Schnelle Ewald-Summation für gemischt periodische Randbedingungen

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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 $\mathcal{I}_M := \{-M/2, \dots, M/2 - 1\}^3$

Fast evaluation of trigonometric sums :

$$\text{NFFT:} \quad f(\boldsymbol{x}_j) \quad := \sum_{\boldsymbol{k} \in \mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \cdot \boldsymbol{x}_j} \qquad \boldsymbol{x}_j \in \mathbb{T}^3, j = 1, \dots, N$$

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

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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 ($\boldsymbol{x}_{ij} := \boldsymbol{x}_i - \boldsymbol{x}_j$):

$$E := \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \frac{q_i q_j}{\|\boldsymbol{x}_{ij}\|}$$

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3d-periodic boundary conditions

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

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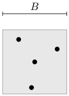

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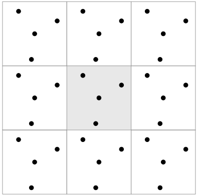

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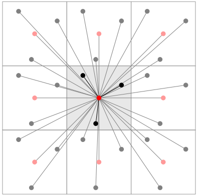
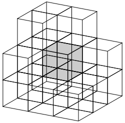


Coulomb energy s.t. periodic boundary conditions

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

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



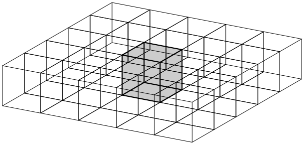
- mixed boundary conditions:

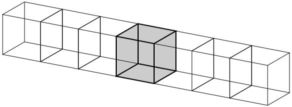
2d-periodic

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

1d-periodic

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





Convergence

$$\phi_{\mathcal{S}}(\boldsymbol{x}_j) := \sum_{\boldsymbol{n}\in\mathcal{S}} \sum_{\substack{i=1 \\ i\neq j \text{ if } \boldsymbol{n}=\boldsymbol{0}}}^{N} \frac{q_i}{\|\boldsymbol{x}_{ij} + B\boldsymbol{n}\|} \quad \mathcal{S} = \mathbb{Z}^3 \,/\, \mathbb{Z}^2 \times \{0\} \,/\, \mathbb{Z} \times \{0\}^2$$

- if $\sum_{j=1}^{N} q_j = 0 \Rightarrow$ we have conditional convergence
- $\Rightarrow$ define the order of summation

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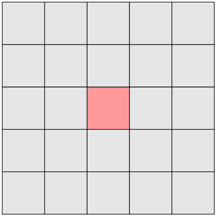

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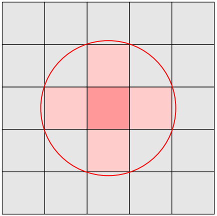

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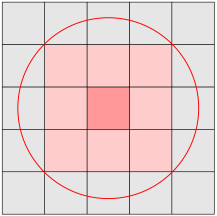

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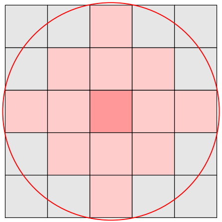

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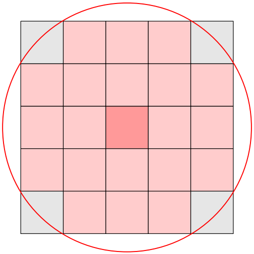

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Non Fourier methods

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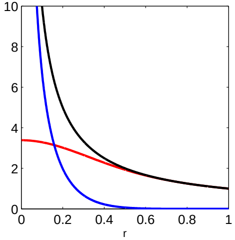
Aim: propose efficient NFFT based methods for 2d- and 1d-periodic b.c.

Ewald's idea

Idea of the Ewald summation [Ewald 1921]:

Ewald splitting

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



- $\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t$ (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
- $\lim_{r\to 0} \frac{\operatorname{erf}(\alpha r)}{r} = \frac{2\alpha}{\sqrt{\pi}} \Rightarrow$ substract self potential
- write the long range part as a sum in Fourier space

3d Ewald Summation - long range part

Long range part of the potential

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

is conditional convergent.

Representation in Fourier space

assume charge neutrality + spherical order of summation to obtain

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

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

3d Ewald Summation - long range part

Long range part of the potential

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

is conditional convergent.

Representation in Fourier space

assume charge neutrality + spherical order of summation to obtain

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

- 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

- choose a good splitting parameter α

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\begin{aligned}
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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} \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}
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- $E_{\mathbb{Z}^3} = \frac{1}{2} \sum_{j=1}^{N} q_j \phi_{\mathbb{Z}^3}(\boldsymbol{x}_j)$

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- $E_{\mathbb{Z}^3} = \frac{1}{2} \sum_{j=1}^{N} q_j \phi_{\mathbb{Z}^3}(\boldsymbol{x}_j)$
- complexity: $\mathcal{O}(N \log N)$, prefactor depends on required accuracy

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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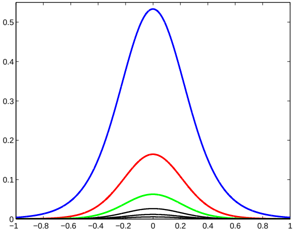

$\Theta^{\mathrm{p2}}(k, r)$

$k = 1$

$k = \sqrt{2}$

$k = \sqrt{3}$

$\ldots$

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

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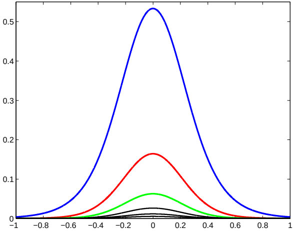

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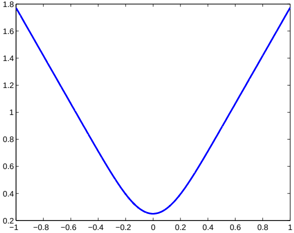

$$\Theta^{\mathrm{p2}}_0(r) = \frac{1}{\alpha}\mathrm{e}^{-\alpha^2 r^2} + r\sqrt{\pi}\operatorname{erf}(\alpha r)$$

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

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

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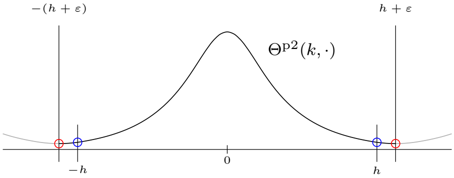
- assume that $|x_{ij,3}| < h$ for all i, j
- choose $\varepsilon > 0$, for each $k = \|\boldsymbol{k}\|$ construct a smooth+periodic function

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



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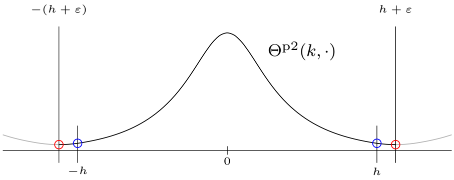
- sufficiently smooth (o o)



A fast algorithm II

- truncate the infinite sum, $\mathbb{Z}^2 \to \mathcal{I}_{\tilde{M}} := \{-\tilde{M}/2\, \dots, \tilde{M}/2 - 1\}^2$
- for $M \in 2\mathbb{N}$ large enough we find for each $k = \|\boldsymbol{k}\| \neq 0$ ($\boldsymbol{k} \in \mathcal{I}_{\tilde{M}}$)

$$R_k(r) \approx \sum_{l=-M/2}^{M/2-1} b_{k,l} \mathrm{e}^{\pi \mathrm{i} l r/(h+\varepsilon)}$$

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

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

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

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- fast computation with NFFTs

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- fast computation with NFFTs
- analog for the $\boldsymbol{k} = \boldsymbol{0}$ term

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

$k = 0$ part

Ewald summation s.t. 1d periodic boundary conditions

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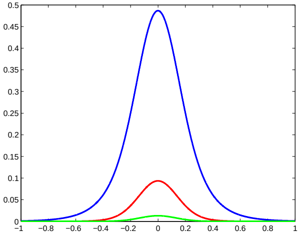

$\Theta^{\mathrm{p1}}(k, r)$

$k = 1$

$k = 2$

$k = 3$

$\dots$

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

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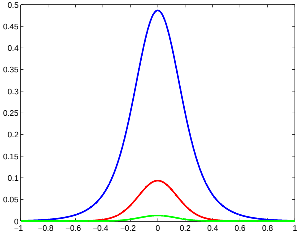
$$\frac{2}{B}\sum_{k\in\mathbb{Z}\setminus\{0\}}\sum_{i=1}^{N} q_i \mathrm{e}^{2\pi\mathrm{i}kx_{ij,1}/B}\Theta^{\mathrm{p1}}(|k|, \|\tilde{\boldsymbol{x}}_{ij}\|) - \frac{1}{B}\sum_{i=1}^{N} q_i \Theta_0^{\mathrm{p1}}(\|\tilde{\boldsymbol{x}}_{ij}\|)$$

1d Fourier series



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

$k = 1$

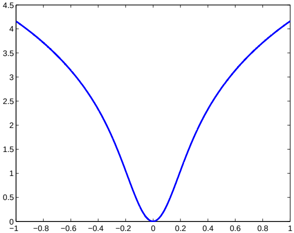
$k = 2$

$k = 3$

$\dots$

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

$k = 0$ part



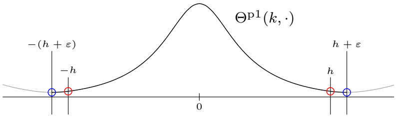
$$\Theta_0^{\mathrm{p1}}(r) = \gamma + \Gamma(0, \alpha^2 r^2) + \ln(\alpha^2 r^2)$$

A fast algorithm

Assume $\|\tilde{\boldsymbol{x}}_{ij}\| < h$ and choose $\varepsilon > 0$.

1d Regularization for each $k > 0$:

$$R_k(r) := \begin{cases} \Theta^{\mathrm{p1}}(k,r) & : |r| \le h \\ B_k(r) & : h < |r| \le h+\varepsilon \end{cases}$$



- sufficiently smooth
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2d Regularization:

- rotate, i.e., consider $R_k^{\mathrm{2d}}(\boldsymbol{x}) := R_k(\|\boldsymbol{x}\|)$
- constant outside the ball $K_{h+\varepsilon}(0,0)$:
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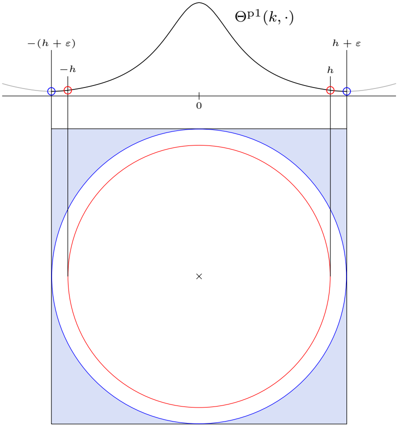
- Approximation by 2d Fourier sum

$$R_k^{\mathrm{2d}}(\boldsymbol{x}) \approx \sum_{l_1,l_2=-M/2}^{M/2-1} b_{k,\boldsymbol{l}} \mathrm{e}^{\pi \mathrm{i} \boldsymbol{l}\cdot\boldsymbol{x}/(h+\varepsilon)}$$



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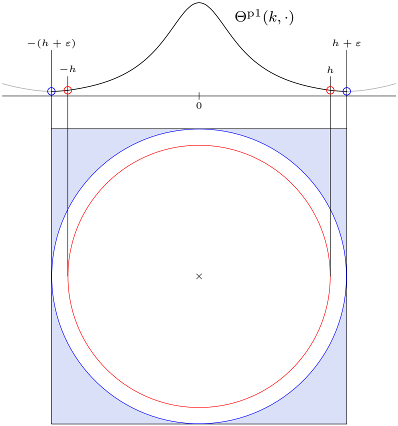
$\rightarrow$ analogously in the case $k = 0$



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Thank you for your attention!