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AutoBZ.jl: Automatic, adaptive Brillouin zone integration using Wannier interpolation

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Summary

AutoBZ.jl is a modular Julia (Bezanson et al., 2017) package implementing efficient algorithms for Brillouin zone (BZ) integration, a fundamental step in electronic structure calculations of physical observables in crystals such as the density of states and the optical conductivity. These capabilities make AutoBZ.jl an extensible framework for computational research on material properties that can compute a broad range of quantities found in experimental spectra or high-throughput screenings using Wannier interpolation and BZ integration (Mostofi et al., 2008). Our BZ integration methods, described in Refs. (Kaye et al., 2023) and (Van Muñoz et al., 2024), are high-order accurate, automatically convergent to a user-specified error tolerance, and if needed, adaptive in momentum space. This allows the resolution of low-temperature properties of strongly interacting systems, using many-body methods such as dynamical mean-field theory (Georges et al., 1996), in which frequency-dependent electronic self-energies may produce scattering rates in the sub-meV regime. The corresponding low-temperature regions of phase diagrams are typically out of reach using traditional integration algorithms, which struggle to resolve localized features in momentum space. AutoBZ.jl can also be used to compute ground-state (i.e. $T = 0$ K) properties of tight-binding models, typically derived from localized Wannier functions, with a given artificial broadening. We expect it to become a widely used tool in the electronic structure community, providing accurate comparisons with experimental spectra, and a robust, automated approach for high-throughput screenings and machine learning of material properties.

Statement of need

Most open-source software packages used for density functional theory plus dynamical mean-field theory, including those compatible with Wannier90 (see, e.g., Refs. (Aichhorn et al., 2016; Romero et al., 2020; Shinaoka et al., 2021; Singh et al., 2021)), employ simple uniform grids for BZ integration, despite the fact that BZ integrands may be highly localized, e.g., near energy isosurfaces for the Green's function. However, these details of electronic structure may sensitively control downstream observables, so it is crucial that BZ integrals be computed in a resolved manner in material-realistic calculations. In practice, this requires using dense uniform integration grids, which become compute or memory-limited in low-temperature calculations involving scattering rates approaching the meV scale. Furthermore, validating uniform integration methods requires careful convergence testing which is not always prioritized, sometimes leading to under-resolved results with spurious features. The algorithms in AutoBZ.jl, which include an optimized uniform grid integration scheme for larger scattering rates, automate convergence testing to provide results to a user-specified error tolerance. For low-temperature calculations, our adaptive integration algorithm has only polylogarithmic

computational complexity with respect to the scattering rate, superior to the polynomial rates of alternative tree-based adaptive methods. These advancements will be crucial for the development of next-generation quantum impurity solvers and the accurate characterization of spectral features for low-temperature phenomena in condensed matter physics.

Design principles

AutoBZ.jl is developed in a modular, Julian fashion involving several components required for integration (Van Muñoz, 2023a) and interpolation (Van Muñoz, 2023c, 2023b) which may be of independent interest in other scientific computing applications. It also contains an extension to SymmetryReduceBZ.jl (Jorgensen et al., 2022) for optimizations involving the lattice symmetry group, including an implementation of a symmetric Monkhorst-Pack grid using the algorithm of Hart et al. (Hart et al., 2019). We use the CommonSolve.jl interface to promote interoperability with existing packages. For example, we provide a routine to compute the electron density that can easily be combined with NonlinearSolve.jl(Pal et al., 2024) to determine the chemical potential. AutoBZ.jl can be called from MATLAB and Python, and includes file-based interfaces to read Wannier90 output, such as Hamiltonian and position operator matrix elements, as well as frequency-dependent self-energy data determined either phenomenologically or using a quantum many-body framework. The modular design of AutoBZ.jl simplifies the addition of new algorithms and problem types, and its interoperatibility and well-documented API enables its use as a scripting tool for many research problems.

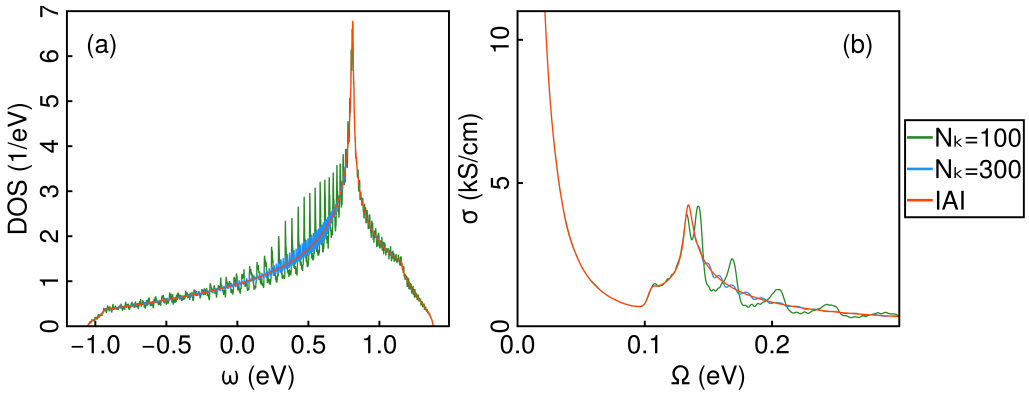

Figure 1: Calculations of various physical observables for a 3-band model of t_{2g} orbitals in the cubic perovskite $SrVO_3$ at a temperature of 24 K, using a Fermi liquid scaling for the scattering rate, which is 1 meV. Panel (a) shows the density of states (DOS) as a function of frequency and panel (b) shows the optical conductivity as a function of excitation frequency at a chemical potential of 12.5 eV. AutoBZ.jl was used to compute the observables at automatically-selected interpolation nodes determined by HChebinterp.jl, yielding a result which can be evaluated on the full domain. We compare the resolved results obtained using adaptive integration with the result of uniform grid integration with N_k momentum space points per dimension.

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