Computing Spectral Properties of Topological Insulators with Disorder

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Abstract

We develop new numerical methods to compute spectral properties of tight-binding Hamiltonians for disordered and defective topological insulators, which characterize their remarkable electronic behavior. Our approach extends a recent framework that uses rational filters to probe the continuous spectrum of infinite-dimensional operators [Colbrook et al., SIAM Rev. 2021].

Keywords: topological insulators, tight-binding models, computational spectral theory

1 Introduction

Topological insulators (TIs) are renowned for their remarkable electronic properties. They exhibit quantised bulk Hall and edge conductances and support electronic transport along edges and interfaces, features that persist even when material defects and disorder are present. These physical characteristics can be understood and quantified through spectral properties of tight-binding Hamiltonian models.

Computing the relevant spectral properties of tight-binding models for disordered and defective TIs in a principled manner poses a significant challenge for two reasons:

1. Transport in the bulk and edge is mediated by a continuum of generalized (non-normalizable) eigenstates associated with bands of continuous spectrum. In general, the tight-binding Hamiltonian's spectrum may contain an exotic mix of continuous and discrete spectral types.

2. Periodic approximations and other artificial truncations of the computational domain may introduce spectral artifacts and, in general, fail to rigorously approximate continuous spectral properties of the Hamiltonian.

Here, we develop numerical methods that overcome both challenges by working within a framework recently proposed to compute discrete and continuous spectral properties of infinite-dimensional operators [1–4]. We compute spectra, approximate eigenstates, spectral measures, spectral projections, transport properties, and conductances of the tight-binding Hamiltonian. Numerical examples are given for the Haldane model, and the techniques extend easily to other TIs in two and three dimensions.

2 The resolvent framework

Let $\mathcal{A} : \mathcal{D}(\mathcal{A}) \to \mathcal{H}$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(\mathcal{L})$. $\mathcal{A}$ has the spectral decomposition

$$\mathcal{A} = \int_{\Lambda(\mathcal{A})} \lambda \, d\mathcal{E}(\lambda), \qquad (1)$$

where $\Lambda(\mathcal{A})$ is the spectrum of $\mathcal{A}$ and $\mathcal{E}$ is the *projection-valued spectral measure*. That is, for each measureable set $\Omega \subset \Lambda(\mathcal{A})$, the spectral projection onto Ω is given by $\mathcal{E}(\Omega) = \int_\Omega d\mathcal{E}(\lambda)$.

The resolvent framework for infinite-dimensional spectral computations uses samples of the resolvent operator,

$$\mathcal{R}(\mathcal{A}, z) = (\mathcal{A} - z\mathcal{I})^{-1} \qquad (2)$$

at points $z_1, \ldots, z_\ell \in \mathbb{C}$ in the complex plane to construct rigorous approximations to both discrete and continuous spectral properties of $\mathcal{A}$.

In practice, this means solving shifted linear equations of the form

$$(\mathcal{A} - z_k\mathcal{I})u_k = f, \qquad k = 1, \ldots, \ell. \qquad (3)$$

For certain spectral properties, one must also compute inner products in $\mathcal{H}$.

2.1 Spectrum and eigenstates

The spectrum $\Lambda(\mathcal{A})$ can be computed with error control [1] by using localization properties of the ϵ-*pseudospectrum*, i.e., the ϵ^{-1} level sets of

$$\|\mathcal{R}(\mathcal{A},z)\|_{\mathcal{H}} = \sup_{f\in\mathcal{H}} \sqrt{\langle \mathcal{R}(\mathcal{A},z)f, f\rangle_{\mathcal{H}}}$$

in the complex z-plane. A sequence of maximizing functions $f_k \in \mathcal{H}$ (e.g., generated by shifted power iterations with $\mathcal{A}$) provide approximating pseudo-eigenstates.

2.2 Spectral measures

We show how to construct spectrally smoothed approximations of the projection-valued spectral measure $\mathcal{E}([a,b])$ using analogs of Stone's theorem:

$$\frac{1}{2\pi \mathrm{i}} \lim_{\epsilon\to 0^+} \int_a^b \left(\mathcal{R}(\mathcal{A},\lambda+i\epsilon) - \mathcal{R}(\mathcal{A},\lambda-i\epsilon)\right) d\lambda \\ = \mathcal{E}([a,b]) - \frac{1}{2}\left(\mathcal{E}(\{a\}) - \mathcal{E}(\{b\})\right).$$

In particular, we remove the endpoint contributions and prove an extension of Stone's theorem to higher-order smoothing kernels that achieve rapid convergence as the smoothing parameter $\epsilon \to 0^+$. We also demonstrate why careful deformations of the integration contour on the left can accelerate the computation of $\mathcal{E}([a,b])$ by orders of magnitude. This work is best understood as an extension of the recent framework for computing smoothed densities of scalar spectral measures $\mu_f = d\langle \mathcal{E}(\lambda)f, f\rangle_{\mathcal{H}}$ [3].

2.3 Functional calculus

In a spirit similar to the projection-valued spectral measure approximations, one can approximate the functional calculus of $\mathcal{A}$ via

$$f(\mathcal{A}) = \int f(\lambda)\, d\mathcal{E}(\lambda), \tag{4}$$

coupled with suitable analogs of Stone's theorem and careful contour deformations into the complex λ-plane [4]. Of particular interest is the time evolution operator for tight-binding Hamiltonians, corresponding to $f_t(\lambda) = \exp(-\mathrm{i}\lambda t)$.

3 Haldane model experiments

The Haldane model describes electrons hopping on a two-dimensional honeycomb lattice in the presence of a periodic magnetic field with zero net flux. When the lattice is pristine (without defects), the infinite-dimensional Hamiltonian's spectral properties can be studied analytically by using Bloch's theorem for periodic media. When the lattice contains edges, defects, or disorder, periodic and truncated approximations are still applied heuristically. However, these may introduce spectral artifacts such as spectral pollution in the gap of the Bloch Hamiltonian.

In place of periodic or truncated approximations of the Haldane Hamiltonian $\mathcal{A}$, we rigorously approximate the action of $\mathcal{R}(\mathcal{A},z)$ on $\mathcal{H}$ by using rectangular sections of a banded infinite-dimensional representation of $\mathcal{A}$ [2]. Applying the resolvent framework for infinite-dimensional spectral computations allows us to rigorously approximate the spectral properties discussed in section 2.

In particular, we use spectral projections to compute bulk and edge conductances of $\mathcal{A}$ and confirm that these are quantized in the presence of weak global disorder, even in the exotic mobility gap regime. The corresponding topological phase diagrams of the Haldane model are computed and wave-packet approximations are constructed to probe generalized eigenstates mediating bulk and edge transport. The functional calculus is applied to compute the time evolution of topologically protected edge states.

References

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