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The Coulomb energy for dense periodic systems

R. Sperb

Research Report No. 98-03
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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

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

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:

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

More precisely, assume that we know that

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

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

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

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

$$C : \Big\{(x,y,z)\Big|\ |x| \le \tfrac{1}{2},\ |y| \le \tfrac{1}{2},\ |z| \le \tfrac{1}{2}\Big\}$$

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

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

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

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

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))

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

with $\hat{Q}_0 = -1.955013\ldots$.

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

$$\widetilde{\rho}_{ij}(\ell,m) = \left(\frac{b}{a}\right)^2 (\eta_i - \eta_j + \ell)^2 + \left(\frac{c}{a}\right)^2 (\zeta_i - \zeta_j + m)^2 \,,$$
$$\widetilde{L}[\eta,\zeta] = \log[1 - 2\, \cos(2\pi\eta)\, e^{-2\pi\,|\zeta|\cdot \frac{c}{b}} + e^{-4\pi\,|\zeta|\cdot\frac{c}{b}}]$$

one now has in the place of (3.2)

$$\begin{aligned} E = \frac{1}{2a} \sum_{i\neq j=1}^{N} q_i q_j \Big\{ & \sum_{m,\ell=-\infty}^{\infty} Be[\widetilde{\rho}_{ij}(\ell,m),\, \xi_i - \xi_j] \\ & - \sum_{n=-\infty}^{\infty} \widetilde{L}[\eta_i - \eta_j, \zeta_i - \zeta_j + n] + 2\pi\, \frac{c}{b}\, ((\zeta_i - \zeta_j)^2 - |\zeta_i - \zeta_j|) \Big\} \\ & + Q_0(a,b,c) \cdot \sum_{i=1}^{N} q_i^2 \end{aligned} \tag{3.4}$$

with

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

where $\gamma \cong 0.577216\ldots$ 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

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

c) If $\rho_{ij}(\ell,m) \to 0$, which is possible for $-1 \le \ell,\, m \le 1$, 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

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

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

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

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

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

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

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

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 $\eta^2+(\zeta+m)^2>0$, $0\le\zeta\le 1$ one has*

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

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

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

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

$$0 < r_1 < r_2 < \ldots < r_N \leq \frac{\sqrt{2}}{2}\ . \tag{3.13}$$

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

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

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:

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

In this notation one gets

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

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:

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

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

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

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

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

where we have set

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

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

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

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

$$\Big|\sum_{p=P+1}^{\infty} K_0(2\pi p\rho)\,\cos(2\pi px)\Big| \le \sum_{p=P+1}^{\infty} K_0(2\pi p\rho) < \int_P^{\infty} K_0(2\pi\rho p)\,dp\ .$$

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

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

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

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

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 $\le 10^{-6}$ one has $R_c \cong 2.24$.

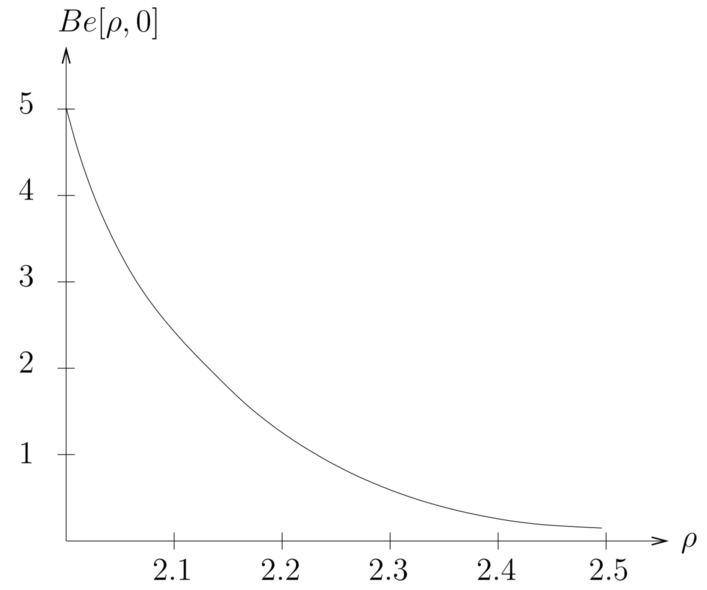

Fig. 1

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

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

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

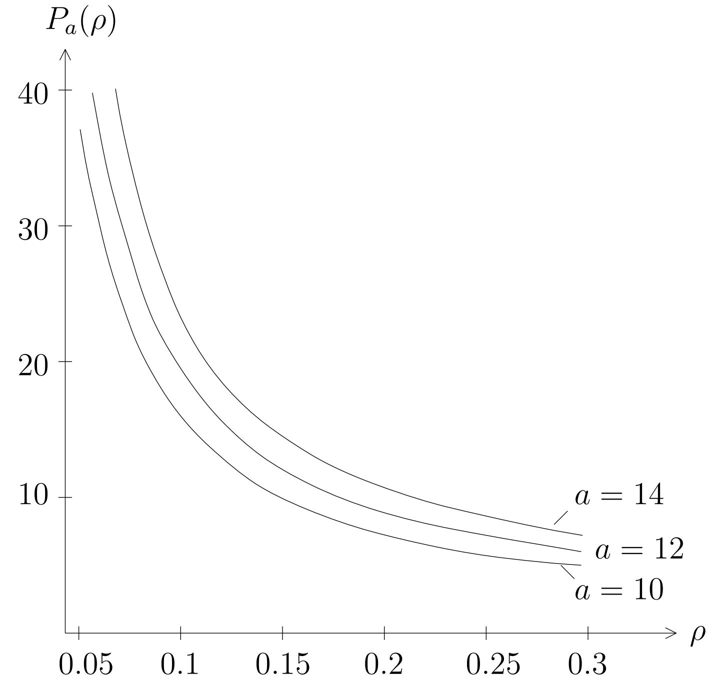

Fig. 2

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

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

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

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

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

where

$$\eta(z) = \sqrt{1+z^2} + \log\Big(\frac{z}{1+\sqrt{1+z^2}}\Big) \tag{4.9}$$

and

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

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

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

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

$$\exp\Big(\nu \cdot \eta\big(\frac{r}{\nu}\big)\Big) \cdot \exp\Big(-\nu\eta\big(\frac{R}{\nu}\big)\Big) =: Pr(\nu, r, R)\ . \tag{4.12}$$

After some rearrangement one finds

$$Pr(\nu, r, R) = \big(\frac{r}{R}\big)^{\nu} \exp\Big[-\nu\Big(w\big(\frac{R}{\nu}\big) - w\big(\frac{R}{\nu}\big)\Big)\Big]\ , \tag{4.13}$$

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:

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

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

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

where we have abbreviated

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

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

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

$$I_\nu(r)\, K_\nu(R) < \frac{1}{2\nu}\,\big(\frac{r}{R}\big)^{\nu}\ . \tag{4.18}$$

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

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

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

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

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

$$\frac{4}{\gamma \cdot \lambda}\, e^{-\gamma \cdot \lambda} \le e^{-a} \; . \tag{4.21}$$

We can put this into a more convenient form. Set

$$f(s) = s + \log(s) \tag{4.22}$$

and let α be the solution of

$$f(s) = a + \log 4 \; . \tag{4.23}$$

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

$$\gamma \ge \frac{\alpha}{\log(\frac{R}{r})} \; . \tag{4.24}$$

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

$$2 \sum_{\ell=L+1}^{\infty} \frac{1}{\ell}\, \exp[-2\pi\ell \cdot d] \le e^{-a} \; , \tag{4.25}$$

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

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

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

$$L \ge \frac{\beta}{2\pi \cdot d} \; , \tag{4.27}$$

where β is the solution of

$$f(s) = a + \log 2 \; . \tag{4.28}$$

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

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

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)

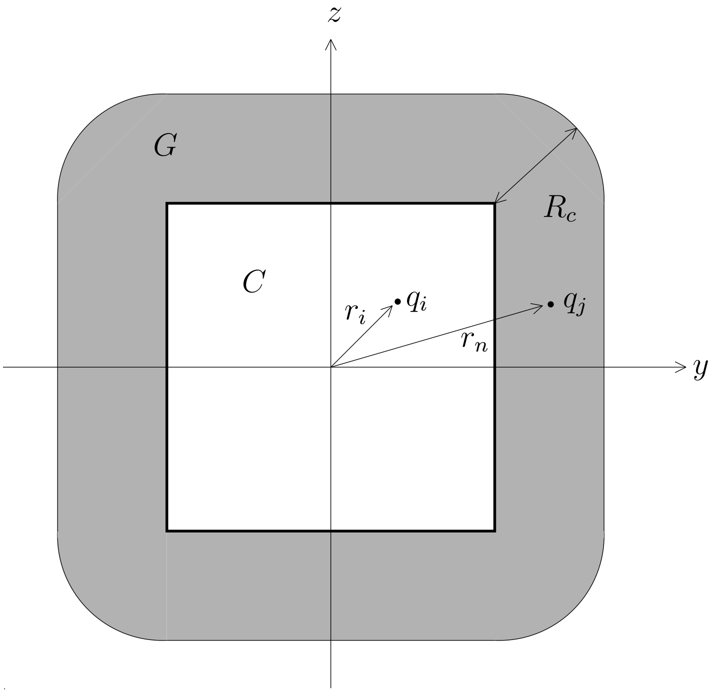

Fig. 3

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

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

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

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

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

$$S_{k\ell} = \{(r, \varphi) | \, r_{k-1} < r \le r_k, \ \varphi_{\ell-1} \le \varphi < \varphi_\ell\} \tag{4.30}$$

and the annular domains

$$S_k = \{(r, \varphi) \, | \, r_{k-1} < r \le r_k\} \tag{4.31}$$

as well as the disk

$$S_0 = \{(r, \varphi) \, | \, r \le r_0\} . \tag{4.32}$$

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

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

Here E_{in} is given by (3.9)

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

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

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

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 $1 \le k < K + 1$ and assume that $q_i \in S_{k-1}$, $q_n \in G \cup C - S_1 \cup S_2 \cup \ldots \cup S_k$, i.e. $r_n > r_k$.

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

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

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

$$Fe[r_k - r_{k-1}, P] \leq e^{-a} \;, \tag{4.35}$$

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

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

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)

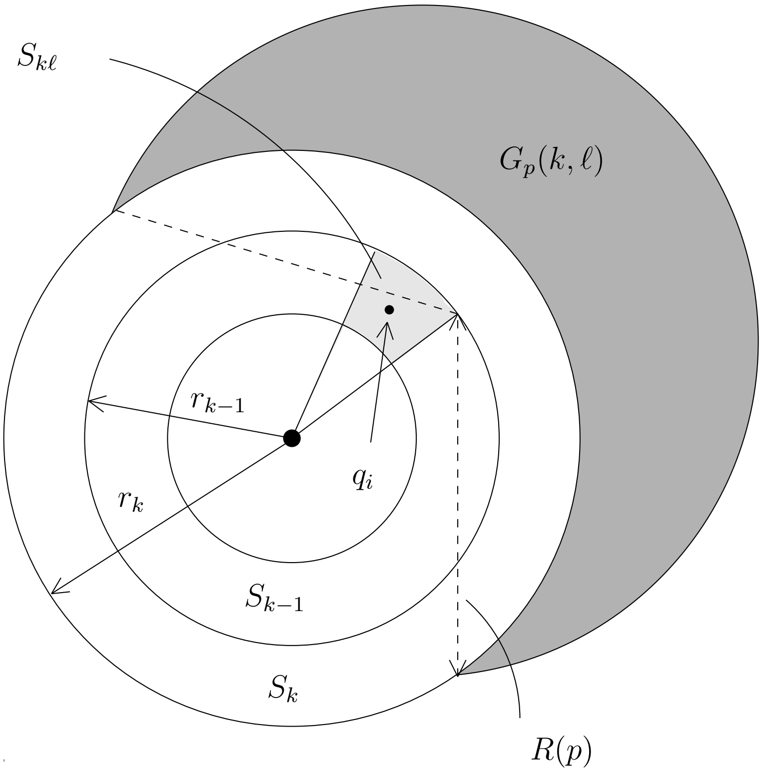

Fig. 4

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

We will also need the intersections

$$I_p(k, \ell) := G_p(k, \ell) \cap G_p(k, \ell + 1) \;. \tag{4.38}$$

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

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

Recursion step: Set

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

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

$$I_p^+(k,\ell) = G_p(k,\ell+1) \backslash I_p(k,\ell) \; , \tag{4.41}$$

$$I_p^-(k,\ell) = G_p(k,\ell) \backslash I_p(k,\ell) \; . \tag{4.42}$$

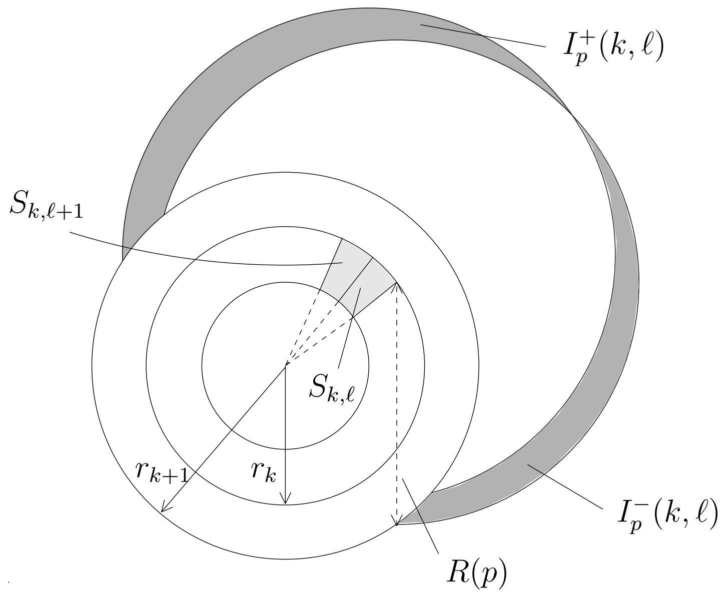

Fig. 5

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

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

The contribution to E_B then is

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

We can repeat the recursions with terms

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

and analogously

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

leading to the corresponding energy contribution

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

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

$$\boldsymbol{E_B^0 = \sum_{k=1}^{K+1}\sum_{p=1}^{P_k} \left(E_B^0(k,p) + \widetilde{E}_B^0(k,p)\right)}\;. \tag{4.48}$$

c) **Recursions for** $1\le\nu$

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 $\nu > R \ge r > 0$ then one has

$$\Big| I_\nu(r)\, K_\nu(R) - \frac{1}{2\nu}\,\Big(\frac{r}{R}\Big)^\nu\Big| \le e^{-a} \tag{4.49}$$

provided

$$\frac{1}{2\nu}\,\Big(\frac{r}{R}\Big)^\nu\,\Big(1-\exp\Big[-\nu\Big(w_0\Big(\frac{R}{\nu}\Big) - w_0\Big(\frac{r}{\nu}\Big)\Big)\Big]\cdot U_1\Big(\frac{r}{\nu}\Big)\, U_2\Big(\frac{R}{\nu}\Big)\Big) \le e^{-a} \tag{4.50}$$

with $w_0(\;)$ 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)

$$H[\nu, r_i, r_n, p] := \frac{1}{2\nu^2}\,\Big(\frac{r_i}{r_n}\Big)^\nu\,\Big[\Big(1+\frac{1}{\nu}\Big)\, r_n^2 - \Big(1-\frac{1}{\nu}\Big)\, r_i^2\Big]\,\pi^2p^2 \le e^{-a}\;, \tag{4.51}$$

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)

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

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

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

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

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

a typical plot looks like figure 6:

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

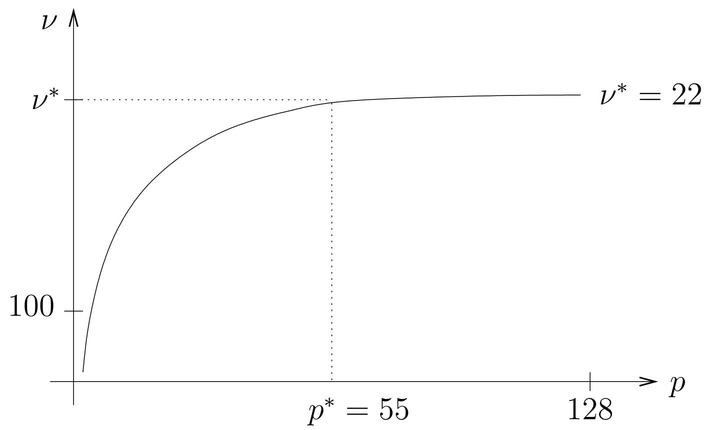

Fig. 6

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

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

and p^* is the value for which

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

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

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

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

$$r_n > r_i\, e^{\frac{\alpha}{\nu}} \,. \tag{4.54}$$

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

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

Then, set in analogy to (4.39)

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

with the same recursion step

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

The associated terms are

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

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

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

Then in the disk

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

one can replace in (4.56)

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

and in (4.58)

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

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:

$$\begin{cases} \widetilde{A}^\nu_p(k,\ell) &= \displaystyle\sum_{q_n \in G_p(k,\ell) \cap C_{k\nu p}} q_n \, s_{pn} \, c^\nu_n \, \hat{K}^\nu_n \\ B^\nu_p(k,\ell) &= \displaystyle\sum_{q_n \in G_p(k,\ell) \cap C_{k\nu p}} q_n \, c_{pn} \, s^\nu_n \, \hat{K}^\nu_n \\ \widetilde{B}^\nu_p(k,\ell) &= \displaystyle\sum_{q_n \in G_p(k,\ell) \cap C_{k\nu p}} q_n \, s_{pn} \, s^\nu_n \, \hat{K}^\nu_n \ . \end{cases} \tag{4.61}$$

The associated terms are then

$$\begin{cases} \widetilde{a}^\nu_p(k,\ell) &= \displaystyle\sum_{q_i \in S_p(k-1,\ell)} q_i \, s_{pi} \, c^\nu_i \, \hat{I}^\nu_i \\ b^\nu_p(k,\ell) &= \displaystyle\sum_{q_i \in S_p(k-1,\ell)} q_i \, c_{pi} \, s^\nu_i \, \hat{I}^\nu_i \\ \widetilde{b}^\nu_p(k,\ell) &= \displaystyle\sum_{q_i \in S_p(k-1,\ell)} q_i \, s_{pi} \, s^\nu_i \, \hat{I}^\nu_i \ . \end{cases} \tag{4.62}$$

The energy contributions are then as in (4.44):

$$E^\nu_B(k,p) = 4 \sum_{\ell=1}^{L} \{a^\nu_p(k,\ell) \, A^\nu_p(k,\ell) + \ldots + \widetilde{b}^\nu_p(k,\ell) \cdot \widetilde{B}^\nu_p(k,\ell)\} \ . \tag{4.63}$$

The total contribution finally is

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

4.3. Procedure for E_L

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

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

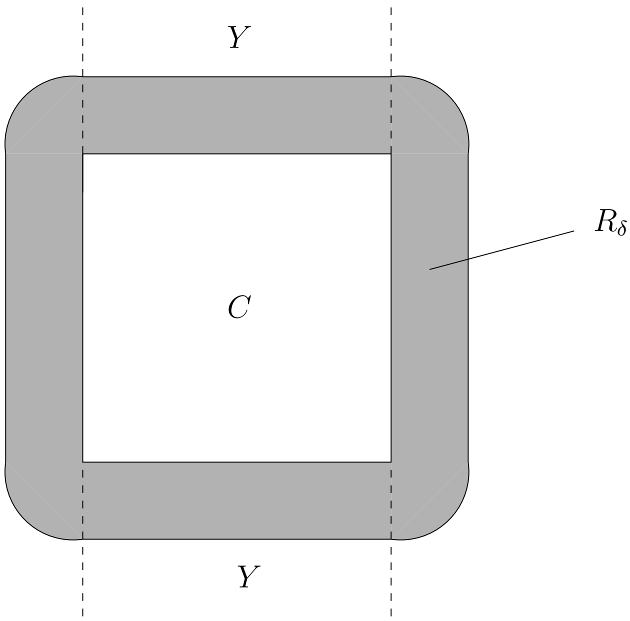

Fig. 7

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

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

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 $\rho(i,j) \le \delta$. This implies that all pairs with $q_i \in C$, $q_j \in R_\delta$, $\rho(i,j) \le \delta$ have been included also, hence we have a correction term

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

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

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

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

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

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

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

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):

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

where β is the solution of

$$f(\beta) := \beta + \log \beta = a + \log 2 \ , \tag{4.72}$$

where $a =$ accuracy parameter.

We can rewrite (4.70) in different form: Set

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

Then we have

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

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

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

with

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

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 $\overline{e}_i$. We define now $\overline{P}(\ell)$ as the smallest integer such that

$$\text{(4.77)} \qquad \overline{P}(\ell) \geq \frac{\beta \cdot M}{2\pi(M - \ell - 1)}$$

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

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

With these quantities two more energy contributions are formed, namely

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

and

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

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

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

where

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

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

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

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):

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

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

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

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

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

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

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

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):

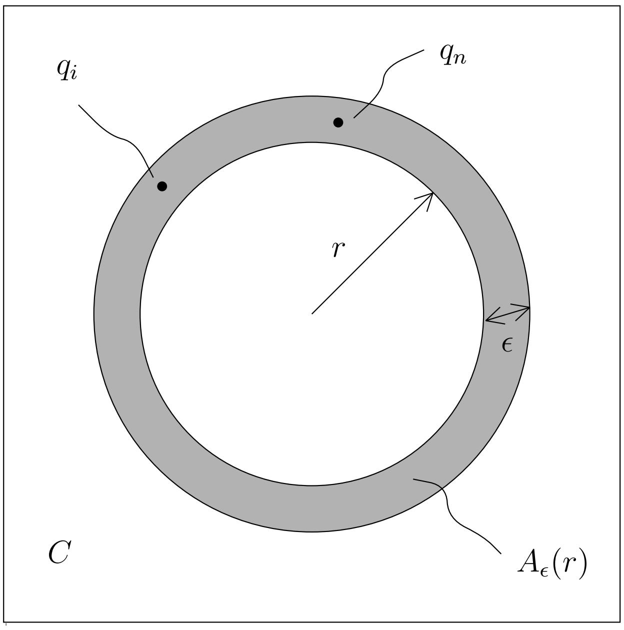

Fig. 8

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 $\frac{1}{2}\,(2\pi\epsilon \cdot r)^2$, $\epsilon =$ small number.

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

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

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:

$$\begin{aligned} E_B \cong \; & 2 \sum_{i=1}^{N} q_i \cdot \sum_{r_n > r_i + \epsilon} q_n \cdot \sum_{p=1}^{P(i,n)} \Big\{ T^{(1)}_{pi} \cdot T^{(2)}_{pn} + \sum_{\nu=1}^{\nu_0(p,i,n)} T^{(3)}_{p\nu i} \, T^{(4)}_{p\nu n} \\ & + \sum_{\nu=\nu_0+1}^{\nu_m(i,n)} \hat{T}^{(3)}_{\nu i} \, \hat{T}^{(4)}_{\nu n} \Big\} \, . \end{aligned} \tag{5.2}$$

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

$$\begin{aligned} T_2(\epsilon, N) \cong \; & N \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r \, dr \Big\{ n_2 \int_{r+\epsilon}^{r+R_c} P(r, \rho) dp + n_3 \int_{p=1}^{P(r,\rho)} \nu_0(p, r, \rho) dp \\ & + n_4 \int_{r+\epsilon}^{R_c} [\nu_m(r, \rho) - \nu_0(1, r, \rho)] dp \Big\} \, . \end{aligned} \tag{5.3}$$

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)

$$P(r, \rho) < \frac{1}{2\pi(\rho - r)} \; \Big\{ a + \log \Big(\frac{1}{\rho - r} \Big) \Big\} \, . \tag{5.4}$$

Therefore one has

$$\begin{aligned} n_2 \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r = \int_{r+\epsilon}^{r+R_c} P(r, \rho) d\rho \, dr < \; & \frac{n_2}{2\pi} \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r \, dr \int_{\epsilon}^{R_c} \Big[\frac{a}{t} + \frac{1}{t} \log \Big(\frac{1}{t} \Big) \Big] dt \\ & < c_2(a) \Big[\log \Big(\frac{1}{\epsilon} \Big) + \log^2 \Big(\frac{1}{\epsilon} \Big) \Big] \, . \end{aligned} \tag{5.5}$$

Next we need an estimate for the expression

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

We use the crude upper bound (see Appendix)

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

which implies

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

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

$$a_0 < c_3(a)\Big[\log\Big(\frac{1}{\epsilon}\Big) + \log^2\Big(\frac{1}{\epsilon}\Big)\Big] \; . \tag{5.9}$$

As a last step we bound the term

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

By (4.24) one has

$$\nu_m(r,\rho) \le \frac{\alpha}{\log(\frac{\rho}{r})} + 1 \; , \tag{5.11}$$

where α is the solution of (4.23).

We estimate as follows:

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

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

$$a_1 < \text{const } \cdot \log\Big(\frac{1}{\epsilon}\Big) \; . \tag{5.12}$$

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

$$T(\epsilon, N) < c_1 \cdot \epsilon^2 \cdot N^2 + N\Big(c_2 \log\Big(\frac{1}{\epsilon}\Big) + c_3 \cdot \log^2\Big(\frac{1}{\epsilon}\Big)\Big) \; . \tag{5.13}$$

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)

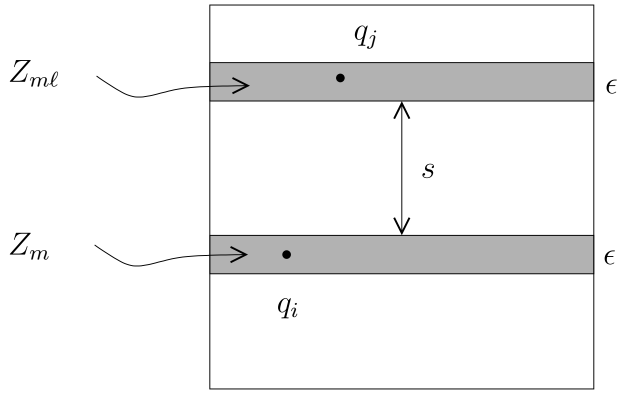

Fig. 9

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^p_m, $d^p_{m\ell}$, $\widetilde{D}^p_m$, $\widetilde{d}^p_{m\ell}$, F^p_m, $f^p_{m\ell}$, $\widetilde{F}^p_m$, $\widetilde{f}^p_{m\ell}$ in (4.78). The summation over p runs from 1 to a value P for which one has the estimate (see (4.27))

$$P \le \frac{\beta}{2\pi \cdot S} \, , \tag{5.14}$$

where β is the solution of (4.28).

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

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

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

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

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

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

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

$$(A2) \qquad s + \frac{1}{2}\; \log s = a + \log\Big(\frac{c}{\rho}\Big).$$

Since $a >> 1$ in applications we certainly have

$$(A3) \qquad s < a + \log\Big(\frac{c}{\rho}\Big) \; ,$$

i.e.

$$(A4) \qquad P < \frac{1}{2\pi\rho}\; \Big(a + \log\Big(\frac{c}{\rho}\Big)\Big) \; .$$

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

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

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

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

which leads to the estimate

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

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

$$(A8) \qquad h[r, R, \nu] = 1 - \exp\Big[-\nu\Big(w_0\Big(\frac{R}{\nu}\Big) - w_0\Big(\frac{r}{\nu}\Big)\Big)\Big] \; U_1\Big(\frac{r}{\nu}\Big) \; U_2\Big(\frac{R}{\nu}\Big)$$

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

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

Hence one has

$$(A10)\qquad \Big|I_\nu(r)\,K_\nu(R)-\frac{1}{2\nu}\,\Big(\frac{r}{R}\Big)^\nu\Big| < \frac{1}{8\nu^2}\,\Big(\frac{r}{R}\Big)^\nu\,\Big\{R^2-r^2+\frac{1}{\nu}\,(R^2+r^2)+O\Big(\frac{1}{\nu^2}\Big)\Big\}$$

which in turn leads to condition (4.51).

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

$$(A11)\qquad \Big|I_\nu(r)\,K_\nu(R)-\frac{1}{2\nu}\,\Big(\frac{r}{R}\Big)^\nu\Big| \le e^{-a}$$

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

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

as used in (4.52).

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