Zeta Expansion For Long-range Interacting Classical And Quantum Lattices

Jonathan K. Busse, Saarbrücken — October 27th, 2025

Math:	**JB**, Buchheit et al., arXiv:2412.16317 (2024)
	JB, Buchheit et al., arXiv:2504.11989 (2025)
Physics:	**JB**, Buchheit et al., arXiv:2509.26274 (2025)
Chemistry:	Robles-Navarro, **JB**, et al., *J. Chem. Phys.* 163, 094104 (2025)

Joint work with A. A. Buchheit; supervised by Prof. Sergej Rjasanow

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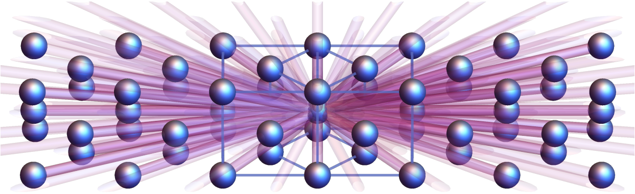
DLR

Long-range interactions appear everywhere in nature

Long-range couplings that decay as a **power-law** with distance $\boldsymbol{r}$ appear everywhere in nature,

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



Computations are hard:

- Huge number of particles (e.g. 10^{23}) makes **exact summation infeasible**.
- **Continuum approximations** require correction terms that account for singularity.
- **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, <u>**zeta functions appear!**</u>

Evaluating large-scale singular lattice sums

The challenge: Evaluate prototypical sums such as

$$S = \sum_{\boldsymbol{z}\in\Lambda}{}' f(\boldsymbol{z}), \qquad f(\boldsymbol{z}) = g(\boldsymbol{z})/|\boldsymbol{z}|^{-\nu}, \quad g : \mathbb{R}^d \to \mathbb{R} \text{ sufficiently smooth}, \quad \nu \in \mathbb{R}^d\,.$$

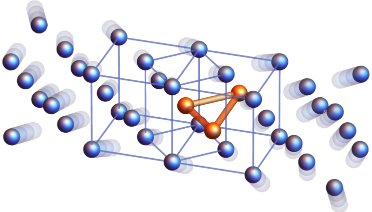
Here, Λ is a d-dimensional lattice, that is $\Lambda = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d\times d}$ regular.

Truncation: $S \approx \sum{}'_{\boldsymbol{z}\in\Lambda,\,|\boldsymbol{z}|<R} f(\boldsymbol{z}) \;\rightsquigarrow\;$ needs arbitrary high $R > 0$ for g constant, $\nu \to d$.

Continuum approximation: $S \approx \frac{1}{|\mathrm{det}(A)|}\int_{\mathbb{R}^d} f(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \;\rightsquigarrow\;$ introduces systematic error.

Solution: Compute S using numerical algorithms based on **generalized zeta functions**, offering full precision at numerical cost independent of particle number.

Broad applicability in long-range interacting lattices

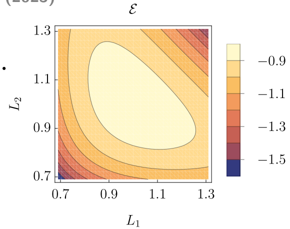


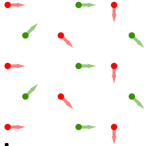
Theoretical chemistry:

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

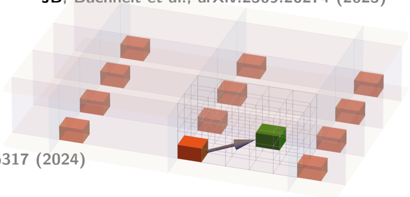
$$U^{(\boldsymbol{m})}(\boldsymbol{r}) = \sum_{\boldsymbol{z}\in L} \int_{\Omega+\boldsymbol{z}} \nabla_{\boldsymbol{r}}^{\boldsymbol{m}} \int_{\Omega+\boldsymbol{r}} |\boldsymbol{r}'-\boldsymbol{r}''|^{-\nu}\,\mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{r}''\,.$$

JB, Buchheit et al., arXiv:2509.26274 (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)

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

Zeta methods for long-range interacting lattices

Two-year research summary on **zeta methods** for **long-range interacting lattices**:

1. Computation and properties of the Epstein zeta function

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

2. Computation of many-body zeta functions

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

3. Stability of matter under inclusion of many-body interactions

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

4. Stable computation high-order generalized zeta derivatives

   JB, Buchheit, (soon on arXiv).

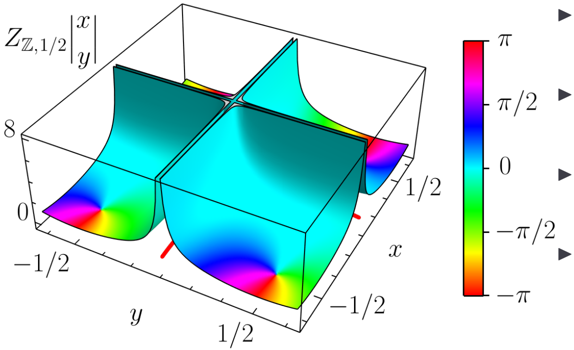
5. Zeta expansion for long-range interactions in micromagnetics

   JB, Buchheit et al., arXiv:2509.26274 (2025).

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 $\nu \in \mathbb{C}$

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



- Foundational work: Epstein

  Epstein, *Math. Ann.* (1903), Epstein, *Math. Ann.* (1906).

- 2D Bessel representation: Chowla–Selberg

  Chowla et al., *Proceedings of the National A. of S.* (1949).

- ND Bessel representation: Elizalde

  Elizalde, *Communications in mathematical physics* (1998).

- Incomplete Gamma representation: Crandall

  Crandall, (2012).

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

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

*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 incomplete Gamma function.

Properties: Functional equation and analyticity

Assume the conditions of the Crandall representation, in particular $\Lambda = A\mathbb{Z}^d$, $\Lambda^* = A^{-T}\mathbb{Z}^d$.

Theorem (Functional equation)

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

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

Theorem (Analyticity)

Let $D_L = \{\boldsymbol{u} \in \mathbb{C}^d : |\mathrm{Re}(\boldsymbol{u}) - \boldsymbol{z}| > |\mathrm{Im}(\boldsymbol{u})| \ \forall \boldsymbol{z} \in L\}$, $L \subseteq \mathbb{R}^d$. *The Epstein zeta function can be holomorphically extended to*

$$(\nu, \boldsymbol{x}, \boldsymbol{y}) \in \mathbb{C} \times D_\Lambda \times D_{\Lambda^*}\,.$$

Epstein zeta exhibits

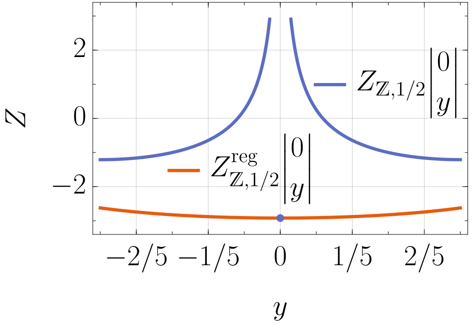
- a simple pole in $\nu \to d$ for $\boldsymbol{y} \in \Lambda^*$,
- a power-law singularities in $\boldsymbol{x} \to \Lambda$ and $\boldsymbol{y} \to \Lambda^*$.

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

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

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

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



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

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);
```

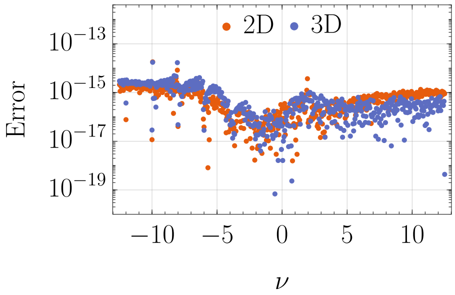
Available on `github.com/epsteinlib`; joint work with: Andreas A. Buchheit, Ruben Gutendorf; DevOps: Jan Schmitz.

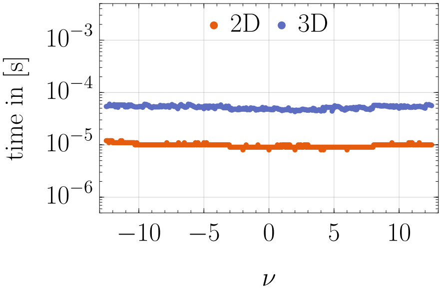
Precision and runtime

```shell
pip install epsteinlib
```

```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))
```





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

EpsteinLib in use by community

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 Ising compound Yadav et al., arXiv:2405.12405 (2025).
- Quantum annealing for competing long-range lattices Koziol et al., arXiv:2511.08336 (2025).

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).

Our work:

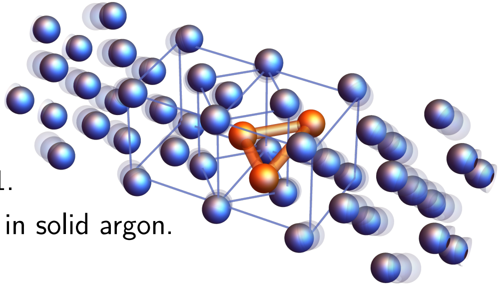
- Computation and properties of the Epstein zeta function **JB**, Buchheit et al., arXiv:2412.16317 (2024).
- Zeta method for many-body lattice sums **JB**, Buchheit et al., arXiv:2504.11989 (2025).
- Three-body interactions in phase transitions Robles-Navarro, **JB**, et al., *J. Chem. Phys.* **163**, 094104 (2025)
- Computation of dipolar interactions with PBC **JB**, Buchheit et al., arXiv:2509.26274 (2025).

Computation of many-body interactions

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

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

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



- 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.

Solution: Restate in terms of n-body zeta functions

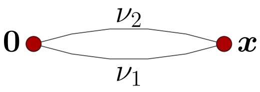
$$\zeta_\Lambda^{(n)}(\nu_1,\dots,\nu_n) = \sum_{\boldsymbol{x}^{(1)},\dots,\boldsymbol{x}^{(n-1)}\in\Lambda}{}' \prod_{j=1}^{n} \frac{1}{|\boldsymbol{x}^{(j)} - \boldsymbol{x}^{(j-1)}|^{\nu_j}}, \qquad \mathrm{Re}(\nu_i) > d,\ \boldsymbol{x}^{(n)} = \boldsymbol{x}^{(0)} \in \Lambda,$$

made efficiently computable in **JB, Buchheit et al., arXiv:2504.11989 (2025)** .

Natural generalization of Epstein zeta to many-body lattice sums

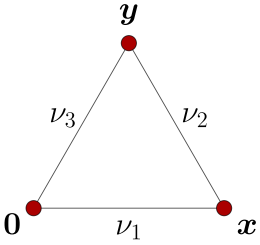
Two-body zeta function

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



Three-body zeta function

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



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

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

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

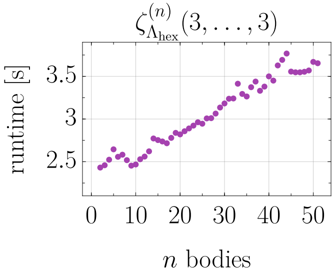
Timing and error

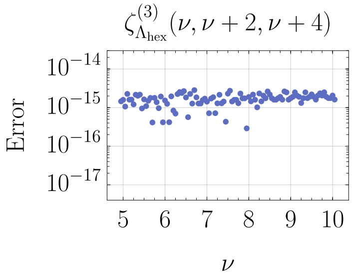
Calculation of *n*-body zeta functions:

- Evaluation of $(n-1)d$-dimensional sums.
- **Direct summation** leads to **exponential** scaling in *n*.
- Ewald-summation not applicable.

Zeta **integral representation**:

- Exponential reduction in runtime (runtime has **linear** scaling in *n*).
- Enables access to meromorphic continuation.
- Achieves machine precision.



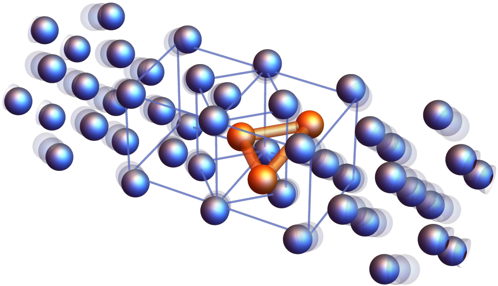


Many-body interactions in phase transitions

Computation of **high-dimensional lattice sums**: through many-body zeta functions!

Example: Many-body pertubative expansion of total cohesive energy E_{coh} with n-body contributions $E_{\mathrm{coh}}^{(n)}$ in theoretical chemistry.

- Before: Only 2-body interactions,
- single 3-body calculation in 3D $=$ **1 month** runtime on a cluster.



Now in 3D on a laptop: 2+3-body term in

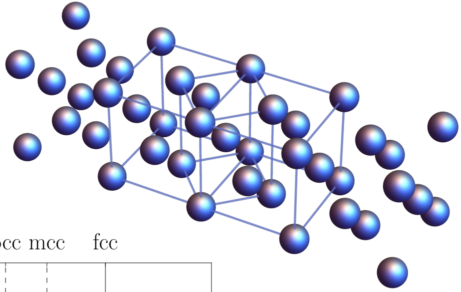
$$E_{\mathrm{coh}} = E_{\mathrm{coh}}^{(2)} + E_{\mathrm{coh}}^{(3)} + \mathrm{h.o.t}\,.$$

Beginning of rigorous investigation into stability of matter in
Robles-Navarro, JB, et al., *J. Chem. Phys.* 163, 094104 (2025).

Bain path

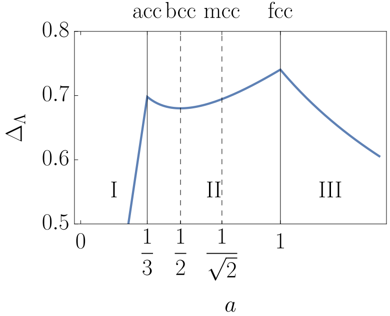
Lattice structure: Let $\Lambda_a = \frac{1}{\sqrt{a+1}} \begin{bmatrix} \sqrt{a} & \sqrt{a} & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \mathbb{Z}^3$

$$\underbrace{\Lambda_{1/3}}_{\text{acc}} \xrightarrow{\text{Bain path}} \underbrace{\Lambda_1}_{\text{fcc}} .$$



Packing density Δ_Λ along **Bain path**,

- acc: axial centered cuboid,
- bcc: body-centered cuboid,
- mcc: mean centered cuboid,
- fcc: face-centered cuboid.



Total Cohesive Energy: 2-body LJ potential

Total **cohesive energy**

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

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

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

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

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

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

Total Cohesive Energy: 3-Body ATM potential

Total **cohesive energy**

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

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

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

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

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

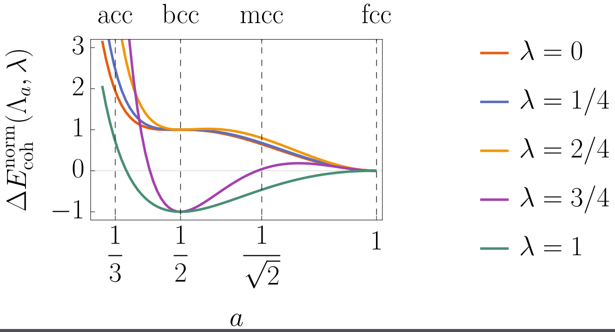
where λ coupling constant, R nearest-neighbour lattice distance.

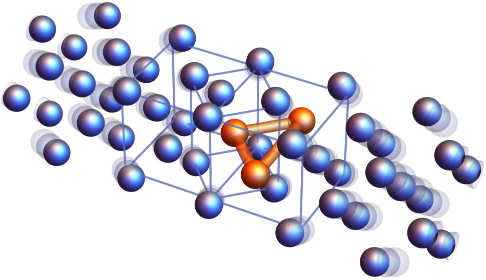
Results: Normalized energy difference alogn Bain path

Total **cohesive energy** along

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

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





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

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

- Normalized energy-difference:

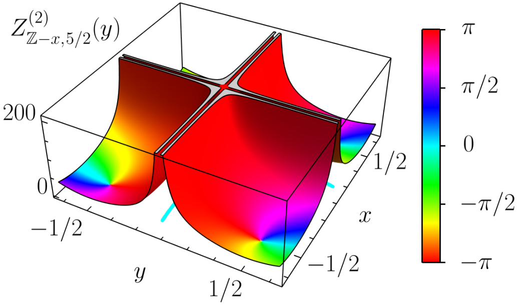
$$\Delta E_{\mathrm{coh}}(\Lambda_a, \lambda) = E_{\mathrm{coh}}(\Lambda_1, \lambda) - E_{\mathrm{coh}}(\Lambda_a, \lambda) ,$$

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

Computation of set zeta derivatives

Let $L \subseteq \mathbb{R}^d$ be uniformly discrete and let $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ be a multi-index. We define the $\boldsymbol{\alpha}$-derivatives of the set zeta function with respect $\boldsymbol{y} \in \mathbb{R}^d$ as meromorphic continuation of the following lattice sum to $\nu \in \mathbb{C}$

$$Z_{L,\nu}^{(\boldsymbol{\alpha})}(\boldsymbol{y}) = \sum_{\boldsymbol{z} \in L}{}' (-2\pi i \boldsymbol{z})^{\boldsymbol{\alpha}} \frac{e^{-2\pi i \boldsymbol{y}\cdot\boldsymbol{z}}}{|\boldsymbol{z}|^{\nu}}, \qquad \mathrm{Re}(\nu) > d + |\boldsymbol{\alpha}|\,.$$



- Generalization of Epstein zeta to derivatives of non-translational invariant point sets

  JB, Buchheit, (soon on arXiv).

- Application: Taylor series with applications in theoretical chemistry

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

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

- Application: Potential in Micromagnetics

  JB, Buchheit et al., arXiv:2509.26274 (2025) .

Crandall representation for set zeta derivatives

Theorem (Set zeta derivatives for shifted lattices)

Let $\Lambda = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d\times d}$ *regular,* $\alpha \in \mathbb{N}_0^d$, $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, *and* $\nu \in \mathbb{C}$ *so that* $\nu \neq d + |\boldsymbol{\alpha}|$ *if* $\boldsymbol{y} \in \Lambda^* = A^{-T}\mathbb{Z}^d$. *Then*

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

Here $G_\nu(\boldsymbol{z}) = \Gamma(\nu/2, \pi\boldsymbol{z}^2)/(\pi\boldsymbol{z}^2)^{\nu/2}$ *is the upper Crandall function with* $\boldsymbol{y}$*-derivatives*

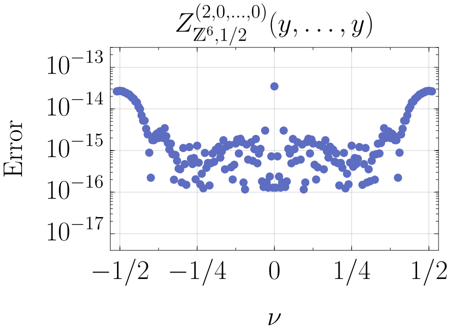
$$G^{(\boldsymbol{\alpha})}_\nu(\boldsymbol{y}) = \sum_{2\boldsymbol{\beta}\leq\boldsymbol{\alpha}} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{y}) G_{\nu+2|\boldsymbol{\alpha}|-2|\boldsymbol{\beta}|}(\boldsymbol{y})$$

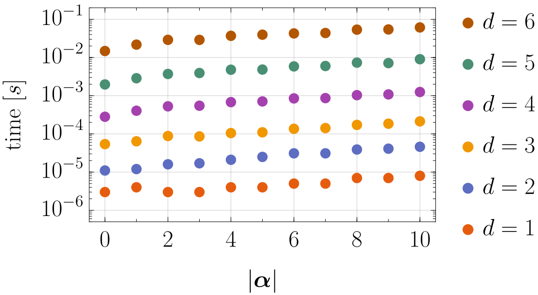
for the monomial $p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{y}) = (-\pi)^{\boldsymbol{\alpha}-\boldsymbol{\beta}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\frac{(\boldsymbol{\alpha}-\boldsymbol{\beta})!}{(\boldsymbol{\alpha}-2\boldsymbol{\beta})!}(2\boldsymbol{y})^{\boldsymbol{\alpha}-2\boldsymbol{\beta}}$.

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'))
```





Applications of zeta derivatives

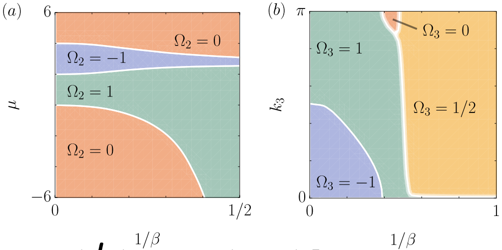
Wide ranging **applications**:

- Exact difference between sum and integral (singular Euler-Maclaurin expansion).
- Stabilization of integrals involving Epstein zeta functions.
- Long-range interactions in micromagnetics,
- and many more!

Superconductivity: Topol. winding number

$$\Omega_2 = \frac{1}{2\pi} \int_{\mathrm{BZ}} \boldsymbol{n}(\boldsymbol{k}) \cdot \Big(\partial_{k_1} \boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_2} \boldsymbol{n}(\boldsymbol{k})\Big) \, \mathrm{d}\boldsymbol{k}$$

where $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{N}(\boldsymbol{k})/|\boldsymbol{N}(\boldsymbol{k})|$ and

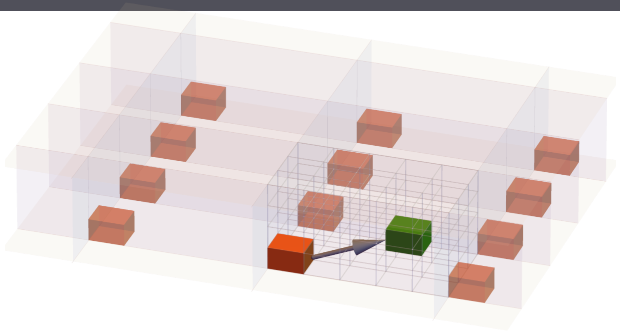


$$\boldsymbol{N}(\boldsymbol{k}) = 2\pi \ \mathrm{Re}\left[\left(Z^{(0,1)}_{\mathbb{Z}^2,\beta+1}\Big(\frac{\boldsymbol{k}}{2\pi}\Big), Z^{(1,0)}_{\mathbb{Z}^2,\beta+1}\Big(\frac{\boldsymbol{k}}{2\pi}\Big), -\Big(Z_{\mathbb{Z}^2,\beta}\Big(\frac{\boldsymbol{k}}{2\pi}\Big) + 2\mu - 4\Big)/2\pi\right)\right].$$

Zeta expansion for long-range interactions 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

$$\boldsymbol{z} + \Omega \xrightarrow{\text{influence}} \boldsymbol{r} + \Omega\,.$$



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., arXiv:2509.26274 (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 oposed to points $\boldsymbol{z}$),
- and partial derivatives of positions ($\partial_{\boldsymbol{r}}^{\boldsymbol{\alpha}}$).

State of the art: **Trunaction** 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).

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 $\boldsymbol{r}$

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

made efficiently computable in **JB, Buchheit et al., arXiv:2509.26274 (2025)** .

Efficiently computable representation for far-field set zeta derivatives

Theorem (Crandall representation)

Let $L = A\mathbb{Z}^n \times \{0\}^{d-n}$, $A \in \mathbb{R}^{n\times n}$ regular, $n \in \mathbb{N}_+$ with $n \le d$, and $\boldsymbol{\alpha} \in \mathbb{N}^d$. For $\boldsymbol{r} \in \mathbb{R}^d$, choose a finite near-field lattice $L_{\mathrm{near}} \subset L$ and set $L_{\mathrm{far}} = L \setminus L_{\mathrm{near}}$. For $\mathrm{Re}(\nu) > n$, we have

$$Z^{(\boldsymbol{\alpha})}_{L_{\mathrm{far}},\nu}(\boldsymbol{r}) = \frac{\pi^{\nu/2}}{\Gamma(\nu/2)}\Bigg[\sum_{\boldsymbol{z}\in L_{\mathrm{far}}} G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}-\boldsymbol{r}) - \sum_{\boldsymbol{z}\in L_{\mathrm{near}}} g^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}-\boldsymbol{r})$$
$$+ \frac{1}{|\det(A)|}\sum_{\boldsymbol{k}\in\Lambda^*}(2\pi i\boldsymbol{k})^{(\alpha_1,\dots,\alpha_n)} e^{2\pi i\boldsymbol{k}\cdot(r_1,\dots,r_n)} G^{(\alpha_{n+1},\dots,\alpha_d)}_{n-\nu}(\boldsymbol{k},(r_{n+1},\dots,r_d))\Bigg].$$

- *Upper Crandall function:* $G_\nu(\boldsymbol{z}) = \Gamma(\nu/2,\pi\boldsymbol{z}^2)/(\pi\boldsymbol{z}^2)^{\nu/2}$.
- *Lower Crandall function:* $g_\nu(\boldsymbol{z}) = \gamma(\nu/2,\pi\boldsymbol{z}^2)/(\pi\boldsymbol{z}^2)^{\nu/2}$.
- ***Incomplete Bessel** function:* $G_\nu(\boldsymbol{k},\boldsymbol{r}) = 2\int_0^1 t^{-\nu-1} e^{-\pi\boldsymbol{k}^2/t^2} e^{-\pi\boldsymbol{r}^2 t^2}\,\mathrm{d}t$.

Here, $\Gamma(\cdot,\cdot)$, $\gamma(\cdot,\cdot)$ upper/lower incomplete Gamma function and $|G_\nu(\boldsymbol{k},\boldsymbol{r})| \le |G_\nu(\boldsymbol{r})|$.

Efficiently computable representation for far-field set zeta derivatives

Theorem (Crandall representation)

Let $L = A\mathbb{Z}^n \times \{0\}^{d-n}$, $n \in \mathbb{N}_+$ *with* $n \le d$, *and* $\boldsymbol{\alpha} \in \mathbb{N}^d$. *For* $\boldsymbol{r} \in \mathbb{R}^d$, *choose a finite near-field lattice* $L_{\mathrm{near}} \subset L$ *and set* $L_{\mathrm{far}} = L \setminus L_{\mathrm{near}}$. *For* $\mathrm{Re}(\nu) > n$, *we have*

$$Z^{(\boldsymbol{\alpha})}_{L_{\mathrm{far}},\nu}(\boldsymbol{r}) = \frac{\pi^{\nu/2}}{\Gamma(\nu/2)}\Bigg[\sum_{\boldsymbol{z}\in L_{\mathrm{far}}} G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}-\boldsymbol{r}) - \sum_{\boldsymbol{z}\in L_{\mathrm{near}}} g^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}-\boldsymbol{r})\,.$$

$$+ \frac{1}{|\det(A)|}\sum_{\boldsymbol{k}\in\Lambda^*} (2\pi i\boldsymbol{k})^{(\alpha_1,\ldots,\alpha_n)} e^{2\pi i\boldsymbol{k}\cdot(r_1,\ldots,r_n)}\, G^{(\alpha_{n+1},\ldots,\alpha_d)}_{n-\nu}(\boldsymbol{k},(r_{n+1},\ldots,r_d))\Bigg]\,.$$

- *Upper Crandall derivatives:* $G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}) = \sum_{|\boldsymbol{\beta}|\le|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r})\, G_{\nu+2|\boldsymbol{\alpha}|-2|\boldsymbol{\beta}|}(\boldsymbol{r})\,.$
- *Lower Crandall derivatives:* $g^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{z}) = \sum_{|\boldsymbol{\beta}|\le|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r})\, g_{\nu+2|\boldsymbol{\alpha}|-2|\boldsymbol{\beta}|}(\boldsymbol{r})\,.$
- ***Incomplete Bessel** derivatives:* $G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{k},\boldsymbol{r}) = \sum_{|\boldsymbol{\beta}|\le|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r})\, G_{\nu-2|\boldsymbol{\alpha}|+2|\boldsymbol{\beta}|}(\boldsymbol{k},\boldsymbol{r})\,.$

Here, $p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r}) = (-\pi)^{\boldsymbol{\alpha}-\boldsymbol{\beta}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\frac{(\boldsymbol{\alpha}-\boldsymbol{\beta})!}{(\boldsymbol{\alpha}-2\boldsymbol{\beta})!}(2\boldsymbol{r})^{\boldsymbol{\alpha}-2\boldsymbol{\beta}}\,.$

JB, Buchheit et al., arXiv:2509.26274 (2025)

Benchmarks

Geometry:

- $\Omega = \prod_{i=1}^{3}[-\frac{c_i}{2}, \frac{c_i}{2}]$,
- $L = \mathbb{Z}^2 \times \{0\}$.

Maximum error over a grid of values:

- $\boldsymbol{r} = (1/4, 1/4, r)$, $r = 0.1, 0.2, \dots, 0.5$,
- $\nu = 10, 10.1, \dots, 14$.

derivatives $\boldsymbol{m}$	cuboid geometry $\boldsymbol{c}$	$\max_{\boldsymbol{r},\nu} E_{\mathrm{rel}}$
$(1,1,0)$	$(1,1,1)/50$	$2.16 \cdot 10^{-16}$
	$(1,1,1)/100$	$2.12 \cdot 10^{-16}$
	$(1,2,3)/100$	$2.20 \cdot 10^{-16}$
$(1,0,1)$	$(1,1,1)/50$	$2.18 \cdot 10^{-16}$
	$(1,1,1)/100$	$2.11 \cdot 10^{-16}$
	$(1,2,3)/100$	$2.16 \cdot 10^{-16}$
$(0,0,2)$	$(1,1,1)/50$	$3.87 \cdot 10^{-16}$
	$(1,1,1)/100$	$2.14 \cdot 10^{-16}$
	$(1,2,3)/100$	$2.19 \cdot 10^{-16}$

Full precision (error $< 4 \cdot 10^{-16}$) over the entire parameter range

at the same **runtime** as low-precision **truncation** schemes.

Demagnetization factor for a 2D Film in 3D

Setting:

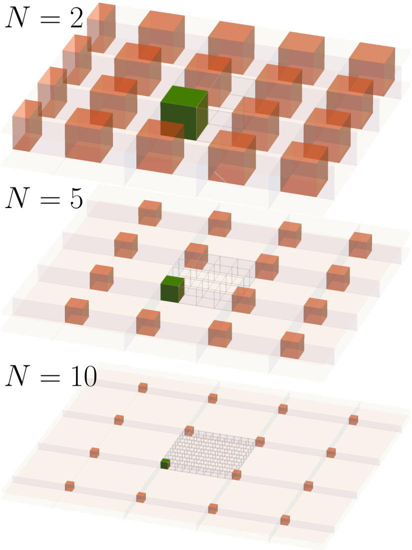
- Cuboids $\Omega = \left(\frac{1}{2}[-\frac{1}{N}, \frac{1}{N}]\right)^3$.
- Number of cuboids per dim. $N \in \mathbb{N}$
- Embedded lattice $L = \mathbb{Z}^2 \times \{0\}$,

$$\color{red}{z + \Omega} \; \xrightarrow{\text{influence}} \; \color{green}{\Omega} \, .$$
$$(z \in L)$$

Zeta expansion for **demagnetization factor** in z-direction:

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

$$D_z^{\mathrm{asym}} = \frac{1}{3} + \frac{Z_{\mathbb{Z}^2,3}(0)}{4\pi}\,\frac{1}{N^3} + \alpha\,\frac{1}{N^7} \, .$$

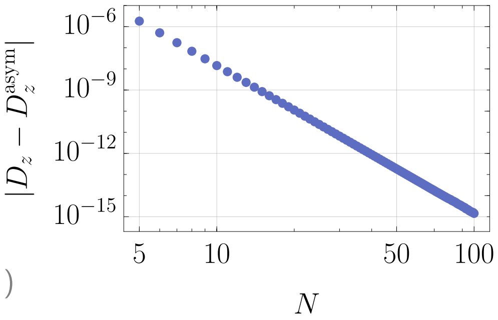


Zeta expansion for **demagnetization factor** in z-direction

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

$$D_z^{\mathrm{asym}} = \frac{1}{3} + \frac{Z_{\mathbb{Z}^2,3}(0)}{4\pi}\,\frac{1}{N^3} + \alpha\,\frac{1}{N^7}$$

$(\ \alpha \approx 0.1441459732\ )$



enabling its **exact computation**

- beyond asymptotic expansions,
- establishing **new ground truth** to test new methods against.

Conclusions

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

- Epstein zeta functions

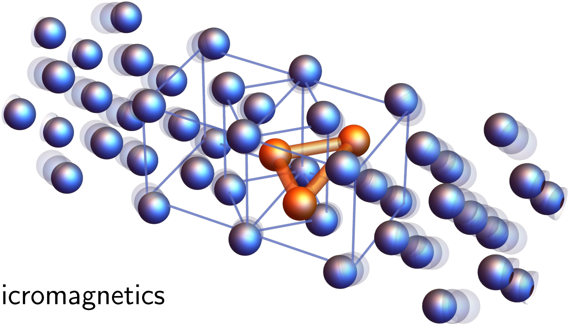
  JB, Buchheit et al., arXiv:2412.16317 (2024) ,

- many-body zeta functions

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

- generalized high-order zeta derivatives

  JB, Buchheit, (soon on arXiv) .



Application of **zeta methods** in:

- Computation of generalized potentials in Micromagnetics

  JB, Buchheit et al., arXiv:2509.26274 (2025) .

- Investigations into the stability of matter in theoretical chemistry

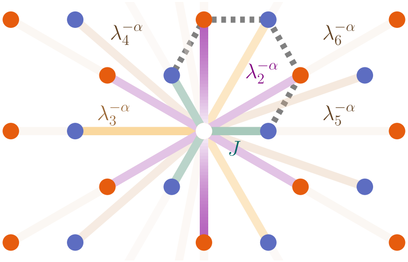
  Robles-Navarro, **JB**, et al., *J. Chem. Phys.* **163**, 094104 (2025) .

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

Outlook

Next steps:

- **Generalizations** of **set zeta derivatives** in condensed matter and theoretical chemistry.
- Inclusion of set zeta derivatives for generalized geometries in **EpsteinLib**.
- Investigations into long-range interacting quantum systems through **graph zeta** functions.



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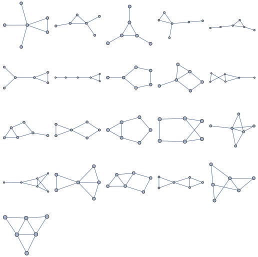

Thank You for Your Attention!

Epstein Zeta Function and Set Zeta Derivatives

Epstein zeta function

$$Z_{\Lambda,\nu}\begin{vmatrix} \boldsymbol{r} \\ 0 \end{vmatrix} = \sum_{\boldsymbol{z}\in\Lambda}{}^{'} |\boldsymbol{z}-\boldsymbol{r}|^{-\nu}, \qquad \Lambda = A\mathbb{Z}^n$$

- Λ: n-dimensional lattice in n-dimensional system ✓
- no derivatives ✓

Set zeta derivatives

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

- L_{far}: n-dimensional lattice in d-dimensional space
- $\nabla^{\boldsymbol{\alpha}}_{\boldsymbol{r}}$: Partial derivatives of positions

Danymical quantum phase transitions

Rate function

$$\lambda(t) = -\frac{4}{\pi}\int_{\mathrm{BZ}} \log(|\mathcal{G}_{(k_1,k_2)}(t)|)\,\mathrm{d}k_1\mathrm{d}k_2, \qquad \mathcal{G}_{\boldsymbol{k}}(t) \text{ Loschmidt echo}$$