Adaptive Brillouin Zone Integration

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Introduction

In solid state physics, an common computational task when studying properties of crystalline materials is integration over the Brillouin Zone (BZ). This region of momentum space is the primitive unit cell of the crystal's reciprocal lattice, which due to Bloch theory is the only region of the momentum space that needs to be studied.

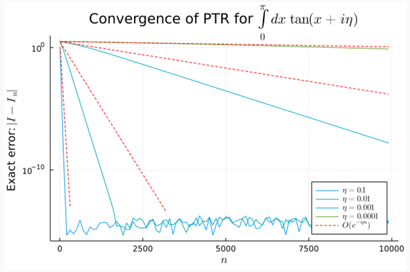
The goal of this internship has been to develop general-purpose numerical tools for efficient Brillouin zone integration, and will result in applications to optical conductivity calculations.

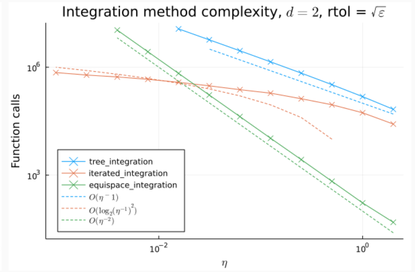
Adaptive integration

The workhorse integration tool for integration is the periodic trapezoidal rule (PTR), which is simply integration with sampling points on an equispace grid. For functions with singularities the convergence is exponential with a rate set by the distance to the nearest singularity in the complex plane.

Adaptive methods utilize higher-order quadrature rules, which for example can exactly integrate fixed-order polynomials. There are both 1D and multi-dimensional quadrature rules, which converge at different rates depending on the details of the problem. The outstanding feature in our integrands is a co-dimension 1 manifold of singularities in the Brillouin zone.

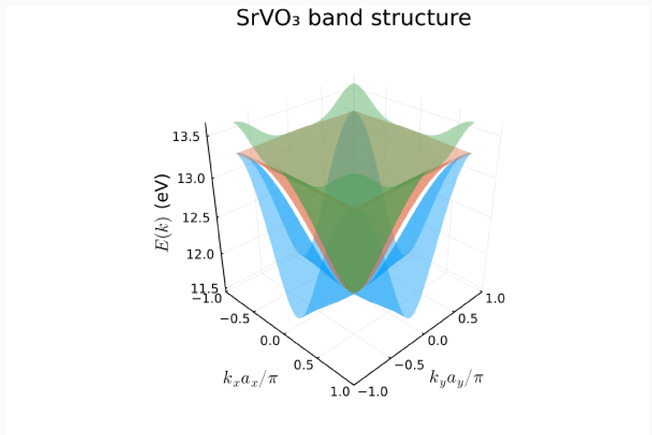
$$\iiint dxdydz\ f(x,y,z) = \int dx \left(\int dy \left(\int dz\ f(x,y,z) \right) \right)$$





Application: Strontium Vanadate

Strontium vanadate, $SrVO_3$, is a perovskite with potential applications to batteries. In our calculations, we obtain the $SrVO_3$ Hamiltonian, $H(\mathbf{k})$ projected onto the lowest energy Wannier orbitals through DFT methods, and then taking interactions into account also calculate the self-energy, $\Sigma(\omega)$, using DMFT methods. We interpolate the Hamiltonian using a Fourier series, whose 3 lowest eigenvalues are plotted below.

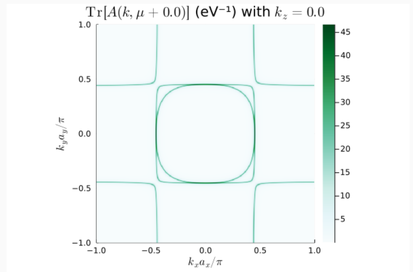


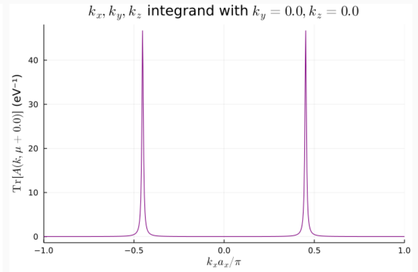
Density of states: structure of integrand

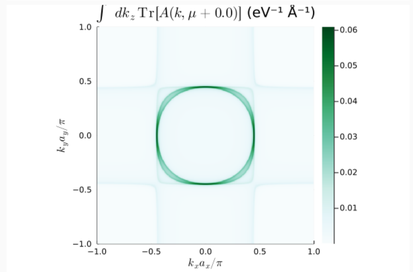
Many properties of a material are governed by its density of states (DOS), a relation between the energy of its electrons and the electronic states available at that energy. We define DOS in terms of $H(\mathbf{k})$, the Green's function, $G(\mathbf{k},\omega)$, and spectral function, $A(\mathbf{k},\omega)$, below:

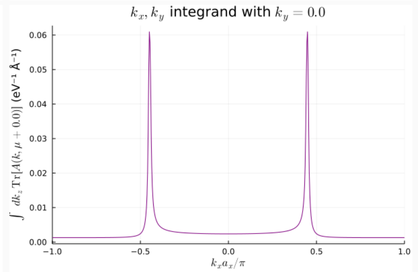
$$G(\mathbf{k},\omega) = ((\omega+\mu)I - H(\mathbf{k}) + \Sigma)^{-1}$$
$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}[G(\mathbf{k},\omega)]$$
$$\mathrm{DOS} = \int_{\mathrm{BZ}} d\mathbf{k}\ \ \mathrm{Tr}[A(\mathbf{k},\omega)]$$

The plots below illustrate the DOS for $SrVO_3$ at a value of $\Sigma = i\eta$ and $\eta = 0.0135$ eV corresponding to a Fermi liquid at $T = 50$ K, and at the Fermi energy $\mu = 12.3958$ eV.

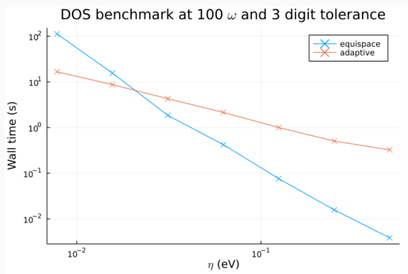


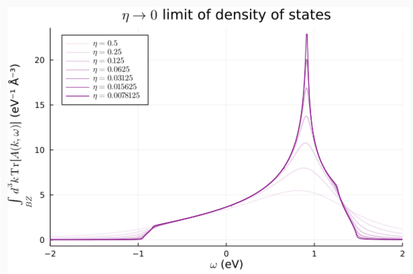






Density of states: calculations





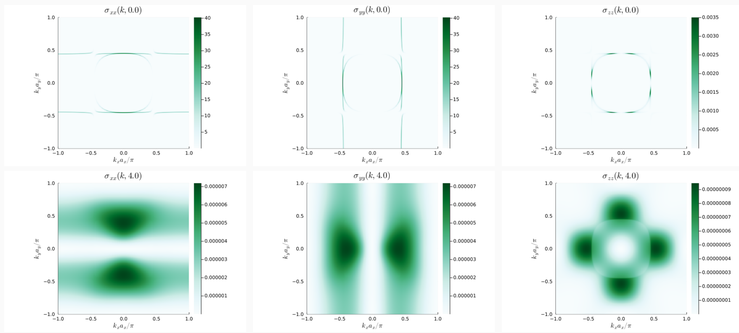
In practice, we have found that adaptive integration beats PTR for η below 1 – 10 meV.

Optical conductivity: structure of integrand

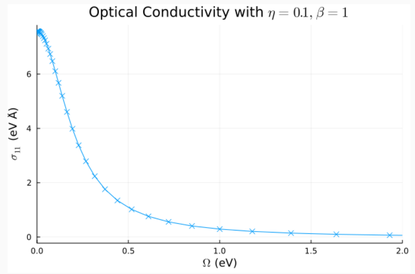
Optical conductivity (OC) describes the probability of an electronic transition given an incident photon of a determined frequency. OC, $\sigma_{\alpha\beta}(\Omega)$, is defined by $A(\mathbf{k},\omega)$, the band velocities $v^\alpha(\mathbf{k})$, and the transport function $\Gamma_{\alpha\beta}(\omega_1,\omega_2)$:[1]

$$\Gamma_{\alpha\beta}(\omega_1,\omega_2) = \int_{\mathrm{BZ}} d\mathbf{k}\ \ \mathrm{Tr}\left[v^\alpha(\mathbf{k})A(\mathbf{k},\omega_1)v^\beta(\mathbf{k})A(\mathbf{k},\omega_2)\right]$$
$$\sigma_{\alpha\beta}(\Omega) = -\left(\frac{e}{2\pi}\right)^2 \int_{-\infty}^{\infty} d\omega\ \frac{f(\omega+\Omega) - f(\omega)}{\beta\Omega}\,\Gamma_{\alpha\beta}(\omega,\omega+\Omega)$$

where $f(\omega) = (1+e^{\beta\omega})^{-1}$ is the Fermi distribution. The plots below show the structure of the integrand for $\Omega = 0$ and 4, and $T = 50$ K when the ω integral is taken first.



Optical conductivity: calculations



Adaptive integration helps efficiently resolve the features at small Ω and low temperature.

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References

[1] E. Assmann, P. Wissgott, J. KuneÅ¡, A. Toschi, P. Blaha, and K. Held, "Woptic: optical conductivity with wannier functions and adaptive k-mesh refinement", Computer Physics Communications **202**, 1–11 (2016).