Computation and Properties of the Epstein Zeta Function

with high-performance implementation in EpsteinLib

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Conference on Simulation of Quantum Matter 2024

github repo: `https://github.com/epsteinlib/epsteinlib`
python wrapper: `pip install epsteinlib`

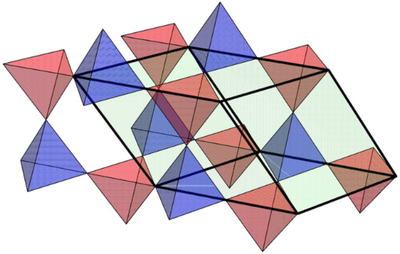
23. August 2024

UNIVERSITÄT DES SAARLANDES

Epstein Zeta Function

Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ and Λ 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:

- Long-range interacting lattices[1]
- Unconventional superconductors
- Spin systems
- High energy physics: Casimir effect

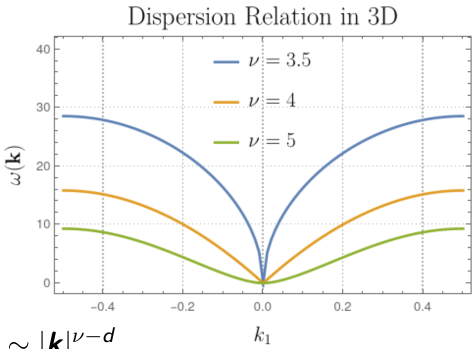
[1] Schwerdtfeger et al., *Journal of Chemical Theory and Computation* **20**, 3379–3405 (May 2024)

Anomalous Quantum Spin Wave Dispersion

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

+ 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 $\omega(\boldsymbol{k}) \sim \boldsymbol{k}^2$

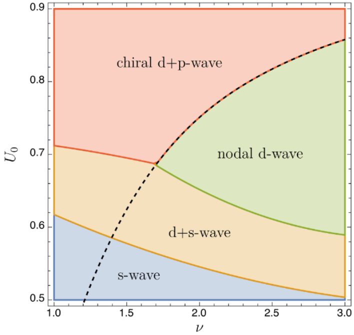
[0] Buchheit et al., *Phys. Rev. Res.* 5, 043065 (Oct. 2023)

Gap Equation for Unconventional Superconductors

Gap Equation:

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

+ fast and efficient computation
+ regularization $\Rightarrow$



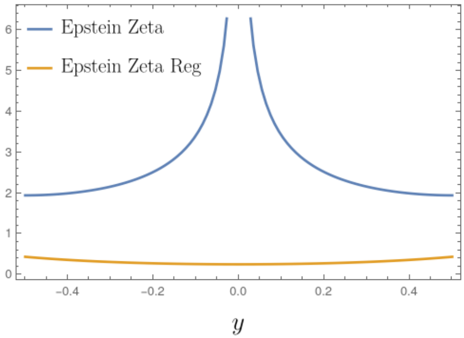
[0] Buchheit et al., *Phys. Rev. Res.* **5**, 043065 (Oct. 2023)

Properties of the (regularized) Epstein Zeta Function

$$Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| \qquad \text{singularity in } \boldsymbol{y} \in \Lambda^*$$

$$Z^{\mathrm{reg}}_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| = e^{2\pi i \boldsymbol{x}\cdot\boldsymbol{y}} Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| - c_\Lambda(\nu)|\boldsymbol{y}|^{\nu-d}$$

smooth in $\boldsymbol{y} \in \mathrm{BZ}$



EpsteinLib

Fast and precise evaluation of

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

of the (regularized) Epstein Zeta function.

```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);
```

https://github.com/epsteinlib/epsteinlib

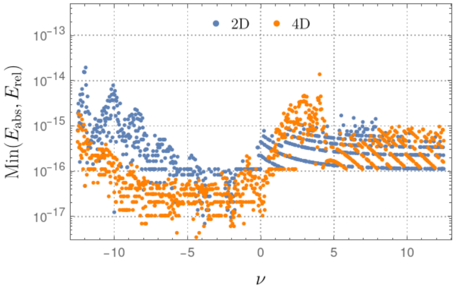
pip install epsteinlib

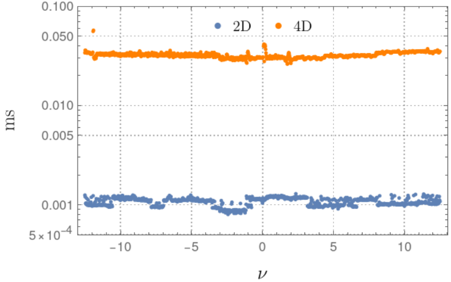
EpsteinLib Benchmark

```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's Representation

Mellin transformation + Riemann splitting + Poisson summation formula leads to

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

where $\lambda > 0$ and

$$G_\nu(\boldsymbol{z}) = \begin{cases} \frac{\Gamma(\nu/2,\pi\boldsymbol{z}^2)}{(\pi\boldsymbol{z}^2)^{\nu/2}}, & \boldsymbol{z}\neq 0,\\ -\frac{1}{\nu/2}, & \boldsymbol{z}=0.\end{cases}$$

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

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$G_\nu(\boldsymbol{z}) \sim \frac{\exp(-\pi\boldsymbol{z}^2)}{(\pi\boldsymbol{z}^2)^{\nu/2}} \Rightarrow$ Truncation

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

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

Round-off Error

- $G_\nu(\boldsymbol{z}) < 10^{-16}$ even for small $\boldsymbol{z}$
- Exponential growth of sphere points in the dimension

Problem: Naive summation neglects too many points!

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Problem: Naive summation neglects too many points!

Way out: More sophisticated routine $\Rightarrow$ compensated summation

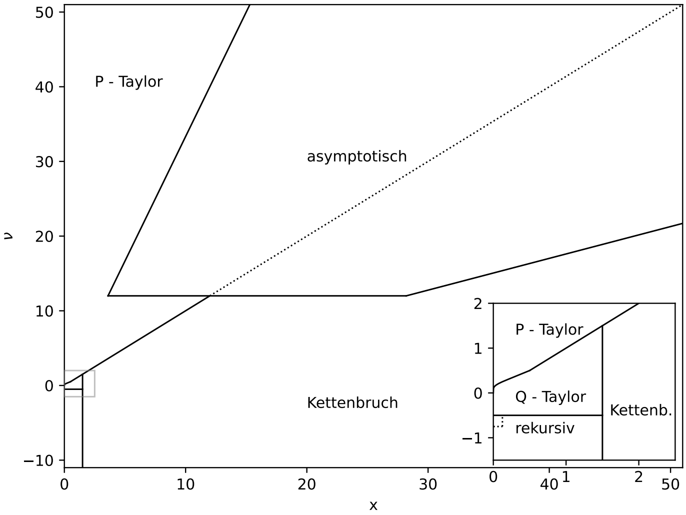
Cutoff

Compensated summation enables better truncation than $G_\nu < 10^{-15}$

Optimal a-priori choice of cutoff by combined numerical and analytical estimation:

- Analytical remainder estimate $\Rightarrow$ upper bound for cutoff
- Bound sum on spherical shells $\Rightarrow$ improved cutoff

Computation of Incomplete Gamma



Error $\leq 10^{-14}$ for $\nu \in (-10, 10)$

Conclusions and Outlook

Done:

- developed high-performance library
- precisely evaluate Epstein zeta for arbitrary real parameters
- discussed analytic properties for real parameters

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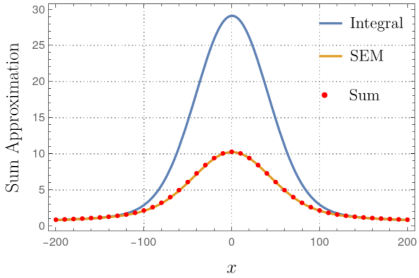
Open questions:

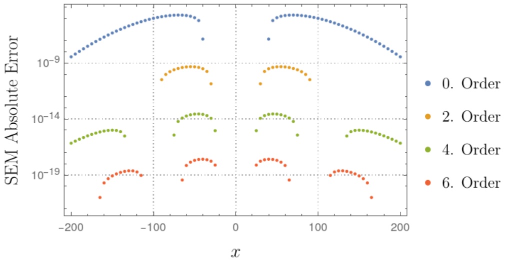
- How to evaluate Epstein zeta for complex arguments?
- How to compute the derivatives?

Danke für Ihre Aufmerksamkeit!

Singular Euler-Maclaurin expansion (SEM) Example

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





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

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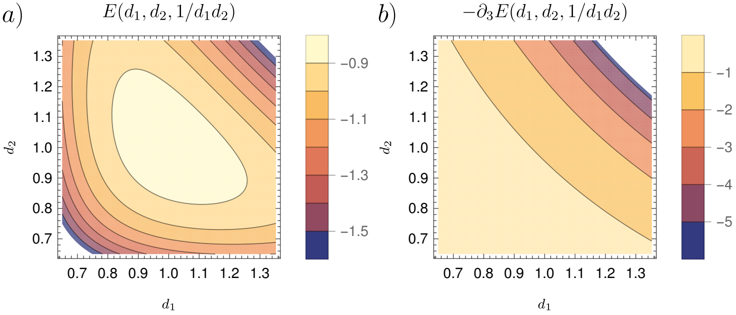
Casimir Effect

Total ground state energy of hypercoboidal region with $d_1, \ldots, d_p$ short sides and q long sides of length $L = L_1 = \ldots = L_q \gg d_1, \ldots, d_p$[1]

$$E(d_1, \ldots, d_p) = -\frac{1}{2} L^q V_\Lambda \pi^{-\frac{p+q+1}{2}} \Gamma\left(\frac{p+q+1}{2}\right) Z_{\Lambda,p+q+1} \begin{vmatrix} 0 \\ 0 \end{vmatrix}$$



[1] J. Ambjørn et al. "Properties of the Vacuum. I. Mechanical and Thermodynamic". In: *Annals of Physics* 147.1 (Aug. 1983), 1–32. ISSN: 00034916. DOI: 10.1016/0003-4916(83)90065-9. (Visited on 05/23/2024).

Unconventional Superconductors

Tight-binding Hamiltonian with power-law long-range interaction[2]

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

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

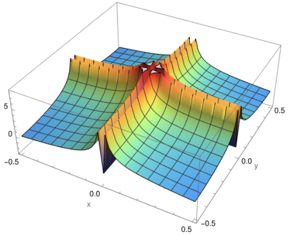
Fouriertransform:

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

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

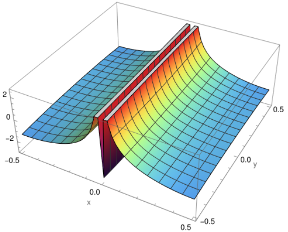
Properties of the (regularized) Epstein Zeta Function

Condition	Epstein Zeta
$\boldsymbol{x} \in \mathbb{R}^d$ and $\boldsymbol{y} \in \mathbb{R}^d$	meromorphic in $\nu \in \mathbb{C} \setminus \{d\}$
$\nu \in \mathbb{C}$ and $\boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda^*$	analytic in $\boldsymbol{x} \in \mathbb{R}^d \setminus \Lambda$
$\nu \in \mathbb{C}$ and $\boldsymbol{x} \in \mathbb{R}^d$	analytic in $\boldsymbol{y} \in \mathbb{R}^d \setminus \Lambda^*$



$$Z^{\mathrm{reg}}_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| = e^{2\pi i \boldsymbol{x}\cdot\boldsymbol{y}} Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| - \frac{\pi^{\nu-\frac{d}{2}}}{V_\Lambda}\frac{\Gamma((d-\nu)/2)}{\Gamma(\nu/2)}|\boldsymbol{y}|^{\nu-d},$$

smooth in $\boldsymbol{y} \in E^*$ if $\nu \in \mathbb{C} \setminus (d + 2\mathbb{N}_0)$

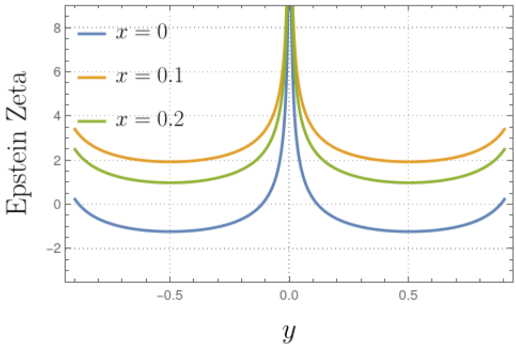


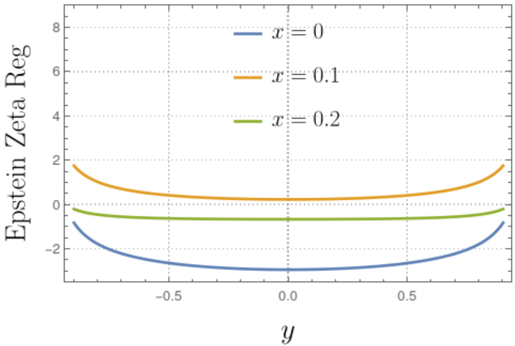
Properties of the (regularized) Epstein Zeta Function

$Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right|$ singularity in $\boldsymbol{y} \in \Lambda^*$

$$Z^{\mathrm{reg}}_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| = e^{2\pi i \boldsymbol{x}\cdot\boldsymbol{y}} Z_{\Lambda,\nu}\left|\begin{matrix}\boldsymbol{x}\\ \boldsymbol{y}\end{matrix}\right| - c_\Lambda(\nu)|\boldsymbol{y}|^{\nu-d}$$

smooth in $\boldsymbol{y} \in \mathrm{BZ}$





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