Computation and Properties of the Epstein Zeta Function

with high-performance implementation in EpsteinLib

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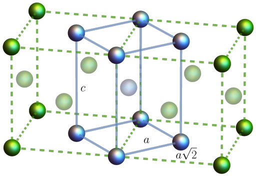
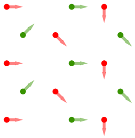
Joint work with Andreas A. Buchheit and Ruben Gutendorf

Python: `pip install epsteinlib`
GitHub: `github.com/epsteinlib`
Preprint: `arXiv:2412.16317`

20. March 2025

Broad Applicability in Long-Range Interacting Lattices





Spin Systems:[3]

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

Theoretical Chemistry:

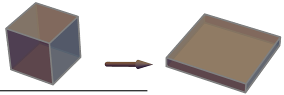
Cohesive energy for Lennard-Jones[1]

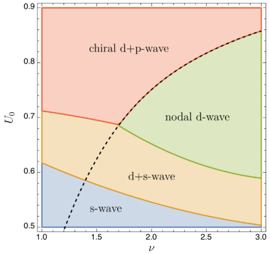
$$E_{\mathrm{LJ}}(\boldsymbol{r}) \propto \frac{1}{n}|\boldsymbol{r}|^{-n} - \frac{1}{m}|\boldsymbol{r}|^{-m}$$

High Energy Physics:

Casimir Energy[2]

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





Superconductivity:

Long range gap equation[4]

$$\Delta(\boldsymbol{k}) = \int_{\mathrm{BZ}} V_{\mathrm{LR}}(\boldsymbol{k}-\boldsymbol{q})\frac{\Delta(\boldsymbol{q})}{2E_{\Delta}(\boldsymbol{q})}\,\mathrm{d}\boldsymbol{q}$$

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[1] Buchheit et al., Computation and Properties of the Epstein Zeta Function (Dec. 2024)

[2] Schwerdtfeger et al., *Journal of Chemical Theory and Computation* **20**, 3379–3405 (May 2024)

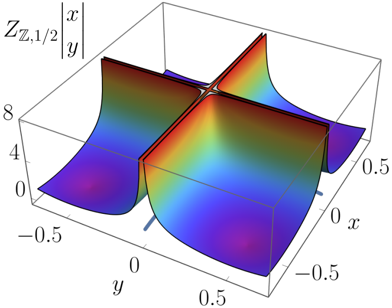
[3] Buchheit et al., *Phys. Rev. Res.* **5**, 043065 (Oct. 2023)

[4] Ambjørn et al., *Annals of Physics* **147**, 1–32 (Aug. 1983)

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 $\nu \in \mathbb{C}$

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



Numerous Applications:

- Spin systems[2]
- Theoretical chemistry[3]
- Unconventional superconductors[4]
- High energy physics: Casimir effect[5]

[5] Buchheit et al., Computation and Properties of the Epstein Zeta Function (Dec. 2024)

[6] Schwerdtfeger et al., *Journal of Chemical Theory and Computation* **20**, 3379–3405 (May 2024)

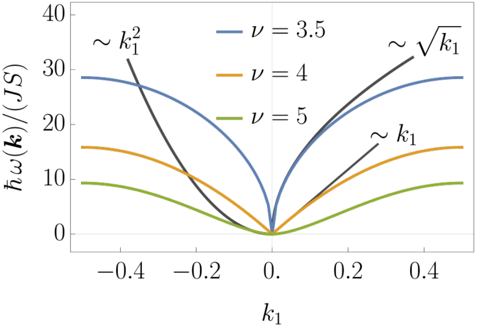
[7] Buchheit et al., *Phys. Rev. Res.* **5**, 043065 (Oct. 2023)

[8] Ambjørn et al., *Annals of Physics* **147**, 1–32 (Aug. 1983)

arXiv:2412.16317 pip install epsteinlib

Example: Anomalous Spin Wave Dispersion[5]

$$H = -c \sum_{\boldsymbol{x},\boldsymbol{y}\in\Lambda}{}' \frac{\boldsymbol{S_x}\cdot\boldsymbol{S_y}}{|\boldsymbol{x}-\boldsymbol{y}|^{\nu}}$$



+ Holstein-Primakoff Transformation
+ Fourier Transformation

$$\omega(\boldsymbol{k}) \sim Z_{\Lambda,\nu}\begin{vmatrix}0\\0\end{vmatrix} - Z_{\Lambda,\nu}\begin{vmatrix}0\\\boldsymbol{k}\end{vmatrix}$$

- $\mathrm{Re}(\nu) < \dim + 2$: Anomalous scaling $\omega(\boldsymbol{k}) \sim |\boldsymbol{k}|^{\nu-d}$
- $\mathrm{Re}(\nu) > \dim + 2$: typical scaling $\omega(\boldsymbol{k}) \sim \boldsymbol{k}^2$

[5] Buchheit et al., Computation and Properties of the Epstein Zeta Function (Dec. 2024)

EpsteinLib

Fast and precise evaluation of Epstein zeta function for

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

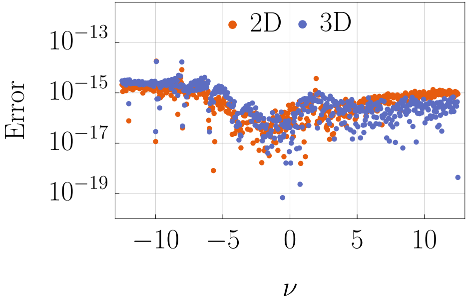
```c
double complex epsteinZeta(double nu, unsigned int dim, const double *A, const double *x, const double *y);
```

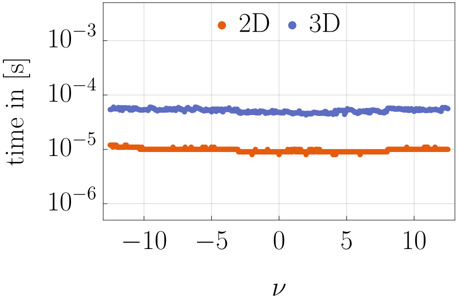
Precision and Runtime

```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))
```





- easy to use
- precise
- ultra fast

Crandall Representation

One algebraically decaying sum $\Rightarrow$ two superexponentially decaying sums

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

with $G_{\nu}(\boldsymbol{z}) \propto \frac{\exp(-\pi\boldsymbol{z}^2)}{(\pi\boldsymbol{z}^2)^{\nu/2}}$ superexponentially decaying.

Crandall + solving numerical challenges = EpsteinLib

[5] Crandall, Unified algorithms for polylogarithm, L-series, and zeta variants (2012)

Epstein Zeta as a new standard function

Now efficiently computable ✓

Analytical properties derived in arxiv:2412.16317 ✓

- Functional Equation.
- Analyticity in all arguments.

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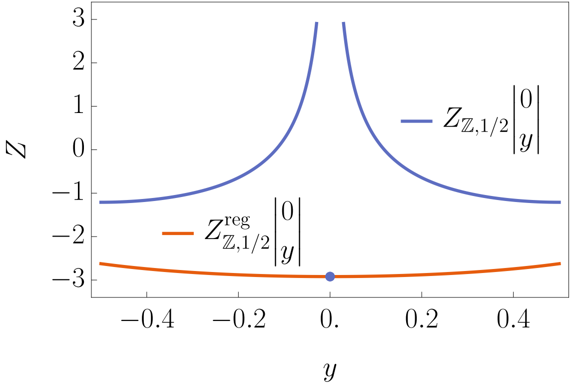
Physically relevant singularities

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



Conclusions

First high-performance library for Epstein zeta function.

- General: Any lattice, any interaction exponent, any shift, any wavevector.
- Fast and precise: exact 3D lattice sums in 10^{-4} seconds, on your laptop.
- Easy-to-use: pip install epsteinlib

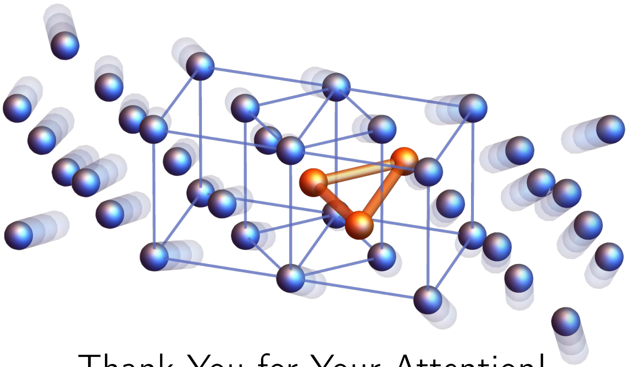
Actively used by the community:

- Long-range interacting hard-core bosons: SciPost Physics 17.4 (2024): 111,
- Long-range Dicke-Ising model: arXiv:2503.02734 (2025).

Outlook

Next steps:

- Multi-body interactions.
- Investigation into stability of matter in theoretical chemistry.



Thank You for Your Attention!

Unconventional Superconductors

Tight-binding Hamiltonian with power-law long-range interaction[6]

$$H = H_0 + H_{\mathrm{int}}$$
$$H_{\mathrm{int}} = \frac{1}{2}\sum_{\sigma,\sigma'} c^\dagger_{\sigma,\boldsymbol{x}} c^\dagger_{\sigma',\boldsymbol{x}-\boldsymbol{y}} V_{\sigma\sigma'}(\boldsymbol{y}) c_{\sigma',\boldsymbol{x}-\boldsymbol{y}} c_{\sigma,\boldsymbol{x}},$$

$$V_{\sigma\sigma'}(\boldsymbol{y}) = \begin{cases} -C_{\sigma\sigma'} \le 0 & \boldsymbol{y} = 0 \\ -\frac{U_{\sigma\sigma'}}{|\boldsymbol{y}|^\nu} \le 0 & \boldsymbol{y} \neq 0 \end{cases}$$

Fouriertransform:

$$H_{\mathrm{int}} = -\frac{V_\Lambda}{2}\sum_{\sigma,\sigma'} \int_{E^*}\int_{E^*} ⨍_{E^*} \left(C_{\sigma\sigma'} + U_{\sigma\sigma'} Z_{\Lambda,\nu}\begin{vmatrix} 0 \\ \boldsymbol{q} \end{vmatrix} \right),$$
$$\times c^\dagger_\sigma(\boldsymbol{k}+\boldsymbol{q}) c^\dagger_{\sigma'}(\boldsymbol{k}'-\boldsymbol{q}) c_{\sigma'}(\boldsymbol{k}') c_\sigma(\boldsymbol{k})\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{k}\,\mathrm{d}\boldsymbol{k}'$$

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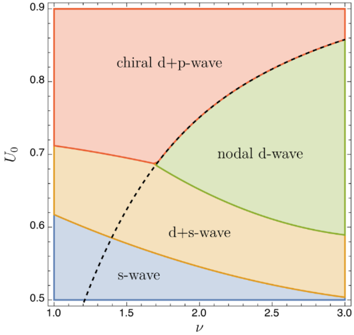
[6] Buchheit et al., *Phys. Rev. Res.* **5**, 043065 (Oct. 2023)

Gap Equation for Unconventional Superconductors

Gap Equation:

$$\Delta(\boldsymbol{k}) = c \int_{\mathrm{BZ}} \Bigg(C_0 + U_0 Z_{\Lambda,\nu} \left| \begin{matrix} 0 \\ \boldsymbol{k} - \boldsymbol{q} \end{matrix} \right| \Bigg) \\ \times \left(\frac{1}{2} \Delta E[\Delta]^{-1}\right)(\boldsymbol{k} - \boldsymbol{q}) \Bigg) \, \mathrm{d}\boldsymbol{q}$$

+ fast and efficient computation
+ regularization $\Rightarrow$



[6] Buchheit et al., *Phys. Rev. Res.* 5, 043065 (Oct. 2023)

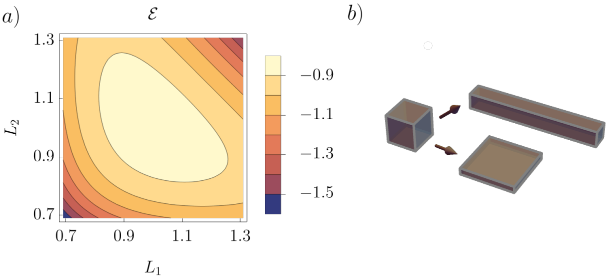
Casimir Effect

Consider Field modes of the klein gordon wave equation

$$\phi(t, \boldsymbol{x}) = e^{-i\lambda_{\boldsymbol{k}} t} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}, \qquad \lambda_{\boldsymbol{k}} = \sqrt{m^2 + \boldsymbol{k}^2}$$

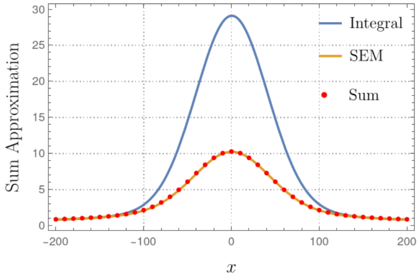
where $\boldsymbol{k} = 2\pi(z_1/L_1, \ldots, z_d/L_d)^T$ for $\boldsymbol{z} \in \mathbb{Z}^d$ and edge-lengths $0 < L_1, \ldots, L_d < \infty$. In the massless case $m = 0$ for $\Lambda^* = \mathrm{diag}(1/L_1, \ldots, 1/L_d)$, the total energy $\mathcal{E}$ is given by

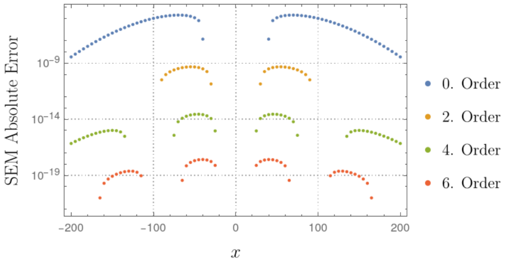
$$\mathcal{E}(\Lambda) = \frac{1}{2} \sum_{\boldsymbol{k}} \lambda_{\boldsymbol{k}}^{-\nu} \Big|_{\nu=-1} = \pi Z_{\Lambda^*,-1} \begin{vmatrix} 0 \\ 0 \end{vmatrix} .$$



Singular Euler-Maclaurin expansion (SEM) Example

$$\overbrace{\sum_{y=-\infty}^{\infty}{}' \frac{g(y)}{|y-x|^{\nu}}}^{\text{sum (exact)}} = \overbrace{\underbrace{\frac{1}{V_\Lambda}\int_{-\infty}^{\infty} \frac{g(y)}{|y-x|^{\nu}}\,\mathrm{d}y}_{\text{integral}} + \underbrace{\sum_{n=0}^{\text{order}} \frac{1}{n}\left(\frac{\partial_y}{-2\pi i}\right)^n Z^{\text{reg}}_{\mathbb{Z},\nu}\left|\begin{matrix}x\\y\end{matrix}\right| \partial_x^n g(x)}_{\text{lattice contribution}}}^{\text{SEM (exact for order } = \infty \text{)}}$$





[6] Buchheit et al., *Nonlinearity* **35**, 3706 (2022)

Computational Challenges

- Stable evaluation close to singularities
- Round-off error in the sum
- Choice of adequate cutoff
- Stable evaluation of incomplete gamma function for negative ν