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

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Contents

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Notation

- define the torus $\mathbb{T} := \mathbb{R}/\mathbb{Z} \simeq [-1/2, 1/2)$
- for $M \in 2\mathbb{N}$ set $\mathcal{I}_M := \{-M/2, \dots, M/2 - 1\}^3$

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Complexity: $\mathcal{O}(|\mathcal{I}_M| \log |\mathcal{I}_M| + N)$

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\text{adjoint NFFT:} & h(\boldsymbol{k}) & := \displaystyle\sum_{j=1}^{N} f_j \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k}\cdot\boldsymbol{x}_j} & \boldsymbol{k} \in \mathcal{I}_M
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Let N charges $q_j \in \mathbb{R}$ at positions $\boldsymbol{x}_j \in \mathbb{R}^3$ be given.
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choose $S := \mathbb{Z}^3$, $\boldsymbol{x}_j \in B\mathbb{T}^3$ and set

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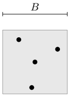

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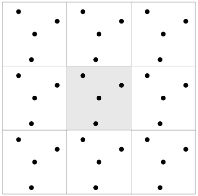

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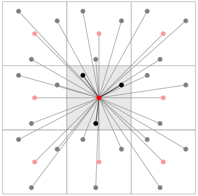

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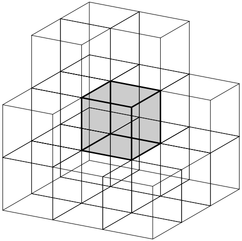

Coulomb energy s.t. periodic boundary conditions

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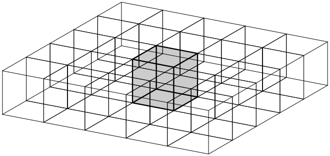
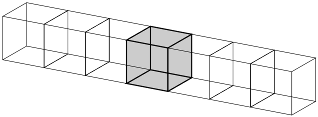
2d-periodic	1d-periodic
$\boldsymbol{x}_j \in B\mathbb{T}^2 \times \mathbb{R},\ \mathcal{S} := \mathbb{Z}^2 \times \{0\}$	$\boldsymbol{x}_j \in B\mathbb{T} \times \mathbb{R}^2,\ \mathcal{S} := \mathbb{Z} \times \{0\}^2$





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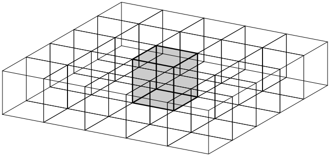

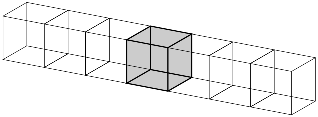

Assume $\sum_{j=1}^{N} q_j = 0 \Rightarrow$ **conditional** convergence

Fast algorithms

Non Fourier methods

- Multigrid, $\mathcal{O}(N)$ [Brandt, Hackbusch, Trottenberg 1977]
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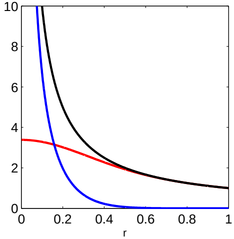
Aim: propose efficient NFFT based methods for 2d- and 1d-periodic b.c.

Ewald's idea

Idea of the Ewald summation [Ewald 1921]:

Ewald splitting

$$\frac{1}{r} = \underbrace{\frac{\operatorname{erf}(\alpha r)}{r}}_{\substack{\text{long ranged,}\\ \text{continuous}}} + \underbrace{\frac{\operatorname{erfc}(\alpha r)}{r}}_{\substack{\text{singular in 0,}\\ \text{short ranged}}}$$



- $\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t$ (error function)
- $\operatorname{erfc}(x) := 1 - \operatorname{erf}(x)$ (complementary error function)
- $\alpha > 0$ (scaling parameter)

3d Ewald Summation

We apply $\frac{1}{r} = \frac{\operatorname{erfc}(\alpha r)}{r} + \frac{\operatorname{erf}(\alpha r)}{r}$ with $r := \|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|$ and obtain

$$\sum_{\boldsymbol{n}\in\mathbb{Z}^3} \sum_{\substack{i,j=1 \\ i\neq j \text{ if } \boldsymbol{n}=\boldsymbol{0}}}^{N} \frac{q_i q_j}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}$$

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- short range part can be obtained via direct evaluation after truncation

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- short range part can be obtained via direct evaluation after truncation
- $\lim_{r\to 0} \frac{\operatorname{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}} \Rightarrow$ substract self energy
- write the long range part as a sum in Fourier space

An efficient algorithm

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- long range part: conditional convergence
  assume: charge neutrality + spherical order of summation

$$\frac{1}{2}\sum_{\boldsymbol{n}\in\mathbb{Z}^3}\sum_{i,j=1}^{N} q_i q_j \frac{\operatorname{erf}(\alpha\|\boldsymbol{x}_i-\boldsymbol{x}_j+B\boldsymbol{n}\|)}{\|\boldsymbol{x}_i-\boldsymbol{x}_j+B\boldsymbol{n}\|}$$

$$= \frac{1}{2\pi B}\sum_{\boldsymbol{k}\in\mathbb{Z}^3\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|^2/(\alpha^2B^2)}}{\|\boldsymbol{k}\|^2}|S(\boldsymbol{k})|^2 + \frac{2\pi}{3B^2}\left\|\sum_{j=1}^{N} q_j\boldsymbol{x}_j\right\|^2,$$

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- truncate the infinite sum ($\mathbb{Z}^3 \to \mathcal{I}_M$)

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$$= \quad \frac{1}{2\pi B}\sum_{\boldsymbol{k}\in\mathbb{Z}^3\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|^2/(\alpha^2B^2)}}{\|\boldsymbol{k}\|^2}|S(\boldsymbol{k})|^2 + \frac{2\pi}{3B^2}\left\|\sum_{j=1}^{N} q_j\boldsymbol{x}_j\right\|^2,$$

  where $S(\boldsymbol{k}) := \sum_{j=1}^{N} q_j \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}_j/B}$
- truncate the infinite sum $(\mathbb{Z}^3 \to \mathcal{I}_M)$
- $S(\boldsymbol{k})$, $\boldsymbol{k}\in\mathcal{I}_M$, by adjoint 3d-NFFT

An efficient algorithm

- calculate the self energy
- compute short range part: direct evaluation
- long range part: conditional convergence
  assume: charge neutrality + spherical order of summation

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- truncate the infinite sum ($\mathbb{Z}^3 \to \mathcal{I}_M$)
- $S(\boldsymbol{k})$, $\boldsymbol{k}\in\mathcal{I}_M$, by adjoint 3d-NFFT
- resulting method: $\mathcal{O}(N\log N)$

Computing the potentials

If we are interested in the potentials:

Write the Fourier part of the potentials in the form

$$\frac{1}{\pi B} \sum_{\boldsymbol{k} \in \mathbb{Z}^3 \setminus \{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2 \|\boldsymbol{k}\|^2/(\alpha^2 B^2)}}{\|\boldsymbol{k}\|^2} \left(\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_i / B} \right) \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_j / B}$$

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. . . and use adjoint NFFT + NFFT

Ewald summation s.t. 2d periodic boundary conditions

Long range part under 2d-periodic b.c. [Grzybowski, Gwóźdź, Bródka 2000]

We define $\boldsymbol{x}_{ij} := \boldsymbol{x}_i - \boldsymbol{x}_j = (\tilde{\boldsymbol{x}}_{ij}, x_{ij,3})$ and obtain

$$\frac{1}{4B} \sum_{\boldsymbol{k}\in\mathbb{Z}^2\setminus\{\boldsymbol{0}\}} \sum_{i,j=1}^{N} q_i q_j \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\tilde{\boldsymbol{x}}_{ij}/B} \Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3}) - \frac{\sqrt{\pi}}{B^2} \sum_{i,j=1}^{N} q_i q_j \Theta_0^{\mathrm{p2}}(x_{ij,3})$$

2d Fourier series

$\boldsymbol{k} = \boldsymbol{0}$ part

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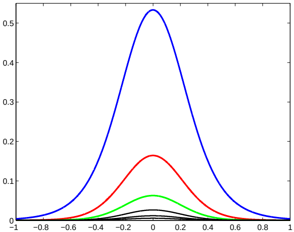

$\Theta^{\mathrm{p2}}(k, r)$

$k = 1$
$k = \sqrt{2}$
$k = \sqrt{3}$
$\ldots$

$$\frac{\mathrm{e}^{2\pi k r/B}\operatorname{erfc}\left(\frac{\pi k}{\alpha B} + \alpha r\right) + \mathrm{e}^{-2\pi k r/B}\operatorname{erfc}\left(\frac{\pi k}{\alpha B} - \alpha r\right)}{k}$$

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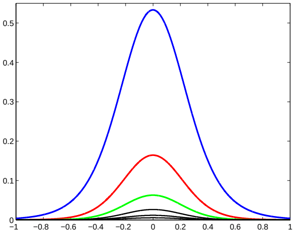

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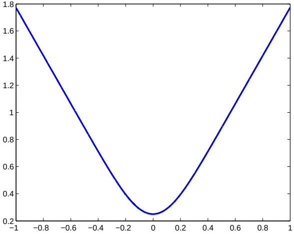

$$\Theta_0^{\mathrm{p2}}(r) = \frac{1}{\alpha} \mathrm{e}^{-\alpha^2 r^2} + r\sqrt{\pi} \operatorname{erf}(\alpha r)$$

A fast algorithm

Long range part

$$\frac{1}{4B} \sum_{\boldsymbol{k} \neq \boldsymbol{0}} \sum_{i,j=1}^{N} q_i q_j \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \tilde{\boldsymbol{x}}_{ij}/B} \Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3}) \qquad - \frac{\sqrt{\pi}}{B^2} \sum_{i,j=1}^{N} q_i q_j \Theta_0^{\mathrm{p2}}(x_{ij,3})$$

- truncate the infinite sum

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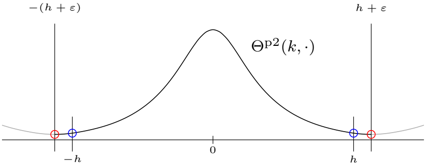
- choose $\varepsilon > 0$, $\forall$ remaining $k = \|\boldsymbol{k}\| \neq 0$ construct a smooth function

$$R_k(r) := \begin{cases} \Theta^{\mathrm{p2}}(k,r) & : |r| \leq h \\ B_k(r) & : h < |r| \leq h+\varepsilon \end{cases}$$



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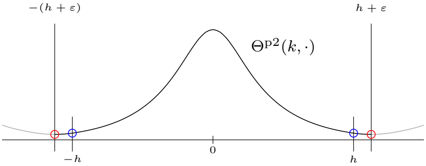

- $m \in 2\mathbb{N}$ sufficiently large

A fast algorithm

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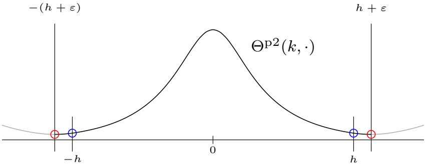

- $m \in 2\mathbb{N}$ sufficiently large
- replace $\Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, \cdot)$ by the Fourier sums

A fast algorithm

Long range part

$$\frac{1}{4B}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\sum_{l=-m/2}^{m/2-1} b_{\|\boldsymbol{k}\|,l}|S(\boldsymbol{k},l)|^2 \qquad -\frac{\sqrt{\pi}}{B^2}\sum_{i,j=1}^{N} q_i q_j \Theta_0^{\mathrm{p}2}(x_{ij,3})$$

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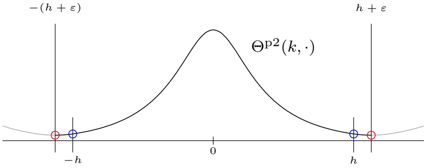

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A fast algorithm

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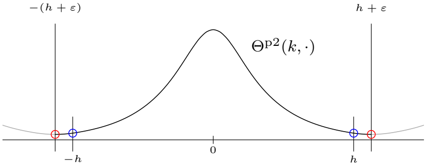

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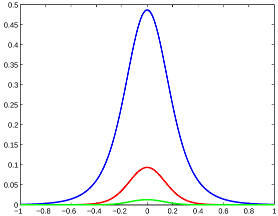
1d-Ewald summation [Porto 2000]

Define $\tilde{\boldsymbol{x}}_{ij} := (x_{i,2} - x_{j,2}, x_{i,3} - x_{j,3})$. Long range part contains a 1d Fourier series with coefficients

$$\Theta^{\mathrm{p1}}(k, \|\tilde{\boldsymbol{x}}_{ij}\|) = \int_0^\alpha \frac{1}{t} \mathrm{e}^{-\pi^2 k^2/(B^2 t^2) - \|\tilde{\boldsymbol{x}}_{ij}\|^2 t^2} \mathrm{d}t \quad (k \neq 0)$$

$+$ extra term for $k = 0$



$k = 1$, $k = 2$, $k = 3$, $\ldots$

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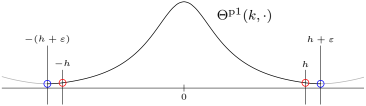

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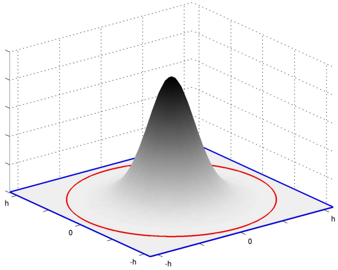

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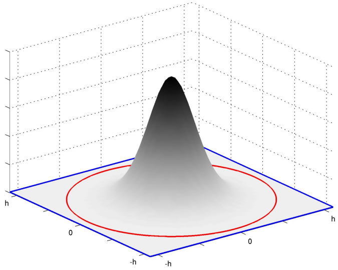

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Thank you for your attention!