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Identifying and classifying localized states in gapless systems using pseudospectral methods

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ABSTRACT

For decades, band theory has been used to understand the physical properties of crystals by leveraging these systems' translational symmetries to determine the spectral range and distribution of their Bloch eigenstates. However, many important phenomena only manifest at a crystal's defects or boundaries where this translational symmetry is broken, such as defect-localized states that appear at color centers, or boundary-localized states whose existence is guaranteed by topology. Although it is possible to extend band theoretic approaches to study these classes of states, these extensions are only applicable in gapped systems, where any localized states are spectrally isolated from the crystal's bulk states. This constraint stems from the fact that the location and localization of a spectrally isolated localized state, $|\psi_{\text{loc}}\rangle$, satisfying $H|\psi_{\text{loc}}\rangle = E_{\text{loc}}|\psi_{\text{loc}}\rangle$ where H is the lattice Hamiltonian, must be calculated using expectation values of the position operator, X, as $\langle\psi_{\text{loc}}|X^n|\psi_{\text{loc}}\rangle$. However, if the system possesses a degenerate bulk eigenstate, $|\psi_{\text{bulk}}\rangle$, these expectation values become meaningless as there is no discriminant for choosing a preferred basis of the system's degenerate subspace.

Instead, pseudospectral methods are based on giving equal treatment to all of a system's relevant operators. Thus, rather than first solving for the eigenstates of H and then calculating expectation values, pseudospectral methods combine these incompatible observables into a single "composite" operator, whose spectrum indicates whether the system has a state approximately localized in the vicinity of some location and at some energy. In essence, by eschewing an exact eigenvalue for any single observable, pseudospectral methods are able to find states that are maximally localized across all observables.

In this project, we developed a new theory for finding localized states in any gapless (or gapped) system based on its pseudospectra. As this theoretical approach directly incorporates information about position and localization alongside spectral information, it is able to inherently identify localized states regardless of the existence of degenerate extended 'bulk' states. Moreover, pseudospectral methods have the added advantage of providing a measure of the states' protection against disorder and are rigorously connected to the system's topology. To confirm our theory, we developed a new numerical method by incorporating Maxwell's equations directly into a system's pseudospectral description to design and optimize cavities in nanophotonic structures possessing higher-order topology (systems which are effectively gapless systems due to their ability to radiate into free-space).

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1. INTRODUCTION

In this project, we developed a new theory for finding localized states in any gapless (or gapped) system based on its multi-operator pseudospectra. As part of this process, we both developed new mathematical theories and then numerically applied them to a variety of physical platforms. Overall, this Laboratory Directed Research and Development project yielded 13 manuscripts, 9 of which have been published at the time this report was prepared, 2 of which are currently in submission, and 2 of which are in preparation. In the following chapters, we provide motivations and brief descriptions of these studies.

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2. SPECTRAL LOCALIZER FOR LINE-GAPPED NON-HERMITIAN SYSTEMS

One drawback of the spectral localizer framework as it is originally developed [9] is that it is restricted to Hermitian systems, prohibiting its application to a variety of physical platforms that have inherent loss, such as photonic structures and dissipative systems. In these contexts, Hamiltonians are non-Hermitian, and the lack of self-adjointness complicates both spectral analysis and the definition of topological invariants. At the same time, interest in non-Hermitian physics is rapidly growing, particularly in photonics; for example, in the design of topological lasers and in systems with absorbing boundary conditions, creating a need for a robust, computable method to diagnose topological phases.

Our work [1] shows that the spectral localizer can be generalized to non-Hermitian Hamiltonians with line-gaps and used to compute strong topological invariants. In particular, we prove that the signature of the localizer equals the Fredholm index associated to the spectral localizer with a non-Hamiltonian, thereby connecting it to established invariants such as Chern numbers. Moreover, we establish conditions under which the localizer retains a line-gap and demonstrate that its signature remains constant under homotopies, making it a reliable topological invariant. Finally, a numerical example based on a lossy Haldane heterostructure illustrates how the method correctly identifies topology changes at interfaces and detects topologically protected edge states, highlighting the framework's applicability to real non-Hermitian photonic systems.

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3. CLASSIFYING TOPOLOGY IN PHOTONIC HETEROSTRUCTURES WITH GAPLESS ENVIRONMENTS

In this study [6], we extend the spectral localizer framework to address the challenge of classifying topology in photonic heterostructures that interface with gapless environments, such as free space. Previous work demonstrates that the spectral localizer provides a robust and computable means of identifying strong topological invariants in both Hermitian and non-Hermitian line-gapped systems. However, many realistic photonic platforms couple directly to the radiative continuum, as free space is gapless above the light line, and the absence of a global band gap prohibits the use of conventional bulk-boundary correspondence arguments. This motivates our investigation of how to define, detect, and quantify topology in systems that lack insulating boundaries.

In particular, we show that the spectral localizer provides a rigorous framework for resolving bulk-boundary correspondence in gapless heterostructures. By reformulating Maxwell's equations into a Hamiltonian form and constructing the spectral localizer as a composite operator, we obtain local markers of topology and spatially resolved measures of protection that remain valid even in radiative environments. Applying this approach to a finite photonic Chern insulator embedded in free space, we demonstrate that the local Chern marker becomes nontrivial at the system's boundary, and the associated closure of the local gap quantifies the emergence of topologically protected resonances. Importantly, we find that approximating radiative outcoupling as material absorption substantially overestimates the degree of protection, underscoring the necessity of a framework that treats radiation channels explicitly.

Altogether, our results reveal that topological photonic systems embedded in gapless environments do exhibit bulk-boundary correspondence, though in the form of boundary-localized resonances rather than strictly bound modes. The spectral localizer provides a quantitative measure of their robustness to disorder and radiative losses. This unified framework thus bridges earlier advances on the spectral localizer framework for Hermitian and non-Hermitian Hamiltonians with the new frontier of gapless topological heterostructures, offering predictive power for the design of robust photonic devices operating in radiative settings.

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4. CLASSIFYING TOPOLOGY IN PHOTONIC CRYSTAL SLABS WITH RADIATIVE ENVIRONMENTS

In this study [11], we address the challenge of realizing and probing Chern insulating phases in photonic slab geometries, where coupling to radiative modes above the light line obscures conventional bulk-edge correspondence. While three-dimensional photonic crystals with complete band gaps have been successfully used to demonstrate topological protection, their complexity and fabrication challenges limit scalability. Slab geometries, by contrast, are technologically versatile and directly compatible with integrated photonics platforms, but the absence of a full gap and the presence of radiation losses raise fundamental questions about the robustness of topological states.

In particular, we show that a properly constructed photonic slab can host a Chern insulating phase despite its intrinsic openness. By analyzing a model system and validating with full-wave simulations, we demonstrate that topological edge states persist below the light line, where they are protected from radiative coupling and remain sharply defined. We further show that coupling to modes above the light line leads to quasi-bound resonances that still inherit topological features, though with finite radiative linewidths. These results establish that slab geometries can support robust topological phases and offer practical routes for probing them in realistic photonic platforms.

Together, our findings bridge the gap between theoretical models of idealized, closed Chern insulators and experimentally relevant photonic slab systems. The framework not only clarifies how bulk-boundary correspondence manifests in open geometries but also provides design principles for observing and harnessing topological phenomena in integrated photonics. This work thus advances the development of scalable topological photonic devices that combine strong topological protection with the technological advantages of planar architectures.

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5. LOCAL MARKERS FOR CRYSTALLINE TOPOLOGY

In this study [5], we introduce a framework of local crystal markers that provides spatially resolved topological diagnostics for crystalline phases. While previous local marker approaches have been successful in identifying bulk topology in disordered and amorphous systems, they do not capture the finer structure of crystalline invariants that arise from spatial symmetries. This limitation poses a barrier to studying higher-order and crystalline topological phases, which are of growing importance in both condensed matter and photonic systems. Our goal is to extend the local marker paradigm to account for the role of crystalline symmetries and thereby enable quantitative probes of topological protection tied to lattice structure.

We show that local crystal markers can be systematically constructed from symmetry representations, and that their spatial distributions faithfully reproduce crystalline topological invariants even in the presence of disorder or in finite systems. These markers allow us to track where topological protection is concentrated in real space, revealing how corner and hinge states arise from underlying lattice symmetries. We validate the approach on prototypical two- and three-dimensional models, where the local crystal markers not only identify the correct topological class but also distinguish between phases with the same bulk invariant yet different crystalline protections. This provides a powerful tool for diagnosing crystalline topological matter beyond conventional band-structure analysis.

Together, our results establish local crystal markers as a unifying diagnostic for crystalline topological phases, bridging symmetry-based classification schemes with spatially resolved observables. This framework opens the door to studying crystalline topology in realistic, disordered, and finite-size systems where momentum-space methods are not applicable, offering new predictive power for both condensed matter platforms and photonic metamaterials.

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6. EVEN SPHERES AS JOINT SPECTRA OF MATRIX MODELS

In this paper [4], we investigate the mathematics of the Clifford spectrum as a joint spectrum for noncommuting Hermitian matrices, motivated by its growing role in physics and its connections to K-theory. While earlier work established the use of the spectral localizer and Clifford spectrum in low-dimensional systems, little was known about what kinds of higher-dimensional spaces could arise as Clifford spectra. This work addresses that gap by systematically analyzing the structures that appear, with particular focus on whether even-dimensional spheres can emerge. The motivation is both mathematical and physical: from a pure perspective, understanding the possible topological shapes of spectra provides insight into noncommutative geometry; from an applied side, these structures have direct implications for models of topological insulators, photonic crystals, and higher-dimensional lattice systems.

In particular, we establish that even spheres can indeed arise as Clifford spectra of certain matrix models, extending the range of known realizable spaces beyond fuzzy two-spheres and toroidal examples. We prove explicit results characterizing when odd vs. even dimensional Clifford algebras lead to trivial vs. nontrivial spectral manifolds, showing that odd-dimensional cases naturally yield unit spheres, while even cases collapse to isolated points unless enriched by additional structure. Importantly, we construct five real symmetric almost-commuting matrices that exhibit a K-theoretic obstruction preventing them from being close to exactly commuting matrices, thereby settling an open question raised in earlier abstract work. Furthermore, we demonstrate that 4D tight-binding lattice models, including those realized in topological electric circuits, provide concrete physical realizations of these spectral spheres, with numerical evidence confirming the appearance of four-spheres in Clifford spectra.

Taken together, the results reveal a systematic connection between Clifford spectra, higher-dimensional spheres, and K-theory invariants. This not only expands the catalog of known spectral geometries but also deepens the interplay between operator algebras and physical models of topological matter. The constructive examples offered here pave the way for future work, including the challenge of defining a "fuzzy four-sphere" built from real symmetric matrices, and highlight the Clifford spectrum as a powerful framework for exploring the geometry of almost commuting operators.

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7. MULTIVARIABLE PSEUDOSPECTRUM IN C^*-ALGEBRAS

In this paper [2], we extend the study of the Clifford spectrum and pseudospectrum to the setting of C^*-algebras and focus on developing robust definitions of multivariable pseudospectra for noncommuting Hermitian operator tuples. The motivation stems from recent applications of spectral localizer methods in photonics, metamaterials, and condensed matter physics, where physically relevant Hamiltonians often involve multiple noncommuting observables. While prior work on Clifford spectra has primarily been restricted to finite-dimensional models, this study emphasizes infinite-dimensional settings and the corresponding algebraic structures that arise, such as the Toeplitz algebra and universal C^*-algebras generated by projections.

Specifically, here we prove several key theoretical results. We show that the Clifford pseudospectrum, defined through the smallest singular value of the spectral localizer, enjoys Lipschitz continuity, ensuring stability under perturbations. We establish spectral permanence in the C*-algebra framework and prove that both Clifford and quadratic pseudospectra are invariant under orthogonal transformations of operator tuples. Furthermore, we derive quantitative inequalities linking the Clifford and quadratic pseudospectra, demonstrating that they remain close when operators nearly commute. Explicit computations for universal pairs of projections reveal striking structures: the quadratic spectrum reduces to four isolated points, while the Clifford spectrum forms a cross-shaped set, illustrating how different definitions capture distinct geometric features of operator tuples.

Finally, the paper provides novel infinite-dimensional examples where the Clifford spectrum exhibits unusual shapes not seen in finite dimensions, including hemispherical and bifurcating structures in three-operator models. These examples highlight the richness of multivariable pseudospectra and their sensitivity to noncommutativity. By situating the analysis within the general framework of C^*-algebras, we lay a mathematical foundation for applying pseudospectral techniques to broad classes of quantum and wave systems, further strengthening the bridge between operator theory and topological physics.

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8. CLASSIFYING PHOTONIC TOPOLOGY USING THE SPECTRAL LOCALIZER AND NUMERICAL K-THEORY

Finally, towards the end of this project, we were invited to write a tutorial on the spectral localizer framework to facilitate its uptake by the broad scientific community. This tutorial is now published [3], and we hope that this provides an accessible point of entry for anyone who is interested in learning about this topic.

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9. CONCLUSION

In conclusion, this project has established a broad and unified framework for diagnosing topology across an unprecedented range of physical and mathematical settings. By extending the spectral localizer framework and related concepts, we have demonstrated their applicability to non-Hermitian systems with loss, photonic heterostructures coupled to gapless environments, and slab geometries subject to radiative coupling. At the same time, we developed new diagnostics such as local crystalline markers and explored fundamental questions in operator theory through the study of Clifford spectra and multivariable pseudospectra in both finite- and infinite-dimensional contexts. Collectively, these efforts not only provide new theoretical foundations but also connect directly to experimentally relevant platforms in photonics and condensed matter, where robustness and disorder tolerance are essential.

Looking ahead, the results of this project open the door to multiple future research directions. On the mathematical side, the constructive examples of higher-dimensional Clifford spectra and the rigorous development of multivariable pseudospectra point toward a deeper interplay between operator algebras, K-theory, and topological physics. On the applied side, our demonstrations of topological protection in open and radiative environments provide practical design principles for scalable photonic devices, while the tutorial on the spectral localizer ensures accessibility to the wider community. Together, these outcomes illustrate the power of combining new mathematics with targeted physical applications, laying the groundwork for further advances in the understanding and utilization of topology in complex quantum and wave systems.

This project also supported a few other studies [7, 8, 12, 10].

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