Fast Ewald summation under 2d- and 1d-periodic boundary conditions based on NFFTs

Franziska Nestler
Chemnitz University of Technology
Faculty of Mathematics
09107 Chemnitz, Germany
Email: franziska.nestler@mathematik.tu-chemnitz.de

Daniel Potts
Chemnitz University of Technology
Faculty of Mathematics
09107 Chemnitz, Germany
Email: potts@mathematik.tu-chemnitz.de

***Abstract*—Ewald summation has established as basic element of fast algorithms evaluating the Coulomb interaction energy of charged particle systems in three dimensions subject to periodic boundary conditions. In this context particle mesh routines, as the P3M method, and the P2NFFT, which is based on nonequispaced fast Fourier transforms (NFFT), should be mentioned. These methods treat the problem efficiently in case that periodic boundary conditions in all three dimensions are assumed. In this paper we present a new approach for the efficient calculation of the Coulomb interaction energy subject to mixed boundary conditions based on NFFTs.**

I. Introduction

Let a set of N charges $q_j \in \mathbb{R}$ at positions $\boldsymbol{x}_j \in \mathbb{R}^3$, $j = 1, \dots, N$, be given. Throughout this paper we assume that the system is electrical neutral, i.e., $\sum_{j=1}^{N} q_j = 0$. The electrostatic energy of the particle system is basically a sum of the form

$$E(\mathcal{S}) := \frac{1}{2} \sum_{i,j=1}^{N} {\sum_{\boldsymbol{n} \in S}}' \frac{q_i q_j}{\|\boldsymbol{x}_i - \boldsymbol{x}_j + B\boldsymbol{n}\|}, \tag{1}$$

where $\mathcal{S} \subseteq \mathbb{Z}^3$ is set according to the given boundary conditions and $B \in \mathbb{R}$ is the edge length of the periodically duplicated simulation box. The prime on the second sum indicates that in the case $\boldsymbol{n} = \boldsymbol{0}$ the terms for $i = j$ are omitted.

If periodic boundary conditions are applied in all three dimensions, the particle positions $\boldsymbol{x}_j$ are commonly assumed to be distributed in a cubic box, i.e., $\boldsymbol{x}_j \in B\mathbb{T}^3$ for some $B > 0$, and $\mathcal{S} := \mathbb{Z}^3$. We thereby define the torus $\mathbb{T} := \mathbb{R}/\mathbb{Z} \simeq [-1/2, 1/2)$. In some applications periodic boundary conditions are assumed in two or one dimension only, where we choose $\mathcal{S} := \mathbb{Z}^2 \times \{0\}$ with $\boldsymbol{x}_j \in B\mathbb{T}^2 \times \mathbb{R}$ and $\mathcal{S} := \mathbb{Z} \times \{0\}^2$ with $\boldsymbol{x}_j \in B\mathbb{T} \times \mathbb{R}^2$, respectively.

It is important to note that in all three cases the infinite sum (1) is only conditionally convergent, i.e., the value of the energy is not well defined unless a precise order of summation is specified.

The well known Ewald summation formulas, which have at first been derived for the fully periodic case, cf. [1], are the principle behind many fast algorithms evaluating the energy (1). The Ewald method is based on the trivial identity

$$\frac{1}{r} = \frac{\operatorname{erf}(\alpha r)}{r} + \frac{\operatorname{erfc}(\alpha r)}{r}, \tag{2}$$

where $\alpha > 0$, $\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t$ is the well known error function and $\operatorname{erfc}(x) := 1 - \operatorname{erf}(x)$ is the complementary error function. If (2) is applied to (1), the poorly converging sum is split into two exponentially converging parts. The first infinite sum, including the erfc-terms, is short ranged and absolutely convergent in spatial domain. Taking a specific summation order into account and exploiting the charge neutrality, the second sum, which is still long ranged, can be transformed into a rapidly converging sum in frequency domain. Usually, the energy (1) is defined over a spherical order of summation, see [4] for a detailed derivation for the fully periodic case. The Ewald summation formulas for 2d- and 1d-periodic boundary conditions are derived in [2] and [3], respectively.

In the fully periodic case, the Ewald method has the complexity $\mathcal{O}(N^{3/2})$ if the splitting parameter α is chosen appropriately. However, the computational effort can be reduced to $\mathcal{O}(N \log N)$ arithmetic operations by evaluating the long range part efficiently using Fast Fourier transforms (FFT). For this purpose, the problem has to be modified in a way that the FFT as a grid transformation can be used. This discretization is performed by replacing the charges q_j by a grid based charge density. This is the basic idea behind Particle Mesh approaches such as the P3M method, see [5] to get an overview over some of these techniques. The same principle is used in the P2NFFT method [6], which is based on nonequispaced fast Fourier transforms (NFFT). Here the discretization process is part of the NFFT algorithms.

For open boundary conditions, i.e., $\mathcal{S} := \{0\}^3$ in (1), fast summation methods [8], [9] based on NFFTs where suggested, too. In this note we aim to close the gap and propose FFT based algorithms also for 2d- and 1d-periodic boundary conditions.

We remark that the fast multipole method can also handle all boundary conditions very efficiently, see [10].

The outline of this paper is as follows. We start with a short introduction to the NFFT. Thereafter we consecutively consider the problem of evaluating (1) subject to 2d- and 1d-periodic boundary conditions. In each case we consider at first the according Ewald summation formula and then present a new approach for the efficient calculation of the Coulomb interaction energy (1) based on NFFTs.

To keep the notation short we define the difference vectors

$\boldsymbol{x}_{ij} := \boldsymbol{x}_i - \boldsymbol{x}_j$. For some $\boldsymbol{M} \in 2\mathbb{N}^d$ we refer to $\mathcal{I}_{\boldsymbol{M}}$ as the index set given by

$$\mathcal{I}_{\boldsymbol{M}} := \left\{ \left[-\tfrac{M_1}{2}, \tfrac{M_1}{2}\right) \times \cdots \times \left[-\tfrac{M_d}{2}, \tfrac{M_d}{2}\right) \right\} \cap \mathbb{Z}^d.$$

Throughout this paper we do not distinguish between row and column vectors and denote by $\boldsymbol{x} \cdot \boldsymbol{y} := x_1 y_1 + \ldots + x_d y_d$ the scalar product and by $\boldsymbol{x} \odot \boldsymbol{y} := (x_1 y_1, \ldots, x_d y_d) \in \mathbb{R}^d$ the component wise product of two vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$. For some $\boldsymbol{x} \in \mathbb{R}^d$ with non-vanishing components we further define the vector $\boldsymbol{x}^{-1} \in \mathbb{R}^d$ by $\boldsymbol{x}^{-1} := (x_1^{-1}, \ldots, x_d^{-1})$.

II. Nonequispaced Fast Fourier Transforms

Let $\boldsymbol{M} \in 2\mathbb{N}^d$, the index set $\mathcal{I}_{\boldsymbol{M}}$ and the coefficients $\hat{f}_{\boldsymbol{k}} \in \mathbb{C}$ for $\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}$ be given. The fast evaluation of a trigonometric polynomial

$$f(\boldsymbol{x}) := \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}}$$

at $N \in \mathbb{N}$ given nodes $\boldsymbol{x}_j \in \mathbb{T}^d$, i.e., the fast computation of $f_j := f(\boldsymbol{x}_j)$, $j = 1, \ldots, N$, is known as d-dimensional NFFT. The algorithm uses an approximation of f in the form

$$f(\boldsymbol{x}) \approx \sum_{\boldsymbol{l} \in \mathcal{I}_{\boldsymbol{m}}} g_{\boldsymbol{l}} \tilde{\varphi}(\boldsymbol{x} - \boldsymbol{l} \odot \boldsymbol{m}^{-1}), \tag{3}$$

where $\tilde{\varphi}$ is a multivariate 1-periodic function, which is well localized in spatial and frequency domain, and $\boldsymbol{m} \in 2\mathbb{N}^d$ with $\boldsymbol{m} > \boldsymbol{M}$ (component wise). It can be shown that it is reasonable to set, cf. [7],

$$g_{\boldsymbol{l}} := \frac{1}{|\mathcal{I}_{\boldsymbol{m}}|} \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \frac{\hat{f}_{\boldsymbol{k}}}{c_{\boldsymbol{k}}(\tilde{\varphi})} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot (\boldsymbol{l} \odot \boldsymbol{m}^{-1})},$$

where $c_{\boldsymbol{k}}(\tilde{\varphi})$ denotes the Fourier coefficient with index $\boldsymbol{k}$ of $\tilde{\varphi}$. Obviously, the coefficients $g_{\boldsymbol{l}} \in \mathbb{C}$ can be calculated using the FFT. The function values $f(\boldsymbol{x}_j)$ are then computed via (3), where the sums can be truncated due to the good localization of $\tilde{\varphi}$ in spatial domain.

Correspondingly, the adjoint NFFT is an algorithm for the efficient calculation of

$$\hat{h}_{\boldsymbol{k}} := \sum_{j=1}^{N} f_j \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_j}, \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}},$$

for N given nodes $\boldsymbol{x}_j \in \mathbb{T}^d$ and coefficients $f_j \in \mathbb{C}$, $j = 1, \ldots, N$. The resulting algorithm has a very similar structure and the same arithmetic complexity of $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}| \log |\mathcal{I}_{\boldsymbol{M}}| + N)$, see [7] for instance. In this reference different choices for the window function $\tilde{\varphi}$ are discussed, too.

III. 2d-periodic systems

For N charges q_j at positions $\boldsymbol{x}_j = (x_{j,1}, x_{j,2}, x_{j,3}) \in B\mathbb{T}^2 \times \mathbb{R}$, $j = 1, \ldots, N$, we define the electrostatic energy subject to periodic boundary conditions in the first two dimensions by $E^{\mathrm{p2}} := E(\mathbb{Z}^2 \times \{0\})$.

At first we review the corresponding Ewald formula, as derived in [2], and then present an NFFT approach for the fast calculation of the energy E^{p2}. In this section we refer to $\tilde{\boldsymbol{x}} := (x_1, x_2) \in B\mathbb{T}^2$ as the vector of the first two components of some $\boldsymbol{x} \in B\mathbb{T}^2 \times \mathbb{R}$.

A. Ewald Formula

If a spherical order of summation is applied, the electrostatic energy E^{p2} can be written in the form, cf. [2],

$$E^{\mathrm{p2}} = E^{\mathrm{p2,S}} + E^{\mathrm{p2,L}} + E^{\mathrm{p2},\boldsymbol{0}} + E^{\mathrm{p2,self}}, \tag{4}$$

where for some $\alpha > 0$

$$E^{\mathrm{p2,S}} := \frac{1}{2} \sum_{\boldsymbol{n} \in \mathbb{Z}^2 \times \{0\}} {\sum_{i,j=1}^{N}}' q_i q_j \frac{\operatorname{erfc}(\alpha \|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|)}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}$$

$$E^{\mathrm{p2,L}} := \frac{1}{4B} \sum_{\boldsymbol{k} \in \mathbb{Z}^2 \setminus \{\boldsymbol{0}\}} \sum_{i,j=1}^{N} q_i q_j \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \tilde{\boldsymbol{x}}_{ij}/B} \Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3})$$

$$E^{\mathrm{p2},\boldsymbol{0}} := -\frac{\sqrt{\pi}}{B^2} \sum_{i,j=1}^{N} q_i q_j \Theta_0^{\mathrm{p2}}(x_{ij,3})$$

$$E^{\mathrm{p2,self}} := -\frac{\alpha}{\sqrt{\pi}} \sum_{j=1}^{N} q_j^2.$$

We thereby define the functions Θ_0^{p2} and Θ^{p2} by

$$\Theta_0^{\mathrm{p2}}(r) := \frac{\mathrm{e}^{-\alpha^2 r^2}}{\alpha} + \sqrt{\pi} r \operatorname{erf}(\alpha r)$$

and

$$\Theta^{\mathrm{p2}}(k, r) := \frac{\Psi(k, r) + \Psi(k, -r)}{k},$$

where we set

$$\Psi(k, r) := \mathrm{e}^{2\pi k r / B} \operatorname{erfc}\left(\tfrac{\pi k}{\alpha B} + \alpha r\right).$$

We immediately see that $\Theta_0^{\mathrm{p2}} \in \mathrm{C}^\infty(\mathbb{R})$ as well as $\Theta^{\mathrm{p2}}(k, \cdot) \in \mathrm{C}^\infty(\mathbb{R})$ for each $k \neq 0$.

Lemma 1. *For arbitrary $r \in \mathbb{R}$ we have $\Theta^{\mathrm{p2}}(k, r) \to 0$ with $\Theta^{\mathrm{p2}}(k, r) \sim k^{-2} \mathrm{e}^{-k^2}$ for $k \to \infty$.*

Proof: The function Θ^{p2} has the integral representation

$$\Theta^{\mathrm{p2}}(k, r) = \frac{4\sqrt{\pi}}{B} \int_0^\alpha \frac{1}{t^2} \exp\left(-\frac{\pi^2 k^2}{B^2 t^2} - r^2 t^2\right) \mathrm{d}t,$$

cf. [11, number 7.4.33]. We now easily see

$$\Theta^{\mathrm{p2}}(k, r) \leq \Theta^{\mathrm{p2}}(k, 0) = \frac{2}{k} \operatorname{erfc}\left(\frac{\pi k}{\alpha B}\right) \approx \frac{2\alpha B}{k^2 \pi^{3/2}} \mathrm{e}^{-\frac{\pi^2 k^2}{\alpha^2 B^2}},$$

which is valid for large k, cf. [11, number 7.1.23]. □

B. An NFFT approach

The infinite sum in $E^{\mathrm{p2,S}}$ is short ranged and can be computed by direct evaluation. Due to Lemma 1 the infinite sum in $E^{\mathrm{p2,L}}$ can be truncated, i.e., we can replace $\mathbb{Z}^2$ by $\mathcal{I}_{\boldsymbol{M}}$ for some appropriate $\boldsymbol{M} \in 2\mathbb{N}^2$.

In the following we choose $h > 0$ and $\varepsilon > 0$ such that $|x_{ij,3}| \leq h(1/2 - \varepsilon)$ for all $i, j = 1, \ldots, N$. In order to compute the far field $E^{\mathrm{p2,L}} + E^{\mathrm{p2},\boldsymbol{0}}$ efficiently we employ the idea of NFFT based fast summation methods [8] and consider the regularization

$$K_{\mathrm{R}}(k, r) := \begin{cases} \frac{1}{4B} \Theta^{\mathrm{p2}}(k, r) & : k \neq 0, |h^{-1} r| \leq 1/2 - \varepsilon \\ \frac{-\sqrt{\pi}}{B^2} \Theta_0^{\mathrm{p2}}(r) & : k = 0, |h^{-1} r| \leq 1/2 - \varepsilon \\ K_{\mathrm{B}}(k, r) & : |h^{-1} r| \in (1/2 - \varepsilon, 1/2] \end{cases},$$

where for each $k \in \{\|\boldsymbol{k}\| : \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}\}$ the function $K_{\mathrm{B}}(k,\cdot)$ is defined such that $K_{\mathrm{R}}(k,\cdot)$ is in the space $\mathrm{C}^p(h\mathbb{T})$ for some $p \in \mathbb{N}$ large enough, i.e., $K_{\mathrm{B}}(k,\cdot)$ fulfills the conditions

$$\begin{aligned} K_{\mathrm{B}}^{(n)}(k, {}^{h}/_{2} - h\varepsilon) &= K_{\mathrm{R}}^{(n)}(k, {}^{h}/_{2} - h\varepsilon) \\ K_{\mathrm{B}}^{(n)}(k, -{}^{h}/_{2} + h\varepsilon) &= K_{\mathrm{R}}^{(n)}(k, -{}^{h}/_{2} + h\varepsilon) \\ &= (-1)^n K_{\mathrm{R}}^{(n)}(k, {}^{h}/_{2} - h\varepsilon) \end{aligned}$$

for all $n = 0, \dots, p$ and is chosen such that

$$K_{\mathrm{R}}^{(n)}(k, {}^{h}/_{2}) = K_{\mathrm{R}}^{(n)}(k, -{}^{h}/_{2}) \quad \forall\, n = 0, \dots, p$$

is satisfied, too. The order p can be chosen arbitrarily large as the functions Θ_0^{p2} and $\Theta^{\mathrm{p2}}(k,\cdot)$ are differentiable for all degrees of differentiation. The resulting functions $K_{\mathrm{R}}(k,\cdot)$ then are h-periodic and smooth. Thus we can find good approximations of the form

$$K_{\mathrm{R}}(k,r) \approx \sum_{l \in \mathcal{I}_{M_3}} b_{k,l} \mathrm{e}^{2\pi \mathrm{i} l r/h}$$

with $M_3 \in 2\mathbb{N}$ large enough and the Fourier coefficients

$$b_{k,l} := \frac{1}{M_3} \sum_{j \in \mathcal{I}_{M_3}} K_{\mathrm{R}}\left(k, {}^{jh}/_{M_3}\right) \mathrm{e}^{-2\pi \mathrm{i} j l/M_3}.$$

With $\boldsymbol{M}^* := (\boldsymbol{M}, M_3) \in 2\mathbb{N}^3$ we obtain

$$\begin{aligned} E^{\mathrm{p2,L}} + E^{\mathrm{p2},\mathbf{0}} &\approx \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \sum_{l \in \mathcal{I}_{M_3}} b_{\|\boldsymbol{k}\|,l} \sum_{i,j=1}^{N} q_i q_j \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v}_{\boldsymbol{k},l} \cdot \boldsymbol{x}_{ij}} \\ &= \sum_{(\boldsymbol{k},l) \in \mathcal{I}_{\boldsymbol{M}^*}} b_{\|\boldsymbol{k}\|,l} |S(\boldsymbol{k},l)|^2, \end{aligned} \tag{5}$$

where we define

$$\boldsymbol{v}_{\boldsymbol{k},l} := \begin{pmatrix} \boldsymbol{k}/B \\ l/h \end{pmatrix} \text{ as well as } S(\boldsymbol{k},l) := \sum_{j=1}^{N} q_j \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v}_{\boldsymbol{k},l} \cdot \boldsymbol{x}_j}.$$

Obviously, the sums $S(\boldsymbol{k},l)$, $(\boldsymbol{k},l) \in \mathcal{I}_{\boldsymbol{M}^*}$, can efficiently be computed by a trivariate adjoint NFFT.

Remark 1. *The energy E^{p2} can also be written in the form $E^{\mathrm{p2}} = \frac{1}{2}\sum_{j=1}^{N} q_j \phi^{\mathrm{p2}}(\boldsymbol{x}_j)$, where for each $\boldsymbol{x}_j$ the potential $\phi^{\mathrm{p2}}(\boldsymbol{x}_j)$ is defined by*

$$\phi^{\mathrm{p2}}(\boldsymbol{x}_j) := \sum_{\boldsymbol{n} \in \mathbb{Z}^2 \times \{0\}} {\sum_{i=1}^{N}}' \frac{q_i}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}.$$

The term $q_j \phi^{\mathrm{p2}}(\boldsymbol{x}_j)$ then represents the energy of the single particle j. It is easy to see that we can write

$$\phi^{\mathrm{p2}}(\boldsymbol{x}_j) = \phi^{\mathrm{p2,S}}(\boldsymbol{x}_j) + \phi^{\mathrm{p2,L}}(\boldsymbol{x}_j) + \phi^{\mathrm{p2},\mathbf{0}}(\boldsymbol{x}_j) + \phi^{\mathrm{p2,self}}(\boldsymbol{x}_j),$$

according to (4)*. By* (5) *we find that the long range part $\phi^{\mathrm{p2,L}}(\boldsymbol{x}_j) + \phi^{\mathrm{p2},\mathbf{0}}(\boldsymbol{x}_j)$ can be approximated by*

$$2 \sum_{(\boldsymbol{k},l) \in \mathcal{I}_{\boldsymbol{M}^*}} b_{\|\boldsymbol{k}\|,l} S(\boldsymbol{k},l) \mathrm{e}^{-2\pi i \boldsymbol{v}_{\boldsymbol{k},l} \cdot \boldsymbol{x}_j}.$$

Having calculated the sums $S(\boldsymbol{k},l)$ the long range parts of the potentials $\phi^{\mathrm{p2}}(\boldsymbol{x}_j)$, $j = 1, \dots, N$, can be computed by a trivariate NFFT. Note that computing this additional NFFT is not necessary if only the total energy E^{p2} is of interest.

IV. 1D-PERIODIC SYSTEMS

For N charges q_j at positions $\boldsymbol{x}_j \in B\mathbb{T} \times \mathbb{R}^2$, $j = 1, \dots, N$, we denote by $E^{\mathrm{p1}} := E(\mathbb{Z} \times \{0\}^2)$ the electrostatic energy (1) subject to periodic boundary conditions in the first dimension.

In this section we refer to $\tilde{\boldsymbol{x}} := (x_2, x_3) \in \mathbb{R}^2$ as the vector of the last two components of some $\boldsymbol{x} \in B\mathbb{T} \times \mathbb{R}^2$. Furthermore we define by

$$\Gamma(s,x) := \int_x^\infty t^{s-1} \mathrm{e}^{-t} \mathrm{d}t$$

the upper incomplete gamma function and by γ the Euler constant.

A. Ewald formula

The Ewald summation formula for the electrostatic energy E^{p1} reads as, cf. [3],

$$E^{\mathrm{p1}} = E^{\mathrm{p1,S}} + E^{\mathrm{p1,L}} + E^{\mathrm{p1},0} + E^{\mathrm{p1,self}},$$

where

$$\begin{aligned} E^{\mathrm{p1,S}} &:= \frac{1}{2} \sum_{\boldsymbol{n} \in \mathbb{Z} \times \{0\}^2} {\sum_{i,j=1}^{N}}' q_i q_j \frac{\operatorname{erfc}(\alpha \|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|)}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|} \\ E^{\mathrm{p1,L}} &:= \frac{1}{B} \sum_{k \in \mathbb{Z} \setminus \{0\}} \sum_{i,j=1}^{N} q_i q_j \mathrm{e}^{2\pi \mathrm{i} k x_{ij,1}/B} \Theta^{\mathrm{p1}}(k, \|\tilde{\boldsymbol{x}}_{ij}\|) \\ E^{\mathrm{p1},0} &:= -\frac{1}{2B} \sum_{\substack{i,j=1 \\ \tilde{\boldsymbol{x}}_{ij} \neq \mathbf{0}}}^{N} q_i q_j \Theta_0^{\mathrm{p1}}(\|\tilde{\boldsymbol{x}}_{ij}\|) \\ E^{\mathrm{p1,self}} &:= -\frac{\alpha}{\sqrt{\pi}} \sum_{j=1}^{N} q_j^2 \end{aligned}$$

for some $\alpha > 0$. Thereby the functions Θ^{p1} and Θ_0^{p1} are defined by

$$\Theta^{\mathrm{p1}}(k,r) := \int_0^\alpha \frac{1}{t} \exp\left(-\frac{\pi^2 k^2}{B^2 t^2} - r^2 t^2\right) \mathrm{d}t$$

and

$$\Theta_0^{\mathrm{p1}}(r) := \gamma + \Gamma(0, \alpha^2 r^2) + \ln(\alpha^2 r^2).$$

It can easily be seen that $\Theta^{\mathrm{p1}}(k,\cdot) \in \mathrm{C}^\infty(\mathbb{R})$ for any k.

Lemma 2. *For arbitrary $r \in \mathbb{R}$ we have $\Theta^{\mathrm{p1}}(k,r) \to 0$ with $\Theta^{\mathrm{p1}}(k,r) \sim k^{-2}\mathrm{e}^{-k^2}$ for $k \to \infty$.*

Proof: We immediately see

$$\Theta^{\mathrm{p1}}(k,r) \leq \Theta^{\mathrm{p1}}(k,0) = \frac{1}{2}\Gamma\left(0, \frac{\pi^2 k^2}{\alpha^2 B^2}\right).$$

The claim follows by applying the asymptotic expansion

$$\Gamma(0,x) \approx \frac{\mathrm{e}^{-x}}{x},$$

cf. [11, number 6.5.32], which holds for large x. □

Lemma 3. *For the univariate function*

$$\vartheta(x) := \begin{cases} 0 & : x = 0 \\ \gamma + \Gamma(0, x^2) + \ln(x^2) & : \textit{else} \end{cases}$$

we have $\vartheta \in \mathrm{C}^\infty(\mathbb{R})$.

Proof: From the identity, cf. [11, number 5.1.11],

$$\gamma + \Gamma(0,t) + \ln(t) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1} t^k}{k!k}, \tag{6}$$

which is fulfilled for all positive t, it can be seen that $\lim_{t\to 0} \Gamma(0,t) + \ln t + \gamma = 0$. Thus, the function ϑ is continuous. Since (6) holds for $t > 0$ we obtain

$$\gamma + \Gamma(0,x^2) + \ln(x^2) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1} x^{2k}}{k!k}$$

for all $x \neq 0$ and conclude

$$\begin{aligned} &\lim_{x\to+0} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(\Gamma(0,x^2) + \ln(x^2)\right) \\ &= \lim_{x\to-0} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(\Gamma(0,x^2) + \ln(x^2)\right) \neq \pm\infty \end{aligned}$$

for all $n \in \mathbb{N}$. □

B. An NFFT approach

Due to Lemma 2 the infinite sum in $E^{\mathrm{p1,L}}$ can be truncated, i.e., we can replace $\mathbb{Z}$ by $\mathcal{I}_{M_0}$ for some appropriate $M_0 \in 2\mathbb{N}$.

In the following we choose $h > 0$ and $\varepsilon > 0$ such that $\|\tilde{\boldsymbol{x}}_{ij}\| \leq h(1/2 - \varepsilon)$ for all $i,j = 1,\dots,N$. In order to compute the far field $E^{\mathrm{p1,L}} + E^{\mathrm{p1,0}}$ efficiently we define the regularization K_{R} by

$$K_{\mathrm{R}}(k,r) := \begin{cases} \frac{1}{B}\Theta^{\mathrm{p1}}(k,r) & : k \neq 0, |h^{-1}r| \leq 1/2 - \varepsilon \\ -\frac{1}{2B}\Theta_0^{\mathrm{p1}}(r) & : k = 0, |h^{-1}r| \leq 1/2 - \varepsilon \\ K_{\mathrm{B}}(k,r) & : |h^{-1}r| \in (1/2 - \varepsilon, 1/2] \end{cases},$$

where for each $k \in \mathbb{N}_0 \cap \mathcal{I}_{M_0}$ the function $K_{\mathrm{B}}(k,\cdot)$ is chosen such that the bivariate function $K_{\mathrm{R}}(k,\|\cdot\|) : h\mathbb{T}^2 \to \mathbb{R}$ is in the space $\mathrm{C}^p(h\mathbb{T}^2)$ for $p \in \mathbb{N}$ sufficiently large, i.e., $K_{\mathrm{B}}(k,\cdot)$ fulfills the conditions

$$\begin{aligned} K_{\mathrm{B}}^{(n)}(k, h/2 - h\varepsilon) &= K_{\mathrm{R}}^{(n)}(k, h/2 - h\varepsilon) \\ K_{\mathrm{B}}^{(n)}(k, -h/2 + h\varepsilon) &= (-1)^n K_{\mathrm{R}}^{(n)}(k, h/2 - h\varepsilon) \end{aligned}$$

for all $n = 0,\dots,p$ and is chosen such that

$$\begin{aligned} K_{\mathrm{R}}(k, h/2) &= K_{\mathrm{R}}(k, -h/2) \\ K_{\mathrm{R}}^{(n)}(k, h/2) &= K_{\mathrm{R}}^{(n)}(k, -h/2) = 0, \quad n = 1,\dots,p. \end{aligned}$$

We further set $K_{\mathrm{R}}(k,\|\boldsymbol{y}\|) := K_{\mathrm{R}}(k, h/2)$ for all $\boldsymbol{y} \in h\mathbb{T}^2$ with $\|\boldsymbol{y}\| > h/2$.

The smooth and periodic functions $K_{\mathrm{R}}(k,\|\cdot\|)$ can then be approximated by a bivariate trigonometric polynomial. To this end, we set $r := \|\boldsymbol{y}\|$, $\boldsymbol{y} \in h\mathbb{T}^2$, and obtain for each $k \in \mathbb{N} \cap \mathcal{I}_{M_0}$ with an appropriate $\boldsymbol{M} \in 2\mathbb{N}^2$

$$K_{\mathrm{R}}(k,\|\boldsymbol{y}\|) \approx \sum_{\boldsymbol{l} \in \mathcal{I}_{\boldsymbol{M}}} b_{k,\boldsymbol{l}} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{l}\cdot\boldsymbol{y}/h}$$

with the Fourier coefficients

$$b_{k,\boldsymbol{l}} := \frac{1}{|\mathcal{I}_{\boldsymbol{M}}|} \sum_{\boldsymbol{j} \in \mathcal{I}_{\boldsymbol{M}}} K_{\mathrm{R}}\left(k, \|\boldsymbol{j} \odot \boldsymbol{M}^{-1}\| h\right) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{j}\cdot(\boldsymbol{l}\odot\boldsymbol{M}^{-1})}.$$

With $\boldsymbol{M}^* := (M_0, \boldsymbol{M}) \in 2\mathbb{N}^3$ we obtain, analogously to (5),

$$\begin{aligned} E^{\mathrm{p1,L}} + E^{\mathrm{p1,0}} &\approx \sum_{(k,\boldsymbol{l}) \in \mathcal{I}_{\boldsymbol{M}^*}} b_{|k|,\boldsymbol{l}} \sum_{i,j=1}^{N} q_i q_j \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{v}_{k,\boldsymbol{l}}\cdot\boldsymbol{x}_{ij}} \\ &= \sum_{(k,\boldsymbol{l}) \in \mathcal{I}_{\boldsymbol{M}^*}} b_{|k|,\boldsymbol{l}} |S(k,\boldsymbol{l})|^2, \end{aligned}$$

where we set

$$S(k,\boldsymbol{l}) := \sum_{j=1}^{N} q_j \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{v}_{k,\boldsymbol{l}}\cdot\boldsymbol{x}_j} \text{ with } \boldsymbol{v}_{k,\boldsymbol{l}} := \begin{pmatrix} k/B \\ \boldsymbol{l}/h \end{pmatrix}.$$

The sums $S(k,\boldsymbol{l})$, $(k,\boldsymbol{l}) \in \mathcal{I}_{\boldsymbol{M}^*}$, can efficiently be evaluated by a trivariate adjoint NFFT. For the 1d-periodic case a similar statement to that in Remark 1 can be given.

V. Conclusion

In this paper we proposed a new approach for the efficient calculation of the Coulomb interaction energy under 2d- and 1d- periodic boundary conditions. The presented methods are based on the corresponding Ewald summation formulas and nonequispaced fast Fourier transforms, where the ansatz is very much related to those of NFFT based fast summation methods. Numerical results of these algorithms will be reported in a further paper, where we aim to set the main focus on the derivation of error estimates as well as concluding statements about the optimal choice of the cutoff parameters and the regularization variables h, ε and p.

References

[1] P. P. Ewald, "Die Berechnung optischer und elektrostatischer Gitterpotentiale," *Annalen der Physik*, vol. 369, no. 3, pp. 253–287, 1921.

[2] A. Grzybowski, E. Gwóźdź, and A. Bródka, "Ewald summation of electrostatic interactions in molecular dynamics of a three-dimensional system with periodicity in two directions," *Phys. Rev. B*, vol. 61, pp. 6706–6712, Mar 2000.

[3] M. Porto, "Ewald summation of electrostatic interactions of systems with finite extent in two of three dimensions," *J. Phys. A*, vol. 33, pp. 6211 – 6218, 2000.

[4] S. W. de Leeuw, J. W. Perram, and E. R. Smith, "Simulation of electrostatic systems in periodic boundary conditions. I. Lattice sums and dielectric constants," *Proc. Roy. Soc. London Ser. A*, vol. 373, no. 1752, pp. 27 – 56, 1980.

[5] M. Deserno and C. Holm, "How to mesh up Ewald sums. I. A theoretical and numerical comparison of various particle mesh routines," *J. Chem. Phys.*, vol. 109, pp. 7678 – 7693, 1998.

[6] M. Pippig and D. Potts, "Particle simulation based on nonequispaced fast Fourier transforms," in *Fast Methods for Long-Range Interactions in Complex Systems*, ser. IAS-Series, G. Sutmann, P. Gibbon, and T. Lippert, Eds. Jülich: Forschungszentrum Jülich, 2011, pp. 131 – 158.

[7] J. Keiner, S. Kunis, and D. Potts, "Using NFFT3 - a software library for various nonequispaced fast Fourier transforms," *ACM Trans. Math. Software*, vol. 36, pp. Article 19, 1 – 30, 2009.

[8] D. Potts and G. Steidl, "Fast summation at nonequispaced knots by NFFTs," *SIAM J. Sci. Comput.*, vol. 24, pp. 2013 – 2037, 2003.

[9] D. Potts, G. Steidl, and A. Nieslony, "Fast convolution with radial kernels at nonequispaced knots," *Numer. Math.*, vol. 98, pp. 329 – 351, 2004.

[10] I. Kabadshow and H. Dachsel, "The Error-Controlled Fast Multipole Method for Open and Periodic Boundary Conditions," in *Fast Methods for Long-Range Interactions in Complex Systems*, ser. IAS-Series, G. Sutmann, P. Gibbon, and T. Lippert, Eds. Jülich: Forschungszentrum Jülich, 2011, pp. 85 – 113.

[11] M. Abramowitz and I. A. Stegun, Eds., *Handbook of Mathematical Functions*. Washington, DC, USA: National Bureau of Standards, 1972.