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cppdlr: Imaginary time calculations using the discrete Lehmann representation

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Summary

Imaginary time Green's functions encode the static and dynamical response of quantum systems at thermal equilibrium to external perturbations, such as applied electromagnetic fields. They therefore represent a direct point of connection between theoretical calculations and experimental measurements. As a consequence, they appear routinely in quantum many-body calculations at finite temperature, both for model systems like the Hubbard model (Hubbard, 1963), and in ab-initio electronic structure calculations beyond density functional theory, e.g., using Hedin's GW method (Golze et al., 2019; Hedin, 1965). Highly compact and accurate representations of imaginary time Green's functions and related imaginary time-dependent response functions are therefore an important ingredient in the development of robust and efficient codes for quantum many-body calculations. However, obtaining such representations has traditionally been challenging, particularly for low temperature calculations, in which the functions develop steep gradients.

In the past several years, significant progress has been achieved using low-rank approximations of the spectral Lehmann representation, which is given by

$$G(\tau) = -\int_{-\infty}^{\infty} d\omega \, \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} \, \rho(\omega).$$

Here, $G(\tau)$ is a fermionic single-particle imaginary time Green's function, and $\rho(\omega)$ is its corresponding spectral function, which encodes information about the single-particle excitations of the underlying quantum many-body system. The spectral function always exists, but is typically not known. However, the existence of this integral representation constrains the space of possible imaginary time Green's functions to lie within the image of the integral operator, which is numerically low-rank, enabling the construction of highly compact basis representations. The intermediate representation (IR) was introduced first, and used the singular value decomposition to obtain an orthogonal but non-explicit basis of imaginary time Green's functions (Chikano et al., 2018; Shinaoka et al., 2017). The recently-introduced discrete Lehmann representation (DLR) uses the interpolative decomposition to obtain a non-orthogonal basis consisting of known exponential functions (Kaye, Chen, & Parcollet, 2022). The number of basis functions required in both representations is similar, and typically significantly less than the previous state-of-the art methods based on orthogonal polynomials (Boehnke et al., 2011; Dong et al., 2020; Gull et al., 2018).

The DLR's use of an explicit basis of simple functions makes many common operations, including interpolation, integration, Fourier transform, and convolution, simple and highly efficient. This has led to a variety of recent algorithmic advances: compact Matsubara frequency meshes in dynamical mean-field theory calculations (Sheng et al., 2023), a stable method to

calculate the single-particle self-energy via the Dyson equation (LaBollita et al., 2023), an improved discretization of the mixing Green's function in the Keldysh formalism (Blommel et al., 2024; Kaye & Strand, 2023), a fast algorithm to evaluate imaginary time Feynman diagrams (Kaye, Huang, et al., 2023), and compact representations of three-point correlation functions (Kiese et al., 2024). It has also yielded immediate applications in computational physics, for example in low-temperature studies of superconductivity (Cai et al., 2022; Hou et al., 2024; Tanjaroon Ly et al., 2023). The DLR can be straightforwardly integrated into existing algorithms and codes, often yielding significant improvements in efficiency, accuracy, and algorithmic simplicity.

Statement of need

`cppdlr` is a C++ library which constructs the DLR and implements its standard operations. The flexible yet high-level interface of `cppdlr` makes it appealing for use both in small-scale applications and in existing large-scale software projects. The DLR has previously been implemented in other programming languages, specifically in Python via `pydlr`, in Fortran via `libdlr`, and in Julia via `Lehmann.jl` (Chen, 2021; Kaye, Chen, & Strand, 2022; Kaye & Strand, 2021; Strand & Kaye, 2021), as well as in the `sparse-ir` library implementing the IR (Wallerberger et al., 2023). `cppdlr` nevertheless provides a needed platform for future developments. First, `cppdlr` is written in C++, a common language used by many large projects in the quantum many-body physics community. Second, it offers a high-level user interface simpler than that of `libdlr`, enabled by the use of C++ templating and the `nda` library ("nda," n.d.) for array types and BLAS/LAPACK compatibility. These features have, for example, enabled the implementation of the DLR in the TRIQS library (Parcollet et al., 2015) for quantum many-body calculations.

`cppdlr` is distributed under the Apache License Version 2.0 through a public Git repository (Kaye, Strand, et al., 2023a). The project documentation (Kaye, Strand, et al., 2023b) is extensive, containing background on the DLR, a user guide describing example programs packaged with the library, and application interface (API) reference documentation for all classes and functions. We envision `cppdlr` as a platform for future algorithmic developments involving the DLR, and as a go-to tool for applications employing the DLR.

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