

Computation of Generalized Zeta Functions

With Applications to Long-Range Interacting Classical and Quantum Lattices

NumPDE Summer Retreat — Wed. June 17, 2026

Jonathan K. Busse

Physics: **JB**, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025)

Math: **JB**, Buchheit et al., arXiv:2504.11989 (2025) (final round in *Numer. Math.*)

JB, Buchheit et al., arXiv:2412.16317 (2024) (accepted in *IMA J. Num. Ana.*)

Chemistry: Robles-Navarro, **JB**, et al., *J. Chem. Phys.* **163**, 094104 (2025)

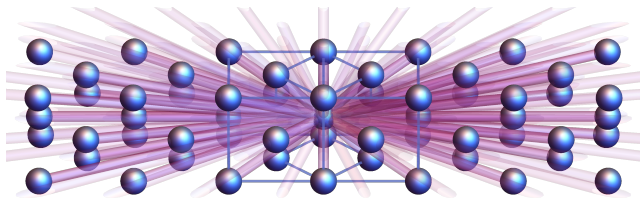
DLR, Inst. of Software Technology, QCA Group & Saarland University; joint work with A. A. Buchheit



Long-range interactions appear everywhere in nature

Long-range couplings that decay as a **power-law** with distance r appear everywhere in nature,

- ▶ Coloumb $\sim 1/r$,
- ▶ dipole-dipole $\sim 1/r^3$,
- ▶ van der Waals $\sim 1/r^6$,
- ▶ in general $\sim 1/r^\alpha$.

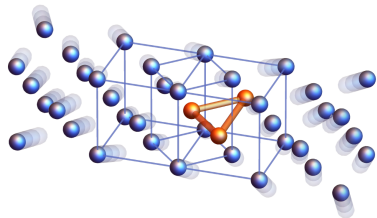


Interesting yet challenging:

- ▶ **Mermin–Wagner theorem not applicable.**
- ▶ **Continuum approximations** require correction terms that account for singularity.
- ▶ **Exact summation infeasible & truncation** introduces exponential numerical work.
- ▶ **Many-body interactions** introduce high-dimensional sums (6D, for 3-body in 3D).

In efficiently computable representations of long-range systems, **zeta functions appear!**

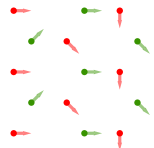
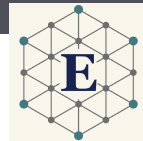
Broad applicability in long-range interacting lattices



Theoretical chemistry: Cohesive energy for Lennard-Jones

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025)

$$E_{\text{LJ}}(\mathbf{r}) \propto \frac{1}{n} |\mathbf{r}|^{-n} - \frac{1}{m} |\mathbf{r}|^{-m}.$$



Spin systems:

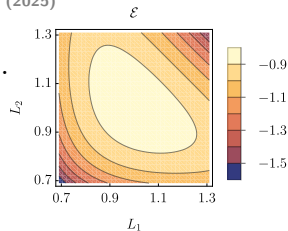
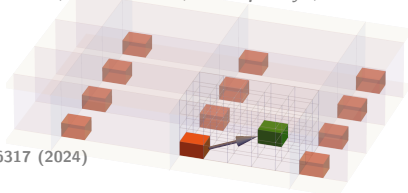
$$H = \sum_{ij \in \Lambda} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$

JB, Buchheit et al., arXiv:2412.16317 (2024)

Micromagnetics: Generalized potential

$$U^{(\alpha)}(\mathbf{r}) = \sum_{\mathbf{z} \in L} \int_{\Omega + \mathbf{z}} \nabla_{\mathbf{r}}^{\alpha} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}''.$$

JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025)



High energy physics: Casimir energy

JB, Buchheit et al., arXiv:2412.16317 (2024)

$$\mathcal{E} = \frac{1}{2} \sum_{\mathbf{k}} \lambda_{\mathbf{k}}^{-\nu} \Big|_{\nu=-1}.$$

Epstein zeta function

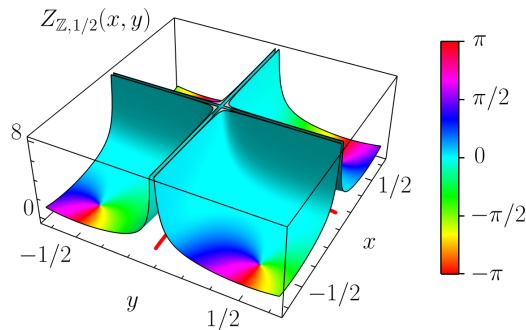
Let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ and $\Lambda = A\mathbb{Z}^d$ be a lattice. The Epstein zeta function is the meromorphic continuation of the following lattice sum to $\nu \in \mathbb{C}$

$$Z_{\Lambda, \nu}(\mathbf{x}, \mathbf{y}) = \sum'_{\mathbf{z} \in \Lambda} \frac{e^{-2\pi i \mathbf{y} \cdot \mathbf{z}}}{|\mathbf{z} - \mathbf{x}|^\nu}, \quad \operatorname{Re}(\nu) > d.$$

Epstein zeta function

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1. Computation of Epstein zeta functions
JB, Buchheit et al., arXiv:2412.16317 (2024)
2. Many-body sums in theoretical chemistry
JB, Buchheit et al., arXiv:2504.11989 (2025)
Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025).
3. Computation of anisotropic lattice sums
JB, Buchheit, (soon on arXiv).
JB, Schmiedinghoff, Fauseweh, Buchheit (ongoing work).
4. Anisotropic lattice sums in micromagnetics
JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025).

Crandall representation of the Epstein zeta function

Theorem (Crandall representation)

Let $\Lambda = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d \times d}$ regular, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, and $\nu \in \mathbb{C}$, $\nu \neq d$ if $\mathbf{y} \in \Lambda^* = A^{-T}\mathbb{Z}^d$. Then

$$Z_{\Lambda, \nu}(\mathbf{x}, \mathbf{y}) = \frac{\pi^{\nu/2}}{\Gamma(\nu/2)} \left[\sum_{\mathbf{z} \in \Lambda} G_{\nu}(\mathbf{z} - \mathbf{x}) e^{-2\pi i \mathbf{y} \cdot \mathbf{z}} + \frac{1}{|\det(A)|} \sum_{\mathbf{k} \in \Lambda^*} G_{d-\nu}(\mathbf{k} + \mathbf{y}) e^{-2\pi i \mathbf{x} \cdot (\mathbf{k} + \mathbf{y})} \right]$$

with **upper Crandall function**

$$G_{\nu}(0) = -\frac{2}{\nu}, \quad G_{\nu}(\mathbf{z}) = \frac{\Gamma(\nu/2, \pi \mathbf{z}^2)}{(\pi \mathbf{z}^2)^{\nu/2}} \propto \frac{\exp(-\pi \mathbf{z}^2)}{(\pi \mathbf{z}^2)^{\nu/2}}.$$

Here, $\Gamma(\cdot)$ is the Gamma function, and $\Gamma(\cdot, \cdot)$ is the upper incomplete Gamma function.

Holomorphy, functional equation and singularities

- **Functional equation:** The parameter transformation $(\Lambda, \nu, \mathbf{x}, \mathbf{y}) \rightarrow (\Lambda^*, d - \nu, \mathbf{y}, -\mathbf{x})$ where $\Lambda = A\mathbb{Z}^d$, $\Lambda^* = A^{-T}\mathbb{Z}^d$ does not change the product

$$\frac{(|\det A|^{2/d}/\pi)^{\nu/2}}{\Gamma((d-\nu)/2)} e^{\pi i \mathbf{x} \cdot \mathbf{y}} Z_{\Lambda, \nu}(\mathbf{x}, \mathbf{y}).$$

- **Jointly holomorphically extendable** in complex neighbourhood of $(\nu, \mathbf{x}, \mathbf{y}) \in \mathbb{R} \setminus \{d\} \times \mathbb{R}^d \setminus \Lambda \times \mathbb{R}^d \setminus \Lambda^*$.

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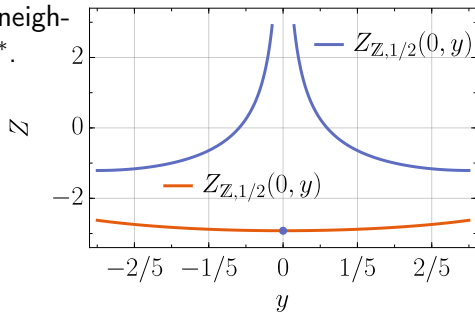
- **Jointly holomorphically extendable** in complex neighbourhood of $(\nu, \mathbf{x}, \mathbf{y}) \in \mathbb{R} \setminus \{d\} \times \mathbb{R}^d \setminus \Lambda \times \mathbb{R}^d \setminus \Lambda^*$.
- **Power-law singularities** in $\mathbf{x} \rightarrow \Lambda$ and $\mathbf{y} \rightarrow \Lambda^*$.

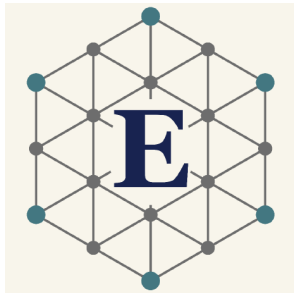
Challenge: Evaluation of integrals near $\mathbf{y} = 0$.

Solution: **Regularization** in $\mathbf{y}$

$$\underbrace{Z_{\Lambda, \nu}(0, \mathbf{y})}_{\substack{\text{singularity} \\ \text{in } \mathbf{y}=0}} = \underbrace{Z_{\Lambda, \nu}^{\text{reg}}(0, \mathbf{y})}_{\substack{\text{smooth} \\ \text{in } \mathbf{y} \in B\mathbb{Z}}} + c_{\Lambda, \nu} |\mathbf{y}|^{\nu-d}$$

$$c_{\Lambda, \nu} = \frac{\pi^{\nu-d/2}}{|\det(A)|} \frac{\Gamma((d-\nu)/2)}{\Gamma(\nu/2)}, \quad \nu \in \mathbb{C} \setminus (d + 2\mathbb{N}_0).$$





C library for the evaluation of the Epstein zeta function for

- ▶ every exponent ν ,
- ▶ every lattice Λ ,
- ▶ every shift vector $\mathbf{x}$,
- ▶ every wavevector $\mathbf{y}$,

including Python, Julia and Mathematica bindings.

```
double complex epsteinZeta(double nu, unsigned int dim, const double *A, const double *x, const double *y);  
double complex epsteinZetaReg(double nu, unsigned int dim, const double *A, const double *x, const double *y);
```

C

Available on github.com/epsteinlib; joint work with: Andreas A. Buchheit, Ruben Gutendorf; DevOps: Jan Schmitz.

Precision and runtime

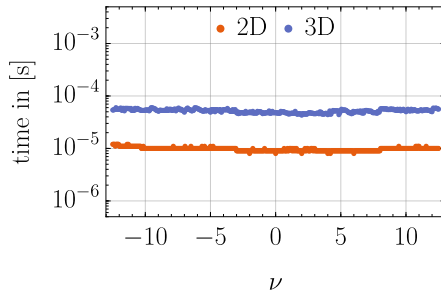
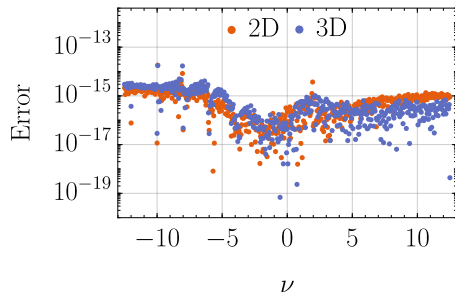
```
pip install epsteinlib
```

Shell

```
import numpy as np
from epsteinlib import epstein_zeta

madelung = epstein_zeta(1.0, np.identity(3), np.zeros(3), np.full(3, 0.5))
```

Python



EpsteinLib in use by community

Our work:

- ▶ Zeta method for many-body lattice sums JB, Buchheit et al., arXiv:2504.11989 (2025).
- ▶ Three-body interactions in phase transitions Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025)
- ▶ Computation of dipolar interactions with PBC JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025).
- ▶ Computation and properties of the Epstein zeta function JB, Buchheit et al., arXiv:2412.16317 (2024).

Condensed matter community:

- ▶ Field-induced magnon decays in dipolar quantum magnets Kim et al., *Physical Review Letters* (2025).
- ▶ Melting of devil's staircases in long-range Dicke-Ising model Koziol et al., *Physical Review B* (2025).
- ▶ Fractional magnetization plateaus in a Shastry–Sutherland Ising compound Yadav et al., *Phys. Rev. X* (2025).
- ▶ Quantum annealing for competing long-range lattices Koziol et al., arXiv:2511.08336 (2025).

Theoretical chemistry:

- ▶ Lattice instabilities in hard- and soft-sphere models Robles-Navarro et al., *Physical Review B* (2026).

High energy physics:

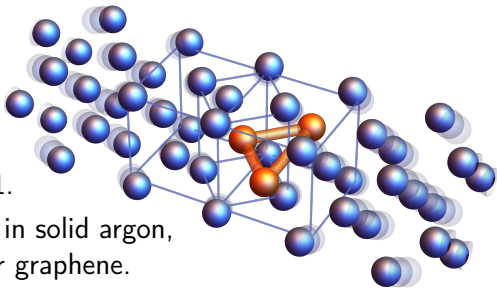
- ▶ Supersymmetry-breaking compactifications Dall'Agata et al., arXiv:2507.02339 (2025).
- ▶ Casimir-Driven de Sitter in M-Theory Bento et al., arXiv:2507.02037 (2025).

Application: Computation of many-body interactions

Many-body perturbative expansion of potential energy E , with n -body components $E^{(n)}$:

$$E = \underbrace{\sum_{\mathbf{x} \in \Lambda} E^{(2)}(\mathbf{x})}_{\text{2-body contributions}} + \underbrace{\sum_{\mathbf{x}, \mathbf{y} \in \Lambda} E^{(3)}(\mathbf{x}, \mathbf{y})}_{\text{3-body contributions}} + \text{h.o.t.},$$

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025)



- ▶ leading to **exponential numerical work** in the number of interaction partners $n \in \mathbb{N}$, $n > 1$.
- ▶ Three-body forces $\approx 10\%$ of total cohesive energy in solid argon, $\approx 51\%$ binding energy of bilayer graphene.

Challenge: Single 3-body calculation in 3D = **1 month** runtime on a single core.

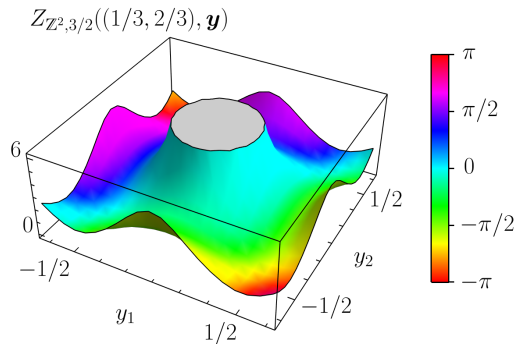
Solution: Restate in terms of **integrals over Epstein zeta functions** made efficiently computable in JB, Buchheit et al., arXiv:2504.11989 (2025).

Reminder: (Isotropic) Epstein zeta function

For a d -dimensional lattice Λ , $\mathbf{y} \in \mathbb{R}^d$, $\boldsymbol{\alpha} \in \mathbb{N}^d$, $\nu \in \mathbb{C}$, meromorphically continue

$$Z_{\Lambda, \nu}(\mathbf{x}, \mathbf{y}) = \sum'_{\mathbf{z} \in \Lambda} e^{-2\pi i \mathbf{y} \cdot \mathbf{z}} V_{\nu}(\mathbf{z} - \mathbf{x}), \quad V_{\nu}(\mathbf{z}) = |\mathbf{z}|^{-\nu}.$$

from $\operatorname{Re}(\nu) > d$ to $\nu \in \mathbb{C}$.

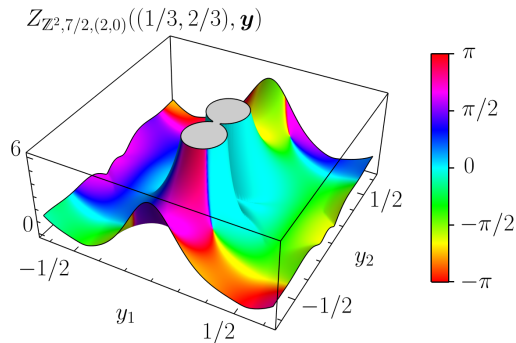


Anisotropic Epstein zeta function

For a d -dimensional lattice Λ , $\mathbf{y} \in \mathbb{R}^d$, $\boldsymbol{\alpha} \in \mathbb{N}^d$, $\nu \in \mathbb{C}$, meromorphically continue

$$Z_{\Lambda, \nu, \boldsymbol{\alpha}}(\mathbf{x}, \mathbf{y}) = \sum'_{\mathbf{z} \in \Lambda} e^{-2\pi i \mathbf{y} \cdot \mathbf{z}} V_{\nu, \boldsymbol{\alpha}}(\mathbf{z} - \mathbf{x}), \quad V_{\nu, \boldsymbol{\alpha}}(\mathbf{z}) = \mathbf{z}^{\boldsymbol{\alpha}} |\mathbf{z}|^{-\nu}$$

from $\operatorname{Re}(\nu) > d + |\boldsymbol{\alpha}|$ to $\nu \in \mathbb{C}$. Connected to **partial derivatives** of Epstein zeta functions,
as $\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} e^{\mathbf{y} \cdot \mathbf{z}} = \mathbf{z}^{\boldsymbol{\alpha}} e^{\mathbf{y} \cdot \mathbf{z}}$ with $\mathbf{z}^{\boldsymbol{\alpha}} = z_1^{\alpha_1} z_2^{\alpha_2} \dots z_d^{\alpha_d}$.

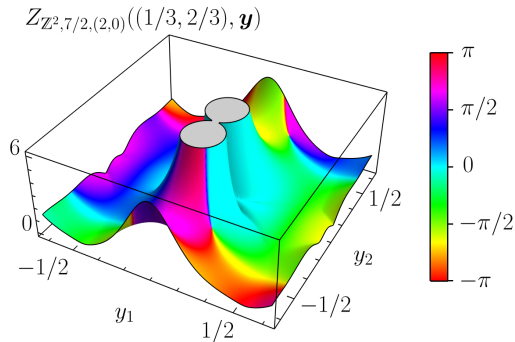


Anisotropic Epstein zeta function

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from $\operatorname{Re}(\nu) > d + |\boldsymbol{\alpha}|$ to $\nu \in \mathbb{C}$. Connected to **partial derivatives** of Epstein zeta functions, as $\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} e^{\mathbf{y} \cdot \mathbf{z}} = \mathbf{z}^{\boldsymbol{\alpha}} e^{\mathbf{y} \cdot \mathbf{z}}$ with $\mathbf{z}^{\boldsymbol{\alpha}} = z_1^{\alpha_1} z_2^{\alpha_2} \dots z_d^{\alpha_d}$.



Applications:

- Taylor series for stable evaluation of integrals over Epstein zeta functions

JB, Buchheit et al., arXiv:2504.11989 (2025)

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025).

- Winding numbers of topological superconductors

JB, Schmiedinghoff, Fauseweh, Buchheit (ongoing work).

- Potential in Micromagnetics

JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025).

Stable computation of anisotropic lattice sums

Theorem (Main result)

Let $\Lambda = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d \times d}$ regular, let $\alpha \in \mathbb{N}^d$, let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ and $\nu \in \mathbb{R}$ so that $\nu \neq d + |\alpha|$ if $\mathbf{y} \in \Lambda^* = A^{-T}\mathbb{Z}^d$. Then it holds that

$$Z_{\Lambda, \nu, \alpha}(\mathbf{x}, \mathbf{y}) = \sum_{k=0}^{\lfloor |\alpha|/2 \rfloor} \frac{\pi^{(\nu-2k)/2}}{\Gamma((\nu-2k)/2)} \left[\sum_{\mathbf{z} \in \Lambda - \mathbf{x}} h_{k, \alpha}(\mathbf{z}) G_{\nu-2k}(\mathbf{z}) e^{-2\pi i \mathbf{y} \cdot (\mathbf{z} + \mathbf{x})} \right. \\ \left. + \frac{(-1)^k}{i^{|\alpha|} |\det A|} \sum_{\mathbf{p} \in \Lambda^* + \mathbf{y}} h_{k, \alpha}(\mathbf{p}) G_{d-\nu+2(|\alpha|-k)}(\mathbf{p}) e^{-2\pi i \mathbf{x} \cdot \mathbf{p}} \right].$$

Here, $h_{k, \alpha}$, $2k \leq |\alpha|$ are homogeneous harmonic polynomials of degree $|\alpha| - 2k$, uniquely defined by

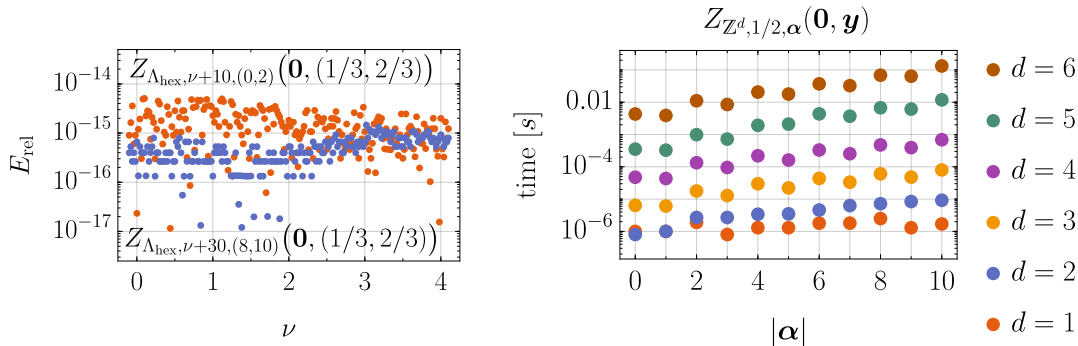
$$\mathbf{z}^\alpha = \sum_{k=0}^{\lfloor |\alpha|/2 \rfloor} |\mathbf{z}|^{2k} h_{k, \alpha}(\mathbf{z}), \quad \mathbf{z} \in \mathbb{R}^d.$$

Precision and runtime

```
import numpy as np
from epsteinlib import epstein_zeta_aniso

madelung = epstein_zeta_aniso(1., np.identity(3), np.zeros(3), np.full(3, 0.5), np.zeros(3, dtype='int'))
```

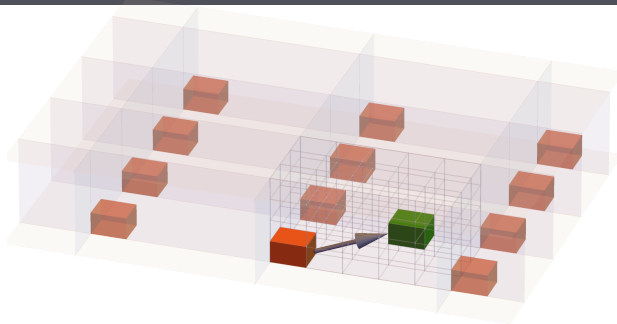
Python



Anisotropic lattice sums in micromagnetics

Consider cuboids Ω at positions $\mathbf{z} \in L = A\mathbb{Z}^n \times \{0\}^{d-n}$, $A \in \mathbb{R}^{n \times n}$ regular and $\mathbf{r} \in \mathbb{R}^d$, where

$$\begin{array}{c} \mathbf{z} + \Omega \\ (z \in L) \end{array} \xrightarrow{\text{influence}} \mathbf{r} + \Omega.$$



Generalized potential with interaction $\nu > d$ and derivative order $\alpha \in \mathbb{N}_0^d$:

$$U^{(\alpha)}(\mathbf{r}) = \sum_{\mathbf{z} \in L} \int_{\Omega + \mathbf{z}} \partial_{\mathbf{r}}^{\alpha} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}''$$

made efficiently computable in **JB**, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025)

State of the art computation long-range interactions in micromagnetics

The computation of the **generalized potential** is challenging, as

$$U^{(\alpha)}(\mathbf{r}) = \sum_{\mathbf{z} \in L} \int_{\Omega + \mathbf{z}} \partial_{\mathbf{r}}^{\alpha} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}''.$$

- ▶ includes n -dimensional lattice in d -dimensional space ($L = A\mathbb{Z}^n \times \{0\}^{d-n}$),
- ▶ interacting geometries Ω (as opposed to points $\mathbf{z}$),
- ▶ and partial derivatives of positions ($\partial_{\mathbf{r}}^{\alpha}$).

State of the art: **Truncation** for truncated lattice $L_{\text{near}} \subset L$:

$$U^{(\alpha)}(\mathbf{r}) \approx \sum_{\mathbf{z} \in L_{\text{near}}} S^{(\alpha)}(\mathbf{r} + \mathbf{z}), \quad S^{(\alpha)}(\mathbf{r}) = \int_{\Omega} \nabla_{\mathbf{r}}^{\alpha} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}''.$$

- ▶ Slow convergence for micromagnetic case ($|\alpha| = 2$ and $\nu = 1$).
- ▶ No convergence for arbitrary $\alpha \in \mathbb{N}_0^d$, $\nu \in \mathbb{R}$ (no meromorphic continuation).

Zeta expansion for long-range interactions in micromagnetics

Solution: **Zeta expansion** for micromagnetics

$$U^{(\alpha)}(\mathbf{r}) = \sum_{\mathbf{z} \in L_{\text{near}}} S^{(\alpha)}(\mathbf{r} + \mathbf{z}) + \sum_{\alpha \geq 0} c_{\alpha} Z_{L_{\text{far}}, \nu}^{(\alpha+2\alpha)}(\mathbf{r})$$

with **exponential** convergence in derivative order α .

Here, c_{α} depend on the geometry and the set zeta derivatives with respect to $\mathbf{r}$

$$Z_{L_{\text{far}}, \nu}^{(\alpha)} = \sum'_{\mathbf{z} \in L_{\text{far}}} \nabla_{\mathbf{r}}^{\alpha} |\mathbf{z} - \mathbf{r}|^{-\nu}, \quad L_{\text{far}} = (A\mathbb{Z}^n \times \{0\}^{d-n}) \setminus L_{\text{near}},$$

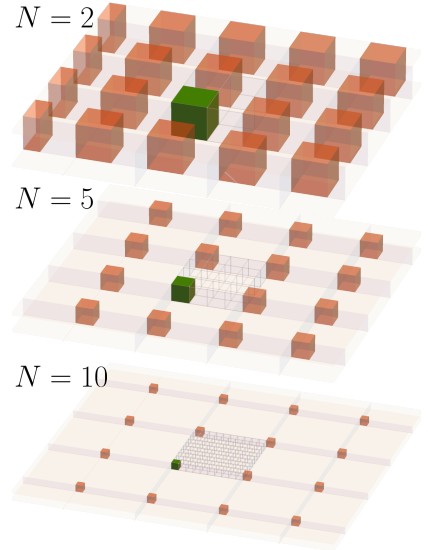
made efficiently computable in **JB**, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025).

Demagnetization factor for a 2D Film in 3D

Zeta expansion for demagnetization factor

$$D_z = 1 + \frac{N^3}{4\pi} \left(U^{(2,0,0)}(0) + U^{(0,2,0)}(0) \right)$$

$$D_z^{\text{asym}} = \frac{1}{3} + \frac{Z_{\mathbb{Z}^2,3}(0)}{4\pi} \frac{1}{N^3}$$



Demagnetization factor for a 2D Film in 3D

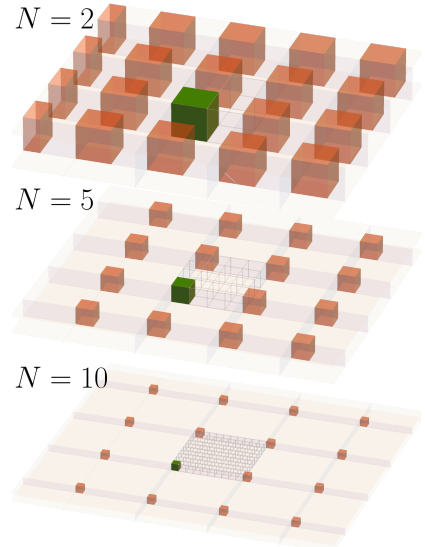
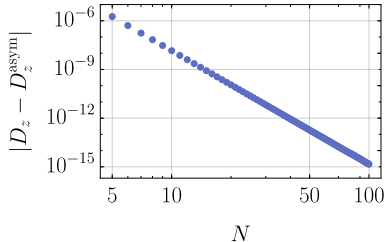
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$(\alpha \approx 0.1441459732)$

enabling its **exact computation**



Conclusions & Outlook

Efficient computation of **large-scale singular** lattice sums, such as

- ▶ Epstein zeta functions

JB, Buchheit et al., arXiv:2412.16317 (2024) ,

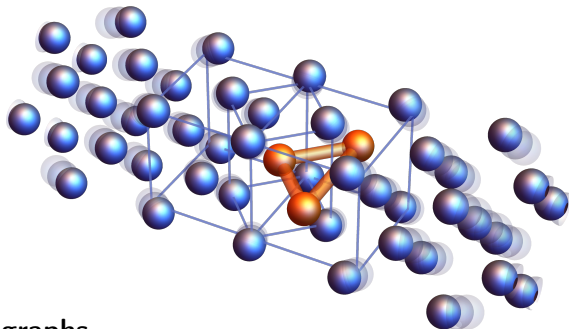
- ▶ high-dimensional lattice sums

JB, Buchheit et al., arXiv:2504.11989 (2025)

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025) ,

- ▶ and anisotropic interactions

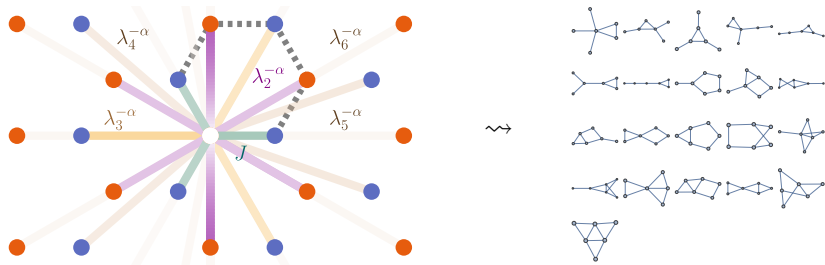
JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025) .



Next steps:

- ▶ Generalization of zeta functions to general **graphs**.
- ▶ Further investigations into the stability of matter through **zeta methods**.

Methods made available to the community through **EpsteinLib**.



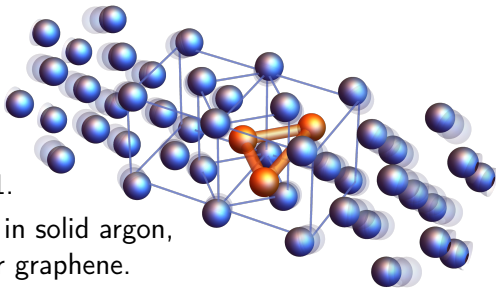
Thank You for Your Attention!

Application: Computation of many-body interactions

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$$E = \underbrace{\sum_{\mathbf{x} \in \Lambda} E^{(2)}(\mathbf{x})}_{\text{2-body contributions}} + \underbrace{\sum_{\mathbf{x}, \mathbf{y} \in \Lambda} E^{(3)}(\mathbf{x}, \mathbf{y})}_{\text{3-body contributions}} + \text{h.o.t.},$$

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025)



- ▶ leading to **exponential numerical work** in the number of interaction partners $n \in \mathbb{N}$, $n > 1$.
- ▶ Three-body forces $\approx 10\%$ of total cohesive energy in solid argon, $\approx 51\%$ binding energy of bilayer graphene.

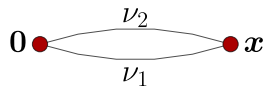
Challenge: Single 3-body calculation in 3D = **1 month** runtime on a single core.

Solution: Restate in terms of integrals over Epstein zeta functions
made efficiently computable in JB, Buchheit et al., arXiv:2504.11989 (2025).

Natural generalization of Epstein zeta to many-body lattice sums

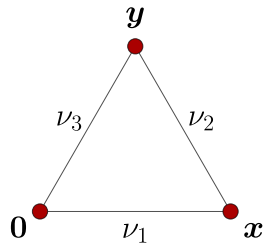
Two-body zeta function

$$Z_{\Lambda, \nu_1 + \nu_2}(0, 0) = \sum'_{\mathbf{x} \in \Lambda} \frac{1}{|\mathbf{x}|^{\nu_1 + \nu_2}} = \zeta_{\Lambda}^{(2)}(\nu_1, \nu_2)$$



Three-body zeta function

$$\zeta_{\Lambda}^{(3)}(\nu_1, \nu_2, \nu_3) = \sum'_{\mathbf{x}, \mathbf{y} \in \Lambda} \frac{1}{|\mathbf{x}|^{\nu_1}} \frac{1}{|\mathbf{x} - \mathbf{y}|^{\nu_2}} \frac{1}{|\mathbf{y}|^{\nu_3}}$$



Truncation: Computation to required precision takes 4 weeks on a single core,

Robles-Navarro, JB, et al., *J. Chem. Phys.* **163**, 094104 (2025).

Computation of many-body zeta functions

Definition (Many-body zeta functions)

Let $\Lambda = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d \times d}$ regular, let $n \in \mathbb{N}_+$, let $\boldsymbol{\nu} \in \mathbb{C}^n$, and let $\mathbf{x}^{(0)} = \mathbf{x}^{(n)} \in \Lambda$, where we adopt the choice $\mathbf{x}^{(0)} = 0$ due to translational invariance. Then, the n -body zeta function is defined as

$$\zeta_{\Lambda}^{(n)}(\boldsymbol{\nu}) = \sum'_{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n-1)} \in \Lambda} \prod_{j=1}^n \frac{1}{|\mathbf{x}^{(j)} - \mathbf{x}^{(j-1)}|^{\nu_j}}, \quad \operatorname{Re}(\nu_i) > d,$$

meromorphically continued to $\boldsymbol{\nu} \in \mathbb{C}^n$.

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Theorem (Integral representation)

Under the conditions of the definition, the n -body zeta function admits the representation

$$\zeta_{\Lambda}^{(n)}(\boldsymbol{\nu}) = |\det(A)| \int \prod_{\text{BZ}} \prod_{i=1}^n Z_{\Lambda, \nu_i}(\mathbf{k}) \, d\mathbf{k}, \quad \operatorname{Re}(\nu_i) > d,$$

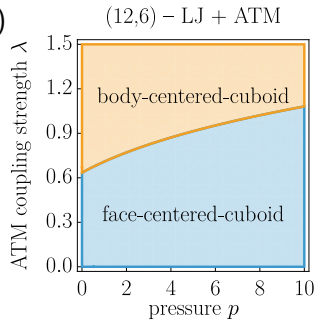
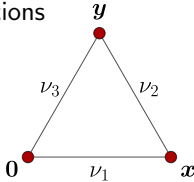
where the Hadamard integral forms the meromorphic continuation to $\boldsymbol{\nu} \in \mathbb{C}^n$.

Example: Total Cohesive Energy

Total cohesive energy $E_{\text{coh}} = \sum_{\mathbf{x} \in \Lambda} E_{\text{LJ}}^{(2)} + \lambda \sum_{\mathbf{x}, \mathbf{y} \in \Lambda} E_{\text{ATM}}^{(3)}(\mathbf{x}, \mathbf{y})$

- ▶ with two-body **Lennard-Jones** (LJ) potential,
 $\rightsquigarrow$ computable through **Epstein zeta** functions,
- ▶ and three-body **Axilrod-Teller-Muto** (ATM) potential,
 $\rightsquigarrow$ computable through **three-body** zeta functions

$$\zeta_{\Lambda}^{(3)}(\nu_1, \nu_2, \nu_3) = \sum'_{\mathbf{x}, \mathbf{y} \in \Lambda} \frac{1}{|\mathbf{x}|^{\nu_1}} \frac{1}{|\mathbf{x} - \mathbf{y}|^{\nu_2}} \frac{1}{|\mathbf{y}|^{\nu_3}}$$

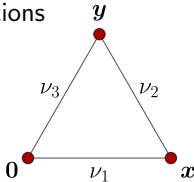


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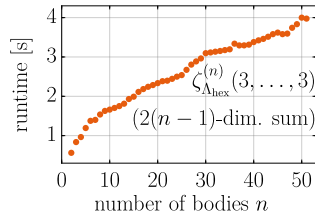
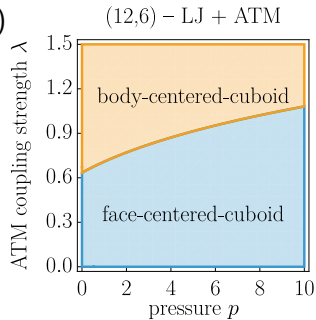
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$$\begin{aligned} \zeta_{\Lambda}^{(3)}(\nu_1, \nu_2, \nu_3) &= \sum'_{\mathbf{x}, \mathbf{y} \in \Lambda} \frac{1}{|\mathbf{x}|^{\nu_1}} \frac{1}{|\mathbf{x} - \mathbf{y}|^{\nu_2}} \frac{1}{|\mathbf{y}|^{\nu_3}} \\ &= |\det(A)| \int_{\text{BZ}} \prod_{i=1}^3 Z_{\Lambda, \nu_i}(\mathbf{k}) d\mathbf{k} \end{aligned}$$



Integral representation:

- ▶ Evaluation of $(n-1)d$ -dimensional sums.
- ▶ **Exponential reduction in runtime** (now **linear** scaling in n).



Total Cohesive Energy: 2-body LJ potential

Total **cohesive energy**

$$E_{\text{coh}} = \sum_{n=2}^{\infty} E_{\text{coh}}^{(n)} = \frac{1}{2} \sum'_{\mathbf{r} \in \Lambda} E_{\text{LJ}}^{(2)}(\mathbf{r}) + \text{h.o.t}$$

with two-body **Lennard-Jones** potential

$$E_{\text{LJ}}^{(2)}(\mathbf{r}) = \frac{nm}{n-m} \left(\frac{1}{n} |\mathbf{r}|^{-n} - \frac{1}{m} |\mathbf{r}|^{-m} \right).$$

In terms of the **Epstein zeta** function:

$$E_{\text{coh}}^{(2)} = \frac{nm}{2(n-m)} \left(\frac{Z_{\Lambda/R,n}}{nR^n} - \frac{Z_{\Lambda/R,m}}{mR^m} \right), \quad Z_{\Lambda,\nu} = Z_{\Lambda,\nu}(0,0),$$

where $n > m > 3$ and R nearest-neighbor lattice distance.

Total Cohesive Energy: 3-Body ATM potential

Total **cohesive energy**

$$E_{\text{coh}} = \sum_{n=2}^{\infty} E_{\text{coh}}^{(n)} = \frac{1}{2} \sum'_{\mathbf{r} \in \Lambda} E_{\text{LJ}}^{(2)}(\mathbf{r}) + \frac{1}{6} \sum'_{\mathbf{x}, \mathbf{y} \in \Lambda} E_{\text{ATM}}^{(3)}(\mathbf{r}) + \text{h.o.t}$$

with three-body **Axilrod–Teller–Muto** potential

$$E_{\text{ATM}}^{(3)}(\mathbf{x}, \mathbf{y}) = \lambda \left(\frac{1}{|\mathbf{x}|^3 |\mathbf{y}|^3 |\mathbf{z}|^3} - 3 \frac{(\mathbf{x} \cdot \mathbf{y})(\mathbf{y} \cdot \mathbf{z})(\mathbf{z} \cdot \mathbf{x})}{|\mathbf{x}|^5 |\mathbf{y}|^5 |\mathbf{z}|^5} \right) \Big|_{\mathbf{z}=\mathbf{y}-\mathbf{x}}.$$

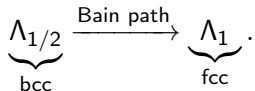
In terms of the **many-body zeta** function:

$$E_{\text{coh}}^{(3)} = \lambda R^{-9} \left(\frac{1}{24} \zeta_{\Lambda/R}^{(3)}(3, 3, 3) - \frac{3}{16} \zeta_{\Lambda/R}^{(3)}(-1, 5, 5) + \frac{3}{8} \zeta_{\Lambda/R}^{(3)}(1, 3, 5) \right)$$

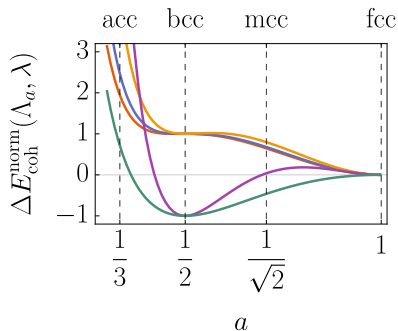
where λ coupling constant, R nearest-neighbour lattice distance.

Results: Normalized energy difference along Bain path

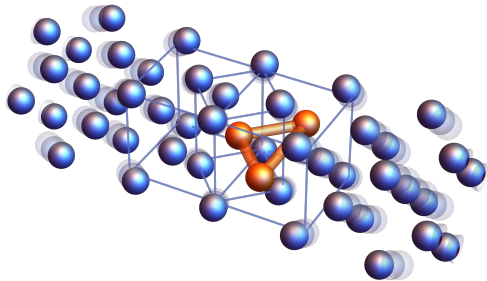
Total cohesive energy along



Normalized energy difference $\Delta E_{\text{coh}}^{\text{norm}}(\Lambda_a, \lambda)$:



- $\lambda = 0$
- $\lambda = 1/4$
- $\lambda = 2/4$
- $\lambda = 3/4$
- $\lambda = 1$



- Three-body coupling strength λ .
- (8,4)-Lennard-Jones potential.

- Minimal nearest-neighbor distance R ,

$$E_{\text{coh}}(\Lambda_a, \lambda) = \min_{R>0} \left(\underbrace{E_{\text{coh}}^{(2)}(R)}_{(8,4)\text{-pot.}} + E_{\text{coh}}^{(3)}(R) \right).$$

- Normalized energy-difference:

$$\Delta E_{\text{coh}}(\Lambda_a, \lambda) = E_{\text{coh}}(\Lambda_1, \lambda) - E_{\text{coh}}(\Lambda_a, \lambda),$$

$$E_{\text{coh}}^{\text{norm}}(\Lambda_a, \lambda) = \Delta E_{\text{coh}}(\Lambda_a, \lambda) / |\Delta E_{\text{coh}}(\Lambda_1, \lambda)|.$$

Example: Topological superconductors with long-range pairing

Long-range chiral **topological superconductor** (class D)

Viyuela et al., *Phys. Rev. Lett.* (2018)

$$H = -\frac{1}{2} \sum'_{\mathbf{r}, \mathbf{r}' \in \mathbb{Z}^2} \left[\tau_\beta(\mathbf{r} - \mathbf{r}') c_{\mathbf{r}}^\dagger c_{\mathbf{r}'} - \Delta_\alpha(\mathbf{r} - \mathbf{r}') c_{\mathbf{r}}^\dagger c_{\mathbf{r}'}^\dagger + \text{h.c.} \right] - (\mu - 2) \sum_{\mathbf{r} \in \mathbb{Z}^2} c_{\mathbf{r}}^\dagger c_{\mathbf{r}}$$

- ▶ with long-range hopping $\tau_\beta(\mathbf{r}) = |\mathbf{r}|^{-\beta}$,
- ▶ long-range pairing $\Delta_\alpha(\mathbf{r}) = (r_1 - ir_2)|\mathbf{r}|^{-(\alpha+1)}$,
- ▶ and chemical potential μ .

Assume periodic boundary conditions, so that in the Nambu-spinor basis of paired fermions

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot (\sigma_x, \sigma_y, \sigma_z), \quad \mathbf{d}(\mathbf{k}) = \begin{pmatrix} -\sum_{\mathbf{r} \in \mathbb{Z}^2} r_2 \sin(\mathbf{k} \cdot \mathbf{r}) / |\mathbf{r}|^{\alpha+1} \\ -\sum_{\mathbf{r} \in \mathbb{Z}^2} r_1 \sin(\mathbf{k} \cdot \mathbf{r}) / |\mathbf{r}|^{\alpha+1} \\ 4 - 2\mu - \sum_{\mathbf{r} \in \mathbb{Z}^2} \cos(\mathbf{k} \cdot \mathbf{r}) / |\mathbf{r}|^\beta \end{pmatrix}, \quad \mathbf{k} \in \text{BZ}.$$

Example: Topological superconductors with long-range pairing in 3D

We compute the winding number

$$\Omega = \frac{1}{4\pi} \int_{\text{BZ}} \mathbf{n}(\mathbf{k}) \cdot \left(\partial_{k_1} \mathbf{n}(\mathbf{k}) \times \partial_{k_2} \mathbf{n}(\mathbf{k}) \right) d\mathbf{k}$$

by writing $\mathbf{n}(\mathbf{k}) = \mathbf{d}(\mathbf{k})/|\mathbf{d}(\mathbf{k})|$ as an anisotropic Epstein zeta function.

Phase diagram replicates the result in Viyuela et al., *Phys. Rev. Lett.* (2018).

Introducing 3D dependency in the long-range hopping

$$\mathbf{d}(\mathbf{k}, k_3) = \begin{pmatrix} -\sum_{\mathbf{r} \in \mathbb{Z}^2} r_2 \sin(\mathbf{k} \cdot \mathbf{r})/|\mathbf{r}|^{\alpha+1} \\ -\sum_{\mathbf{r} \in \mathbb{Z}^2} r_1 \sin(\mathbf{k} \cdot \mathbf{r})/|\mathbf{r}|^{\alpha+1} \\ \sum_{\mathbf{z} \in \mathbb{Z}^3} \cos((\mathbf{k}, k_3)^T \cdot \mathbf{z})/|\mathbf{z}|^\beta \end{pmatrix}$$

for $\mu = 2$ yields **fractional winding numbers** in phase diagram.

