# The Coulomb energy for dense periodic systems 

## Report

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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 $1 / 2 \mathrm{~N}^{*}(\mathrm{~N}-1)$ 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

$$
\begin{equation*}
S=\sum_{i, j=1}^{N} f\left(x^{i}, x^{j}\right) \tag{2.1}
\end{equation*}
$$

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:

$$
\begin{equation*}
f\left(x^{i}, x^{j}\right)=\sum_{\ell=1}^{\infty} p_{\ell}\left(x^{i}\right) \cdot q_{\ell}\left(x^{j}\right) . \tag{2.2}
\end{equation*}
$$

More precisely, assume that we know that

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

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

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

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

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

and the $N$ charges $q_{i} \subset C$ have coordinates $\left(x_{i}, y_{i}, z_{i}\right)$. We then introduce the following notations

$$
\left\{\begin{align*}
\rho_{i j}(\ell, m) & =\left[\left(y_{i}-y_{j}+\ell\right)^{2}+\left(z_{i}-z_{j}+m^{2}\right]^{\frac{1}{2}},\right. & & \ell, m \in \mathbb{Z}  \tag{3.1}\\
B e[\rho, x] & =4 \sum_{p=1}^{\infty} K_{0}(2 \pi p \cdot \rho) \cos (2 \pi p x), & & \rho>0 \\
L[y, z] & =\log \left\{1-2 \cos (2 \pi y) e^{-2 \pi|z|}+e^{-4 \pi|z|}\right\} & & K_{0}=\text { Bessel function } \\
Q_{0} & =-1.942248 \ldots & &
\end{align*}\right.
$$

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

$$
\begin{align*}
E= & \frac{1}{2} \sum_{i \neq j=1}^{N} q_{i} q_{j}\left\{\sum_{m, \ell=-\infty}^{\infty} B e\left[\rho_{i j}(\ell, m), x_{i}-x_{j}\right]\right. \\
& -\sum_{n=-\infty}^{\infty} L\left[y_{i}-y_{j}, z_{i}-z_{j}+n\right]  \tag{3.2}\\
& \left.+\frac{2 \pi}{3}\left(\sum_{i=1}^{N} q_{i} \vec{x}_{i}\right)^{2}+2 \pi\left(\left(z_{i}-z_{j}\right)^{2}-\left|z_{i}-z_{j}\right|\right)\right\}+Q_{0} \cdot \sum_{i=1}^{N} q_{i}^{2} \\
= & E_{B}+E_{L}+\frac{2 \pi}{3} D^{2}+E_{z}+Q_{0} \cdot \sum_{i=1}^{N} q_{i}^{2},
\end{align*}
$$

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))

$$
\begin{align*}
E=\frac{1}{2} \sum_{i \neq j=1}^{N} q_{i} q_{j}\{ & \sum_{\ell=-\infty}^{\infty} B e\left[\rho_{i j}(\ell, 0), x_{i}-x_{j}\right]-L\left[y_{i}-y_{j}, z_{i}-z_{j}\right] \\
& \left.-2 \pi\left|z_{i}-z_{j}\right|\right\}+\hat{Q}_{0} \cdot \sum_{i=1}^{N} q_{i}^{2} \tag{3.3}
\end{align*}
$$

$$
\text { with } \hat{Q}_{0}=-1.955013 \ldots
$$

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

$$
\begin{aligned}
& \tilde{\rho}_{i j}(\ell, m)=\left(\frac{b}{a}\right)^{2}\left(\eta_{i}-\eta_{j}+\ell\right)^{2}+\left(\frac{c}{a}\right)^{2}\left(\zeta_{i}-\zeta_{j}+m\right)^{2}, \\
& \widetilde{L}[\eta, \zeta]=\log \left[1-2 \cos (2 \pi \eta) e^{-2 \pi|\zeta| \cdot \frac{c}{b}}+e^{-4 \pi|\zeta| \cdot \frac{c}{b}}\right]
\end{aligned}
$$

one now has in the place of (3.2)

$$
\begin{align*}
E= & \frac{1}{2 a} \sum_{i \neq j=1}^{N} q_{i} q_{j}\left\{\sum_{m, \ell=-\infty}^{\infty} B e\left[\widetilde{\rho}_{i j}(\ell, m), \xi_{i}-\xi_{j}\right]\right. \\
& \left.-\sum_{n=-\infty}^{\infty} \widetilde{L}\left[\eta_{i}-\eta_{j}, \zeta_{i}-\zeta_{j}+n\right]+2 \pi \frac{c}{b}\left(\left(\zeta_{i}-\zeta_{j}\right)^{2}-\left|\zeta_{i}-\zeta_{j}\right|\right)\right\}  \tag{3.4}\\
& +Q_{0}(a, b, c) \cdot \sum_{i=1}^{N} q_{i}^{2}
\end{align*}
$$

with

$$
\begin{align*}
Q_{0}(a, b, c)= & 2 \sum_{\ell=1}^{\infty} \sum_{m, n=-\infty}^{\infty}, K_{0}\left(\frac{2 \pi \ell}{a} \sqrt{(b \cdot m)^{2}+(c \cdot n)^{2}}\right) \\
& -2 \sum_{n=1}^{\infty} \log \left(1-e^{-2 \pi n \frac{c}{b}}\right)+\gamma-\log \left(4 \pi \frac{a}{b}\right), \tag{3.5}
\end{align*}
$$

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

$$
\begin{equation*}
\hat{Q}(a, b)=4 \sum_{\ell, m=1}^{\infty} K_{0}\left(2 \pi \ell \cdot m \cdot \frac{b}{a}\right)+\gamma-\log \left(4 \pi \frac{a}{b}\right) . \tag{3.6}
\end{equation*}
$$

c) If $\rho_{i j}(\ell, m) \rightarrow 0$, which is possible for $-1 \leq \ell, m \leq 1$, then the two terms $B e[$,$] and$ $L[$,$] in (3.2) or (3.3) that become singular have to be combined and yield a regular$
term. One is led to the following result: Set

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

where $\psi$ 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

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

If $\rho_{i j}(\ell, m)$ becomes small (say $<0.1$ ) then the combination $B e\left[\rho_{i j}(\ell, m), x_{i}-x_{j}\right]-$ $L\left[y_{i}-y_{j}, z_{i}-z_{j}+m\right]$ in (3.3) may be replaced by

$$
\begin{align*}
E_{i j}:=G & {\left[\rho_{i j}(\ell, m), x_{i}-x_{j}\right]+H\left[\pi\left(y_{i}-y_{j}+\ell\right), \pi\left(z_{i}-z_{j}+m\right)\right] }  \tag{3.9}\\
& -5.0620485 .
\end{align*}
$$

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

$$
\begin{equation*}
K_{0}\left[\sqrt{R^{2}+r^{2}-2 r R \cos \varphi}\right]=K_{0}(R) I_{0}(r)+2 \sum_{\nu=1}^{\infty} K_{\nu}(R) I_{\nu}(r) \cos (\nu \varphi) . \tag{3.10}
\end{equation*}
$$

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 $L\left[y_{i}-y_{j}, z_{i}-z_{j}+m\right]$ we can use identities (3.9) and (3.10) of [5] which lead to the identity given in

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

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

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 $\varphi$ polar coordinates in the $(y, z)$-plane so that the distance between $q_{i}$ and $q_{n}$ is given by

$$
\begin{equation*}
\rho(i, n)=\sqrt{r_{i}^{2}+r_{n}^{2}-2 r_{i} r_{n} \cos \left(\varphi_{i}-\varphi_{n}\right)} . \tag{3.12}
\end{equation*}
$$

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

$$
\begin{equation*}
0<r_{1}<r_{2}<\ldots<r_{N} \leq \frac{\sqrt{2}}{2} . \tag{3.13}
\end{equation*}
$$

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

$$
\begin{equation*}
E_{B}=\frac{1}{2} \sum_{i=1}^{N} q_{i} \sum_{n>i} q_{n} B e\left[\rho(i, n), x_{i}-x_{n}\right] . \tag{3.14}
\end{equation*}
$$

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:

$$
\left\{\begin{align*}
c_{p i} & =\cos \left(2 \pi p x_{i}\right)  \tag{3.15}\\
s_{p i} & =\sin \left(2 \pi p x_{i}\right) \\
c_{i}^{\nu} & =\cos \left(\nu \cdot \varphi_{i}\right) \\
s_{i}^{\nu} & =\sin \left(\nu \cdot \varphi_{i}\right) \\
K_{p i}^{\nu} & =K_{\nu}\left(2 \pi p \cdot r_{i}\right) \\
I_{p i}^{\nu} & =I_{\nu}\left(2 \pi p \cdot r_{i}\right) .
\end{align*}\right.
$$

In this notation one gets

$$
\begin{align*}
\operatorname{Be}\left[\rho(i, n), x_{i}-x_{n}\right]= & 4 \sum_{p=1}^{\infty}\left(c_{p i} c_{p n}+s_{p i} \cdot s_{p n}\right)\left\{K_{p n}^{0} \cdot I_{p i}^{0}+\right.  \tag{3.16}\\
& \left.+2 \sum_{\nu=1}^{\infty} K_{p n}^{\nu} \cdot I_{p i}^{\nu}\left(c_{i}^{\nu} \cdot c_{n}^{\nu}+s_{i}^{\nu} \cdot s_{n}^{\nu}\right)\right\} .
\end{align*}
$$

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

$$
L_{i j}:=-\sum_{n=-\infty}^{\infty} L\left[y_{i}-y_{j}, z_{i}-z_{j}+n\right] .
$$

It is again convenient to introduce the following abbreviations:

$$
\left\{\begin{array}{l}
e_{0}=\exp (-2 \pi)  \tag{3.17}\\
e_{i}=\exp \left(-2 \pi z_{i}\right) \\
\bar{e}_{i}=\exp \left(-2 \pi\left(1-z_{i}\right)\right) \\
\hat{c}_{p i}=\cos \left(2 \pi p y_{i}\right) \\
\hat{s}_{p i}=\sin \left(2 \pi p y_{i}\right) .
\end{array}\right.
$$

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

$$
\begin{equation*}
L_{i j}=2 \sum_{p=1}^{\infty} \frac{1}{p\left(1-\left(e_{0}\right)^{p}\right)}\left\{\left(e_{i} \cdot \bar{e}_{j}\right)^{p}+\left(\frac{e_{j}}{e_{i}}\right)^{p}\right\}\left(\hat{c}_{p i} \cdot \hat{c}_{p j}+\hat{s}_{p i} \cdot \hat{s}_{p j}\right) . \tag{3.18}
\end{equation*}
$$

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

$$
\frac{1}{2} \sum_{i \neq j} q_{i} q_{j}\left(\left(z_{i}-z_{j}\right)^{2}-\left|z_{i}-z_{j}\right|\right)=: E_{z}
$$

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

$$
\begin{equation*}
E_{z}=2 \pi\left[\sum_{i=1}^{N-1} q_{i}\left(D_{z}^{i}+Q_{i} z_{i}\right)-D_{z}^{2}\right] \tag{3.19}
\end{equation*}
$$

where we have set

$$
\begin{equation*}
D_{z}=\sum_{i=1}^{N} q_{i} z_{i}, \quad D_{z}^{i}=\sum_{j=i+1}^{N} q_{j} z_{j}, \quad Q_{i}=\sum_{j=1}^{i} q_{j} \tag{3.20}
\end{equation*}
$$

## 4. Calculation of the Coulomb energy

### 4.1. Estimates for truncation errors

We first analyze the convergence behaviour of the term $\operatorname{Be}\left[\rho(i, n), x_{i}-x_{n}\right]$ 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

$$
\begin{equation*}
B e[\rho, x]=4 \sum_{p=1}^{\infty} K_{0}(2 \pi p \rho) \cos (2 \pi p x), \tag{4.1}
\end{equation*}
$$

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

$$
\left|\sum_{p=P+1}^{\infty} K_{0}(2 \pi p \rho) \cos (2 \pi p x)\right| \leq \sum_{p=P+1}^{\infty} K_{0}(2 \pi p \rho)<\int_{P}^{\infty} K_{0}(2 \pi \rho p) d p .
$$

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

$$
\begin{equation*}
4 \sum_{p=P+1}^{\infty} K_{0}(2 \pi p \rho)<\frac{5.016}{2 \pi \rho} \frac{1}{\sqrt{2 \pi \rho \cdot P}} \exp (-2 \pi \rho \cdot P)=: F e[\rho, P] . \tag{4.2}
\end{equation*}
$$

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

$$
\begin{equation*}
B e[\rho, 0] \leq e^{-a} \tag{4.3}
\end{equation*}
$$

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 $10^{6} \cdot B e[\rho, 0]$. 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 $\rho$ on the other hand the number $P$ giving the term $B e[\rho, x]$ with the required accuracy is defined by the smallest number $P=P_{a}(\rho) \in \mathbb{N}$ such that

$$
\begin{equation*}
F e[\rho, P] \leq e^{-a} . \tag{4.4}
\end{equation*}
$$

As an illustration we show in Figure 2 some typical curves $P_{a}(\rho)$


Fig. 2

The next important information concerns the number of $\nu$-terms needed in the GegenbauerTheorem (3.10). This now requires by (3.16) that

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

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

$$
\begin{gather*}
I_{\nu}(\nu \cdot z)=\frac{1}{\sqrt{2 \pi \nu}} \frac{e^{\nu \eta(z)}}{\left(1+z^{2}\right)^{\frac{1}{4}}}\left\{1+\sum_{k=1}^{\infty} \frac{u_{k}(t(z))}{\nu^{k}}\right\}  \tag{4.7}\\
K_{\nu}(\nu \cdot z)=\sqrt{\frac{\pi}{2 \nu}} \frac{e^{-\nu \eta(z)}}{\left(1+z^{2}\right)^{\frac{1}{4}}}\left\{1+\sum_{k=1}^{\infty}(-1)^{k} \frac{u_{k}(t(z))}{\nu^{k}}\right\}, \tag{4.8}
\end{gather*}
$$

where

$$
\begin{equation*}
\eta(z)=\sqrt{1+z^{2}}+\log \left(\frac{z}{1+\sqrt{1+z^{2}}}\right) \tag{4.9}
\end{equation*}
$$

and

$$
\begin{equation*}
t(z)=\left(1+z^{2}\right)^{-1 / 2} \tag{4.10}
\end{equation*}
$$

The functions $u_{k}(t)$ are given in [1], p. 366, \#9.3.9. The first three are

$$
\begin{equation*}
u_{0}=1, u_{1}(t)=\frac{3 t-5 t^{3}}{24}, u_{2}(t)=\frac{8\left(t^{2}-462 t^{4}+385 t^{6}\right)}{1152} \tag{4.11}
\end{equation*}
$$

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

$$
\begin{equation*}
\exp \left(\nu \cdot \eta\left(\frac{r}{\nu}\right)\right) \cdot \exp \left(-\nu \eta\left(\frac{R}{\nu}\right)\right)=: \operatorname{Pr}(\nu, r, R) . \tag{4.12}
\end{equation*}
$$

After some rearrangement one finds

$$
\begin{equation*}
\operatorname{Pr}(\nu, r, R)=\left(\frac{r}{R}\right)^{\nu} \exp \left[-\nu\left(w\left(\frac{R}{\nu}\right)-w\left(\frac{R}{\nu}\right)\right)\right] \tag{4.13}
\end{equation*}
$$

where $w(s)=\sqrt{1+s^{2}}-\log \left(1+\sqrt{1+s^{2}}\right)$.
For $|s|<1$ we can expand $w(s)$ in a power series:

$$
\begin{align*}
w(s) & =1-\log 2+\frac{s^{2}}{4}-\frac{s^{4}}{32}+\frac{s^{6}}{96}-\frac{5 \cdot s^{8}}{1024}+\ldots  \tag{4.14}\\
& =1-\log 2+w_{0}(s)
\end{align*}
$$

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

$$
\begin{equation*}
I_{\nu}(r) \cdot K_{\nu}(R)=\frac{1}{2 \nu}\left(\frac{r}{R}\right)^{\nu} \cdot \exp \left[-\nu\left(w_{0}\left(\frac{R}{\nu}\right)-w_{0}\left(\frac{r}{\nu}\right)\right)\right] \cdot U_{1}\left(\frac{r}{\nu}\right) \cdot U_{2}\left(\frac{R}{\nu}\right) \tag{4.15}
\end{equation*}
$$

where we have abbreviated

$$
\begin{gather*}
U_{1}(s)=\left(1+s^{2}\right)^{-\frac{1}{4}} \cdot\left\{1+\sum_{k=1}^{\infty} \frac{u_{k}(t(s))}{\nu^{k}}\right\}  \tag{4.16}\\
U_{2}(s)=\left(1+s^{2}\right)^{-\frac{1}{4}} \cdot\left\{1+\sum_{k=1}^{\infty}(-1)^{k} \frac{u_{k}(t(s))}{\nu^{k}}\right\} . \tag{4.17}
\end{gather*}
$$

Note that $U_{1}(s), U_{2}(s)$ are close to 1 for $s$ small, i.e. for large $\nu$.
For $\nu>R>r \geq 0$ one has the simple estimate

$$
\begin{equation*}
I_{\nu}(r) K_{\nu}(R)<\frac{1}{2 \nu}\left(\frac{r}{R}\right)^{\nu} . \tag{4.18}
\end{equation*}
$$

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

$$
\begin{equation*}
8 \sum_{\nu=\gamma+1}^{\infty} K_{\nu}(R) I_{\nu}(r)<4 \int_{\gamma}^{\infty} \frac{1}{\nu}\left(\frac{r}{R}\right)^{\nu} d \nu=4 \cdot E_{1}\left(\gamma \log \left(\frac{R}{r}\right)\right) \tag{4.19}
\end{equation*}
$$

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

$$
\begin{equation*}
E_{1}(s)<\frac{1}{s} e^{-s} . \tag{4.20}
\end{equation*}
$$

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

$$
\begin{equation*}
\frac{4}{\gamma \cdot \lambda} e^{-\gamma \cdot \lambda} \leq e^{-a} \tag{4.21}
\end{equation*}
$$

We can put this into a more convenient form. Set

$$
\begin{equation*}
f(s)=s+\log (s) \tag{4.22}
\end{equation*}
$$

and let $\alpha$ be the solution of

$$
\begin{equation*}
f(s)=a+\log 4 \tag{4.23}
\end{equation*}
$$

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

$$
\begin{equation*}
\gamma \geq \frac{\alpha}{\log \left(\frac{R}{r}\right)} . \tag{4.24}
\end{equation*}
$$

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

$$
\begin{equation*}
2 \sum_{\ell=L+1}^{\infty} \frac{1}{\ell} \exp [-2 \pi \ell \cdot d] \leq e^{-a} \tag{4.25}
\end{equation*}
$$

with $d=\left|z_{j}-z_{i}\right|$ or $d=1-\left|z_{j}-z_{i}\right|$. Again we have

$$
\begin{equation*}
2 \sum_{\ell=L+1}^{\infty} \frac{1}{\ell} \exp [-2 \pi \ell \cdot d]<2 \int_{L}^{\infty} \frac{1}{\ell} \exp [-2 \pi d \cdot \ell] d \ell=2 E_{1}(2 \pi d \cdot L) \tag{4.26}
\end{equation*}
$$

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

$$
\begin{equation*}
L \geq \frac{\beta}{2 \pi \cdot d} \tag{4.27}
\end{equation*}
$$

where $\beta$ is the solution of

$$
\begin{equation*}
f(s)=a+\log 2 . \tag{4.28}
\end{equation*}
$$

### 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

$$
\begin{align*}
E_{B}= & 2 \sum_{i=1}^{N} q_{i} \sum_{r_{n} \geq r_{i}} q_{n} \sum_{p=1}^{\infty}\left(c_{p i} c_{p n}+s_{p i} s_{p n}\right)\left\{K_{p n}^{0} I_{p i}^{0}+\right.  \tag{4.29}\\
& \left.+2 \sum_{\nu=1}^{\infty} K_{p n}^{\nu} I_{p i}^{\nu}\left(c_{i}^{\nu} c_{n}^{\nu}+s_{i}^{\nu} s_{n}^{\nu}\right)\right\}
\end{align*}
$$

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 $(r, \varphi)$ 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

$$
\begin{equation*}
S_{k \ell}=\left\{(r, \varphi) \mid r_{k-1}<r \leq r_{k}, \varphi_{\ell-1} \leq \varphi<\varphi_{\ell}\right\} \tag{4.30}
\end{equation*}
$$

and the annular domains

$$
\begin{equation*}
S_{k}=\left\{(r, \varphi) \mid r_{k-1}<r \leq r_{k}\right\} \tag{4.31}
\end{equation*}
$$

as well as the disk

$$
\begin{equation*}
S_{0}=\left\{(r, \varphi) \mid r \leq r_{0}\right\} . \tag{4.32}
\end{equation*}
$$

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 $E_{B P}$ which can be calculated as

$$
\begin{equation*}
E_{B P}=2 \sum_{k=1}^{K} \sum_{\substack{q_{i} \in S_{k-1} \cap C \\ q_{n} \in S_{k-1} \cup S_{k}}} q_{i} q_{n} E_{i n} . \tag{4.33}
\end{equation*}
$$

Here $E_{i n}$ is given by (3.9)

$$
\begin{equation*}
E_{i n}=G\left[\rho(i, n), x_{i}-x_{n}\right]+H\left[\left(y_{i}-y_{n}\right) \cdot \pi,\left(z_{i}-z_{n}\right) \cdot \pi\right]-5.0620485 \tag{4.34a}
\end{equation*}
$$

if $\rho(i, n)=\sqrt{r_{i}^{2}+r_{n}^{2}-2 r_{i} r_{n} \cos \left(\varphi_{i}-\varphi_{n}\right)} \leq \delta$ and

$$
\begin{equation*}
E_{\text {in }}=\frac{1}{2} B e\left[\rho(i, n), x_{i}-x_{n}\right] \tag{4.34b}
\end{equation*}
$$

if $\rho(i, n)>\delta$. Here $\delta \cong 0.1$ may be chosen and the functions $G[], H[]$ and $B e[]$ 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 $q_{i} \in S_{k-1}, q_{n} \in G \cup C-$ $S_{1} \cup S_{2} \cup \ldots \cup S_{k}$, i.e. $r_{n}>r_{k}$.

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

$$
2 \sum_{q_{i} \in S_{k-1}} q_{i} \sum_{r_{n}>r_{k}} q_{n} \sum_{p=1}^{P}\left(c_{p i} c_{p n}+S_{p i} S_{p n}\right) K_{p n}^{0} I_{p i}^{0},
$$

where the limit $P$ is determined by inequality (4.4) with $\rho=\sqrt{r_{n}^{2}+r_{i}^{2}-2 r_{n} r_{i} \cos \left(\varphi_{n}-\varphi_{i}\right)}$ there. This can be done in the following way: Let $P_{k}$ be the smallest number satisfying

$$
\begin{equation*}
F e\left[r_{k}-r_{k-1}, P\right] \leq e^{-a}, \tag{4.35}
\end{equation*}
$$

with $F e$ [ ] defined in (4.2). For any $1 \leq p \leq P_{k}$ let $R(p)$ the solution of

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

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

$$
\begin{equation*}
G_{p}(k, \ell)=\left\{(r, \varphi) \mid r>r_{k} \wedge r^{2}+r_{k-1}^{2}-2 r r_{k-1} \cos \left(\varphi-\varphi_{\ell}\right) \leq R^{2}(p)\right\} \tag{4.37}
\end{equation*}
$$

We will also need the intersections

$$
\begin{equation*}
I_{p}(k, \ell):=G_{p}(k, \ell) \cap G_{p}(k, \ell+1) . \tag{4.38}
\end{equation*}
$$

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

$$
\begin{equation*}
A_{p}^{0}(k, 1)=\sum_{q_{n} \in G_{p}(k, 1)} q_{n} c_{p n} K_{p n}^{0} . \tag{4.39}
\end{equation*}
$$

Recursion step: Set

$$
\begin{equation*}
A_{p}^{0}(k, \ell+1)=A_{p}^{0}(k, \ell)+\sum_{q_{n} \in I_{p}^{+}(k, \ell)} q_{n} c_{p n} K_{p n}^{0}-\sum_{q_{n} \in I_{p}^{-}(k, \ell)} q_{n} c_{p n} K_{p n}^{0} . \tag{4.40}
\end{equation*}
$$

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

$$
\begin{equation*}
I_{p}^{+}(k, \ell)=G_{p}(k, \ell+1) \backslash I_{p}(k, \ell), \tag{4.41}
\end{equation*}
$$

$$
\begin{equation*}
I_{p}^{-}(k, \ell)=G_{p}(k, \ell) \backslash I_{p}(k, \ell) . \tag{4.42}
\end{equation*}
$$



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

$$
\begin{equation*}
a_{p}^{0}(k, \ell)=\sum_{q_{i} \in S(k-1, \ell)} q_{i} c_{p i} I_{p i}^{0} \tag{4.43}
\end{equation*}
$$

The contribution to $E_{B}$ then is

$$
\begin{equation*}
E_{B}^{0}(k, p)=2 \sum_{\ell=1}^{L} a_{p}^{0}(k, \ell) A_{p}^{0}(k, \ell) \tag{4.44}
\end{equation*}
$$

We can repeat the recursions with terms

$$
\begin{equation*}
\widetilde{a}_{p}^{0}(k, \ell)=\sum_{q_{i} \in S(k, \ell)} q_{i} s_{p i} I_{p i}^{0} \tag{4.45}
\end{equation*}
$$

and analogously

$$
\begin{equation*}
\widetilde{A}_{p}^{0}(k, \ell)=\sum_{q_{n} \in G_{p}(k, \ell)} q_{n} s_{p n} K_{p n}^{0} \tag{4.46}
\end{equation*}
$$

leading to the corresponding energy contribution

$$
\begin{equation*}
\widetilde{E}_{B}^{0}(k, p)=2 \sum_{\ell=1}^{L} \widetilde{a}_{p}^{0}(k, \ell) \widetilde{A}_{p}^{0}(k, \ell) \tag{4.47}
\end{equation*}
$$

The energy contribution to $E_{B}$ stemming from the product decomposition then finally is

$$
\begin{equation*}
E_{B}^{0}=\sum_{k=1}^{K+1} \sum_{p=1}^{P_{k}}\left(E_{B}^{0}(k, p)+\widetilde{E}_{B}^{0}(k, p)\right) \tag{4.48}
\end{equation*}
$$

c) Recursions for $1 \leq \nu$

There is one additional difficulty arising in the calculations involving the Bessel functions $I_{\nu}, K_{\nu}$ : both numbers may be huge or extremely small if $\nu$ 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

$$
\begin{equation*}
\left|I_{\nu}(r) K_{\nu}(R)-\frac{1}{2 \nu}\left(\frac{r}{R}\right)^{\nu}\right| \leq e^{-a} \tag{4.49}
\end{equation*}
$$

provided

$$
\begin{equation*}
\frac{1}{2 \nu}\left(\frac{r}{R}\right)^{\nu}\left(1-\exp \left[-\nu\left(w_{0}\left(\frac{R}{\nu}\right)-w_{0}\left(\frac{r}{\nu}\right)\right)\right] \cdot U_{1}\left(\frac{r}{\nu}\right) U_{2}\left(\frac{R}{\nu}\right)\right) \leq e^{-a} \tag{4.50}
\end{equation*}
$$

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)

$$
\begin{equation*}
H\left[\nu, r_{i}, r_{n}, p\right]:=\frac{1}{2 \nu^{2}}\left(\frac{r_{i}}{r_{n}}\right)^{\nu}\left[\left(1+\frac{1}{\nu}\right) r_{n}^{2}-\left(1-\frac{1}{\nu}\right) r_{i}^{2}\right] \pi^{2} p^{2} \leq e^{-a} \tag{4.51}
\end{equation*}
$$

where it is assumed that $\nu>2 \pi\left(R_{c}+\frac{\sqrt{2}}{2}\right) \geq 2 \pi p \cdot r_{n}$ and $r_{n}>r_{i}$.
As a simple approximation one may take (see Section 5)

$$
\begin{equation*}
\nu \geq \nu_{0}\left(r_{n}, p\right)=\left(r_{n}^{2} \pi^{2} p^{2} e^{a}\right)^{1 / 3} \tag{4.52}
\end{equation*}
$$

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

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

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

$$
H_{a}\left[\nu, r_{i}, r_{n}, p\right]=\left(\frac{1}{2 \nu}\left(\frac{r_{i}}{r_{n}}\right)^{\nu}-K_{\nu}\left(\pi p r_{n}\right) \cdot I_{\nu}\left(\pi p r_{i}\right)\right) e^{a}
$$

a typical plot looks like figure 6:
level line $H_{a}\left[\nu, r_{i}, r_{n}, p\right]=1$
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)
$\nu^{*}$ is the smallest integer satisfying

$$
\begin{equation*}
\frac{1}{2 \nu}\left(\frac{r_{i}}{r_{n}}\right)^{\nu} \leq e^{-a} \tag{4.52a}
\end{equation*}
$$

and $p^{*}$ is the value for which

$$
\begin{equation*}
K_{\nu}\left(\pi p r_{k}\right) I_{\nu}\left(\pi p r_{i}\right) \leq e^{-a} \tag{4.52b}
\end{equation*}
$$

Note that $\nu^{*}$ 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 $\nu$-values given by (4.24): if $r_{n}>r_{i}$ and

$$
\begin{equation*}
\nu \geq \nu_{m} \geq \frac{\alpha}{\log \left(\frac{r_{n}}{r_{i}}\right)} \tag{4.53}
\end{equation*}
$$

then these values of $\nu$ 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

$$
\begin{equation*}
r_{n}>r_{i} e^{\frac{\alpha}{\nu}} \tag{4.54}
\end{equation*}
$$

Here $\alpha$ 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

$$
\begin{equation*}
C_{k \nu}=\left\{(r, \varphi) \left\lvert\, r \leq r_{k} e^{\frac{\alpha}{\nu}}\right.\right\} \tag{4.55}
\end{equation*}
$$

Then, set in analogy to (4.39)

$$
\begin{equation*}
A_{p}^{\nu}(k, 1)=\sum_{q_{n} \in G_{p}(k, 1) \cap C_{k \nu}} q_{n} c_{p n} c_{n}^{\nu} K_{p n}^{\nu} \tag{4.56}
\end{equation*}
$$

with the same recursion step

$$
\begin{equation*}
A_{p}^{\nu}(k, \ell+1)=A_{p}^{\nu}(k, \ell)+\sum_{q_{n} \in I^{+}(k, \ell) \cap C_{k \nu}} q_{n} c_{p n} c_{n}^{\nu} K_{p n}^{\nu}-\sum_{q_{n} \in I^{-}(k, \ell) \cap C_{k \nu}} q_{n} c_{p n} c_{n}^{\nu} K_{p n}^{\nu} \tag{4.57}
\end{equation*}
$$

The associated terms are

$$
\begin{equation*}
a_{p}^{\nu}(k, \ell)=\sum_{q_{i} \in S(k-1, \ell)} q_{i} c_{p i} c_{i}^{\nu} I_{p i}^{\nu} . \tag{4.58}
\end{equation*}
$$

The recursions run for all values of $\nu$ from $\nu=1$ to $\nu=\nu_{m}(k) \leq \frac{\alpha}{\log \left(\frac{r_{k}}{r_{k-1}}\right)}$.
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

$$
\begin{equation*}
H\left[\nu, r_{k}, R, p\right]=e^{-a} . \tag{4.59}
\end{equation*}
$$

Then in the disk

$$
\begin{equation*}
C_{\nu k p}=\left\{(r, \varphi) \mid r \leq R_{k}(\nu, p)\right\} \tag{4.60}
\end{equation*}
$$

one can replace in (4.56)

$$
K_{p n}^{\nu} \text { by } \hat{K}_{n}^{\nu}:=r_{n}^{-2 \nu}
$$

and in (4.58)

$$
I_{p i}^{\nu} \text { by } \hat{I}_{i}^{\nu}:=\frac{1}{2 \nu} \cdot r_{i}^{2 \nu} .
$$

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:

$$
\left\{\begin{align*}
\widetilde{A}_{p}^{\nu}(k, \ell) & =\sum_{q_{n} \in G_{p}(k, \ell) \cap C_{k \nu p}} q_{n} s_{p n} c_{n}^{\nu} \hat{K}_{n}^{\nu}  \tag{4.61}\\
B_{p}^{\nu}(k, \ell) & =\sum_{q_{n} \in G_{p}(k, \ell) \cap C_{k \nu p}} q_{n} c_{p n} s_{n}^{\nu} \hat{K}_{n}^{\nu} \\
\widetilde{B}_{p}^{\nu}(k, \ell) & =\sum_{q_{n} \in G_{p}(k, \ell) \cap C_{k \nu p}} q_{n} s_{p n} s_{n}^{\nu} \hat{K}_{n}^{\nu} .
\end{align*}\right.
$$

The associated terms are then

$$
\left\{\begin{array}{l}
\widetilde{a}_{p}^{\nu}(k, \ell)=\sum_{q_{i} \in S_{p}(k-1, \ell)} q_{i} s_{p i} c_{i}^{\nu} \hat{I}_{i}^{\nu}  \tag{4.62}\\
b_{p}^{\nu}(k, \ell)=\sum_{q_{i} \in S_{p}(k-1, \ell)} q_{i} c_{p i} s_{i}^{\nu} \hat{I}_{i}^{\nu} \\
\widetilde{b}_{p}^{\nu}(k, \ell)=\sum_{q_{i} \in S_{p}(k-1, \ell)} q_{i} s_{p i} s_{i}^{\nu} \hat{I}_{i}^{\nu} .
\end{array}\right.
$$

The energy contributions are then as in (4.44):

$$
\begin{equation*}
E_{B}^{\nu}(k, p)=4 \sum_{\ell=1}^{L}\left\{a_{p}^{\nu}(k, \ell) A_{p}^{\nu}(k, \ell)+\ldots+\widetilde{b}_{p}^{\nu}(k, \ell) \cdot \widetilde{B}_{p}^{\nu}(k, \ell)\right\} \tag{4.63}
\end{equation*}
$$

The total contribution finally is

$$
\begin{equation*}
E_{B}=E_{B}^{0}+\sum_{k=1}^{K} \sum_{p=1}^{P_{k}} \sum_{\nu=1}^{\nu_{m}(k)} E_{B}^{\nu}(k, p) \tag{4.64}
\end{equation*}
$$

### 4.3. Procedure for $E_{L}$

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

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



Fig. 7

According to (3.2) the energy contribution denoted as $E_{L}$ may be written as

$$
\begin{equation*}
E_{L}=-\frac{1}{2} \sum_{q_{i} \in C} \sum_{q_{j} \in C \cup Y} q_{i} q_{j} L\left[y_{i}-y_{j}, z_{i}-z_{j}\right] . \tag{4.66}
\end{equation*}
$$

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

$$
\begin{equation*}
E_{\delta}=\frac{1}{2} \sum_{\substack{q_{i} \in C \\ \rho(i, j) \leq \delta}} \sum_{q_{j} \in R_{\delta}} q_{i} q_{j} L\left[y_{i}-y_{j}, z_{i}-z_{j}\right] . \tag{4.67}
\end{equation*}
$$

It remains therefore to calculate the remaining terms of $E_{L}$ in (4.66), that is

$$
\begin{equation*}
\hat{E}_{L}=-\frac{1}{2} \sum_{\substack{q_{i} \in C \\ \rho(i, j)>\delta}} \sum_{\substack{q_{j} \in C \cup Y}} L\left[y_{i}-y_{j}, z_{i}-z_{j}\right] . \tag{4.68}
\end{equation*}
$$

The calculation of $\hat{E}_{L}$, i.e. the approximation with given accuracy, is split up into two parts: for all pairs $\left(q_{i}, q_{j}\right) \in C$ such that

$$
\epsilon<\left|z_{i}-z_{j}\right|<1-\epsilon
$$

we will apply the product decomposition as given in (3.18). For all pairs in $C$ with $\left|z_{i}-z_{j}\right| \leq \epsilon$ or $\left|z_{i}-z_{j}\right| \geq 1-\epsilon$ the energy contributions will be calculated pairwise. The choice of $\epsilon$ 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

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

We now make use of (3.18) and consider first the terms denoted $e_{i}\left(=\exp \left(-2 \pi \cdot z_{i}\right)\right)$. 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

$$
\begin{equation*}
\sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_{p} \sum_{q_{i} \in Z_{m}} q_{i} \hat{c}_{p i} e_{i}^{-p} \sum_{q_{i} \in Z_{m+\ell}} q_{i} \hat{c}_{p j} e_{j}^{p}=E_{L}^{(1)} . \tag{4.70}
\end{equation*}
$$

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):

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

where $\beta$ is the solution of

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

where $a=$ accuracy parameter.
We can rewrite (4.70) in different form: Set

$$
\left\{\begin{align*}
D_{m}^{p} & =\sum_{q_{i} \in Z_{m}} q_{i} \hat{c}_{p i} e_{i}^{-p}  \tag{4.73}\\
d_{m \ell}^{p} & =\sum_{q_{j} \in Z_{m+\ell}} q_{j} \hat{c}_{p j} e_{j}^{p}
\end{align*}\right.
$$

Then we have

$$
\begin{equation*}
E_{L}^{(1)}=\sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_{p} D_{m}^{p} d_{m \ell}^{p} . \tag{4.75}
\end{equation*}
$$

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

$$
\begin{equation*}
E_{L}^{(2)}=\sum_{m=1}^{M-2} \sum_{\ell=2}^{M-m} \sum_{p=1}^{P(\ell)} \alpha_{p} \widetilde{D}_{m}^{p} \widetilde{d}_{m \ell}^{p}, \tag{4.75}
\end{equation*}
$$

with

$$
\left\{\begin{array}{l}
\widetilde{D}_{m}^{p}=\sum_{q_{i} \in Z_{m}} q_{i} \hat{s}_{p i} e_{i}^{-p}  \tag{4.76}\\
\widetilde{d}_{m \ell}^{p}=\sum_{q_{j} \in Z_{m+\ell}} q_{j} \hat{s}_{p j} e_{j}^{p} .
\end{array}\right.
$$

In the expressions $E_{L}^{(1)}, E_{L}^{(2)}$ the charges are chosen in different stripes such that $\left|z_{i}-z_{j}\right| \geq \epsilon=\frac{1}{M}$. Next we choose the positions such that $1-\left|z_{i}-z_{j}\right| \geq \epsilon$ 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

$$
\begin{equation*}
\bar{P}(\ell) \geq \frac{\beta \cdot M}{2 \pi(M-\ell-1)} \tag{4.77}
\end{equation*}
$$

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

$$
\left\{\begin{align*}
F_{m}^{p} & =\sum_{q_{i} \in Z_{m}} q_{i} \hat{c}_{p i}\left(\bar{e}_{i}\right)^{p}, \widetilde{F}_{m}^{p}=\sum_{q_{i} \in Z_{m}} q_{i} \hat{s}_{p i}\left(\bar{e}_{i}\right)^{p}  \tag{4.78}\\
f_{m \ell}^{p} & =\sum_{q_{j} \in Z_{m+\ell}} q_{j} \hat{c}_{p j}\left(e_{j}\right)^{p}, \tilde{f}_{m \ell}^{p}=\sum_{q_{j} \in Z_{m+\ell}} q_{j} \hat{s}_{p j} e_{j}^{p} .
\end{align*}\right.
$$

With these quantities two more energy contributions are formed, namely

$$
\begin{equation*}
E_{L}^{(3)}=\sum_{m=2}^{M} \sum_{\ell=0}^{M-m} \sum_{p=1}^{\bar{P}(\ell)} \alpha_{p} F_{m}^{p} \cdot f_{m \ell}^{p}, \tag{4.79}
\end{equation*}
$$

and

$$
\begin{equation*}
E_{L}^{(4)}=\sum_{m=2}^{M} \sum_{\ell=0}^{M-m} \sum_{p=1}^{\bar{P}(\ell)} \alpha_{p} \widetilde{F}_{m}^{p} \cdot \widetilde{f}_{m \ell}^{p} . \tag{4.80}
\end{equation*}
$$

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 $\left|z_{i}-z_{j}\right| \leq \epsilon$ or $1-\left|z_{i}-z_{j}\right| \leq \epsilon=\frac{1}{M}$. Thus the last contribution to $E_{L}$ is

$$
\begin{equation*}
E_{L}^{\delta}=-\frac{1}{2} \sum_{q_{i}, q_{j} \in C \cap Z_{\delta, \epsilon}} q_{i} q_{j} \sum_{s=-S}^{S} L\left[y_{i}-y_{i}, z_{i}-z_{j}+s\right] \tag{4.81}
\end{equation*}
$$

where

$$
\begin{equation*}
Z_{\delta, \epsilon}=\left\{\text { pairs }\left(q_{i}, q_{j}\right)\left|\rho(i, j)>\delta,\left|z_{i}-z_{j}\right| \leq \epsilon \vee 1-\left|z_{i}-z_{j}\right| \leq \epsilon\right\}\right. \tag{4.82}
\end{equation*}
$$

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

$$
\begin{equation*}
G=\left\{(y, z)| | y \left\lvert\, \leq \frac{1}{2}+R_{c}\right., 0 \leq z \leq 1\right\} \tag{4.83}
\end{equation*}
$$

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):

$$
\begin{equation*}
-L\left[y_{j}-y_{i}, z_{j}-z_{i}\right]=2 \sum_{p=1}^{\infty} \frac{1}{p} \exp \left[-2 \pi p\left|z_{j}-z_{i}\right|\right] \cos \left[2 \pi p\left(y_{i}-y_{j}\right)\right] \tag{4.84}
\end{equation*}
$$

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

$$
\begin{equation*}
-L\left[y_{j}-y_{i}, z_{j}-z_{i}\right]=2 \sum_{p=1}^{\infty} \frac{1}{p}\left(\frac{e_{j}}{e_{i}}\right)^{p}\left(c_{p i} \cdot c_{p j}+s_{p i} \cdot s_{p j}\right) \tag{4.85}
\end{equation*}
$$

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

$$
\begin{equation*}
E_{L}^{\delta}=-\frac{1}{2} \sum_{\substack{q_{i}, q_{j} \in C \\ \rho(i, j)>\delta}} q_{i} q_{j} L\left[y_{i}-y_{j}, z_{i}-z_{j}\right] . \tag{4.86}
\end{equation*}
$$

Finally, the correction term $E_{\delta}$ given in (4.67) is the same except that the set $R_{\delta}$ there has to be replaced by

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

## 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 $E_{B P}$ can thus be estimated as follows

$$
\begin{equation*}
T_{1}(\epsilon, N) \cong n_{1}(a) \cdot 2 \pi^{2} \cdot \epsilon^{2} N^{2} \int_{0}^{\frac{\sqrt{2}}{2}} r^{3} d r=c_{1}(a) \cdot \epsilon^{2} \cdot N^{2} \tag{5.1}
\end{equation*}
$$

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:

$$
\begin{align*}
E_{B} \cong & 2 \sum_{i=1}^{N} q_{i} \cdot \sum_{r_{n}>r_{i}+\epsilon} q_{n} \cdot \sum_{p=1}^{P(i, n)}\left\{T_{p i}^{(1)} \cdot T_{p n}^{(2)}+\sum_{\nu=1}^{\nu_{0}(p, i, n)} T_{p \nu i}^{(3)} T_{p \nu n}^{(4)}\right. \\
& \left.+\sum_{\nu=\nu_{0}+1}^{\nu_{m}(i, n)} \hat{T}_{\nu i}^{(3)} \hat{T}_{\nu n}^{(4)}\right\} . \tag{5.2}
\end{align*}
$$

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 $\rho$ the same for $q_{n}$.

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

$$
\begin{align*}
T_{2}(\epsilon, N) \cong & N \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r d r\left\{n_{2} \int_{r+\epsilon}^{r+R_{c}} P(r, \rho) d p+n_{3} \int_{p=1}^{P(r, \rho)} \nu_{0}(p, r, \rho) d p\right.  \tag{5.3}\\
& \left.+n_{4} \int_{r+\epsilon}^{R_{c}}\left[\nu_{m}(r, \rho)-\nu_{0}(1, r, \rho)\right] d p\right\}
\end{align*}
$$

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 $\rho$ replaced by $\rho-r$ there. One finds (see Appendix)

$$
\begin{equation*}
P(r, \rho)<\frac{1}{2 \pi(\rho-r)}\left\{a+\log \left(\frac{1}{\rho-r}\right)\right\} . \tag{5.4}
\end{equation*}
$$

Therefore one has

$$
\begin{align*}
n_{2} \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r=\int_{r+\epsilon}^{r+R_{c}} P(r, \rho) d \rho d r< & \frac{n_{2}}{2 \pi} \int_{\epsilon}^{\frac{\sqrt{2}}{2}} r d r \int_{\epsilon}^{R_{c}}\left[\frac{a}{t}+\frac{1}{t} \log \left(\frac{1}{t}\right)\right] d t  \tag{5.5}\\
& <c_{2}(a)\left[\log \left(\frac{1}{\epsilon}\right)+\log ^{2}\left(\frac{1}{\epsilon}\right)\right]
\end{align*}
$$

Next we need an estimate for the expression

$$
\begin{equation*}
a_{0} \equiv \int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_{c}} \int_{p=1}^{P(r, \rho)} \nu_{0}(p, r, \rho) d p d \rho d r \tag{5.6}
\end{equation*}
$$

We use the crude upper bound (see Appendix)

$$
\begin{equation*}
\nu_{0}(p, r, \rho)<\left[e^{a}(\pi p \rho)^{2}\right]^{1 / 3} \tag{5.7}
\end{equation*}
$$

which implies

$$
\begin{align*}
& \int_{p=1}^{P(r, \rho)} \nu_{0}(p, r, \rho) d p<\frac{3}{5} e^{a / 3}(\pi \rho)^{2 / 3} \cdot P(r, \rho)^{5 / 3}  \tag{5.8}\\
& =\frac{3}{5} e^{a / 3} \cdot(\pi P(r, \rho) \cdot \rho)^{2 / 3} \cdot P(r, \rho)<\frac{3}{5} e^{a / 3}\left(\pi\left(\frac{\sqrt{2}}{2}+R_{c}\right)\right)^{2 / 3} \cdot P(r, \rho) .
\end{align*}
$$

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

$$
\begin{equation*}
a_{0}<c_{3}(a)\left[\log \left(\frac{1}{\epsilon}\right)+\log ^{2}\left(\frac{1}{\epsilon}\right)\right] . \tag{5.9}
\end{equation*}
$$

As a last step we bound the term

$$
\begin{equation*}
a_{1} \equiv \int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_{c}}\left(\nu_{m}(r, \rho)-\nu_{0}(1, r, \rho)\right) d \rho d r<\int_{\epsilon}^{\frac{\sqrt{2}}{2}} \int_{r+\epsilon}^{r+R_{c}} \nu_{m}(r, \rho) d \rho d r \tag{5.10}
\end{equation*}
$$

By (4.24) one has

$$
\begin{equation*}
\nu_{m}(r, \rho) \leq \frac{\alpha}{\log \left(\frac{\rho}{r}\right)}+1 \tag{5.11}
\end{equation*}
$$

where $\alpha$ is the solution of (4.23).
We estimate as follows:

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

so that one has the crude estimate (for small $\epsilon$ !)

$$
\begin{equation*}
a_{1}<\text { const } \cdot \log \left(\frac{1}{\epsilon}\right) . \tag{5.12}
\end{equation*}
$$

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

$$
\begin{equation*}
T(\epsilon, N)<c_{1} \cdot \epsilon^{2} \cdot N^{2}+N\left(c_{2} \log \left(\frac{1}{\epsilon}\right)+c_{3} \cdot \log ^{2}\left(\frac{1}{\epsilon}\right)\right) . \tag{5.13}
\end{equation*}
$$

Here $\epsilon$ 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 $\epsilon$-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))

$$
\begin{equation*}
P \leq \frac{\beta}{2 \pi \cdot S} \tag{5.14}
\end{equation*}
$$

where $\beta$ is the solution of (4.28).
Hence the number of terms needed for the calculation of $E_{L}$ allows the estimate

$$
\begin{equation*}
T^{(5)}(\epsilon, N)<c_{5} \int_{\epsilon}^{1-\epsilon} \frac{\beta}{2 \pi \cdot s} d s<c_{5} \cdot \frac{\beta}{2 \pi} \log \left(\frac{1}{\epsilon}\right) \cdot N . \tag{5.15}
\end{equation*}
$$

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

We can now make an optimal choice of $\epsilon$ 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

$$
\begin{equation*}
\underline{T(\epsilon, N)<N\left(C_{1}+C_{2} \cdot \log N+C_{3}(\log N)^{2}\right) .} \tag{5.16}
\end{equation*}
$$

If one optimizes the value of $\epsilon$ 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

$$
\begin{equation*}
\frac{5.016}{2 \pi \rho} \frac{1}{\sqrt{2 \pi \rho \cdot P}} \exp (-2 \pi \rho P)=e^{-a} \tag{A1}
\end{equation*}
$$

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

$$
\begin{equation*}
s+\frac{1}{2} \log s=a+\log \left(\frac{c}{\rho}\right) . \tag{A2}
\end{equation*}
$$

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

$$
\begin{equation*}
s<a+\log \left(\frac{c}{\rho}\right), \tag{A3}
\end{equation*}
$$

i.e.

$$
\begin{equation*}
P<\frac{1}{2 \pi \rho}\left(a+\log \left(\frac{c}{\rho}\right)\right) . \tag{A4}
\end{equation*}
$$

One can give a very sharp estimate in the following way. We set $s_{0}=a+\log \left(\frac{c}{\rho}\right)$ and $s=s_{0}(1-t)$. Then insertion into (A2) and reduction yields

$$
\begin{equation*}
s_{0} \cdot t+\frac{1}{2} \log (1-t)=\frac{1}{2} \log s_{0} . \tag{A5}
\end{equation*}
$$

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

$$
\begin{equation*}
t=\frac{1}{2} \frac{\log s_{0}}{s_{0}+\frac{1}{2}} \tag{A6}
\end{equation*}
$$

which leads to the estimate

$$
\begin{equation*}
P \cong \frac{1}{2 \pi \rho} s_{0}\left[1-\frac{\frac{1}{2} \log s_{0}}{s_{0}+\frac{1}{2}}\right], s_{0}=a+\log \left(\frac{5.016}{2 \pi \rho}\right) . \tag{A7}
\end{equation*}
$$

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

$$
\begin{equation*}
h[r, R, \nu]=1-\exp \left[-\nu\left(w_{0}\left(\frac{R}{\nu}\right)-w_{0}\left(\frac{r}{\nu}\right)\right)\right] U_{1}\left(\frac{r}{\nu}\right) U_{2}\left(\frac{R}{\nu}\right) \tag{A8}
\end{equation*}
$$

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

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

Hence one has

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

which in turn leads to condition (4.51).
In order to find a crude approximation $\nu_{0}$ for the value of $\nu$ for which

$$
\begin{equation*}
\left|I_{\nu}(r) K_{\nu}(R)-\frac{1}{2 \nu}\left(\frac{r}{R}\right)^{\nu}\right| \leq e^{-a} \tag{A11}
\end{equation*}
$$

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

$$
\begin{equation*}
\nu \cong \nu_{0}=\left(r_{n} \pi p\right)^{2 / 3} \cdot e^{a / 3}, \tag{A12}
\end{equation*}
$$

as used in (4.52).

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