

# Zeta Expansion for Long-Range Interactions under Periodic Boundary Conditions with Applications to Micromagnetics

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Joint work with Andreas A. Buchheit

Preprint: [arXiv:2509.26274](https://arxiv.org/abs/2509.26274)

Python: `pip install epsteinlib`

GitHub: [github.com/epsteinlib](https://github.com/epsteinlib)

October 2 2025

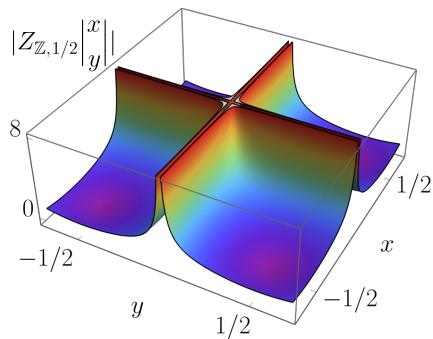


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# Epstein Zeta Function

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  $\nu \in \mathbb{C}$

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



- ▶ Private notes: Hurwitz<sup>a</sup>
- ▶ Foundational work: Epstein<sup>b</sup>
- ▶ 2D Bessel representation: Chowla–Selberg<sup>c</sup>
- ▶ ND Bessel representation: Elizalde<sup>d</sup>
- ▶ Incomplete Gamma representation: Crandall<sup>e</sup>

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<sup>a</sup>Oswald et al. (2016), *From Arithmetic to Zeta-Functions: ...*

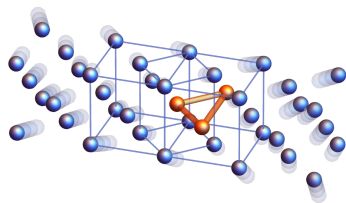
<sup>b</sup>Epstein (1903), *Math. Ann.* Epstein (1906), *Math. Ann.*

<sup>c</sup>Chowla et al. (1949), *Proceedings of the National Academy of Sciences*

<sup>d</sup>Elizalde (1998), *Communications in mathematical physics*

<sup>e</sup>Crandall (2012)

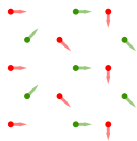
# Broad Applicability in Long-Range Interacting Lattices



## Theoretical Chemistry: Cohesive energy for Lennard-Jones

Robles-Navarro, Busse, et al. (2025), *The Journal of Chemical Physics*

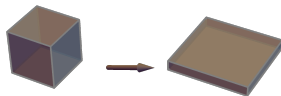
$$E_{\text{LJ}}(\mathbf{r}) \propto \frac{1}{n} |\mathbf{r}|^{-n} - \frac{1}{m} |\mathbf{r}|^{-m}$$



## High Energy Physics: Casimir Energy

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

$$E_{\text{cas}} = \frac{1}{2} \sum_{\mathbf{k}} \lambda_{\mathbf{k}}^{-\nu} \Big|_{\nu=-1}$$

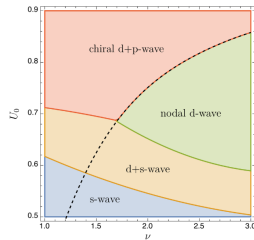


## Spin Systems:

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

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

arXiv:2509.26274

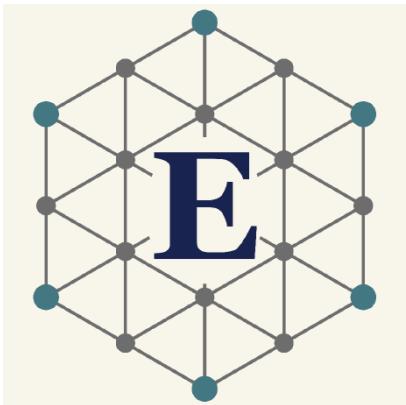


## Superconductivity: Long range gap equation

Buchheit et al. (2023), *Phys. Rev. Res.*

$$\Delta(\mathbf{k}) = \int_{\text{BZ}} V_{\text{LR}}(\mathbf{k} - \mathbf{q}) \frac{\Delta(\mathbf{q})}{2E_{\Delta}(\mathbf{q})} d\mathbf{q}$$

`pip install epsteinlib`



Evaluation of Epstein zeta function for

- ▶ every exponent  $\nu$ ,
- ▶ every lattice  $\Lambda$ ,
- ▶ every shift vector  $\mathbf{x}$ ,
- ▶ every wavevector  $\mathbf{y}$ .

In use by community:<sup>abcd</sup>

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<sup>a</sup> Koziol et al. (2025), *Physical Review B*

<sup>b</sup> Kim et al. (2025), *Physical Review Letters*

<sup>c</sup> Dall'Agata et al. (2025) arXiv:2507.02339

<sup>d</sup> Yadav et al. (2025) arXiv:2405.12405

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

C

# Precision and Runtime

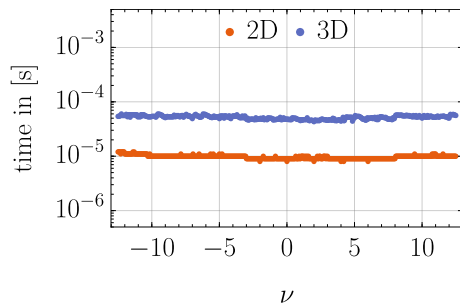
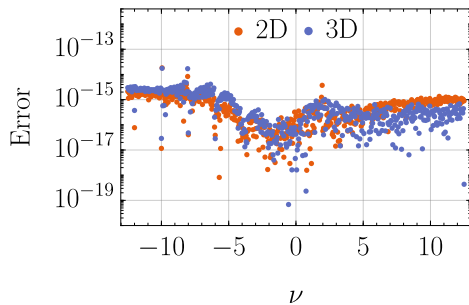
```
pip install epsteinlib
```

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



# 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  $\mathbf{y} \in \Lambda^* = A^{-T}\mathbb{Z}^d$ )

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

with **upper Crandall function**

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

( incomplete Gamma function  $\Gamma(\cdot, \cdot)$  )

# Epstein Zeta as a New Standard Function

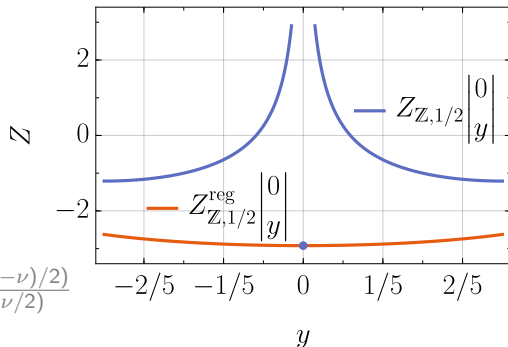
Epstein zeta efficiently computable ✓

Analytical properties derived in arxiv:2412.16317 ✓

- ▶ Symmetries.
- ▶ Functional Equation.
- ▶ Joint holomorphy all arguments.

Singularity structure ✓

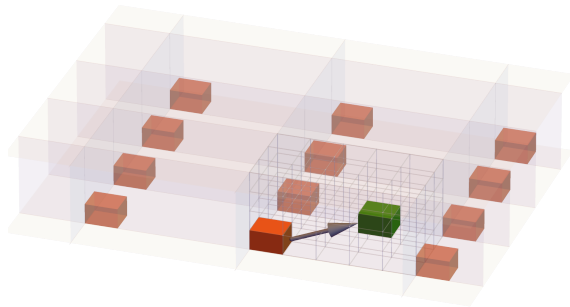
$$\underbrace{Z_{\Lambda,\nu}\left|\begin{smallmatrix} 0 \\ \mathbf{y} \end{smallmatrix}\right|}_{\text{singularity in } \mathbf{y}=0} = \underbrace{Z_{\Lambda,\nu}^{\text{reg}}\left|\begin{smallmatrix} 0 \\ \mathbf{y} \end{smallmatrix}\right|}_{\text{smooth in } \mathbf{y}\in\text{BZ}} + c_{\Lambda,\nu}|\mathbf{y}|^{\nu-d}$$
$$c_{\Lambda,\nu} = \frac{\pi^{\nu-d/2}}{|\det(A)|} \frac{\Gamma((d-\nu)/2)}{\Gamma(\nu/2)}$$



# Micromagnetics of a 2D Film in 3D

Consider Cuboids  $\Omega$  at positions  $\mathbf{z} \in L = A\mathbb{Z}^2 \times \{0\}$ ,  $A \in \mathbb{R}^{2 \times 2}$  regular and  $\mathbf{r} \in \mathbb{R}^d$ , where

$$\mathbf{z} + \Omega \xrightarrow{\text{influence}} \mathbf{r} + \Omega$$



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

Generalized potential ( multi-index notation  $\nabla_{\mathbf{r}}^{\mathbf{m}} = \partial_{r_1}^{m_1} \dots \partial_{r_d}^{m_d}$  )

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

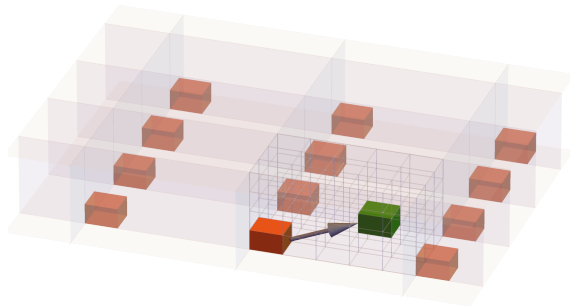
with interaction  $\nu > d$  and derivative order  $\mathbf{m} \in \mathbb{N}^d$ .



# Micromagnetics of a 2D Film in 3D

Consider Cuboids  $\Omega$  at positions  $\mathbf{z} \in L = A\mathbb{Z}^2 \times \{0\}$ ,  $A \in \mathbb{R}^{2 \times 2}$  regular and  $\mathbf{r} \in \mathbb{R}^d$ , where

$$\mathbf{z} + \Omega \xrightarrow{\text{influence}} \mathbf{r} + \Omega$$



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

Generalized potential zeta decomposition for  $L_{\text{near}} \subset L$

$$U^{(\mathbf{m})}(\mathbf{r}) \approx \sum_{\mathbf{z} \in L_{\text{near}}} S^{(\mathbf{m})}(\mathbf{r} + \mathbf{z})$$

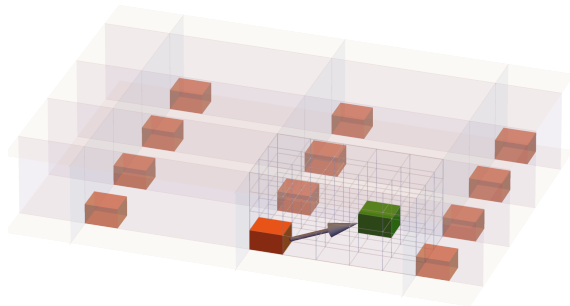
with interaction  $\nu > d$  and derivative order  $\mathbf{m} \in \mathbb{N}^d$

$$S^{(\mathbf{m})}(\mathbf{r}) = \int_{\Omega} \nabla_{\mathbf{r}}^{\mathbf{m}} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}'' .$$

# Micromagnetics of a 2D Film in 3D

Consider Cuboids  $\Omega$  at positions  $\mathbf{z} \in L = A\mathbb{Z}^2 \times \{0\}$ ,  $A \in \mathbb{R}^{2 \times 2}$  regular and  $\mathbf{r} \in \mathbb{R}^d$ , where

$$\mathbf{z} + \Omega \xrightarrow{\text{influence}} \mathbf{r} + \Omega$$



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

Generalized potential zeta decomposition for  $L_{\text{far}} = L \setminus \{L_{\text{near}}\}$

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

with interaction  $\nu > d$  and derivative order  $\mathbf{m} \in \mathbb{N}^d$

$$S^{(\mathbf{m})}(\mathbf{r}) = \int_{\Omega} \nabla_{\mathbf{r}}^{\mathbf{m}} \int_{\Omega + \mathbf{r}} |\mathbf{r}' - \mathbf{r}''|^{-\nu} d\mathbf{r}' d\mathbf{r}'' \quad Z_{L_{\text{far}}, \nu}(\mathbf{r}) = \sum'_{\mathbf{z} \in L_{\text{far}}} \frac{1}{|\mathbf{z} - \mathbf{r}|^{\nu}}.$$

# Epstein Zeta Function and Set Zeta Derivatives

## Epstein zeta function

$$Z_{\Lambda, \nu} \left| \begin{matrix} \mathbf{r} \\ 0 \end{matrix} \right| = \sum'_{\mathbf{z} \in \Lambda} |\mathbf{z} - \mathbf{r}|^{-\nu}, \quad \Lambda = A\mathbb{Z}^n$$

- ▶  $\Lambda$ :  $n$ -dimensional lattice in  $n$ -dimensional system ✓
- ▶ no derivatives ✓

# Epstein Zeta Function and Set Zeta Derivatives

## Epstein zeta function

$$Z_{\Lambda, \nu} \left| \begin{matrix} \mathbf{r} \\ 0 \end{matrix} \right| = \sum'_{\mathbf{z} \in \Lambda} |\mathbf{z} - \mathbf{r}|^{-\nu}, \quad \Lambda = A\mathbb{Z}^n$$

- ▶  $\Lambda$ :  $n$ -dimensional lattice in  $n$ -dimensional system ✓
- ▶ no derivatives ✓

## Set zeta derivatives

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

- ▶  $L_{\text{far}}$ :  $n$ -dimensional lattice in  $d$ -dimensional space
- ▶  $\nabla_{\mathbf{r}}^{\alpha}$ : Partial derivatives of positions

# Crandall Representation for 2D Film in 3D

## Theorem (Crandall representation)

Let  $\Lambda = A\mathbb{Z}^2$ ,  $A \in \mathbb{R}^{2 \times 2}$  regular,  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$ ,  $\nu \in \mathbb{C}$  and  $L_{\text{far}} = (\Lambda \times \{0\}) \setminus L_{\text{near}}$   
( $\nu \neq 3$  if  $\mathbf{y} \in \Lambda^* = A^{-T}\mathbb{Z}^3$ )

$$Z_{L_{\text{far}}, \nu}^{(\alpha)}(\mathbf{r}) = \frac{\pi^{\nu/2}}{\Gamma(\nu/2)} \left[ \sum_{\mathbf{z} \in L_{\text{far}}} G_{\nu}^{(\alpha)}(\mathbf{z} - \mathbf{r}) - \sum_{\mathbf{z} \in L_{\text{near}}} g_{\nu}^{(\alpha)}(\mathbf{z} - \mathbf{r}) \right. \\ \left. + \frac{1}{|\det(A)|} \sum_{\mathbf{k} \in \Lambda^*} (2\pi i \mathbf{k})^{(\alpha_1, \alpha_2)} e^{2\pi i \mathbf{k} \cdot (\mathbf{r}_1, \mathbf{r}_2)} G_{1-\nu}^{(\alpha_3)}(\mathbf{k}, \mathbf{r}_3) \right].$$

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

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

# Crandall Representation for 2D Film in 3D

## Theorem (Crandall representation)

Let  $\Lambda = A\mathbb{Z}^2$ ,  $A \in \mathbb{R}^{2 \times 2}$  regular,  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$ ,  $\nu \in \mathbb{C}$  and  $L_{\text{far}} = (\Lambda \times \{0\}) \setminus L_{\text{near}}$   
( $\nu \neq 3$  if  $\mathbf{y} \in \Lambda^* = A^{-T}\mathbb{Z}^3$ )

$$Z_{L_{\text{far}}, \nu}^{(\alpha)}(\mathbf{r}) = \frac{\pi^{\nu/2}}{\Gamma(\nu/2)} \left[ \sum_{\mathbf{z} \in L_{\text{far}}} G_{\nu}^{(\alpha)}(\mathbf{z} - \mathbf{r}) - \sum_{\mathbf{z} \in L_{\text{near}}} g_{\nu}^{(\alpha)}(\mathbf{z} - \mathbf{r}) \right. \\ \left. + \frac{1}{|\det(A)|} \sum_{\mathbf{k} \in \Lambda^*} (2\pi i \mathbf{k})^{(\alpha_1, \alpha_2)} e^{2\pi i \mathbf{k} \cdot (\mathbf{r}_1, \mathbf{r}_2)} G_{1-\nu}^{(\alpha_3)}(\mathbf{k}, \mathbf{r}_3) \right].$$

- ▶ Upper Crandall derivatives  $G_{\nu}^{(\alpha)}(\mathbf{z}) = \sum_{|\beta| \leq |\alpha|/2} p_{\alpha, \beta}(\mathbf{r}) G_{\nu+2|\alpha|-2|\beta|}(\mathbf{r}),$
- ▶ Lower Crandall derivatives  $g_{\nu}^{(\alpha)}(\mathbf{z}) = \sum_{|\beta| \leq |\alpha|/2} p_{\alpha, \beta}(\mathbf{r}) g_{\nu+2|\alpha|-2|\beta|}(\mathbf{r}),$
- ▶ Incomplete Bessel derivatives  $G_{\nu}^{(\alpha)}(\mathbf{k}, \mathbf{r}) = \sum_{|\beta| \leq |\alpha|/2} p_{\alpha, \beta}(\mathbf{r}) G_{\nu-2|\alpha|+2|\beta|}(\mathbf{k}, \mathbf{r}).$

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

# 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:

►  $\mathbf{r} = (1/4, 1/4, r)$ ,  $r = 0.1, 0.2, \dots, 0.5$

►  $\nu = 10, 10.1, \dots, 14$

derivatives $\mathbf{m}$	cuboid geometry $\mathbf{c}$	$\max_{\mathbf{r}, \nu} E_{\text{rel}}$
(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	$2.19 \cdot 10^{-16}$

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

## Demagnetization factor for a 2D Film in 3D

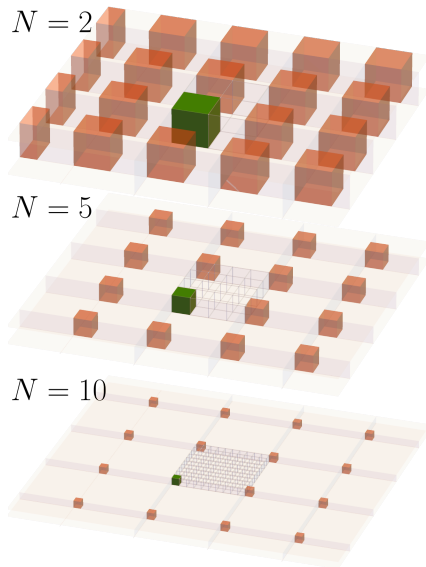
- ▶ Cuboids  $\Omega = (\frac{1}{2}[-\frac{1}{N}, \frac{1}{N}])^3$
- ▶ Nb. of Cuboids per dim.  $N \in \mathbb{N}$
- ▶ Embedded lattice  $L = \mathbb{Z}^2 \times \{0\}$

$$\begin{array}{ccc} \textcolor{red}{z} + \textcolor{red}{\Omega} & \xrightarrow{\text{influence}} & \textcolor{green}{\Omega} \\ (z \in L) & & \end{array}$$

Demagnetization factor in z-direction

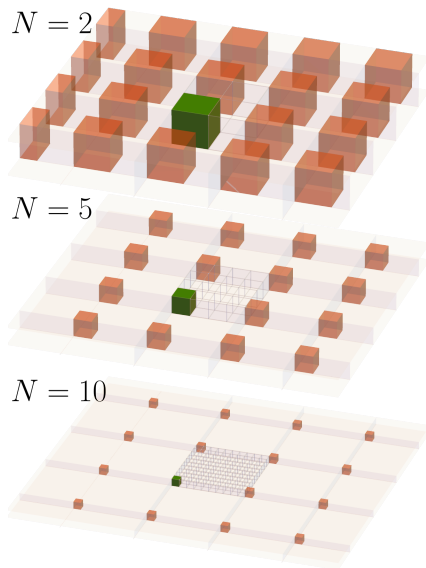
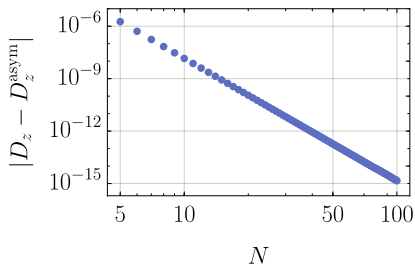
$$D_z = 1 + \frac{N^3}{4\pi} \left( U^{(2,0,0)}(0) + U^{(0,2,0)}(0) \right)$$

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





# Demagnetization factor for a 2D Film in 3D



Demagnetization factor in z-direction

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

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

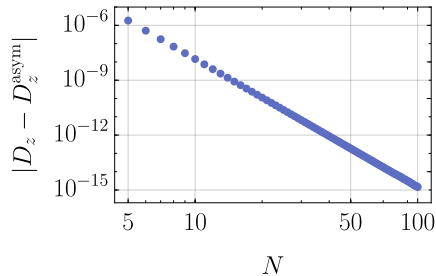
(  $\alpha \approx 0.1441459732$  )

# Conclusions

## Efficient computation of:

- ▶  $n$ -dimensional lattice sums in  $d$ -dimensional systems
- ▶ including any partial derivatives
- ▶ for any geometry
- ▶ beyond machine-precision

$N$	$D_z$
2	0.4222 0496 3454 0001 7334 0215 3861 9290
5	0.3390 8248 7690 9804 5966 0589 1398 9491
10	0.3340 5219 1717 7249 3459 0417 7785 8568
50	0.3333 3908 4315 3283 8944 2139 2339 3160
100	0.3333 3405 2206 1043 3571 9460 7573 5189

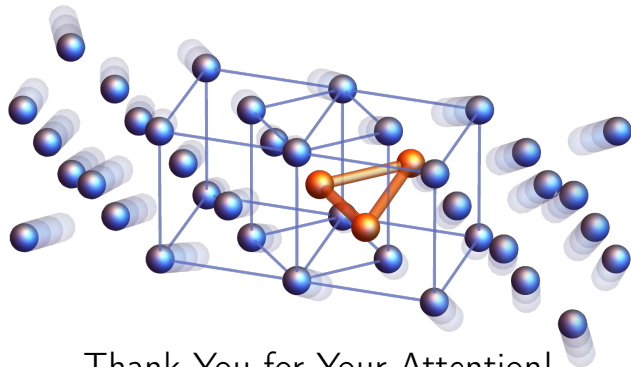


Reuse your code + apply correction

# Outlook

## Next steps:

- ▶ Rigorous discussion of set zeta derivatives
- ▶ Include set zeta derivatives in EpsteinLib
- ▶ Investigations into stability of matter

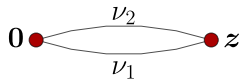


Thank You for Your Attention!

# Generalization to many-body lattice sums

## Two-body zeta function

$$Z_{\Lambda, \nu_1 + \nu_2} \left| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \right| = \sum'_{z \in \Lambda} \frac{1}{|z|^{\nu_1}} \frac{1}{|z|^{\nu_2}} = \zeta_{\Lambda}^{(2)}(\nu_1, \nu_2)$$

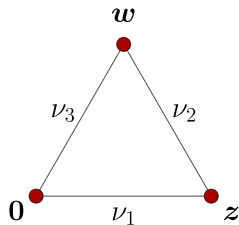


Buchheit et al. (2025)

## Three-body zeta function

$$\zeta_{\Lambda}^{(3)}(\nu_1, \nu_2, \nu_3) = \sum'_{\substack{z \in \Lambda \\ w \in \Lambda}} \frac{1}{|z|^{\nu_1}} \frac{1}{|w - z|^{\nu_2}} \frac{1}{|w|^{\nu_3}}$$

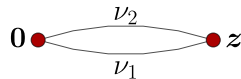
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# Generalization to many-body lattice sums

## Two-body zeta function

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



Buchheit et al. (2025)

## Three-body zeta function

$$\zeta_{\Lambda}^{(3)}(\nu_1, \nu_2, \nu_3) = \text{Vol}(\Lambda) \int_{\text{BZ}} Z_{\Lambda, \nu_1} \begin{vmatrix} 0 \\ \mathbf{y} \end{vmatrix} Z_{\Lambda, \nu_2} \begin{vmatrix} 0 \\ \mathbf{y} \end{vmatrix} Z_{\Lambda, \nu_3} \begin{vmatrix} 0 \\ \mathbf{y} \end{vmatrix} d\mathbf{y}$$

...

