Zeta expansion

for long-range interacting lattice systems

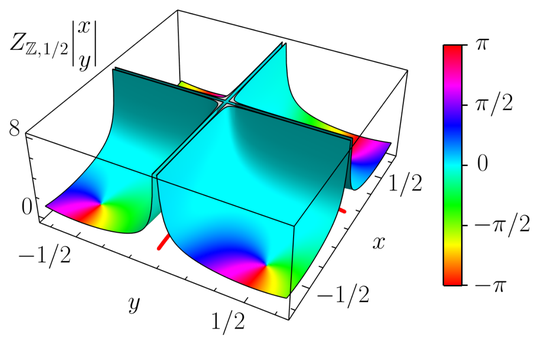
Jonathan K. Busse – joint work with Andreas A. Buchheit

jonathan@jbusse.de

Isotropic Lattice Sums: Epstein Zeta Function

Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ and let Λ be a lattice. The Epstein Zeta function is the holomorphic continuation of the following **lattice sum** to $\nu \in \mathbb{C} \setminus \{d\}$

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





Paul Epstein 1871–1939. Source: tinyurl.com/449ts2ed (Visited 08/28/2024)

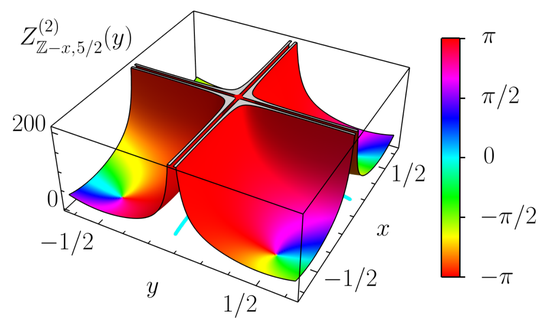
Applications:

- **Spin systems** [1].
- High-dimensional **many-body** interactions [3].
- Stability of matter in **theoretical chemistry** [4].
- **Casimir effect** in high-energy physics [1].

Anisotropic Lattice Sums: 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 to $\boldsymbol{y} \in \mathbb{R}^d$ as the meromorphic continuation of the following lattice sum to $\nu \in \mathbb{C}$

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



Multi-index notation:

$$|\boldsymbol{\alpha}| = \alpha_1 + \ldots + \alpha_d, \qquad \boldsymbol{z}^{\boldsymbol{\alpha}} = z_1^{\alpha_1} z_2^{\alpha_2} \ldots z_d^{\alpha_d}\,.$$

Applications:

- Taylor series stabilizes computations in **theoretical chemistry** [3, 4].
- Forces in **micromagnetics** [2].
- **Topological superconductors** (*ongoing*).

Application: Many-Body Lattice Sums [3, 4]

Total **cohesive energy**

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

- with two-body (n,m)-**Lennard-Jones** (LJ) potential, $n > m > 3$,

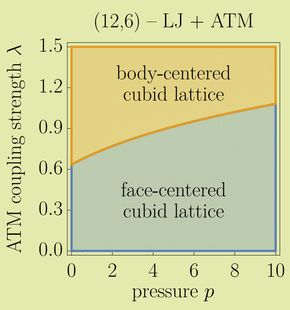
$$E^{(2)}_{\mathrm{LJ}}(\boldsymbol{r}) = \tfrac{nm}{n-m}\left(\tfrac{1}{n}|\boldsymbol{r}|^{-n} - \tfrac{1}{m}|\boldsymbol{r}|^{-m}\right),$$

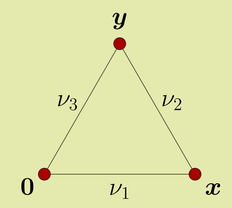
  ⇝ computable through **Epstein zeta** functions,
- and three-body **Axilrod–Teller–Muto** (ATM) potential,

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

  ⇝ computable through **three-body** zeta functions

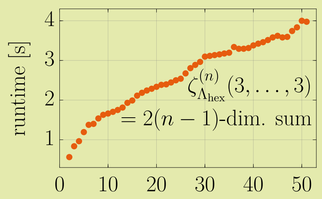
$$\zeta^{(3)}_{\Lambda}(\nu_1,\nu_2,\nu_3) = \sum_{\boldsymbol{x},\boldsymbol{y}\in\Lambda}{}' \frac{1}{|\boldsymbol{x}|^{\nu_1}}\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu_2}}\frac{1}{|\boldsymbol{y}|^{\nu_3}} = |\det(A)| \int_{\mathrm{BZ}} \prod_{i=1}^{3} Z_{\Lambda,\nu_i}\left|\begin{matrix}\boldsymbol{0}\\ \boldsymbol{k}\end{matrix}\right| \mathrm{d}\boldsymbol{k}\,.$$





Integral representation:

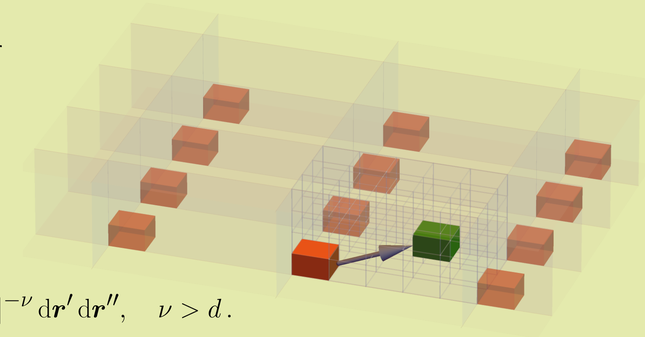
- Evaluation of $(n-1)d$-dimensional sums.
- **Exponential reduction in runtime**, now **linear** scaling in number of bodies.



Application: Forces in Micromagnetics [2]

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

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



Generalized potential with derivative order $\boldsymbol{m} \in \mathbb{N}_0^d$

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

Made efficiently computable through **set zeta derivatives** in [2].

Zeta Expansion for Micromagnetics

Split potential into near-field and far-field lattices

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

with **exponential** convergence in derivative order $|\boldsymbol{\alpha}|$. Here, $c_{\boldsymbol{\alpha}}$ depend on the geometry and

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

are the set zeta derivatives with respect to $\boldsymbol{r}$, efficiently computable through the Crandall representation.

Theorem: Crandall Representation

Let $L = A\mathbb{Z}^n \times \{0\}^{d-n}$, $n \in \mathbb{N}_+$ with $n \leq d$, and $\boldsymbol{\alpha} \in \mathbb{N}_0^d$. 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

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

with upper Crandall derivatives

$$G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{r}) = \textstyle\sum_{|\boldsymbol{\beta}|\leq|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r}) G_{\nu+2|\boldsymbol{\alpha}|-2|\boldsymbol{\beta}|}(\boldsymbol{r}), \qquad G_{\nu}(\boldsymbol{r}) = \Gamma(\nu/2, \pi\boldsymbol{r}^2)/(\pi\boldsymbol{r}^2)^{\nu/2}$$

where $\Gamma(\cdot,\cdot)$ the upper incomplete Gamma function; with lower Crandall derivatives

$$g^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{r}) = \textstyle\sum_{|\boldsymbol{\beta}|\leq|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r}) g_{\nu+2|\boldsymbol{\alpha}|-2|\boldsymbol{\beta}|}(\boldsymbol{r}), \qquad g_{\nu}(\boldsymbol{r}) = \gamma(\nu/2, \pi\boldsymbol{r}^2)/(\pi\boldsymbol{r}^2)^{\nu/2}$$

where $\gamma(\cdot,\cdot)$ the lower incomplete Gamma function; and with incomplete Bessel derivatives

$$G_{\nu}(\boldsymbol{k},\boldsymbol{r}) = 2\textstyle\int_0^1 t^{-\nu-1} e^{-\pi\boldsymbol{k}^2/t^2} e^{-\pi\boldsymbol{r}^2 t^2}\,\mathrm{d}t, \qquad G^{(\boldsymbol{\alpha})}_{\nu}(\boldsymbol{k},\boldsymbol{r}) = \textstyle\sum_{|\boldsymbol{\beta}|\leq|\boldsymbol{\alpha}|/2} p_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{r}) G_{\nu-2|\boldsymbol{\alpha}|+2|\boldsymbol{\beta}|}(\boldsymbol{k},\boldsymbol{r}).$$

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

EpsteinLib



High-Performance C library for

- every real exponent ν
- every lattice Λ
- every offset $\boldsymbol{x}$
- every wavevector $\boldsymbol{y}$

of the **(regularized) Epstein Zeta** function, including **high-order derivatives** in development branch.

With **Python**, **Julia**, and **Mathematica** wrappers.

Github: `https://github.com/epsteinlib/epsteinlib`

EpsteinLib: C Library

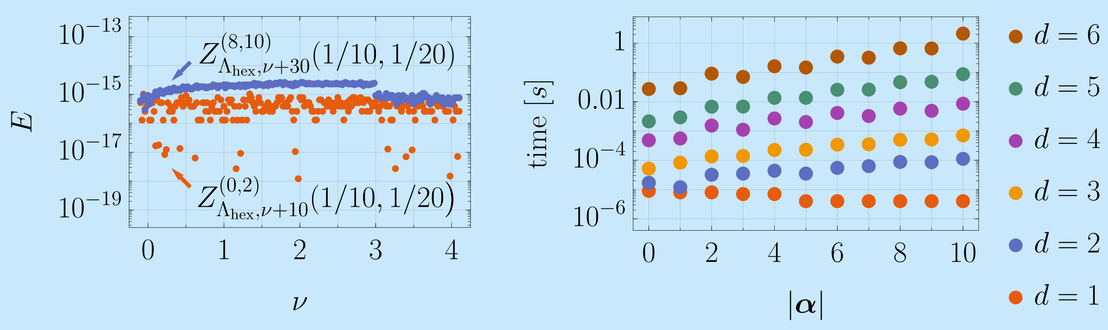
```c
double complex epsteinZeta(double nu, unsigned int dim, double *A, double *x, double *y)
double complex epsteinZetaReg(double nu, unsigned int dim, double *A, double *x, double *y)
double complex setZetaDer(double nu, unsigned int dim, double *A, double *x, double *y, unsigned int *alpha)
```
C

EpsteinLib: Python Wrapper

```
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

Benchmark: Eighteen 3D Derivatives at Machine Precision in Under One Millisecond



Benchmark: Full Precision at Runtime of Low-Precision Truncation Schemes

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:

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

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

References

[1] A. A. Buchheit, **J. K. Busse** et al. **Computation and Properties of the Epstein Zeta Function with High-Performance Implementation in EpsteinLib**. arXiv:2509.26274 (2025).

[2] A. A. Buchheit, **J. K. Busse** et al. **Zeta Expansion for Long-Range Interactions under Periodic Boundary Conditions with Applications to Micromagnetics**. *J. Comp. Phys.*, **114885**, DOI: 10.1016/j.jcp.2026.114885 (2026).

[3] A. A. Buchheit and **J. K. Busse** **Epstein Zeta Method for Many-Body Lattice Sums**. arXiv:2504.11989 (2025).

[4] A. Robles-Navarro, **J. K. Busse** et al. **Exact Lattice Summations for Lennard-Jones Potentials Coupled to a Three-Body Axilrod–Teller–Muto Term Applied to Cuboidal Phase Transitions**. *J. Chem. Phys.* **163**, 094104, DOI: 10.1063/5.0276677 (2025).

[5] A. A. Buchheit, **J. K. Busse** et al. **Epsteinlib**. URL: https://github.com/epsteinlib/ (2026).

Group Quantum Computing Applications
Department High-Performance Computing

DLR Institute of Software Technology

SAARLAND UNIVERSITY