aligned} H[y, z] &= \log(y^2 + z^2) - L[y, z] + \log(4\pi^2) \\ &= 2 \cdot z + \frac{1}{3} (y^2 - z^2) + \frac{1}{90} (y^4 - 6y^2 z^2 + z^4) \\ &\quad + \frac{2}{2835} (y^6 - 15y^4 z^2 + 15y^2 z^4 - z^6) + \text{higher order terms} . \end{aligned}$$

If $\rho_{ij}(\ell, m)$ becomes small (say < 0.1) then the combination $Be[\rho_{ij}(\ell, m), x_i - x_j] - L[y_i - y_j, z_i - z_j + m]$ in (3.3) may be replaced by

$$(3.9) \quad \begin{aligned} E_{ij} &:= G[\rho_{ij}(\ell, m), x_i - x_j] + H[\pi(y_i - y_j + \ell), \pi(z_i - z_j + m)] \\ &\quad - 5.0620485 . \end{aligned}$$

We now develop the product decomposition for the Coulomb energy as defined by (3.2). For the term involving the Bessel function this is based on

Lemma 1 (*Gegenbauer's Addition Theorem*)

Assume that $R > r > 0$. Then one has

$$(3.10) \quad K_0 \left[\sqrt{R^2 + r^2 - 2rR \cos \varphi} \right] = K_0(R) I_0(r) + 2 \sum_{\nu=1}^{\infty} K_{\nu}(R) I_{\nu}(r) \cos(\nu \varphi) .$$

For the proof of (3.10) and related theorems the interested reader is referred to the classical book of Watson [6].

For the terms of the form $L[y_i - y_j, z_i - z_j + m]$ we can use identities (3.9) and (3.10) of [5] which lead to the identity given in

Lemma 2 For any η, ζ with $\eta^2 + (\zeta + m)^2 > 0$, $0 \leq \zeta \leq 1$ one has

$$(3.11) \quad - \sum_{m=-\infty}^{\infty} L[\eta, \zeta + m] = 2 \sum_{\ell=1}^{\infty} \frac{1}{\ell(1 - \exp(-2\pi\ell))} \left\{ \exp[-2\pi\ell(1 - |\zeta|)] \right. \\ \left. + \exp[-2\pi\ell|\zeta|] \right\} \cos(2\pi\ell\eta) .$$

Lemmas 1 and 2 are the basis for the complete product decomposition of the Coulomb energy. First we now derive the general expression and then in a separate section the actual calculation is developed.

Let q_i be a charge in the basic cell C and q_n another charge which may be in C or any periodic image of a charge in C . Denote by r and φ polar coordinates in the (y, z) -plane so that the distance between q_i and q_n is given by

$$(3.12) \quad \rho(i, n) = \sqrt{r_i^2 + r_n^2 - 2r_i r_n \cos(\varphi_i - \varphi_n)} .$$

For the moment a convenient assumption is that all charges in the basic cell C are ordered according to their distance to the center in the (y, z) -plane and one has

$$(3.13) \quad 0 < r_1 < r_2 < \dots < r_N \leq \frac{\sqrt{2}}{2} .$$

We will skip the strict inequality signs later on. In this notation the part of the Coulomb energy in (3.2) involving the Bessel functions may be written as

$$(3.14) \quad E_B = \frac{1}{2} \sum_{i=1}^N q_i \sum_{n>i} q_n Be[\rho(i, n), x_i - x_n] .$$

We can then apply Lemma 1 and the addition theorem for cosines to find the complete product decomposition in (3.14). To this end, it is convenient to introduce the following abbreviations:

$$(3.15) \quad \left\{ \begin{array}{lcl} c_{pi} & = & \cos(2\pi p x_i) \\ s_{pi} & = & \sin(2\pi p x_i) \\ c_i^\nu & = & \cos(\nu \cdot \varphi_i) \\ s_i^\nu & = & \sin(\nu \cdot \varphi_i) \\ K_{pi}^\nu & = & K_\nu(2\pi p \cdot r_i) \\ I_{pi}^\nu & = & I_\nu(2\pi p \cdot r_i) . \end{array} \right.$$

In this notation one gets

$$(3.16) \quad \begin{aligned} Be[\rho(i, n), x_i - x_n] &= 4 \sum_{p=1}^{\infty} (c_{pi} c_{pn} + s_{pi} \cdot s_{pn}) \left\{ K_{pn}^0 \cdot I_{pi}^0 + \right. \\ &\quad \left. + 2 \sum_{\nu=1}^{\infty} K_{pn}^\nu \cdot I_{pi}^\nu (c_i^\nu \cdot c_n^\nu + s_i^\nu \cdot s_n^\nu) \right\} . \end{aligned}$$

For the application of (3.16) a rather careful analysis is necessary and this will be carried out in Section 4.

We also need the product decomposition of the term

$$L_{ij} := - \sum_{n=-\infty}^{\infty} L[y_i - y_j, z_i - z_j + n] .$$

It is again convenient to introduce the following abbreviations:

$$(3.17) \quad \begin{cases} e_0 &= \exp(-2\pi) \\ e_i &= \exp(-2\pi z_i) \\ \bar{e}_i &= \exp(-2\pi(1 - z_i)) \\ \hat{c}_{pi} &= \cos(2\pi p y_i) \\ \hat{s}_{pi} &= \sin(2\pi p y_i) . \end{cases}$$

Then Lemma 2 and the addition theorem for cosines immediately lead to

$$(3.18) \quad L_{ij} = 2 \sum_{p=1}^{\infty} \frac{1}{p(1 - (e_0)^p)} \left\{ (e_i \cdot \bar{e}_j)^p + \left(\frac{e_j}{e_i} \right)^p \right\} (\hat{c}_{pi} \cdot \hat{c}_{pj} + \hat{s}_{pi} \cdot \hat{s}_{pj}) .$$

Of course this is only defined if $0 \leq z_i < z_j \leq 1$. Finally the contribution to the energy stemming from the term

$$\frac{1}{2} \sum_{i \neq j} q_i q_j ((z_i - z_j)^2 - |z_i - z_j|) =: E_z$$

can be rewritten such that $\frac{1}{2} N(N-1)$ pairs (i, j) are avoided:

Using the charge neutrality some algebra shows that one can write

$$(3.19) \quad E_z = 2\pi \left[\sum_{i=1}^{N-1} q_i (D_z^i + Q_i z_i) - D_z^2 \right]$$

where we have set

$$(3.20) \quad D_z = \sum_{i=1}^N q_i z_i, \quad D_z^i = \sum_{j=i+1}^N q_j z_j, \quad Q_i = \sum_{j=1}^i q_j .$$

4. Calculation of the Coulomb energy

4.1. Estimates for truncation errors

We first analyze the convergence behaviour of the term $Be[\rho(i, n), x_i - x_n]$ in (3.14). Since we are dealing with sums of alternating signs it seems sensible to assume that if all terms occurring are given with an error less than e^{-a} , where a is a measure for the accuracy required, then the total sum has the same accuracy.

Now

$$(4.1) \quad Be[\rho, x] = 4 \sum_{p=1}^{\infty} K_0(2\pi p \rho) \cos(2\pi p x) ,$$

and the error if we truncate the series at $p = P$ can be estimated as follows

$$\left| \sum_{p=P+1}^{\infty} K_0(2\pi p\rho) \cos(2\pi p x) \right| \leq \sum_{p=P+1}^{\infty} K_0(2\pi p\rho) < \int_P^{\infty} K_0(2\pi \rho p) dp .$$

For the integral we can use the estimates given in [1], p. 481, # 11.1.18 leading to the bound

$$(4.2) \quad 4 \sum_{p=P+1}^{\infty} K_0(2\pi p\rho) < \frac{5.016}{2\pi\rho} \frac{1}{\sqrt{2\pi\rho \cdot P}} \exp(-2\pi\rho \cdot P) =: Fe[\rho, P] .$$

The estimate (4.2) is not applicable for $P = 0$. For this case one can determine the values ρ directly for which

$$(4.3) \quad Be[\rho, 0] \leq e^{-a} .$$

This condition determines the cut-off distance R_c : if $\rho(i, n) > R_c$ then all charges q_n may be neglected whose distance to q_i is greater than R_c .

In figure 1 we show a plot of $10^6 \cdot Be[\rho, 0]$. It tells us e.g. that for an error $\leq 10^{-6}$ one has $R_c \cong 2.24$.

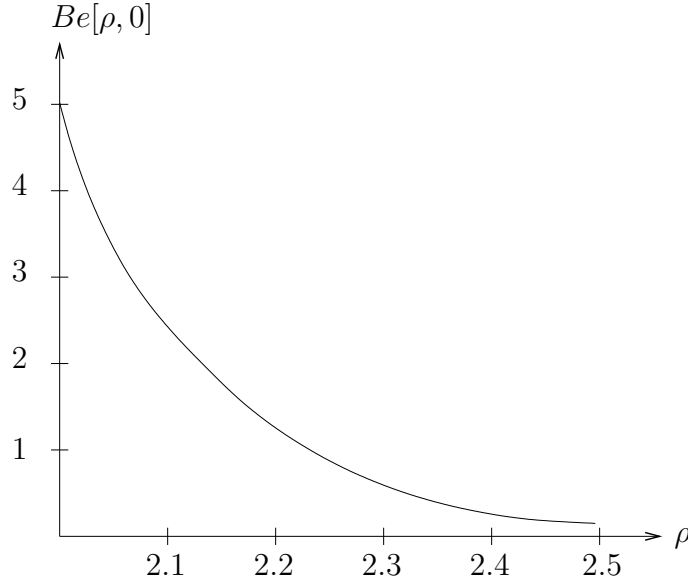


Fig. 1

For a given distance ρ on the other hand the number P giving the term $Be[\rho, x]$ with the required accuracy is defined by the smallest number $P = P_a(\rho) \in \mathbb{N}$ such that

$$(4.4) \quad Fe[\rho, P] \leq e^{-a} .$$

As an illustration we show in Figure 2 some typical curves $P_a(\rho)$

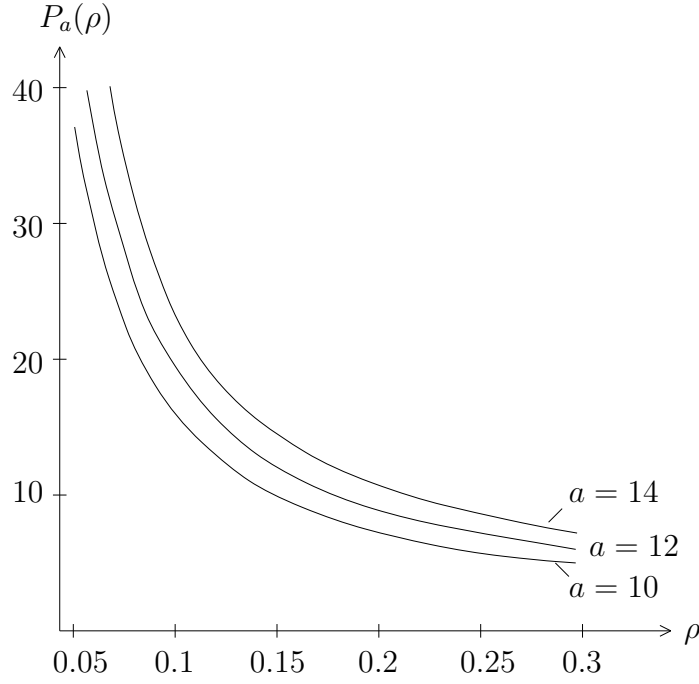


Fig. 2

The next important information concerns the number of ν -terms needed in the Gegenbauer-Theorem (3.10). This now requires by (3.16) that

$$(4.6) \quad 8 \sum_{\nu=\gamma+1}^{\infty} K_{\nu}(R) I_{\nu}(r) \leq e^{-a} .$$

In our applications typically $0 \leq r < R < 15$ so that we may assume that $\gamma > R$ and the asymptotic expansions for large ν are valid as given in [1], p. 378, # 9.7.7 and 9.7.8. reading

$$(4.7) \quad I_{\nu}(\nu \cdot z) = \frac{1}{\sqrt{2\pi\nu}} \frac{e^{\nu\eta(z)}}{(1+z^2)^{\frac{1}{4}}} \left\{ 1 + \sum_{k=1}^{\infty} \frac{u_k(t(z))}{\nu^k} \right\}$$

$$(4.8) \quad K_{\nu}(\nu \cdot z) = \sqrt{\frac{\pi}{2\nu}} \frac{e^{-\nu\eta(z)}}{(1+z^2)^{\frac{1}{4}}} \left\{ 1 + \sum_{k=1}^{\infty} (-1)^k \frac{u_k(t(z))}{\nu^k} \right\} ,$$

where

$$(4.9) \quad \eta(z) = \sqrt{1+z^2} + \log \left(\frac{z}{1+\sqrt{1+z^2}} \right)$$

and

$$(4.10) \quad t(z) = (1+z^2)^{-1/2} .$$

The functions $u_k(t)$ are given in [1], p. 366, #9.3.9. The first three are

$$(4.11) \quad u_0 = 1, \quad u_1(t) = \frac{3t - 5t^3}{24}, \quad u_2(t) = \frac{8(t^2 - 462t^4 + 385t^6)}{1152}.$$

We now set $\nu \cdot z = r$ in (4.7) and $\nu \cdot z = R$ in (4.8). The important term now is the combination

$$(4.12) \quad \exp\left(\nu \cdot \eta\left(\frac{r}{\nu}\right)\right) \cdot \exp\left(-\nu \eta\left(\frac{R}{\nu}\right)\right) =: Pr(\nu, r, R).$$

After some rearrangement one finds

$$(4.13) \quad Pr(\nu, r, R) = \left(\frac{r}{R}\right)^\nu \exp\left[-\nu\left(w\left(\frac{R}{\nu}\right) - w\left(\frac{r}{\nu}\right)\right)\right],$$

where $w(s) = \sqrt{1+s^2} - \log(1 + \sqrt{1+s^2})$.

For $|s| < 1$ we can expand $w(s)$ in a power series:

$$(4.14) \quad \begin{aligned} w(s) &= 1 - \log 2 + \frac{s^2}{4} - \frac{s^4}{32} + \frac{s^6}{96} - \frac{5 \cdot s^8}{1024} + \dots \\ &= 1 - \log 2 + w_0(s) \end{aligned}$$

with the obvious definition of $w_0(s)$. The important point now is that the “large” term $\nu(1 - \log 2)$ cancels, and we can write

$$(4.15) \quad I_\nu(r) \cdot K_\nu(R) = \frac{1}{2\nu} \left(\frac{r}{R}\right)^\nu \cdot \exp\left[-\nu\left(w_0\left(\frac{R}{\nu}\right) - w_0\left(\frac{r}{\nu}\right)\right)\right] \cdot U_1\left(\frac{r}{\nu}\right) \cdot U_2\left(\frac{R}{\nu}\right),$$

where we have abbreviated

$$(4.16) \quad U_1(s) = (1 + s^2)^{-\frac{1}{4}} \cdot \left\{1 + \sum_{k=1}^{\infty} \frac{u_k(t(s))}{\nu^k}\right\}$$

$$(4.17) \quad U_2(s) = (1 + s^2)^{-\frac{1}{4}} \cdot \left\{1 + \sum_{k=1}^{\infty} (-1)^k \frac{u_k(t(s))}{\nu^k}\right\}.$$

Note that $U_1(s)$, $U_2(s)$ are close to 1 for s small, i.e. for large ν .

For $\nu > R > r \geq 0$ one has the simple estimate

$$(4.18) \quad I_\nu(r) K_\nu(R) < \frac{1}{2\nu} \left(\frac{r}{R}\right)^\nu.$$

We now return to (4.6) and use the bound (4.18) to deduce

$$(4.19) \quad 8 \sum_{\nu=\gamma+1}^{\infty} K_\nu(R) I_\nu(r) < 4 \int_{\gamma}^{\infty} \frac{1}{\nu} \left(\frac{r}{R}\right)^\nu d\nu = 4 \cdot E_1\left(\gamma \log\left(\frac{R}{r}\right)\right),$$

where $E_1(s)$ denotes the exponential integral (see [1], p. 228) for which we may use the bound ([1], p. 231)

$$(4.20) \quad E_1(s) < \frac{1}{s} e^{-s} .$$

Combining (4.19) and (4.20) we arrive at the truncation condition for γ (setting $\lambda = \log(\frac{R}{r})$)

$$(4.21) \quad \frac{4}{\gamma \cdot \lambda} e^{-\gamma \cdot \lambda} \leq e^{-a} .$$

We can put this into a more convenient form. Set

$$(4.22) \quad f(s) = s + \log(s)$$

and let α be the solution of

$$(4.23) \quad f(s) = a + \log 4 .$$

Then the cut-off condition for the largest values $\nu = \gamma$ to be taken for given accuracy a is

$$(4.24) \quad \gamma \geq \frac{\alpha}{\log(\frac{R}{r})} .$$

As a last item we need the cut-off condition for the sum on the right of (3.11). This requires

$$(4.25) \quad 2 \sum_{\ell=L+1}^{\infty} \frac{1}{\ell} \exp[-2\pi\ell \cdot d] \leq e^{-a} ,$$

with $d = |z_j - z_i|$ or $d = 1 - |z_j - z_i|$. Again we have

$$(4.26) \quad 2 \sum_{\ell=L+1}^{\infty} \frac{1}{\ell} \exp[-2\pi\ell \cdot d] < 2 \int_L^{\infty} \frac{1}{\ell} \exp[-2\pi d \cdot \ell] d\ell = 2E_1(2\pi d \cdot L) ,$$

and therefore the calculation leading to (4.24) can be repeated and one arrives at

$$(4.27) \quad L \geq \frac{\beta}{2\pi \cdot d} ,$$

where β is the solution of

$$(4.28) \quad f(s) = a + \log 2 .$$

4.2. Procedure for E_B

The main issue of this work is the calculation of the energy contribution E_B defined by (3.14) - (3.16) as

$$(4.29) \quad E_B = 2 \sum_{i=1}^N q_i \sum_{r_n \geq r_i} q_n \sum_{p=1}^{\infty} (c_{pi} c_{pn} + s_{pi} s_{pn}) \left\{ K_{pn}^0 I_{pi}^0 + \right. \\ \left. + 2 \sum_{\nu=1}^{\infty} K_{pn}^{\nu} I_{pi}^{\nu} (c_i^{\nu} c_n^{\nu} + s_i^{\nu} s_n^{\nu}) \right\}.$$

We assume that the accuracy required is given by the condition that the error is to be at most e^{-a} , a = accuracy parameter. Since a will usually be chosen once for all we omit the dependence of various quantities on a later on.

The first information we use concerns the “influence region” given by condition (4.3): only charges q_n within the region $G \cup C$ have to be considered in (4.29) (see Figure 2)

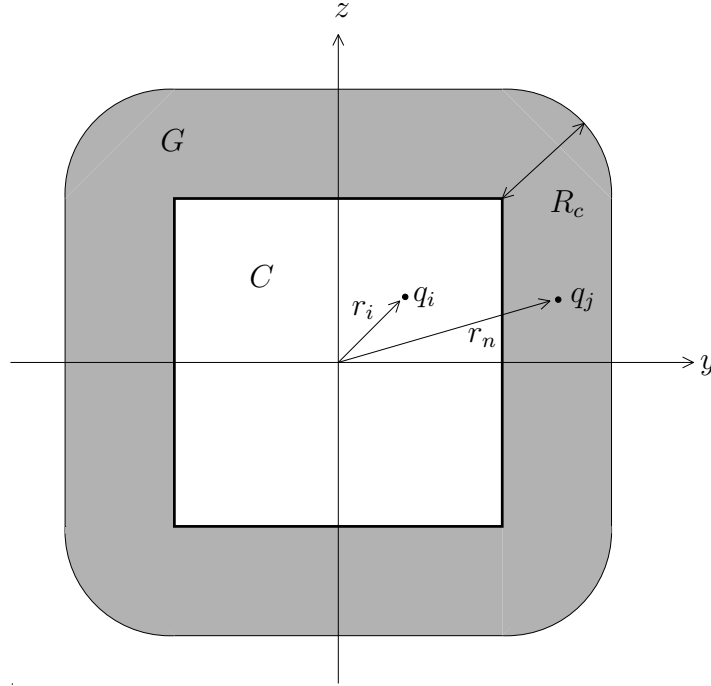


Fig. 3

The cut-off distance R_c is given in equation (4.3).

In C we introduce a partition into sectorial domains as follows:

Let (r, φ) be polar coordinates in the (y, z) -plane. Set

$$\varphi_{\ell} = \frac{2\pi}{L} \cdot \ell, \quad \ell = 1, \dots, L,$$

where L will be chosen depending on the number N of charges in C . Further select a sequence

$$0 < r_0 < r_1 < \dots < r_K = \frac{\sqrt{2}}{2} < r_{K+1} ,$$

where K will also depend on N . We then define the domains

$$(4.30) \quad S_{k\ell} = \{(r, \varphi) \mid r_{k-1} < r \leq r_k, \varphi_{\ell-1} \leq \varphi < \varphi_\ell\}$$

and the annular domains

$$(4.31) \quad S_k = \{(r, \varphi) \mid r_{k-1} < r \leq r_k\}$$

as well as the disk

$$(4.32) \quad S_0 = \{(r, \varphi) \mid r \leq r_0\} .$$

The calculation of E_B consists of two parts: for all charges $q_i \in C$, $q_n \in C \cup G$ whose distances r_i, r_n to the origin differ only slightly we calculate pairwise, and for the other pairs the product decomposition is applied.

a) **Pairwise calculation**

We denote the associated energy contribution by E_{BP} which can be calculated as

$$(4.33) \quad E_{BP} = 2 \sum_{k=1}^K \sum_{\substack{q_i \in S_{k-1} \cap C \\ q_n \in S_{k-1} \cup S_k}} q_i q_n E_{in} .$$

Here E_{in} is given by (3.9)

$$(4.34a) \quad E_{in} = G[\rho(i, n), x_i - x_n] + H[(y_i - y_n) \cdot \pi, (z_i - z_n) \cdot \pi] - 5.0620485$$

if $\rho(i, n) = \sqrt{r_i^2 + r_n^2 - 2r_i r_n \cos(\varphi_i - \varphi_n)} \leq \delta$ and

$$(4.34b) \quad E_{in} = \frac{1}{2} Be[\rho(i, n), x_i - x_n]$$

if $\rho(i, n) > \delta$. Here $\delta \cong 0.1$ may be chosen and the functions $G[]$, $H[]$ and $Be[]$ are defined in (3.7), (3.8) and (3.1).

b) **Product decomposition: Recursions for $\nu = 0$**

We now consider any k with $1 \leq k < K + 1$ and assume that $q_i \in S_{k-1}$, $q_n \in G \cup C - S_1 \cup S_2 \cup \dots \cup S_k$, i.e. $r_n > r_k$.

Our aim now is to calculate of (4.29) the sums

$$2 \sum_{q_i \in S_{k-1}} q_i \sum_{r_n > r_k} q_n \sum_{p=1}^P (c_{pi} c_{pn} + S_{pi} S_{pn}) K_{pn}^0 I_{pi}^0 ,$$

where the limit P is determined by inequality (4.4) with $\rho = \sqrt{r_n^2 + r_i^2 - 2r_n r_i \cos(\varphi_n - \varphi_i)}$ there. This can be done in the following way: Let P_k be the smallest number satisfying

$$(4.35) \quad Fe[r_k - r_{k-1}, P] \leq e^{-a} ,$$

with $Fe[\]$ defined in (4.2). For any $1 \leq p \leq P_k$ let $R(p)$ the solution of

$$Fe[R, p] = e^{-a} , \quad (R = r_k - r_{k-1}) .$$

Note that roughly one has $R(p) = \frac{\text{const.}}{p}$. For any sectorial domain $S_{k\ell}$ we now define a domain $G_p(k, \ell)$ containing the charges q_n that are sufficiently far from $S_{k\ell}$ (see Fig. 3)

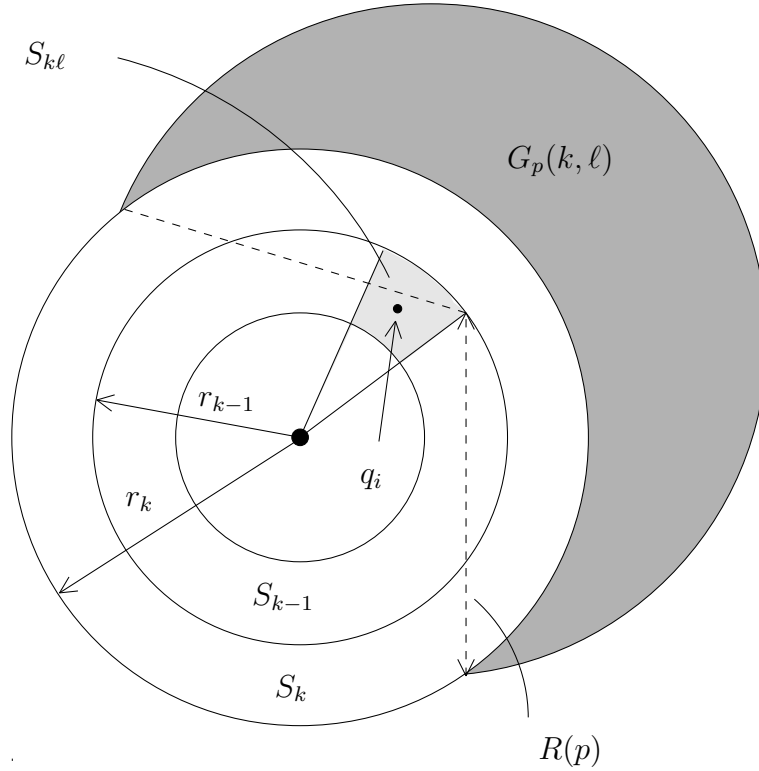


Fig. 4

$$(4.37) \quad G_p(k, \ell) = \{(r, \varphi) \mid r > r_k \wedge r^2 + r_{k-1}^2 - 2r r_{k-1} \cos(\varphi - \varphi_\ell) \leq R^2(p)\} .$$

We will also need the intersections

$$(4.38) \quad I_p(k, \ell) := G_p(k, \ell) \cap G_p(k, \ell + 1) .$$

We now define a recursion for fixed k and p , with $1 \leq k \leq K + 1$, $1 \leq p \leq P_k$.

Start of the recursion: Set

$$(4.39) \quad A_p^0(k, 1) = \sum_{q_n \in G_p(k, 1)} q_n c_{pn} K_{pn}^0 .$$

Recursion step: Set

$$(4.40) \quad A_p^0(k, \ell + 1) = A_p^0(k, \ell) + \sum_{q_n \in I_p^+(k, \ell)} q_n c_{pn} K_{pn}^0 - \sum_{q_n \in I_p^-(k, \ell)} q_n c_{pn} K_{pn}^0 .$$

Here the regions $I_p^+(k, \ell)$, $I_p^-(k, \ell)$ (see Fig. 5) are defined by

$$(4.41) \quad I_p^+(k, \ell) = G_p(k, \ell + 1) \setminus I_p(k, \ell) ,$$

$$(4.42) \quad I_p^-(k, \ell) = G_p(k, \ell) \setminus I_p(k, \ell) .$$

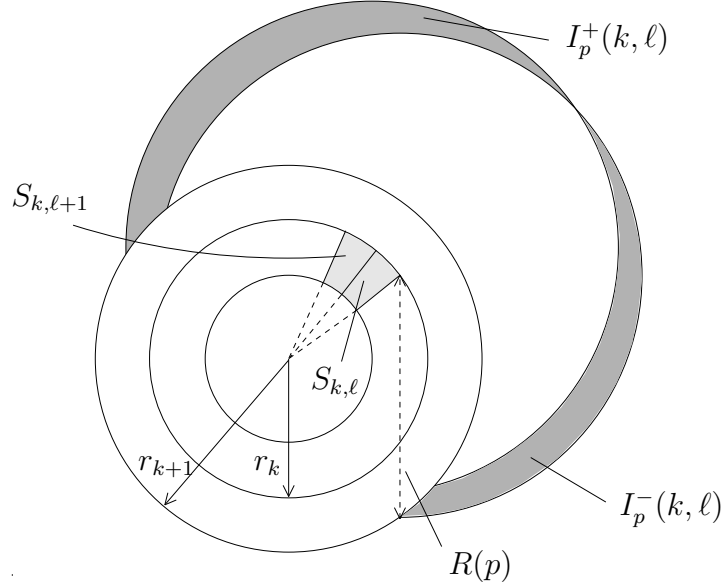


Fig. 5

Remark: a) The recursion scheme avoids unnecessary overlaps in the sums arising from (4.29) and the domains $G_p(k, \ell)$ ensure that no terms are calculated whose contribution to the energy would be smaller than e^{-a} .

b) The domains S_k , $S_{k, \ell}$, $G_p(k, \ell)$, $I_p^\pm(k, \ell)$ have to be determined only once and remain the same for possibly many calculations.

We also need the associated terms

$$(4.43) \quad a_p^0(k, \ell) = \sum_{q_i \in S(k-1, \ell)} q_i c_{pi} I_{pi}^0 .$$

The contribution to E_B then is

$$(4.44) \quad E_B^0(k, p) = 2 \sum_{\ell=1}^L a_p^0(k, \ell) A_p^0(k, \ell) .$$

We can repeat the recursions with terms

$$(4.45) \quad \tilde{a}_p^0(k, \ell) = \sum_{q_i \in S(k, \ell)} q_i s_{pi} I_{pi}^0$$

and analogously

$$(4.46) \quad \tilde{A}_p^0(k, \ell) = \sum_{q_n \in G_p(k, \ell)} q_n s_{pn} K_{pn}^0 ,$$

leading to the corresponding energy contribution

$$(4.47) \quad \tilde{E}_B^0(k, p) = 2 \sum_{\ell=1}^L \tilde{a}_p^0(k, \ell) \tilde{A}_p^0(k, \ell) .$$

The energy contribution to E_B stemming from the product decomposition then finally is

$$(4.48) \quad \mathbf{E}_B^0 = \sum_{k=1}^{K+1} \sum_{p=1}^{P_k} (\mathbf{E}_B^0(\mathbf{k}, p) + \tilde{\mathbf{E}}_B^0(\mathbf{k}, p)) .$$

c) Recursions for $1 \leq \nu$

There is one additional difficulty arising in the calculations involving the Bessel functions I_ν , K_ν : both numbers may be huge or extremely small if ν is large. Products of the two terms however will in our case stay moderate. We now can take advantage of the asymptotic behavior described by formula (4.15).

If $\nu > R \geq r > 0$ then one has

$$(4.49) \quad \left| I_\nu(r) K_\nu(R) - \frac{1}{2\nu} \left(\frac{r}{R} \right)^\nu \right| \leq e^{-a}$$

provided

$$(4.50) \quad \frac{1}{2\nu} \left(\frac{r}{R} \right)^\nu \left(1 - \exp \left[-\nu \left(w_0 \left(\frac{R}{\nu} \right) - w_0 \left(\frac{r}{\nu} \right) \right) \right] \cdot U_1 \left(\frac{r}{\nu} \right) U_2 \left(\frac{R}{\nu} \right) \right) \leq e^{-a}$$

with $w_0(\cdot)$ defined in (4.14) and U_1, U_2 in (4.16), (4.17).

If we replace R by $2\pi p r_n$, r by $2\pi p \cdot r_i$ then a sufficient condition for the validity of (4.50) is (see Appendix)

$$(4.51) \quad H[\nu, r_i, r_n, p] := \frac{1}{2\nu^2} \left(\frac{r_i}{r_n} \right)^\nu \left[\left(1 + \frac{1}{\nu} \right) r_n^2 - \left(1 - \frac{1}{\nu} \right) r_i^2 \right] \pi^2 p^2 \leq e^{-a} ,$$

where it is assumed that $\nu > 2\pi(R_c + \frac{\sqrt{2}}{2}) \geq 2\pi p \cdot r_n$ and $r_n > r_i$.

As a simple approximation one may take (see Section 5)

$$(4.52) \quad \nu \geq \nu_0(r_n, p) = (r_n^2 \pi^2 p^2 e^a)^{1/3} .$$

As an illustration we give a numerical example:

Choose $a = 10$, so that $e^{-10} \cong 0.0000454$,

$r_i = 0.2$, $r_n = 0.22$, $p = 3$.

From (4.52) one finds that for $\nu \geq 28$ one has

$$\left\{ \frac{1}{2\nu} \left(\frac{r_i}{r_n} \right)^{2\nu} - K_\nu(2\pi p r_n) I_\nu(2\pi p r_i) \right\} \leq 0.0000454$$

while in fact $\{ \} \cong 0.0000444$.

The approximation (4.52) yields $\nu = 46$ as the critical value.

The condition (4.51) is useful as long as p is not too large (which is possible if $r_n - r_i$ is small).

Setting

$$H_a[\nu, r_i, r_n, p] = \left(\frac{1}{2\nu} \left(\frac{r_i}{r_n} \right)^\nu - K_\nu(\pi p r_n) \cdot I_\nu(\pi p r_i) \right) e^a$$

a typical plot looks like figure 6:

level line $H_a[\nu, r_i, r_n, p] = 1$
for $r_i = 0.58$, $r_n = 0.6$, $e^a = 10^6$

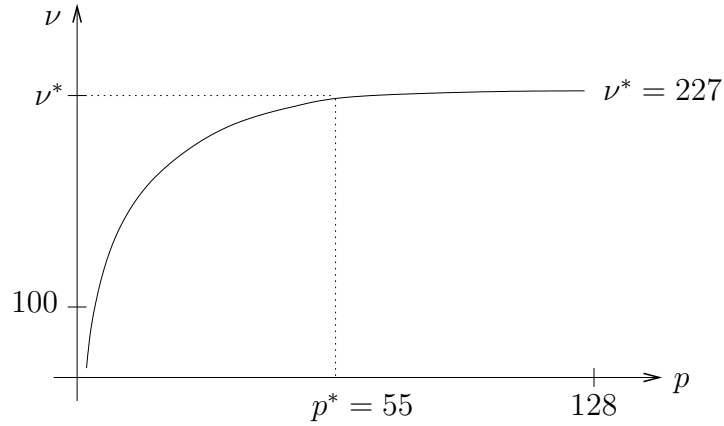


Fig. 6

Values for error $\leq 10^{-6}$:

$y = 440$: condition (4.24)

$P_a(0.02) = 128$: condition (4.4)

ν^* is the smallest integer satisfying

$$(4.52a) \quad \frac{1}{2\nu} \left(\frac{r_i}{r_n} \right)^\nu \leq e^{-a} ,$$

and p^* is the value for which

$$(4.52b) \quad K_\nu(\pi p r_k) I_\nu(\pi p r_i) \leq e^{-a} .$$

Note that ν^* and p^* are substantially smaller than the associated values y and $P_a(\rho)$.

We now can define the recursions involving the Bessel functions of index $\nu \geq 1$.

We first use the cut-off condition for the ν -values given by (4.24): if $r_n > r_i$ and

$$(4.53) \quad \nu \geq \nu_m \geq \frac{\alpha}{\log\left(\frac{r_n}{r_i}\right)} ,$$

then these values of ν may be neglected.

We turn this condition around in the following way: any charge q_n with distance r_n from the center may be neglected if

$$(4.54) \quad r_n > r_i e^{\frac{\alpha}{\nu}} .$$

Here α is determined by (4.23) and depends only on the accuracy parameter a . The recursion scheme is thus as follows.

Take a fixed value of k , fixed value of $p \leq P_k$ and define the disk $C_{k\nu}$ as

$$(4.55) \quad C_{k\nu} = \left\{ (r, \varphi) \mid r \leq r_k e^{\frac{\alpha}{\nu}} \right\} .$$

Then, set in analogy to (4.39)

$$(4.56) \quad A_p^\nu(k, 1) = \sum_{q_n \in G_p(k, 1) \cap C_{k\nu}} q_n c_{pn} c_n^\nu K_{pn}^\nu ,$$

with the same recursion step

$$(4.57) \quad A_p^\nu(k, \ell + 1) = A_p^\nu(k, \ell) + \sum_{q_n \in I^+(k, \ell) \cap C_{k\nu}} q_n c_{pn} c_n^\nu K_{pn}^\nu - \sum_{q_n \in I^-(k, \ell) \cap C_{k\nu}} q_n c_{pn} c_n^\nu K_{pn}^\nu .$$

The associated terms are

$$(4.58) \quad a_p^\nu(k, \ell) = \sum_{q_i \in S(k-1, \ell)} q_i c_{pi} c_i^\nu I_{pi}^\nu .$$

The recursions run for all values of ν from $\nu = 1$ to $\nu = \nu_m(k) \leq \frac{\alpha}{\log(\frac{r_k}{r_{k-1}})}$.

The value of $\nu_m(k)$ may be rather large and one can therefore use the simplification suggested by inequality (4.49): for given $\nu \leq \nu_m(k)$ let $R_k(\nu, p)$ the solution of

$$(4.59) \quad H[\nu, r_k, R, p] = e^{-a}.$$

Then in the disk

$$(4.60) \quad C_{\nu kp} = \{(r, \varphi) \mid r \leq R_k(\nu, p)\}$$

one can replace in (4.56)

$$K_{pn}^\nu \text{ by } \hat{K}_n^\nu := r_n^{-2\nu}$$

and in (4.58)

$$I_{pi}^\nu \text{ by } \hat{I}_i^\nu := \frac{1}{2\nu} \cdot r_i^{2\nu}.$$

The recursions for $\nu \geq 1$ have to be repeated for slightly modified terms which we get from the expressions in (3.16) according to the following list:

$$(4.61) \quad \begin{cases} \tilde{A}_p^\nu(k, \ell) &= \sum_{q_n \in G_p(k, \ell) \cap C_{k\nu p}} q_n s_{pn} c_n^\nu \hat{K}_n^\nu \\ B_p^\nu(k, \ell) &= \sum_{q_n \in G_p(k, \ell) \cap C_{k\nu p}} q_n c_{pn} s_n^\nu \hat{K}_n^\nu \\ \tilde{B}_p^\nu(k, \ell) &= \sum_{q_n \in G_p(k, \ell) \cap C_{k\nu p}} q_n s_{pn} s_n^\nu \hat{K}_n^\nu. \end{cases}$$

The associated terms are then

$$(4.62) \quad \begin{cases} \tilde{a}_p^\nu(k, \ell) &= \sum_{q_i \in S_p(k-1, \ell)} q_i s_{pi} c_i^\nu \hat{I}_i^\nu \\ b_p^\nu(k, \ell) &= \sum_{q_i \in S_p(k-1, \ell)} q_i c_{pi} s_i^\nu \hat{I}_i^\nu \\ \tilde{b}_p^\nu(k, \ell) &= \sum_{q_i \in S_p(k-1, \ell)} q_i s_{pi} s_i^\nu \hat{I}_i^\nu. \end{cases}$$

The energy contributions are then as in (4.44):

$$(4.63) \quad E_B^\nu(k, p) = 4 \sum_{\ell=1}^L \{a_p^\nu(k, \ell) A_p^\nu(k, \ell) + \dots + \tilde{b}_p^\nu(k, \ell) \cdot \tilde{B}_p^\nu(k, \ell)\}.$$

The total contribution finally is

$$(4.64) \quad E_B = E_B^0 + \sum_{k=1}^K \sum_{p=1}^{P_k} \sum_{\nu=1}^{\nu_m(k)} E_B^\nu(k, p) .$$

4.3. Procedure for E_L

It is convenient for the subsequent analysis to introduce two more sets (see Fig. 6)

$$(4.65) \quad \begin{aligned} Y &= \left\{ (y, z) \mid |y| \leq \frac{1}{2}, |z| > \frac{1}{2} \right\} \\ R_\delta &= \left\{ (y, z) \mid (y, z) \in \mathbb{R}^2 - C, \text{dist}\{(y, z), C\} \leq \delta \right\} . \end{aligned}$$

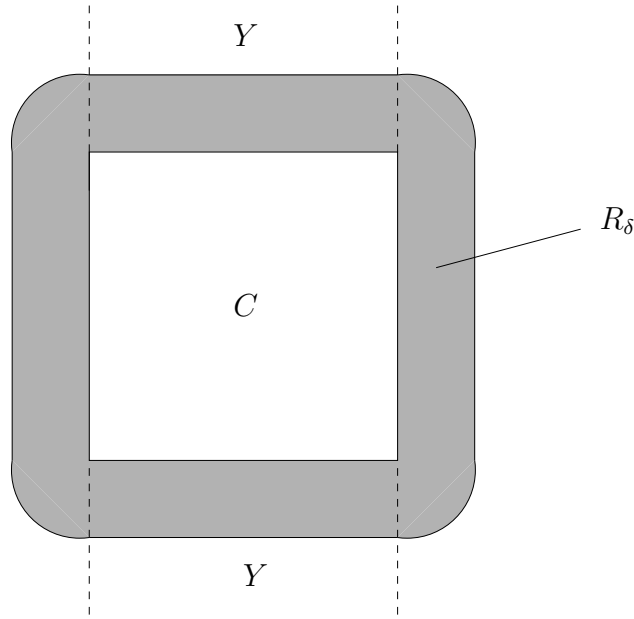


Fig. 7

According to (3.2) the energy contribution denoted as E_L may be written as

$$(4.66) \quad E_L = -\frac{1}{2} \sum_{q_i \in C} \sum_{q_j \in C \cup Y} q_i q_j L[y_i - y_j, z_i - z_j] .$$

We now have to take into account that some terms of E_L have already been included in E_B : the terms that were needed in (4.33). These are all the pairs q_i, q_j where $q_i \in C$, $q_j \in G \cup C$ with $\rho(i, j) \leq \delta$. This implies that all pairs with $q_i \in C$, $q_j \in R_\delta$, $\rho(i, j) \leq \delta$ have been included also, hence we have a correction term

$$(4.67) \quad E_\delta = \frac{1}{2} \sum_{q_i \in C} \sum_{\substack{q_j \in R_\delta \\ \rho(i, j) \leq \delta}} q_i q_j L[y_i - y_j, z_i - z_j] .$$

It remains therefore to calculate the remaining terms of E_L in (4.66), that is

$$(4.68) \quad \hat{E}_L = -\frac{1}{2} \sum_{q_i \in C} \sum_{\substack{q_j \in C \cup Y \\ \rho(i,j) > \delta}} L[y_i - y_j, z_i - z_j] .$$

The calculation of \hat{E}_L , i.e. the approximation with given accuracy, is split up into two parts: for all pairs $(q_i, q_j) \in C$ such that

$$\epsilon < |z_i - z_j| < 1 - \epsilon$$

we will apply the product decomposition as given in (3.18). For all pairs in C with $|z_i - z_j| \leq \epsilon$ or $|z_i - z_j| \geq 1 - \epsilon$ the energy contributions will be calculated pairwise. The choice of ϵ will be discussed later on.

a) **Product decomposition of $E_L(\rho(i, j) > \delta)$**

We split up the basic cell C into M stripes

$$(4.69) \quad \left\{ \begin{array}{l} Z_m = \left\{ (y, z) \mid |y| \leq \frac{1}{2}, \frac{m-1}{M} \leq z < \frac{m}{M} \right\}, \quad m = 1, \dots, M-1 \\ \text{and} \\ Z_M = \left\{ (y, z) \mid |y| \leq \frac{1}{2}, \frac{M-1}{M} \leq z \leq 1 \right\} . \end{array} \right.$$

We now make use of (3.18) and consider first the terms denoted $e_i (= \exp(-2\pi \cdot z_i))$. Choose $q_i \in Z_m$ and $q_j \in Z_{m+\ell}$, $\ell \geq 2$. Then the associated energy contribution can be written as

$$(4.70) \quad \sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_p \sum_{q_i \in Z_m} q_i \hat{c}_{pi} e_i^{-p} \sum_{q_j \in Z_{m+\ell}} q_j \hat{c}_{pj} e_j^p = E_L^{(1)} .$$

Here $\alpha_p = \frac{1}{p(1-\exp(-2\pi p))}$ and the number $P(\ell)$ is determined by the accuracy; this was derived in (4.26) - (4.28):

$$(4.71) \quad P(\ell) \geq \frac{\beta \cdot M}{2\pi(\ell - 1)}$$

where β is the solution of

$$(4.72) \quad f(\beta) := \beta + \log \beta = a + \log 2 ,$$

where a = accuracy parameter.

We can rewrite (4.70) in different form: Set

$$(4.73) \quad \begin{cases} D_m^p &= \sum_{q_i \in Z_m} q_i \hat{c}_{pi} e_i^{-p} \\ d_{m\ell}^p &= \sum_{q_j \in Z_{m+\ell}} q_j \hat{c}_{pj} e_j^p . \end{cases}$$

Then we have

$$(4.75) \quad E_L^{(1)} = \sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_p D_m^p d_{m\ell}^p .$$

There is then a similar expression involving the sinus terms \hat{s}_{pi} :

$$(4.75) \quad E_L^{(2)} = \sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_p \widetilde{D}_m^p \widetilde{d}_{m\ell}^p ,$$

with

$$(4.76) \quad \begin{cases} \widetilde{D}_m^p &= \sum_{q_i \in Z_m} q_i \hat{s}_{pi} e_i^{-p} \\ \widetilde{d}_{m\ell}^p &= \sum_{q_j \in Z_{m+\ell}} q_j \hat{s}_{pj} e_j^p . \end{cases}$$

In the expressions $E_L^{(1)}$, $E_L^{(2)}$ the charges are chosen in different stripes such that $|z_i - z_j| \geq \epsilon = \frac{1}{M}$. Next we choose the positions such that $1 - |z_i - z_j| \geq \epsilon$ in order to apply the product decomposition formula involving the terms \bar{e}_i . We define now $\bar{P}(\ell)$ as the smallest integer such that

$$(4.77) \quad \bar{P}(\ell) \geq \frac{\beta \cdot M}{2\pi(M - \ell - 1)}$$

and introduce in analogy to (4.73), (4.76) the quantities

$$(4.78) \quad \begin{cases} F_m^p &= \sum_{q_i \in Z_m} q_i \hat{c}_{pi} (\bar{e}_i)^p, \quad \widetilde{F}_m^p = \sum_{q_i \in Z_m} q_i \hat{s}_{pi} (\bar{e}_i)^p \\ f_{m\ell}^p &= \sum_{q_j \in Z_{m+\ell}} q_j \hat{c}_{pj} (e_j)^p, \quad \widetilde{f}_{m\ell}^p = \sum_{q_j \in Z_{m+\ell}} q_j \hat{s}_{pj} e_j^p . \end{cases}$$

With these quantities two more energy contributions are formed, namely

$$(4.79) \quad E_L^{(3)} = \sum_{m=2}^M \sum_{\ell=0}^{M-m} \sum_{p=1}^{\bar{P}(\ell)} \alpha_p F_m^p \cdot f_{m\ell}^p ,$$

and

$$(4.80) \quad E_L^{(4)} = \sum_{m=2}^M \sum_{\ell=0}^{M-m} \sum_{p=1}^{\bar{P}(\ell)} \alpha_p \widetilde{F}_m^p \cdot \widetilde{f}_{m\ell}^p .$$

The total energy contribution stemming from the product decomposition of E_L from charges q_i, q_j in C with $\rho(i, j) > \delta$ is thus $E_L^{(1)} + E_L^{(2)} + E_L^{(3)} + E_L^{(4)}$.

b) Pairwise calculation

The remaining pairs that have not been calculated so far are pairs q_i, q_j with $\rho(i, j) > \delta$ but $|z_i - z_j| \leq \epsilon$ or $1 - |z_i - z_j| \leq \epsilon = \frac{1}{M}$. Thus the last contribution to E_L is

$$(4.81) \quad E_L^\delta = -\frac{1}{2} \sum_{q_i, q_j \in C \cap Z_{\delta, \epsilon}} q_i q_j \sum_{s=-S}^S L[y_i - y_i, z_i - z_j + s]$$

where

$$(4.82) \quad Z_{\delta, \epsilon} = \{\text{pairs } (q_i, q_j) \mid \rho(i, j) > \delta, |z_i - z_j| \leq \epsilon \vee 1 - |z_i - z_j| \leq \epsilon\}.$$

The number S in (4.81) depends again on the accuracy. For most practical purposes $S = 2$ or 3 will suffice.

4.4. Modifications for the two-dimensional case

There is very little that has to be changed if the basic system is only periodic in x and y direction and z ranges in a finite height (see Remark a) following Eq. (3.2)). In this case the charges q_n are located in the rectangle

$$(4.83) \quad G = \left\{ (y, z) \mid |y| \leq \frac{1}{2} + R_c, 0 \leq z \leq 1 \right\}$$

where the cut-off distance R_c is still given by (4.3).

All formulae for the calculation of E_B remain valid under the restriction that $q_n \in G$, G now being defined by (4.83).

For the calculation of E_L we need the counterpart of the product decomposition formula (3.18). We can now make use of another identity given in [5] (#(3.16) there):

$$(4.84) \quad -L[y_j - y_i, z_j - z_i] = 2 \sum_{p=1}^{\infty} \frac{1}{p} \exp[-2\pi p |z_j - z_i|] \cos[2\pi p (y_i - y_j)].$$

One readily checks that the counterpart of (3.18) now reads (in the notation introduced in (3.17))

$$(4.85) \quad -L[y_j - y_i, z_j - z_i] = 2 \sum_{p=1}^{\infty} \frac{1}{p} \left(\frac{e_j}{e_i} \right)^p (c_{pi} \cdot c_{pj} + s_{pi} \cdot s_{pj}).$$

One now has only the corresponding energy contributions $E_L^{(1)}$ and $E_L^{(2)}$ as defined in (4.74)-(4.76), with now $\alpha_p = \frac{1}{p}$.

In the pairwise calculation the analog of formula (4.81) now is

$$(4.86) \quad E_L^\delta = -\frac{1}{2} \sum_{\substack{q_i, q_j \in C \\ \rho(i, j) > \delta}} q_i q_j L[y_i - y_j, z_i - z_j].$$

Finally, the correction term E_δ given in (4.67) is the same except that the set R_δ there has to be replaced by

$$(4.87) \quad R_\delta = \left\{ (y, z) \mid \frac{1}{2} < |y| \leq \frac{1}{2} + \delta \right\}.$$

5. Estimate for the number of terms

The main issue of this section is to derive a bound for number of terms involved as function of the number N of the charges located in the basic cell C , with N being rather large. We will use a number of simplifications in the following which should have only a minor effect on the final result.

It is clear that only numerical tests will give a precise answer, but such tests depend very much on the way this method is programmed. Nevertheless one can get a good idea about how the number of terms to be calculated will increase as N increases.

We concentrate fully on N keeping the accuracy a fixed in a range which seems of practical importance, say $6 \leq a \leq 15$.

a) Pairwise calculation

We assume that in (4.31) $r_0 = r_k - r_{k-1} = \epsilon$ for all k and estimate first the number of terms occurring in (4.33). Formula (4.33) has the following geometrical interpretation (see Figure 6):

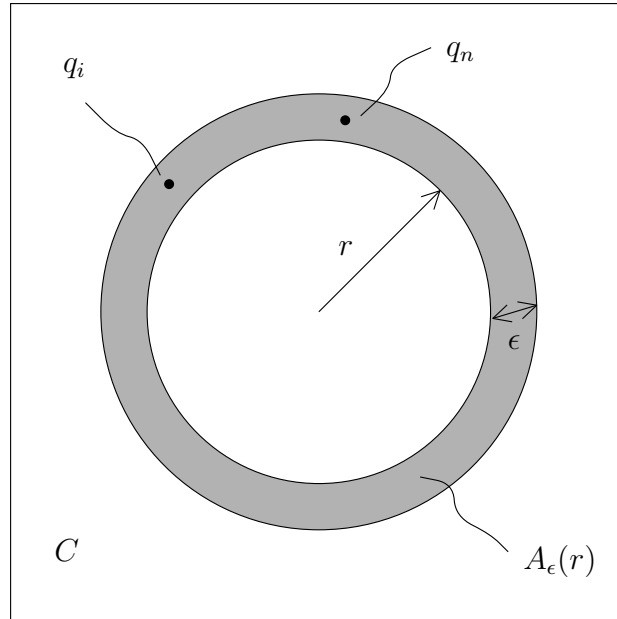


Fig. 8

For fixed r one has to calculate the interaction of all charge pairs q_i, q_n in the annulus $A_\epsilon(r)$. Since there are N charges in C (volume of $C = 1$) the number of pairs contained in $A_\epsilon(r)$ can be approximated by $\frac{1}{2} (2\pi\epsilon \cdot r)^2$, $\epsilon = \text{small number}$.

The number $T_1(\epsilon, N)$ of terms necessary for E_{BP} can thus be estimated as follows

$$(5.1) \quad T_1(\epsilon, N) \cong n_1(a) \cdot 2\pi^2 \cdot \epsilon^2 N^2 \int_0^{\frac{\sqrt{2}}{2}} r^3 dr = c_1(a) \cdot \epsilon^2 \cdot N^2$$

where $n_1(a)$ is a number which depends only on the accuracy a . The correction term given in (4.67) can be incorporated in (5.1) as well.

b) Product decomposition for E_B

We first rewrite the basic product decomposition formula (4.29) in the way it is applied in our procedure:

$$(5.2) \quad E_B \cong 2 \sum_{i=1}^N q_i \cdot \sum_{r_n > r_i + \epsilon} q_n \cdot \sum_{p=1}^{P(i,n)} \left\{ T_{pi}^{(1)} \cdot T_{pn}^{(2)} + \sum_{\nu=1}^{\nu_0(p,i,n)} T_{p\nu i}^{(3)} T_{p\nu n}^{(4)} \right. \\ \left. + \sum_{\nu=\nu_0+1}^{\nu_m(i,n)} \hat{T}_{\nu i}^{(3)} \hat{T}_{\nu n}^{(4)} \right\}.$$

Here the $T^{(i)}$ -terms stand for the types of terms contained in (4.29).

In the following we shall approximate the sums by integrals and the summation limits $P(i, n)$, $\nu_0(p, i, n)$ by continuous functions. Let r be the distance to the origin in the (y, z) -plane of a charge q_i and ρ the same for q_n .

Then the number of terms involved in (5.2) can be approximated as

$$(5.3) \quad T_2(\epsilon, N) \cong N \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r dr \left\{ n_2 \int_{r+\epsilon}^{r+R_c} P(r, \rho) d\rho + n_3 \int_{p=1}^{P(r,\rho)} \nu_0(p, r, \rho) dp \right. \\ \left. + n_4 \int_{r+\epsilon}^{R_c} [\nu_m(r, \rho) - \nu_0(1, r, \rho)] d\rho \right\}.$$

Here n_2, n_3, n_4 count the number of trigonometric and Bessel functions involved.

We now need an upper bound for $P(r, \rho)$ and this is determined in (4.4) with ρ replaced by $\rho - r$ there. One finds (see Appendix)

$$(5.4) \quad P(r, \rho) < \frac{1}{2\pi(\rho - r)} \left\{ a + \log \left(\frac{1}{\rho - r} \right) \right\}.$$

Therefore one has

$$(5.5) \quad n_2 \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r dr = \int_{r+\epsilon}^{r+R_c} P(r, \rho) d\rho dr < \frac{n_2}{2\pi} \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r dr \int_{\epsilon}^{R_c} \left[\frac{a}{t} + \frac{1}{t} \log \left(\frac{1}{t} \right) \right] dt \\ < c_2(a) \left[\log \left(\frac{1}{\epsilon} \right) + \log^2 \left(\frac{1}{\epsilon} \right) \right].$$

Next we need an estimate for the expression

$$(5.6) \quad a_0 \equiv \int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_c} \int_{p=1}^{P(r,\rho)} \nu_0(p, r, \rho) dp d\rho dr .$$

We use the crude upper bound (see Appendix)

$$(5.7) \quad \nu_0(p, r, \rho) < [e^a (\pi p \rho)^2]^{1/3}$$

which implies

$$(5.8) \quad \begin{aligned} \int_{p=1}^{P(r,\rho)} \nu_0(p, r, \rho) dp &< \frac{3}{5} e^{a/3} (\pi \rho)^{2/3} \cdot P(r, \rho)^{5/3} \\ &= \frac{3}{5} e^{a/3} \cdot (\pi P(r, \rho) \cdot \rho)^{2/3} \cdot P(r, \rho) < \frac{3}{5} e^{a/3} \left(\pi \left(\frac{\sqrt{2}}{2} + R_c \right) \right)^{2/3} \cdot P(r, \rho) . \end{aligned}$$

The combination of (5.8) and (5.5) shows that

$$(5.9) \quad a_0 < c_3(a) \left[\log \left(\frac{1}{\epsilon} \right) + \log^2 \left(\frac{1}{\epsilon} \right) \right] .$$

As a last step we bound the term

$$(5.10) \quad a_1 \equiv \int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_c} (\nu_m(r, \rho) - \nu_0(1, r, \rho)) d\rho dr < \int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_c} \nu_m(r, \rho) d\rho dr .$$

By (4.24) one has

$$(5.11) \quad \nu_m(r, \rho) \leq \frac{\alpha}{\log(\frac{\rho}{r})} + 1 ,$$

where α is the solution of (4.23).

We estimate as follows:

$$\int_{r+\epsilon}^{r+R_c} \frac{d\rho}{\log(\frac{\rho}{r})} = \int_{\epsilon}^{R_c} \frac{d\rho}{\log(1 + \frac{t}{r})} < \int_{\epsilon}^{R_c} \frac{r+t}{t} dt = r \log \left(\frac{R_c}{\epsilon} \right) + R_c - \epsilon$$

so that one has the crude estimate (for small ϵ !)

$$(5.12) \quad a_1 < \text{const} \cdot \log \left(\frac{1}{\epsilon} \right) .$$

Combining (5.1), (5.3), (5.5), (5.9) and (5.12) we see that the total number of terms needed for the calculation of E_B can be estimated in the form

$$(5.13) \quad T(\epsilon, N) < c_1 \cdot \epsilon^2 \cdot N^2 + N \left(c_2 \log \left(\frac{1}{\epsilon} \right) + c_3 \cdot \log^2 \left(\frac{1}{\epsilon} \right) \right) .$$

Here ϵ is the width of the annulus shown in Figure 6.

c) Product decomposition of E_L

The procedure explained in (4.69) and the sequel can be summarized as follows (see Fig. 9)

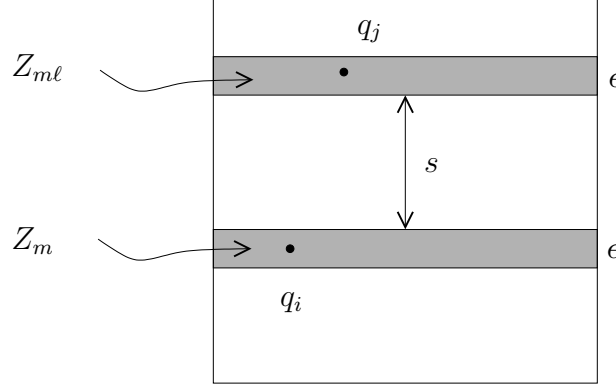


Fig. 9

For any charge pair q_i in the ϵ -strip Z_m , q_j in $Z_{m\ell}$ one has to calculate the sums denoted by $D_m^p, d_{m\ell}^p, \widetilde{D}_m^p, \widetilde{d}_{m\ell}^p, F_m^p, f_{m\ell}^p, \widetilde{F}_m^p, \widetilde{f}_{m\ell}^p$ in (4.78). The summation over p runs from 1 to a value P for which one has the estimate (see (4.27))

$$(5.14) \quad P \leq \frac{\beta}{2\pi \cdot S},$$

where β is the solution of (4.28).

Hence the number of terms needed for the calculation of E_L allows the estimate

$$(5.15) \quad T^{(5)}(\epsilon, N) < c_5 \int_{\epsilon}^{1-\epsilon} \frac{\beta}{2\pi \cdot s} ds < c_5 \cdot \frac{\beta}{2\pi} \log\left(\frac{1}{\epsilon}\right) \cdot N.$$

Hence for the total number of terms needed for the calculation of the Coulomb energy the estimate (5.13) holds with the meaning of ϵ described in Figures 6 and 7.

We can now make an optimal choice of ϵ which will depend on the constants c_1, c_2 and c_3 in (5.13). They have not been determined yet since this should be based on the CPU time required. If we choose $\epsilon = c \cdot N^{-1/2}$ we see that

$$(5.16) \quad \underline{T(\epsilon, N) < N(C_1 + C_2 \cdot \log N + C_3(\log N)^2)}.$$

If one optimizes the value of ϵ in (5.13) there is no significant improvement of the estimate (5.16).

Appendix

A.1 Estimate for the solution of (4.4)

We first derive an upper bound for the solution of

$$(A1) \quad \frac{5.016}{2\pi\rho} \frac{1}{\sqrt{2\pi\rho \cdot P}} \exp(-2\pi\rho P) = e^{-a} .$$

Setting $c = \frac{5.016}{2\pi}$ and $2\pi\rho P = s$ we rewrite the equation in the form

$$(A2) \quad s + \frac{1}{2} \log s = a + \log\left(\frac{c}{\rho}\right) .$$

Since $a \gg 1$ in applications we certainly have

$$(A3) \quad s < a + \log\left(\frac{c}{\rho}\right) ,$$

i.e.

$$(A4) \quad P < \frac{1}{2\pi\rho} \left(a + \log\left(\frac{c}{\rho}\right) \right) .$$

One can give a very sharp estimate in the following way. We set $s_0 = a + \log(\frac{c}{\rho})$ and $s = s_0(1 - t)$. Then insertion into (A2) and reduction yields

$$(A5) \quad s_0 \cdot t + \frac{1}{2} \log(1 - t) = \frac{1}{2} \log s_0 .$$

Since t is close to zero we may expand the logarithm. First order approximation then gives

$$(A6) \quad t = \frac{1}{2} \frac{\log s_0}{s_0 + \frac{1}{2}} ,$$

which leads to the estimate

$$(A7) \quad P \cong \frac{1}{2\pi\rho} s_0 \left[1 - \frac{\frac{1}{2} \log s_0}{s_0 + \frac{1}{2}} \right] , \quad s_0 = a + \log\left(\frac{5.016}{2\pi\rho}\right) .$$

Numerical tests show that this approximation is surprisingly sharp. There is however no significant improvement of the estimate given in (5.5) resulting from this sharper estimate for P .

A.2. Derivation of condition (4.51)

A series expansion of the term

$$(A8) \quad h[r, R, \nu] = 1 - \exp \left[-\nu \left(w_0\left(\frac{R}{\nu}\right) - w_0\left(\frac{r}{\nu}\right) \right) \right] U_1\left(\frac{r}{\nu}\right) U_2\left(\frac{R}{\nu}\right)$$

in powers of $\frac{1}{\nu}$ yields

$$(A9) \quad \begin{aligned} h[r, R, \nu] &= \frac{1}{4\nu} \left(R^2 - r^2 + \frac{1}{\nu} (R^2 + r^2) - \frac{1}{32} (R^2 - r^2) \frac{1}{\nu} + O\left(\frac{1}{\nu^2}\right) \right) \\ &< \frac{1}{4\nu} (R^2 - r^2) + \frac{1}{\nu} (R^2 + r^2) + O\left(\frac{1}{\nu^2}\right). \end{aligned}$$

Hence one has

$$(A10) \quad \left| I_\nu(r) K_\nu(R) - \frac{1}{2\nu} \left(\frac{r}{R} \right)^\nu \right| < \frac{1}{8\nu^2} \left(\frac{r}{R} \right)^\nu \left\{ R^2 - r^2 + \frac{1}{\nu} (R^2 + r^2) + O\left(\frac{1}{\nu^2}\right) \right\}$$

which in turn leads to condition (4.51).

In order to find a crude approximation ν_0 for the value of ν for which

$$(A11) \quad \left| I_\nu(r) K_\nu(R) - \frac{1}{2\nu} \left(\frac{r}{R} \right)^\nu \right| \leq e^{-a}$$

we choose $r = R = 2\pi p r_n$ and use (A10). This leads to the estimate

$$(A12) \quad \nu \cong \nu_0 = (r_n \pi p)^{2/3} \cdot e^{a/3},$$

as used in (4.52).

References

- [1] Abramowitz M., Stegun I., Handbook of Mathematical Functions. Dover, N.Y., (1970).
- [2] Ewald P.P., Die Berechnung optischer und elektrostatischer Gitterpotentiale. Ann. Phys, **64**, 253-287.
- [3] Lekner J., Summation of Coulomb fields in computer simulated disordered systems. Physica A, 176, (1991), 524-532.
- [4] Lekner J., Coulomb forces and potentials in systems with an orthorhombic unit cell. Molecular Simulation, to appear.
- [5] Sperb R., An alternative to Ewald sums. Part I: Identities for sums. Molecular Simulation, **20**, (1998), 171-200.
- [6] Watson G.N., A treatise on the theory of Bessel functions. Cambridge Univ. Press.

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