Computation of Generalized Zeta Functions

With Applications to Long-Range Interacting Classical and Quantum Lattices

Workshop on Quantum Technologies, RWTH Aachen — Tue. May 12, 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)

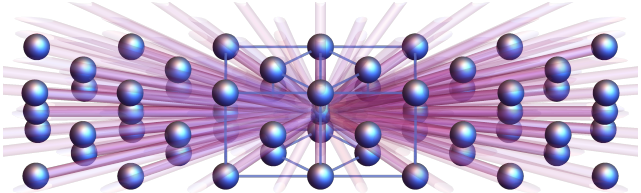
DLR, Inst. of Software Technology, QCA Group & Saarland University; joint work with A. A. Buchheit

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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 $\sim 1/r^\alpha$.

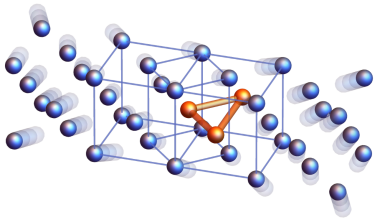


Interesting yet challenging:

- **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!**

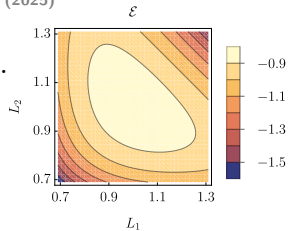
Broad applicability in long-range interacting lattices

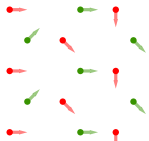


Theoretical chemistry:
Cohesive energy for Lennard-Jones

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

$$E_{\mathrm{LJ}}(\boldsymbol{r}) \propto \frac{1}{n}|\boldsymbol{r}|^{-n} - \frac{1}{m}|\boldsymbol{r}|^{-m}\,.$$





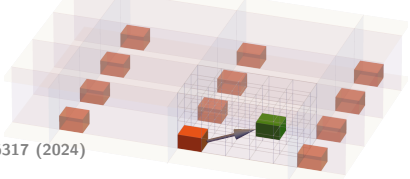
Micromagnetics: Generalized potential

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

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

Spin systems:

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



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

High energy physics:
Casimir energy

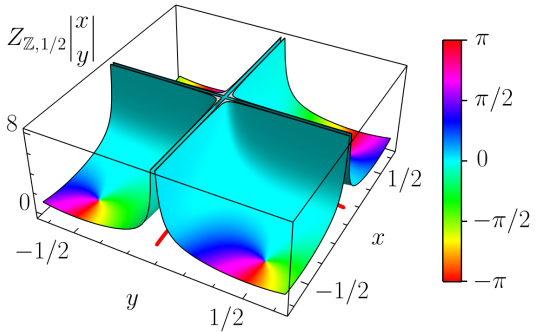
JB, Buchheit et al., arXiv:2412.16317 (2024)

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

Epstein zeta function

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

$$Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| = \sum_{\boldsymbol{z}\in\Lambda}{}' \frac{e^{-2\pi i \boldsymbol{y}\cdot\boldsymbol{z}}}{|\boldsymbol{z}-\boldsymbol{x}|^{\nu}}, \qquad \mathrm{Re}(\nu) > d.$$



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

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

with ***upper Crandall*** *function*

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

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 $(\Lambda, \nu, \boldsymbol{x}, \boldsymbol{y}) \to (\Lambda^*, d-\nu, \boldsymbol{y}, -\boldsymbol{x})$ does not change the product

$$\frac{(|\det A|^{2/d}/\pi)^{\nu/2}}{\Gamma\big((d-\nu)/2\big)} e^{\pi i \boldsymbol{x}\cdot\boldsymbol{y}} Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right|.$$

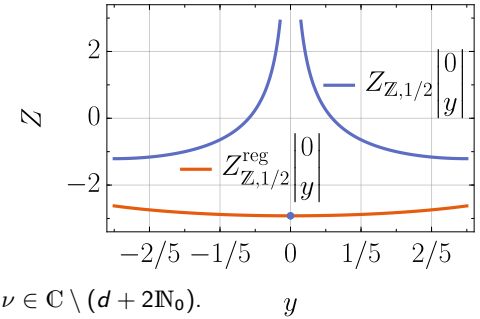
- **Joint holomorphy** in $(\nu, \boldsymbol{x}, \boldsymbol{y}) \in \mathbb{C} \times D_\Lambda \times D_{\Lambda^*}$.
- **Power-law singularities** in $\boldsymbol{x} \to \Lambda$ and $\boldsymbol{y} \to \Lambda^*$.

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

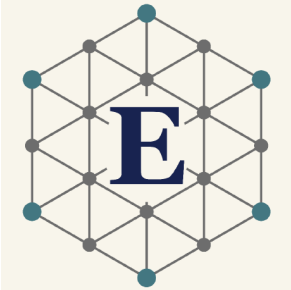
Solution: **Regularization** in $\boldsymbol{y}$

$$\underbrace{Z_{\Lambda,\nu}\left|\begin{matrix}0\\ \boldsymbol{y}\end{matrix}\right|}_{\substack{\textbf{singularity}\\ \text{in } \boldsymbol{y}=0}} = \underbrace{Z^{\mathrm{reg}}_{\Lambda,\nu}\left|\begin{matrix}0\\ \boldsymbol{y}\end{matrix}\right|}_{\substack{\textbf{smooth}\\ \text{in } \boldsymbol{y}\in\mathrm{BZ}}} + c_{\Lambda,\nu}|\boldsymbol{y}|^{\nu-d}$$

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



EpsteinLib



C library for the evaluation of the Epstein zeta function for

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

including Python, Julia and Mathematica bindings.

```c
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

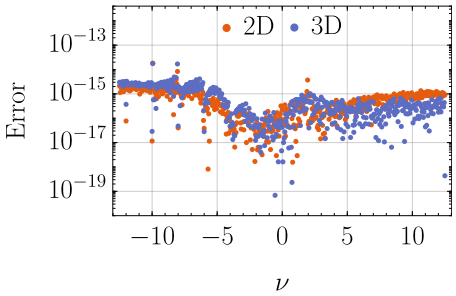
```shell
pip install epsteinlib
```

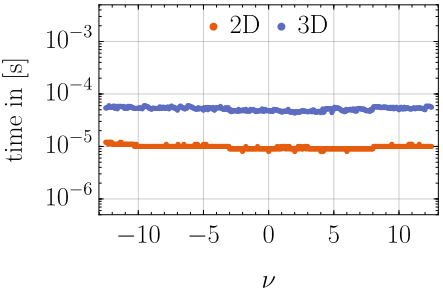
Shell

```python
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:

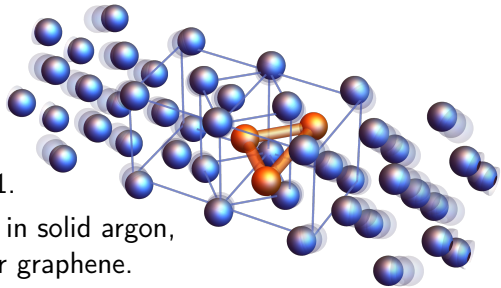
- Supersymmetry-breaking compactifications Dall'Agata et al., arXiv:2507.02339 (2025).
- Casimir-Driven de Sitter in M-Theory Bento et al., arXiv:2507.02037 (2025).

Application: Computation of many-body interactions

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

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

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.

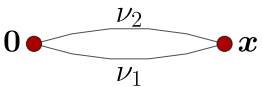
Challenge: Single 3-body calculation in 3D = **1 month** runtime on a single core.

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

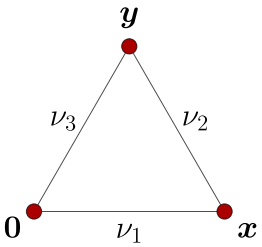
Two-body zeta function

$$Z_{\Lambda,\nu_1+\nu_2}\left|\begin{matrix}0\\0\end{matrix}\right| = \sum_{\boldsymbol{x}\in\Lambda}{}' \frac{1}{|\boldsymbol{x}|^{\nu_1+\nu_2}} = \zeta_\Lambda^{(2)}(\nu_1,\nu_2)$$



Three-body zeta function

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



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 $\boldsymbol{x}^{(0)} = \boldsymbol{x}^{(n)} \in \Lambda$, where we adopt the choice $\boldsymbol{x}^{(0)} = 0$ due to translational invariance. Then, the n-body zeta function is defined as

$$\zeta_\Lambda^{(n)}(\boldsymbol{\nu}) = {\sum_{\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n-1)}\in\Lambda}}' \prod_{j=1}^{n} \frac{1}{|\boldsymbol{x}^{(j)} - \boldsymbol{x}^{(j-1)}|^{\nu_j}}, \quad \mathrm{Re}(\nu_i) > d\,,$$

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

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

Theorem (Integral representation)

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

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

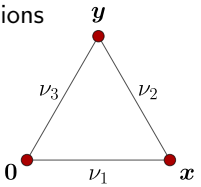
where the Hadamard integral forms the meromorphic continuation to $\boldsymbol{\nu} \in \mathbb{C}^n$.

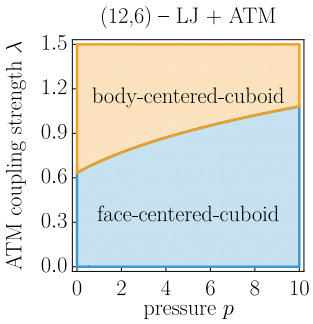
Example: Total Cohesive Energy

Total **cohesive energy** $E_{\mathrm{coh}} = \sum_{\boldsymbol{x}\in\Lambda} E^{(2)}_{\mathrm{LJ}} + \lambda \sum_{\boldsymbol{x},\boldsymbol{y}\in\Lambda} E^{(3)}_{\mathrm{ATM}}(\boldsymbol{x},\boldsymbol{y})$

- 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

$$\zeta^{(3)}_{\Lambda}(\nu_1,\nu_2,\nu_3) = \sum_{\boldsymbol{x},\boldsymbol{y}\in\Lambda}{}' \frac{1}{|\boldsymbol{x}|^{\nu_1}} \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu_2}} \frac{1}{|\boldsymbol{y}|^{\nu_3}}$$





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

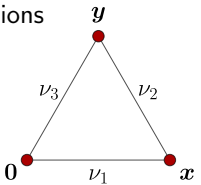
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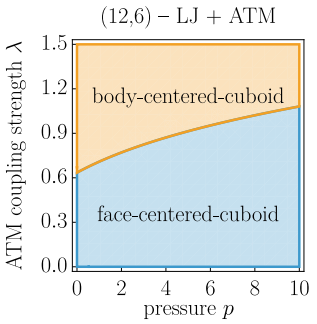
$$\zeta^{(3)}_{\Lambda}(\nu_1,\nu_2,\nu_3) = \sum_{\boldsymbol{x},\boldsymbol{y}\in\Lambda}{}' \frac{1}{|\boldsymbol{x}|^{\nu_1}} \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu_2}} \frac{1}{|\boldsymbol{y}|^{\nu_3}}$$

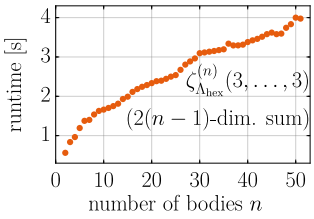
$$= |\det(A)| \int_{\mathrm{BZ}} \prod_{i=1}^{3} Z_{\Lambda,\nu_i}(\boldsymbol{k})\,\mathrm{d}\boldsymbol{k}$$



Integral representation:

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





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

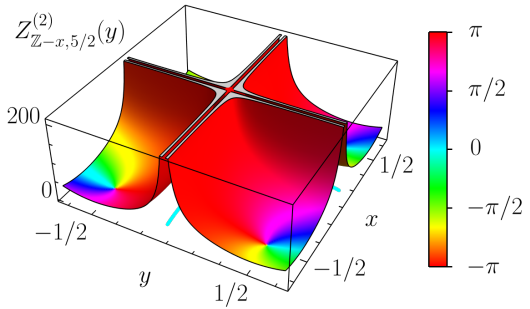
Robles-Navarro, **JB**, et al., *J. Chem. Phys.* **163**, 094104 (2025)

Computation of anisotropic lattice sums

For a d-dimensional lattice Λ, $\boldsymbol{y} \in \mathbb{R}^d$, $\boldsymbol{\alpha} \in \mathbb{N}^d$ and $\mathrm{Re}(\nu) > d + |\boldsymbol{\alpha}|$ consider

$$Z^{(\boldsymbol{\alpha})}_{\Lambda,\nu}(\boldsymbol{y}) = (-2\pi i)^{|\boldsymbol{\alpha}|} \sum_{\boldsymbol{z}\in\Lambda}{}' z_1^{\alpha_1} z_2^{\alpha_2} \dots z_d^{\alpha_d} \frac{e^{-2\pi i \boldsymbol{y}\cdot\boldsymbol{z}}}{|\boldsymbol{z}|^{\nu}}.$$

These are the **$\boldsymbol{\alpha}$-derivatives of Epstein zeta functions** with respect to $\boldsymbol{y}$.



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).

Theorem (Main result)

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

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

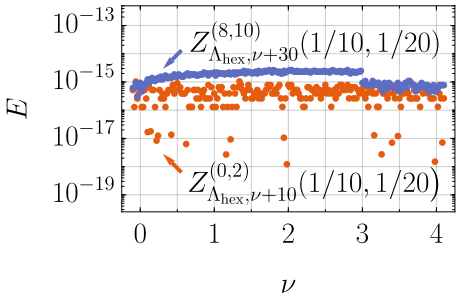
Here, $h_{k,\boldsymbol{\alpha}}$, $2k \le |\boldsymbol{\alpha}|$ are homogeneous harmonic polynomials of degree $|\boldsymbol{\alpha}| - 2k$, uniquely defined by

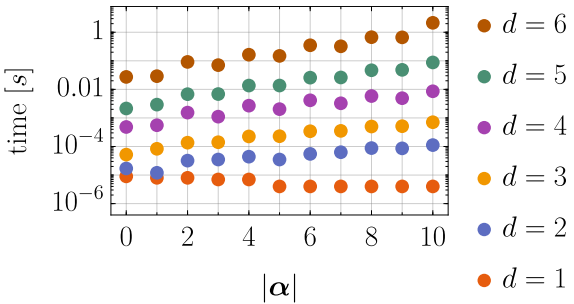
$$\boldsymbol{z}^{\boldsymbol{\alpha}} = \sum_{k=0}^{\lfloor|\boldsymbol{\alpha}|/2\rfloor} |\boldsymbol{z}|^{2k} h_{k,\boldsymbol{\alpha}}(\boldsymbol{z}), \qquad \boldsymbol{z} \in \mathbb{R}^d.$$

Precision and runtime

```python
import numpy as np
from epsteinlib import set_zeta_der

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

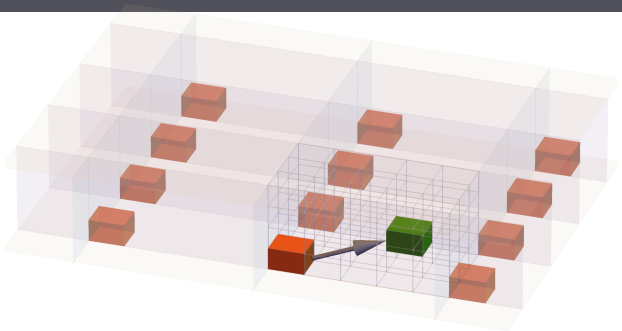




Extension: Anisotropic lattice sums in micromagnetics

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

$$\underset{(\boldsymbol{z} \in L\ )}{\boldsymbol{z}+\Omega} \xrightarrow{\text{influence}} \boldsymbol{r}+\Omega\,.$$



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

$$U^{(\boldsymbol{m})}(\boldsymbol{r}) = \sum_{\boldsymbol{z}\in L} \int_{\Omega+\boldsymbol{z}} \partial_{\boldsymbol{r}}^{\boldsymbol{m}} \int_{\Omega+\boldsymbol{r}} |\boldsymbol{r}' - \boldsymbol{r}''|^{-\nu}\, \mathrm{d}\boldsymbol{r}'\, \mathrm{d}\boldsymbol{r}''$$

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

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

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

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

$$U^{(\boldsymbol{m})}(\boldsymbol{r}) \approx \sum_{\boldsymbol{z}\in L_{\mathrm{near}}} S^{(\boldsymbol{m})}(\boldsymbol{r}+\boldsymbol{z}), \qquad S^{(\boldsymbol{m})}(\boldsymbol{r}) = \int_{\Omega} \nabla_{\boldsymbol{r}}^{\boldsymbol{m}} \int_{\Omega+\boldsymbol{r}} |\boldsymbol{r}' - \boldsymbol{r}''|^{-\nu} \,\mathrm{d}\boldsymbol{r}' \,\mathrm{d}\boldsymbol{r}'' \,.$$

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

Zeta expansion for long-range interactions in micromagnetics

Solution: **Zeta expansion** for micromagnetics

$$U^{(\boldsymbol{m})}(\boldsymbol{r}) = \sum_{\boldsymbol{z}\in L_{\mathrm{near}}} S^{(\boldsymbol{m})}(\boldsymbol{r}+\boldsymbol{z}) + \sum_{\boldsymbol{\alpha}\geq 0} c_{\boldsymbol{\alpha}} Z^{(\boldsymbol{m}+2\boldsymbol{\alpha})}_{L_{\mathrm{far}},\nu}(\boldsymbol{r})$$

with **exponential** convergence in derivative order $\boldsymbol{\alpha}$.

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

$$Z^{(\boldsymbol{\alpha})}_{L_{\mathrm{far}},\nu} = \sum_{\boldsymbol{z}\in L_{\mathrm{far}}}{}' \nabla^{\boldsymbol{\alpha}}_{\boldsymbol{r}} |\boldsymbol{z}-\boldsymbol{r}|^{-\nu}, \qquad L_{\mathrm{far}} = (A\mathbb{Z}^n \times \{0\}^{d-n}) \setminus L_{\mathrm{near}},$$

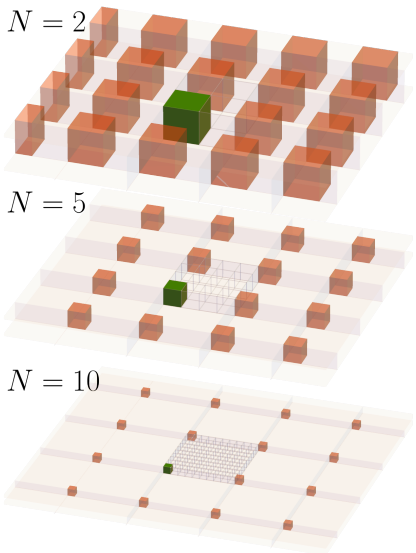
made efficiently computable in **JB**, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025).

Demagnetization factor for a 2D Film in 3D

Zeta expansion for **demagnetization factor**

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

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



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

Demagnetization factor for a 2D Film in 3D

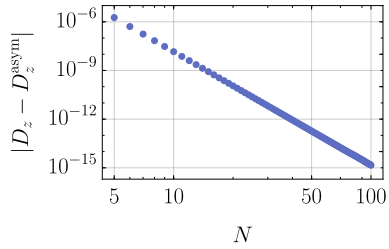
Zeta expansion for **demagnetization factor**

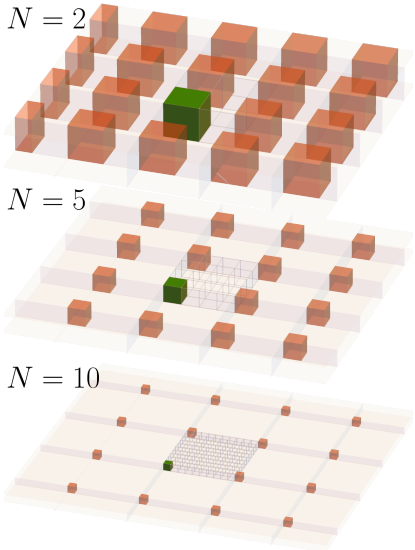
$$D_z = 1 + \frac{N^3}{4\pi}\left(U^{(2,0,0)}(0) + U^{(0,2,0)}(0)\right)$$

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

($\alpha \approx 0.1441459732$)

enabling its **exact computation**





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

Conclusions & Outlook

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

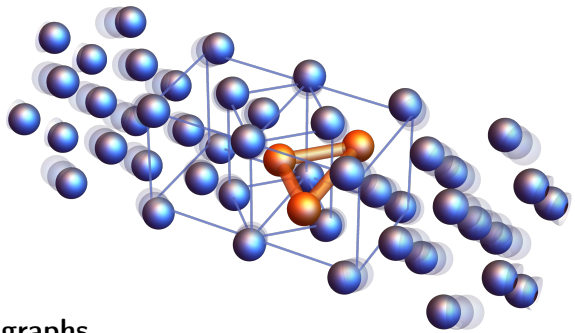
- Epstein zeta functions

  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

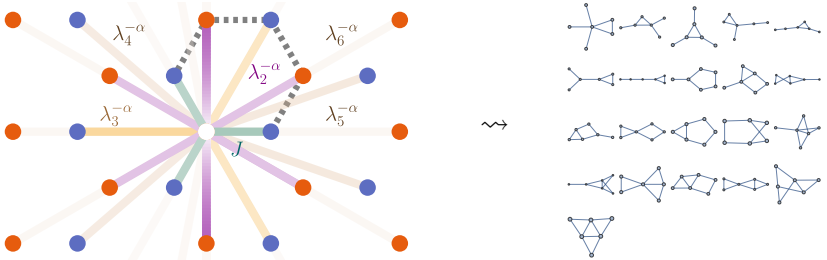
  JB, Buchheit et al., *J. Comp. Phys.*, **559** 114885 (2025) .



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 throught **EpsteinLib.**



Thank You for Your Attention!

Total Cohesive Energy: 2-body LJ potential

Total **cohesive energy**

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

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

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

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

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

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

Total Cohesive Energy: 3-Body ATM potential

Total **cohesive energy**

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

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

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

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

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

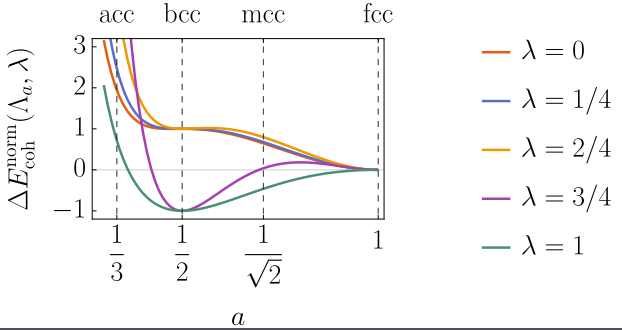
where λ coupling constant, R nearest-neighbour lattice distance.

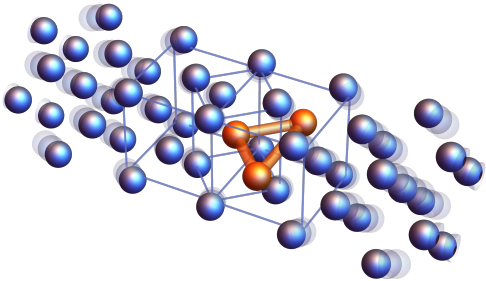
Results: Normalized energy difference along Bain path

Total **cohesive energy** along

$$\underbrace{\Lambda_{1/2}}_{\text{bcc}} \xrightarrow{\text{Bain path}} \underbrace{\Lambda_1}_{\text{fcc}} .$$

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





- Three-body coupling strength λ.
- (8,4)-Lennard–Jones potential.
- Minimal nearest-neighbor distance R,

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

- Normalized energy-difference:

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

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

Example: Topological superconductors with long-range pairing

Long-range chiral **topological superconductor** (class D) Viyuela et al., *Phys. Rev. Lett.* (2018)

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

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

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

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

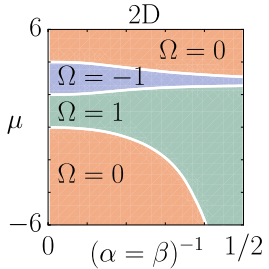
Example: Topological superconductors with long-range pairing in 3D

We compute the winding number

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

by writing $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{d}(\boldsymbol{k})/|\boldsymbol{d}(\boldsymbol{k})|$ as an Epstein zeta derivative.

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



Introducing 3D dependency in the long-range hopping

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

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

