NFFT basierte schnelle Ewald-Summation für gemischt periodische Randbedingungen

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Definition of the Coulomb interaction energy

Let N charges $q_j \in \mathbb{R}$ at positions $\boldsymbol{x}_j \in \mathbb{R}^3$ be given.
Coulomb interaction energy ($\boldsymbol{x}_{ij} := \boldsymbol{x}_i - \boldsymbol{x}_j$):

$$E := \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \frac{q_i q_j}{\|\boldsymbol{x}_{ij}\|} = \frac{1}{2} \sum_{j=1}^{N} q_j \phi(\boldsymbol{x}_j) \quad \text{with} \quad \phi(\boldsymbol{x}_j) := \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij}\|}.$$

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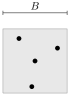
3d-periodic boundary conditions

choose $S := \mathbb{Z}^3$, $\boldsymbol{x}_j \in B\mathbb{T}^3$ and set

$$\phi(\boldsymbol{x}_j) := \phi_{\mathcal{S}}(\boldsymbol{x}_j)$$

$$:= \sum_{\boldsymbol{n} \in \mathcal{S}} \sum_{\substack{i=1 \\ i \neq j \text{ if } \boldsymbol{n}=\boldsymbol{0}}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}$$

$\mathbb{T} := \mathbb{R}/\mathbb{Z} \simeq [-1/2, 1/2)$



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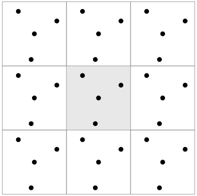

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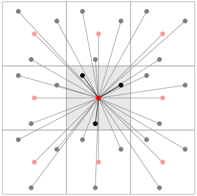
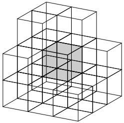


Coulomb energy s.t. periodic boundary conditions

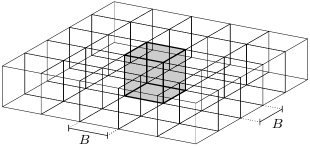
$$E(\mathcal{S}) := \frac{1}{2}\sum_{j=1}^{N} q_j \phi_{\mathcal{S}}(\boldsymbol{x}_j) \quad \text{with} \quad \phi_{\mathcal{S}}(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{\substack{i=1 \\ i\neq j \text{ if } \boldsymbol{n}=\boldsymbol{0}}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}$$

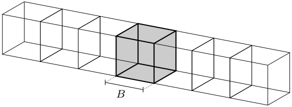
- fully periodic: $\boldsymbol{x}_j \in B\mathbb{T}^3$, $\mathcal{S} := \mathbb{Z}^3$



- mixed boundary conditions:

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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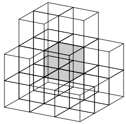

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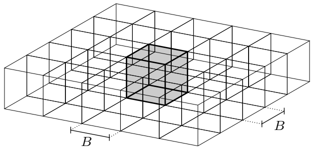
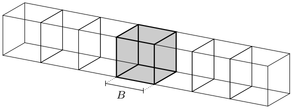




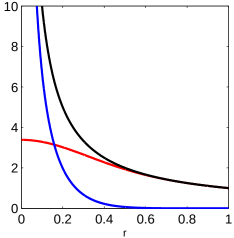
Assume $\sum_{j=1}^{N} q_j = 0 \Rightarrow$ conditional convergence

Ewald's idea

Idea of the Ewald summation [Ewald 1921]:

Ewald splitting

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



- $\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t$ (error function)
- $\mathrm{erfc}(x) := 1 - \mathrm{erf}(x)$ (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

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

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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
- $\lim_{r\to 0} \frac{\mathrm{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}} \Rightarrow$ substract self potential
- write the long range part as a sum in Fourier space
  $\to$ use the FFT for nonequispaced data (NFFT)

The 3d-NFFT

Notation

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

$$\text{FFT:} \qquad f(\boldsymbol{j}) \quad := \sum_{\boldsymbol{k}\in\mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{j}/M} \qquad \boldsymbol{j} \in \mathcal{I}_M$$

[Dutt, Rokhlin 1993] [Beylkin 1995]
[Potts, Steidl, Tasche 2001] [Greengard, Lee 2004]

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

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\text{adjoint NFFT:} \quad & h(\boldsymbol{k}) &:= \sum_{j=1}^{N} f_j \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}_j} \qquad & \boldsymbol{k} \in \mathcal{I}_M
\end{aligned}$$

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3d Ewald Summation - long range part

Long range part of the potential

$$\phi^{\mathrm{L}}_{\mathbb{Z}^3}(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \sum_{i=1}^{N} q_i \frac{\operatorname{erf}(\alpha\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|)}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|}$$

is conditional convergent.

Representation in Fourier space

assume charge neutrality + spherical order of summation to obtain

$$\phi^{\mathrm{L}}_{\mathbb{Z}^3}(\boldsymbol{x}_j) = \frac{1}{\pi B} \sum_{\boldsymbol{k}\in\mathbb{Z}^3\setminus\{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2\|\boldsymbol{k}\|^2/(\alpha^2 B^2)}}{\|\boldsymbol{k}\|^2} \sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}_{ij}/B} + \frac{4\pi}{3B^2}\left(\sum_{i=1}^{N} q_i \boldsymbol{x}_i\right)\cdot\boldsymbol{x}_j$$

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- Fourier coefficients tend to zero exponentially fast
- Fourier coefficients are singular in $\boldsymbol{k}=\boldsymbol{0}$

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- Fourier coefficients tend to zero exponentially fast
- Fourier coefficients are singular in $\boldsymbol{k} = \boldsymbol{0}$
- the $\boldsymbol{k} = \boldsymbol{0}$ term represents the order of summation

Fast Algorithm: P^2NFFT $\mathcal{O}(N \log N)$ [Pippig, Potts 2011]

$\mathcal{O}(N \log N)$ Algorithm:

- Fourier part:

$$\begin{aligned} &\frac{1}{\pi B} \sum_{\boldsymbol{k} \in \mathbb{Z}^3 \setminus \{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2 \|\boldsymbol{k}\|^2/(\alpha^2 B^2)}}{\|\boldsymbol{k}\|^2} \sum_{i=1}^{N} q_i \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_{ij}/B} \\ =&\frac{1}{\pi B} \sum_{\boldsymbol{k} \in \mathbb{Z}^3 \setminus \{\boldsymbol{0}\}} \frac{\mathrm{e}^{-\pi^2 \|\boldsymbol{k}\|^2/(\alpha^2 B^2)}}{\|\boldsymbol{k}\|^2} \left(\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_{i}/B} \right) \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_{j}/B} \end{aligned}$$

- direct: short range part, self potentials, $\boldsymbol{k} = \boldsymbol{0}$ terms

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$\mathcal{O}(N \log N)$ Algorithm:

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

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

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Ewald summation s.t. 2d-periodic boundary conditions

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

We write $\boldsymbol{x}_{ij} = (\tilde{\boldsymbol{x}}_{ij}, x_{ij,3})$ and obtain for $\phi^{\mathrm{L}}_{\mathbb{Z}^2\times\{0\}}(\boldsymbol{x}_j)$

$$\frac{1}{2B}\sum_{\boldsymbol{k}\in\mathbb{Z}^2\setminus\{\boldsymbol{0}\}}\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\tilde{\boldsymbol{x}}_{ij}/B}\Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3}) - \frac{2\sqrt{\pi}}{B^2}\sum_{i=1}^{N} q_i \Theta^{\mathrm{p2}}_0(x_{ij,3})$$

2d Fourier series

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

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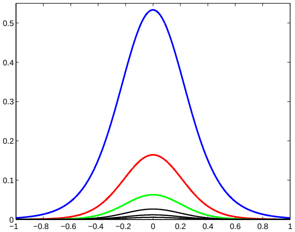

$\Theta^{\mathrm{p2}}(k,r)$

$k=1$

$k=\sqrt{2}$

$k=\sqrt{3}$

$\dots$

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

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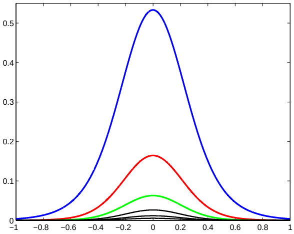
2d Fourier series



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

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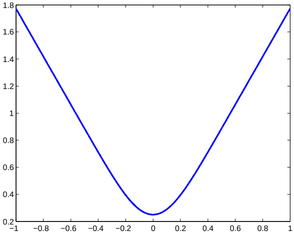
$k=\sqrt{3}$
$\dots$

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

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



$$\Theta^{\mathrm{p2}}_0(r) = \frac{1}{\alpha}\mathrm{e}^{-\alpha^2 r^2} + r\sqrt{\pi}\operatorname{erf}(\alpha r)$$

A fast algorithm I

The 2d Fourier sum

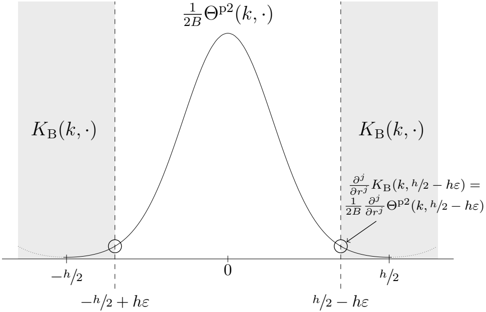
$$\frac{1}{2B}\sum_{\boldsymbol{k}\in\mathbb{Z}^2\setminus\{\boldsymbol{0}\}}\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\cdot\tilde{\boldsymbol{x}}_{ij}/B}\Theta^{\mathrm{p2}}(\|\boldsymbol{k}\|, x_{ij,3})$$

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

- $\forall\, r : \Theta^{\mathrm{p2}}(k,r) \sim k^{-2}\mathrm{e}^{-k^2}$ as $k\to\infty$
- $\forall\, k : \Theta^{\mathrm{p2}}(k,\cdot) \in \mathrm{C}^\infty(\mathbb{R})$

Regularization:

- $x_{ij,3}$ are absolutely bounded
- we are just interested in $\Theta^{\mathrm{p2}}(k,\cdot)$ over a finite interval (white area)



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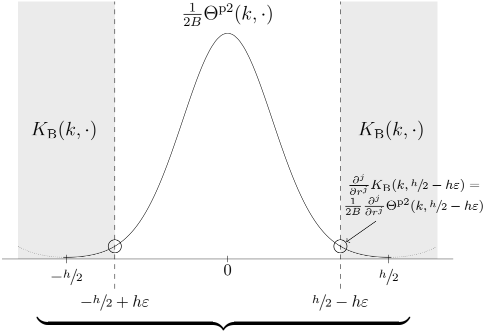
Regularization:

- $x_{ij,3}$ are absolutely bounded
- we are just interested in $\Theta^{\mathrm{p2}}(k,\cdot)$ over a finite interval (white area)
- construct a smooth and periodic function $K_{\mathrm{R}}(k,\cdot)$



$K_{\mathrm{R}}(k,\cdot) : h\mathbb{T} \to \mathbb{R}$

$\to \varepsilon \in (0, 1/2)$ determines the size of the areas at the boundaries

A fast algorithm II

The 2d Fourier sum (∗)

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

- truncate the infinite sum, $\mathbb{Z}^2 \to \mathcal{I}_{\tilde{M}} := \{-\tilde{M}/2 \ldots, \tilde{M}/2 - 1\}^2$

A fast algorithm II

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- for $M \in 2\mathbb{N}$ large enough we find for each $k = \|\boldsymbol{k}\| \neq 0$ ($\boldsymbol{k} \in \mathcal{I}_{\tilde{M}}$)

$$\Theta^{\mathrm{p2}}(k, x_{ij,3}) = K_{\mathrm{R}}(k, x_{ij,3}) \approx \sum_{l=-M/2}^{M/2-1} b_{k,l}\mathrm{e}^{2\pi\mathrm{i}l x_{ij,3}/h}$$

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- we obtain with $\hat{\boldsymbol{x}}_i := \left(\frac{x_{i,1}}{B}, \frac{x_{i,2}}{B}, \frac{x_{i,3}}{h}\right)$ the approximation

$$(*) \approx \sum_{\boldsymbol{k}\in\mathcal{I}_{\tilde{M}}\setminus\{\boldsymbol{0}\}}\sum_{l=-M/2}^{M/2-1} b_{\|\boldsymbol{k}\|,l}\left(\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}\begin{bmatrix}k_1\\k_2\\l\end{bmatrix}\cdot\hat{\boldsymbol{x}}_i}\right)\mathrm{e}^{-2\pi\mathrm{i}\begin{bmatrix}k_1\\k_2\\l\end{bmatrix}\cdot\hat{\boldsymbol{x}}_j}$$

A fast algorithm II

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- analog for the $\boldsymbol{k} = \boldsymbol{0}$ term

Some numerical results

- optimal choice of the parameters? (especially ε)
- to obtain first numerical results: tuned ε by hand
- we obtain acceptable errors in comparison to the 3d-periodic method

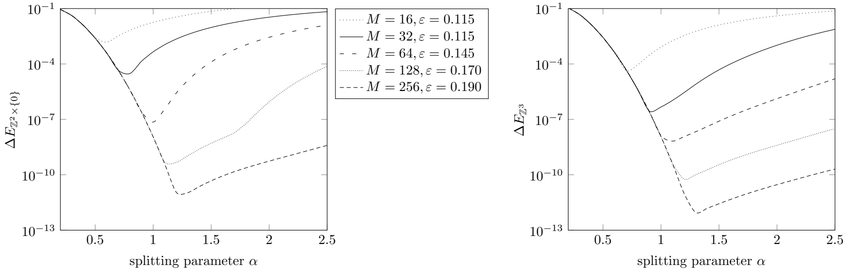


Figure : Achieved rms errors for a 2d-periodic (left) and the corresponding 3d-periodic computation (right) with $N = 300$ particles.

Structure is the same as for 3d-periodic systems

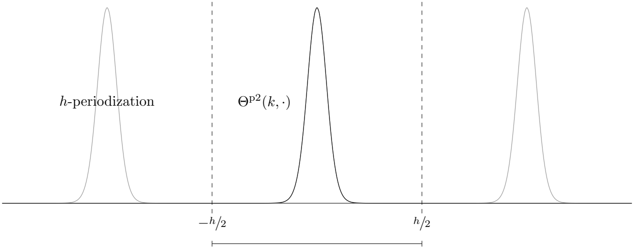
- Near field, self interactions
- Far field
  1. adjoint 3d NFFT
  2. Multiplikation with the Fourier coefficients
  3. 3d NFFT

Problems

- for each $\|\mathbf{k}\|$ we have to construct the regularization and compute the Fourier coefficients via the FFT
  $\rightarrow$ many precomputation steps
- more parameters: degree of smoothness, regularization parameter ε, ...
  $\rightarrow$ optimal choice? exact error control?

How to reduce precomputation costs?

For k large enough:



$$\Theta^{\mathrm{p2}}(k,r) \approx \sum_{n=-\infty}^{\infty} \Theta^{\mathrm{p2}}(k, r+nh)$$

Poisson summation:

$$\sum_{n=-\infty}^{\infty} \Theta^{\mathrm{p2}}(k, r+nh) = \frac{1}{h} \sum_{l=-\infty}^{\infty} \frac{2Bh^2}{\pi(h^2k^2 + B^2l^2)} \mathrm{e}^{-\pi^2 l^2/(\alpha^2 h^2) - \pi^2 k^2/(\alpha^2 B^2)} \mathrm{e}^{2\pi \mathrm{i} l r/h}$$

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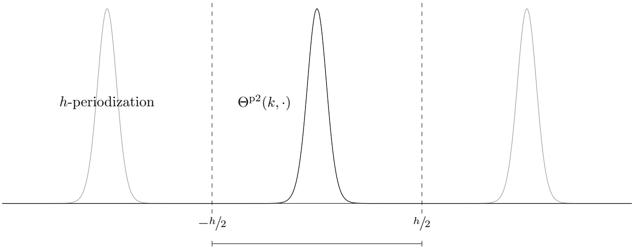

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$\rightarrow$ Fourier coefficients are given analytically

Ewald summation s.t. 1d periodic boundary conditions

Long range part under 1d-periodic b.c. [Porto 2000]

We write $\boldsymbol{x}_{ij} = (x_{ij,1}, \tilde{\boldsymbol{x}}_{ij})$ and obtain for $\phi^{\mathrm{L}}_{\mathbb{Z}\times\{0\}^2}(\boldsymbol{x}_j)$

$$\frac{2}{B}\sum_{k\in\mathbb{Z}\setminus\{0\}}\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}kx_{ij,1}/B}\Theta^{\mathrm{p1}}(|k|,\|\tilde{\boldsymbol{x}}_{ij}\|) - \frac{1}{B}\sum_{i=1}^{N} q_i \Theta^{\mathrm{p1}}_0(\|\tilde{\boldsymbol{x}}_{ij}\|)$$

1d Fourier series $\qquad\qquad$ $k = 0$ part

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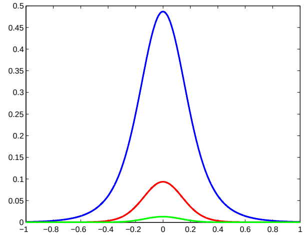

$\Theta^{\mathrm{p1}}(k, r)$

$k = 1$

$k = 2$

$k = 3$

$\dots$

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

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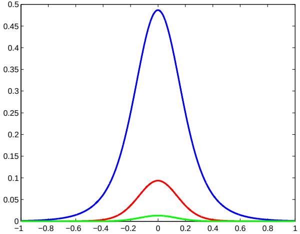

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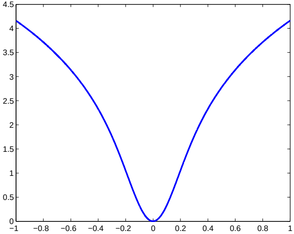

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$$\Theta^{\mathrm{p1}}_0(r) = \gamma + \Gamma(0, \alpha^2 r^2) + \ln(\alpha^2 r^2)$$

A fast algorithm

The 1d Fourier sum

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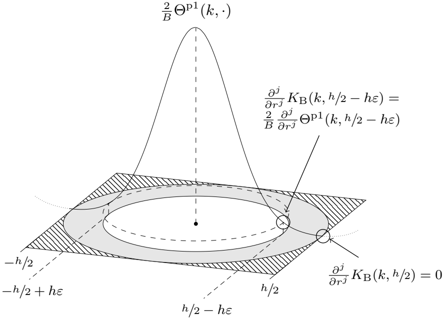
- regularization of $\Theta^{\mathrm{p1}}(|k|,\cdot)$ on $[-h/2, h/2]$



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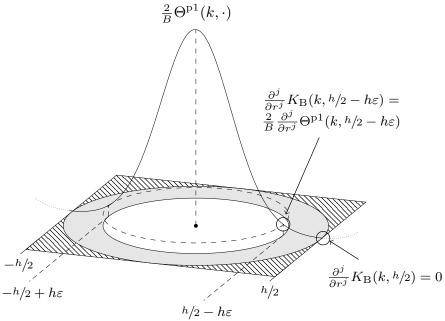
- regularization of $\Theta^{\mathrm{p1}}(|k|,\cdot)$ on $[-h/2, h/2]$
- claim vanishing derivatives at the boundary
- rotate and extend the function to the torus $h\mathbb{T}^2$ (constant value over the striped area)



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- claim vanishing derivatives at the boundary
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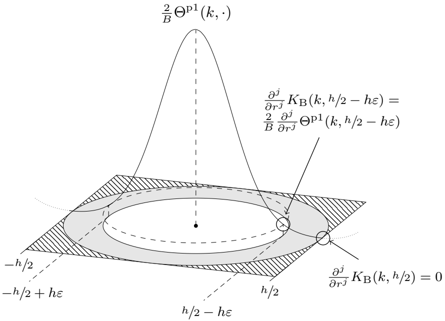
- result: periodically smooth function in 2 variables
- approximate by bivariate trigonometric polynomials
- proceed as for 2d-periodic b.c.



Conclusion

- 3d-periodic: Ewald + NFFT $\rightarrow$ fast algorithm [Pippig, Potts 2011]
- open boundary conditions: NFFT based fast summation [Potts, Steidl 2003]

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- new approach to fast Ewald summation under mixed boundary conditions: [Nestler, Pippig, Potts 2013 (Preprint)]
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Thank you for your attention!