

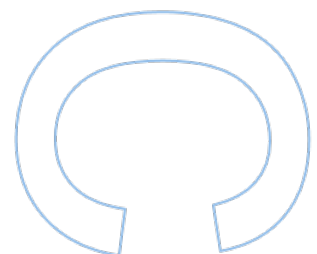
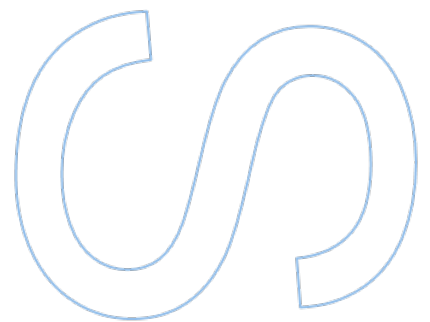
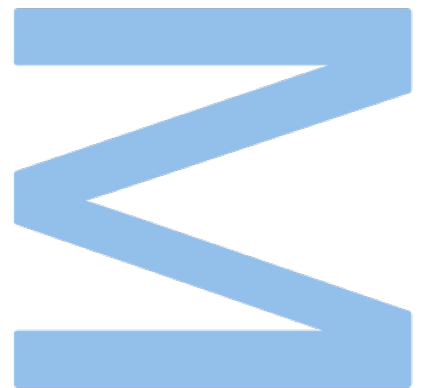
Incommensurability effects on a Second Order Topological Insulator

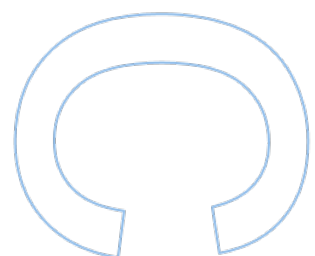
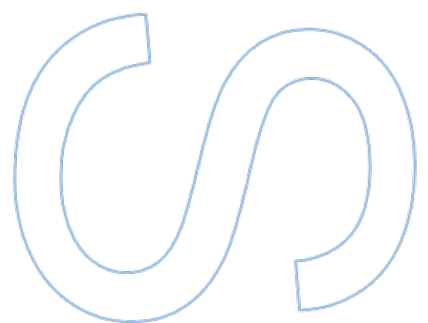
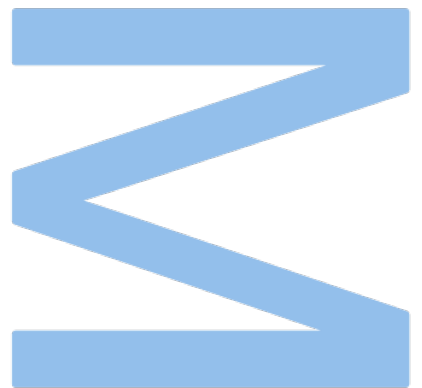
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Abstract

Symmetry-protected quantum phases in topological systems have recently been extended to higher-order. Concurrently, the intricate localization properties of quasi-periodic systems and their impact on topological insulators have gathered significant attention. Nonetheless, the characterization of quasi-periodic higher-order topological insulators remains unexplored. In this thesis, we bridge these two areas by studying the effects of quasi-periodic modulations on the prototypical Benalcazar-Bernevig-Hughes (BBH) model for higher-order topology at half filling.

In order to build our intuition on the interplay between quasi-periodicity and topology, we start with a first-order topological insulator. Thus, we characterize a Chern insulator with Quadratic Band Crossing Points (QBCP) under the effect of a 1D quasi-periodic modulation, where it is shown that clean limit Chern phases ($C = \pm 2$) are robust to QP modulations. However, stronger modulations can induce topological phase transitions in gap closing and opening fashion into topological regimes ($C = \pm 1$) not accessible in the clean limit. Afterwards we discuss the BBH model and its disordered version to gain insight on the effects of translational symmetry breaking on higher-order topological phases. The main results are for the chiral Quasi-Periodic Quadrupole Insulator (QPQI) where the effects of quasi-periodicity in the BBH model are vastly characterized, thus performing the first study of a QP higher-order topological insulator. We demonstrate that clean limit quadrupole insulating (QI) phases with zero-energy corner modes are robust to quasi-periodic modulations. Moreover, we encounter the first gapped QP-induced QI phase (QPQI) described by intricate dynamics between the zero-energy corner modes and edge states that disperse with varying phase shifts. A gapless QPQI regime was also encountered with localized states at the Fermi level, similar to higher-order topological Anderson insulating (HOTAI) phases. This study is accompanied by a detailed classification of topological, spectral and localization properties throughout the several observed phases.

In this thesis, we broaden the scope of chiral QI phases by incorporating QP modulations in the BBH model, providing verification that QI phases are robust to QP modulations. Furthermore, we demonstrate the emergence of QPQI phases with dynamics absent in the clean limit. This expansion results in a diverse phase diagram, encompassing QI topological phases, trivial and Anderson insulators, and even critical metals.

Resumo

As fases quânticas protegidas por simetria em sistemas topológicos foram recentemente estendidas para uma ordem superior. Ao mesmo tempo, as complexas propriedades de localização de sistemas quase periódicos e o seu impacto em isoladores topológicos têm atraído atenção significativa. No entanto, o efeito de quase-periodicidade em isoladores topológicos de ordem superior permanece inexplorado. Nesta tese fazemos a ponte entre estas duas áreas, estudando os efeitos de modulações quase periódicas no modelo prototípico de Benalcazar-Bernevig-Hughes (BBH) para topologia de ordem superior com meio preenchimento.

Para construir a nossa intuição sobre a interação entre quase periodicidade e topologia, começamos com um isolador topológico de primeira ordem. Assim, caracterizamos um isolador Chern com pontos de cruzamento de banda quadrática (QBCP) sob o efeito de uma modulação quase periódica 1D, no qual é mostrado que as fases Chern do limite limpo ($C = \pm 2$) são robustas a modulações QP. No entanto, modulações mais fortes podem induzir transições de fase topológicas, em abertura e fecho do hiato de energia, para regimes topológicos ($C = \pm 1$) não acessíveis no limite limpo. Posteriormente discutimos o modelo BBH e sua versão desordenada para estudar o efeito da quebra de simetria de translação em fases topológicas de ordem superior. Os principais resultados são para o isolador de momento quadrupolar quase periódico quiral (QPQI) no qual os efeitos da quase periodicidade no modelo BBH são amplamente caracterizados, realizando assim o primeiro estudo de um isolador topológico QP de ordem superior. Demonstramos que as fases isoladoras de momento quadrupolar de limite limpo (QI) caracterizadas por modos de canto de energia zero, são robustas a modulações quase periódicas. Além disso, encontramos a primeira fase QI induzida por QP (QPQI) descrita por uma dinâmica complexa entre os modos de canto de energia zero e estados de fronteira que dispersam com mudanças de fases do potencial. Um regime QPQI sem hiato de energia também foi encontrado com estados localizados no nível de Fermi, semelhante a fases isoladores topológicos de Anderson de ordem superior (HOTAI). Este estudo é acompanhado por uma classificação detalhada das propriedades topológicas, espectrais e de localização ao longo das diversas fases observadas.

Nesta tese, apresentamos novas fases QI quirais incorporando modulações QP no modelo BBH, fornecendo a verificação de que as fases QI são robustas a modulações quase-perioódicas. Além disso, demonstramos o surgimento de fases QPQI com dinâmica ausente no limite limpo. Esta expansão resulta em um diagrama de fases diversificado, abrangendo fases topológicas QI, isoladores triviais e de Anderson e até metais críticos.

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Chapter 1

Introduction

Condensed matter is an area of physics concerned with studying properties of materials. Its diverse phenomenon range from descriptions of phase transitions to quantum descriptions of superconductivity, ferromagnetic and antiferromagnetic phases, condensates and many other interesting and complex properties. It is safe to say that without our understanding of condensed matter physics, most of the technology that surrounds us, would not be possible.

This said, we do a brief recap of important hallmarks of condensed matter. In 1900 Paul Drude proposed the first theoretical model for a classical electron gas on a solid metal. This model allowed for the calculation of several quantities in terms of the mean free time (τ), revealing its success with the explanation of the Hall effect, discovered fifty years earlier by Edwin Hall. This physicist showed that a transverse voltage to the applied current appeared in a conductor when it was subjected to a perpendicular magnetic field (B).

A century passed, and in 1980, Klaus von Klitzing and collaborators [2] discovered that the Hall conductance was quantized to integers of e^2/h , with this new behavior being robust to system contaminations and deformations. The linear dependence of the Hall resistivity (ρ_{xy}) at low fields gives way to a plateau insulating behavior, accompanied by zero longitudinal resistivity (ρ_{xx}), as shown in figure 1.1. Another remarkable physicist that shaped the course of physics, Lev Landau made contributions in the field of quantum mechanics, where he developed the theory of Landau quantization. Landau theorized that the band structure of materials, when subjected to a uniform perpendicular magnetic field, degenerated into energy levels, known

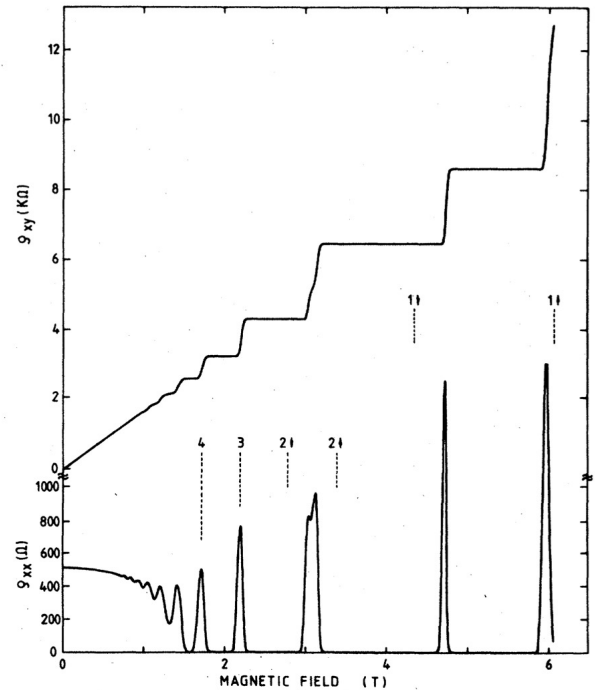


Figure 1.1: Hall resistivity ρ_{xy} and longitudinal resistivity ρ_{xx} as a function of magnetic field strength (T). Image taken from [1].

as Landau levels. This theory set the fundamentals needed for the understanding of the quantum Hall effect (QHE).

It was not until 1982 that Thouless and collaborators [3], shed some light on the underlying mechanism behind the QHE. The Hall conductivity $\sigma_{xy} = \frac{e^2}{h}n$ was not proportional to a “random” integer but to a quantized topological invariant that emerges from band topology, the first Chern number, to be discussed later. Another six years were needed after Thouless’s new insights on QHE, for Haldane to propose a model [4], where quantum Hall phases could be observed in the absence of a magnetic field. The anomalous quantum Hall effect (AQHE) was born. All this inspiring work performed in the 70s and 80s paved the way to the field of topology in condensed matter physics.

1.1 Topological Insulators

Topology is an area of mathematics that studies “spaces”¹ and the way that they are linked through slow and continuous deformations. From a topology perspective, a donut and a mug are exactly the same object, which we call a torus, which is any closed surface that contains one single handle (or, more colloquially, one hole). We can adiabatically deform a mug into a donut and vice versa. However, we cannot deform a donut into a sphere since it has no holes. In this manner, the number of holes in a manifold emerges as a topological invariant, the genus. Topological phases of matter share the same phenomenology. A system in a given topological phase can be adiabatically deformed into any new configuration, keeping its topological properties, as long as the system remains in the same topological phase. For this reason, topological phases of matter are robust to the introduction of deformations and impurities in the system. A new characterization of phases of matter emerges, having in mind concepts of topology. In these novel phases, a quantized bulk property is the hallmark of a finite topological invariant.

In crystalline systems with translation invariance, the inherent topological behavior of systems comes from the underlying band structure. A fundamental consequence of topological phases in gapped band structures is the existence of gapless conducting states at the interfaces, where the topological invariant changes. For 2 dimensional systems, these edge states were first analyzed by Halperin in 1982,[5]. These electronic states are chiral since they only propagate in one direction along the topological vacuum boundary. This is the celebrated bulk boundary correspondence [6, 7]. In 1D, there are also interesting examples of topological systems, with a paradigmatic example being the tight binding model of polyacetylene proposed by Su, Schrieffer and Heeger more commonly referred to as the SSH model [8]. This model presents a quantized bulk electronic polarization alongside zero-energy gapless boundary states. Due to their exotic insulating properties, they have gained particular attention in research [6, 9, 10, 11].

In contrast with the Landau paradigm, where phase transitions are associated with symmetry breaking, topological phases are associated with the presence of a given symmetry of the system or the absence thereof. Time reversal symmetry ($\mathcal{T}$), particle-hole² symmetry ($\mathcal{C}$) and chiral symmetry³ (Π), turn out to be of major importance, which became clear in 2008 when Schnyder and collaborators completed the work done by Altland and Zirnbauer [12], linking the presence of these discrete symmetries to topological

¹This can be any structure in a generalized dimension, in condensed matter physics the relevant space is usually the first Brillouin zone (FBZ), although, some topological invariants are defined in more complex and not so trivial geometries.

²Also known as charge conjugation

³Also known as sub-lattice symmetry

constrains [13]. Besides discrete symmetries, a material can have a set of crystalline symmetries that give rise to topological character. These types of materials are known as topological crystalline insulators [14, 15], which have their own set of topological invariants.

1.2 The Chern Number and AQHE

In order to gain some intuition on the characterization of topological systems, we dive succinctly into the 2D Chern insulators.

A 2D gapped system with a valence and a conduction band is considered. In these types of systems, if time reversal symmetry is broken, the topological invariant is the Chern number. Let $\{|u_{\mathbf{k}}^-\rangle\}$ be the Bloch states of the valence band, then these states define the Berry connection of the band $\mathcal{A}(\mathbf{k}) = i \langle u_{\mathbf{k}}^- | \nabla_{\mathbf{k}} u_{\mathbf{k}}^- \rangle$. We can now ask, what phase does a state accumulate when we take it adiabatically across a given path over the first Brillouin zone (FBZ). The Abelian Wilson loop over a path C in the FBZ is defined by:

$$\mathcal{W}[C] = \exp \left(i \oint_C \mathcal{A}(\mathbf{k}) \cdot d^2\mathbf{k} \right). \quad (1.2.1)$$

The exponent of the Wilson loop is known as the Berry phase (or geometric phase) [16]. Making use of Stokes' theorem, the line integral over $C = \partial S$ can be rewritten as a surface integral over the surface S ,

$$\gamma = \oint_{\partial S} \mathcal{A}(\mathbf{k}) \cdot d^2\mathbf{k} = \int_S \nabla \times \mathcal{A}(\mathbf{k}) \cdot d\mathbf{S} = \int_S \Omega(\mathbf{k}) \cdot d\mathbf{S}. \quad (1.2.2)$$

The surface integral form reveals itself to be more illuminating regarding how this mathematical object “sees” the band structure of the system. A new quantity is then introduced $\Omega(\mathbf{k}) = \nabla \times \mathcal{A}(\mathbf{k})$, the Berry curvature. For 2 dimensional systems, if the integration is performed over the entire FBZ, the topological invariant of the system is defined, the first Chern number $C \in \mathbb{Z}$,

$$C = \frac{1}{2\pi} \int_{FBZ} \Omega(\mathbf{k}) \cdot d\mathbf{S}. \quad (1.2.3)$$

The Chern number shares an intimate relation with the transversal conductivity of the system, with $\sigma_{xy} = \frac{e^2}{h} C$. Chern insulators need to have broken-time reversal symmetry. This concludes the bridge between topological phases of matter and the anomalous quantum Hall effect. In other dimensions, the Berry phase is identically defined, though the associated topological invariant may be different. These topological invariants are quantized by symmetries, and because they are Gauge invariant, manifest as observables of the system. In the case of 1D systems, such as the SSH model, one possible topological invariant is the winding number ν , that quantizes the bulk electronic polarization of the system. The particular choice of topological invariant comes from the underlying symmetries we choose to fix a priori. In the case of multiple filled bands and if the Berry Connection is non-diagonal, a non-Abelian formulation is required.

1.3 Disorder and Topological Insulators

We now take a look at the effects of a disordered potential. At first glance, disorder might seem an awkward addition to our system. As it turns out, disorder is omnipresent in experimental realizations since it can be understood as lattice deformations or impurities. In the clean limit, crystalline symmetry is present, and so the Bloch Hamiltonian fully describes the system. However, with the introduction of disorder, spatial symmetries are broken. For this reason, disordered metallic systems manifest a finite resistivity, even at $T = 0$, with the resistivity rising as disorder increases. In fact, we can paint an intuitive picture of what happens when a local disordered potential is added: a part of the wave is scattered from $k \rightarrow -k$.⁴ If we keep adding scattering centers randomly distributed, destructive interference of the waves will occur in most of the lattice but for one small region where all the spectral weight of the wave function is concentrated, or more simply put, the wave function becomes confined to a small region of space. This localization phenomenon was first discovered by P. W. Anderson in 1958 [17] and is referred to as Anderson localization. A material is said to be an Anderson insulator if its insulating capabilities are provided by the existence of Anderson localized states at the Fermi level, even if the system is gapless.

Later contributions to disordered electronic systems showed that for the orthogonal symmetry class at $D \leq 2$, any amount of disorder leads to Anderson localization [18, 19, 20]. This is a surprising result that shows disorder cannot be treated as perturbations to Bloch waves since the crystalline momenta k is no longer a good quantum number. The same cannot be said about 3-dimensional systems, whereas, as a function of energy, the states change from being localized to extended. This energy is called the mobility edge of the system. For a critical value of disorder (W_c) all the spectrum becomes Anderson localized. In this thesis, we will focus on low-dimensional systems with $D \leq 2$.

As stated, topological properties are symmetry-protected, so, as long as the effective disordered Hamiltonian preserves the relevant symmetries, topological phases can occur. In fact, disorder plays a key role on the QHE, since the plateaus of constant Hall resistivity only appear in the presence of disorder. Moreover, the original experiment was realized on a contaminated sample [2]. This shows that in the presence of weak disorder, topological properties are robust. In these regimes, a system in a topological phase exhibits Anderson localized states. However, the topology is entirely carried by a few critical states⁵. Topological phase transitions can also be induced by disorder, since disorder can lead to a gap-closing transition [21]. Furthermore, in the presence of disorder, gapless topological phases are usually observed, with the topological phase transitions (TPT) occurring through the “levitation and annihilation” mechanism [22, 23, 24, 25]. In this manner, disorder-induced topological phases are referred to as topological Anderson insulators (TAI) [26].

1.4 Quasi-Periodicity and Topological Insulators

Disordered electronic systems are proficiently classified, either with experimental realizations of TAI, numerical work or analytical proofs regarding localization properties and their interplay with topology. Another class of systems that break translational invariance are quasi-periodic systems. Aubry and

⁴For 1-dimensional (1D) materials.

⁵A critical state is an intermediary characterization between extended and localized, more concretely is a state with a fractal dimension smaller than 1 but not localized

André proposed the first instance of these types of systems, which displayed a quasi-periodic modulation in a simple 1-dimensional (1D) tight binding chain [27]. In contrast with Anderson disorder, extended, critical and localized phases can arise even in 1D [28, 29, 30]. Away from one-dimensional systems, higher-dimensional models also display diverse localization phenomena, gaining special attention on the interplay between Moiré physics and localization [31, 32, 33]. An example of exotic behavior in uncorrelated quasi-periodic systems is the existence of mixed localized and extended spectra in 2-dimensional (2D) systems [34].

Quasi-periodicity also shows its potential in topological matter, where it unveils new topological behavior [35, 36] with far richer localization properties than their disordered cousins. Different types of Chern insulating phases have been shown to be induced by quasi-periodic modulations [37, 38].

These types of systems were first considered in cold atoms experiments, while more recently they have gained attention in Moiré materials and in many-body localization phenomenon [39, 40]. Furthermore, systems with quasi-periodic modulations can be realized on widely different platforms, including optical lattices [41, 42], photonic [43, 44] and phononic [45, 46] metamaterials, and moiré materials [47, 48].

1.5 higher-order Topological Insulators

In the last six years, higher-order topological insulators (HOTIs) have drawn great interest among condensed matter physicists. Unlike the more conventional first-order topological insulators, for which bulk-boundary correspondence guarantees the existence of $D - 1$ dimensional boundary states, HOTIs are characterized by boundary states with lower dimensionality. In particular, an m^{th} order topological insulator has $D - m$ dimensional gapless boundary modes for a D dimensional system [49]. For example, a second-order topological insulator (SOTI) in a 2-dimensional system has zero-energy corner modes. In these higher-order generalizations, bulk boundary correspondence holds, as the presence of a bulk quantized property manifests in gapless boundary modes. In contrast with first-order TIs that exhibit a trivial boundary, HOTIs exhibit a more intricate bulk-boundary correspondence, featuring successive lower-dimensional TIs in their boundaries. This complexity gives rise to a nested hierarchy of topological insulators. Consequently, an m^{th} order topological insulator is characterized by an $(m - 1)^{\text{th}}$ order TI in the boundary. Moreover, symmetries are equally important for higher-order topology, with HOTIs phases protected by either discrete symmetries⁶ or by crystalline symmetries.

The first theorized model was introduced in 2017 by Bernevig, Benalcazar and Hughes [49] (BBH model) and reveals to be a clever higher-dimensional generalization of the known SSH model. It acts as the building block for most of the newly proposed HOTIs. The family of BBH models consist of a 2 dimensional SOTI and a 3 dimensional third-order topological insulator (TOTI). The first one is characterized by gapless corner states with a quantized bulk quadrupole moment, boundary dipole moment and corner charges. As for the BBH TOTI, it displays a quantized bulk octupole moment, quadrupole boundary moment, hinge dipole moment and corner charges. This boundary hierarchy paints a clear picture of classical electromagnetism, with the emergence of canonical boundary signatures of quadrupole and octupole moments.

Since the introduction of the BBH model, new higher-order topological models have been proposed,

⁶The tenfold way no longer applies in these higher-order generalizations.

such as its equivalent model [50], the breathing kagome lattice as presented in Refs. [51, 52], twisted Moiré superlattice's [53], generalizations of the Haldane model [54] and many others. Considerable efforts have been made to unveil the symmetries behind the protection of these topological phases and to understand their robustness against weak disorder. Furthermore, these new topological regimes have been experimentally realized in phononic metamaterials [55], electric circuits [56, 57] and even real solid-state materials [58]. Some disordered HOTIs have been studied [59, 60] and have been experimentally observed [57]. Although some work has been performed on quasicrystals with higher-order phases [61, 62], the effects of quasi-periodicity in higher-order topology remain vastly unstudied.

1.6 Discrete Symmetries

In this section, we make some quick remarks about the three different discrete symmetries that allow for the definition of each symmetry class in the tenfold way [12, 13]. We follow the book on topology by Miguel Araújo and Pedro Sacramento [63].

1.6.1 Time Reversal Symmetry

Time reversal is defined by the following condition: for every ψ that satisfies the Schrödinger equation, then $T\psi^*$ also satisfies the Schrödinger equation with the substitution $t \rightarrow -t$, where T is unitary. In this manner, we can write:

$$i\hbar\partial_t\psi = \mathcal{H}\psi \leftrightarrow -i\hbar\partial_t\psi^* = \mathcal{H}^*\psi^* \leftrightarrow -i\hbar\partial_t(T\psi^*) = T\mathcal{H}^*T^\dagger(T\psi^*). \quad (1.6.1)$$

Then the time reversal operation is given by the following substitutions:

$$\psi \rightarrow T\psi^* \quad (1.6.2)$$

$$\mathcal{H} \rightarrow T\mathcal{H}^*T^\dagger. \quad (1.6.3)$$

A given theory is time symmetric if $T\mathcal{H}^*T^\dagger = \mathcal{H}$.

1.6.2 Particle-Hole Symmetry

Particle-hole or charge conjugation symmetry is defined by the condition: if there exists a unitary matrix C such that $C\psi^*$ satisfies the Schrödinger equation, then $C\mathcal{H}^*C^\dagger = -\mathcal{H}$.

1.6.3 Chiral Symmetry

Chiral or sub-lattice symmetry is defined by:

$$\exists \Pi : \Pi\mathcal{H}\Pi^\dagger = -\mathcal{H} \quad (1.6.4)$$

This definition implies that $\{\mathcal{H}, \Pi\} = 0$ so that if $|\psi_n\rangle$ is an eigenstate of $\mathcal{H}$ with energy E_n , then $\Pi|\psi_n\rangle$ is also an eigenstate of $\mathcal{H}$ with energy $-E_n$. So, any Hamiltonian that preserves chiral symmetry has

a symmetric spectrum. Any Hamiltonian that preserves chiral symmetry can be written as an anti-diagonal matrix. The chiral operator is then $\Sigma_z = \sigma_z \otimes I_{N/2}$, however it's possible that for a given basis the Hamiltonian does not present this structure despite being chiral symmetric. In these cases, a unitary transformation U can be considered that rotates the Hamiltonian to anti-diagonal form:

$$U\mathcal{H}U^\dagger = \begin{pmatrix} 0 & h \\ h^\dagger & 0 \end{pmatrix} \quad (1.6.5)$$

where h is a given matrix with half the dimension of the Hilbert Space, $(N/2)$. This can be achieved in real space by identifying two decoupled sub-lattices and proceeding to properly order the real-space basis. This said, Π can be constructed from U in the following manner:

$$\begin{aligned} \Sigma_z U\mathcal{H}U^\dagger \Sigma_z &= -U\mathcal{H}U^\dagger \leftrightarrow \\ \leftrightarrow U^\dagger \Sigma_z U\mathcal{H}U^\dagger \Sigma_z U &= -\mathcal{H}. \end{aligned} \quad (1.6.6)$$

From this we make the identification $\Pi = U^\dagger \Sigma_z U = \Pi^\dagger$ concluding that $\Pi^2 = \Pi\Pi^\dagger = 1$.

Let us consider a system with time reversal symmetry ($T\mathcal{H}^*T^\dagger = \mathcal{H}$), and charge conjugation ($C\mathcal{H}^*C^\dagger = -\mathcal{H}$). From the charge conjugation symmetry and using C unitarity one can invert the relation and obtain $\mathcal{H}^* = -C^\dagger \mathcal{H} C$. We can then insert this relation into the time reversal condition:

$$T\mathcal{H}^*T^\dagger = -TC^\dagger \mathcal{H} C T^\dagger = \mathcal{H} \leftrightarrow (TC^\dagger) \mathcal{H} (CT^\dagger) = -\mathcal{H}. \quad (1.6.7)$$

It is clear that a system with charge conjugation and time reversal symmetry also preserves chiral symmetry with $\Pi = TC^\dagger = CT^\dagger$. A system can preserve chiral symmetry even if it does not preserve the other two.

Before concluding this section, we explore some of the properties of this symmetry. Assuming a chiral symmetric Hamiltonian in anti-diagonal form 1.6.5, its eigenvectors can be written as $|\psi\rangle = \frac{1}{\sqrt{2}}(\psi_A, \psi_B)$ such that $\{\psi_A, \psi_B\}$ are normalized to 1, thus $\Pi|\psi\rangle = \frac{1}{\sqrt{2}}(\psi_A, -\psi_B)$. Either of the $|\psi_{A,B}\rangle$ obey an eigenvalue equation that involves diagonalizing some lower-dimensional operator. For this, we consider the following eigenvalue problem:

$$\mathcal{H}^2 |\psi_n\rangle = E_n^2 |\psi_n\rangle. \quad (1.6.8)$$

Assuming $\mathcal{H}$ to be in the form of eq. 1.6.5 then it follows:

$$\begin{cases} (hh^\dagger) \psi_A^n = E_n^2 \psi_A^n \\ (h^\dagger h) \psi_B^n = E_n^2 \psi_B^n \end{cases}. \quad (1.6.9)$$

Out of the three discrete symmetries we have introduced, chiral symmetry will play an important role in the work that follows. In this manner, it is only fitting that we have made a more detailed characterization of this symmetry. In the chapter that follows, we move away from the introduction and focus on essential methods to study the vast properties of topological electronic systems.

Chapter 2

Methods

2.1 Wannier Functions, Wannier Centers and Boundary Hamiltonian through Wilson Loops

Wilson loops are a powerful tool when tackling topological properties. They allow us to compute several quantities, such as bulk polarizations, Chern numbers, etc. They are closely connected to topology and define the Wannier functions, which are a localized basis for the Hamiltonian interpreted as the tight binding atomic orbitals. More recently, Wilson loop operators were shown to be adiabatically connected to the boundary Hamiltonian [64] allowing for the study of boundary topology.

2.1.1 Polarization in 1D crystals

In insulators, the electronic contribution to polarization comes from the displacements of electrons relative to the atomic positive charges inside the unit cells of the system. These shifts are the so-called Wannier centers, which can be computed via diagonalization of the projected position operators.

The position operator in a 1D crystal with L_x unit cells and N_{orb} orbitals per UC may be defined following the work in Ref. [65]:

$$\hat{x} = \sum_{R,\alpha} c_{R,\alpha}^\dagger |0\rangle e^{-i\Delta k(R+r_\alpha)} \langle 0| c_{R,\alpha}, \quad (2.1.1)$$

where $\Delta k = \frac{2\pi}{L_x}$ and r_α are the relative positions of the orbitals inside the unit cell. Making use of a discrete Fourier transform, one can pass from real space to reciprocal space and thus $\hat{x}$ takes the form:

$$\hat{x} = \sum_{k,\alpha} c_{k+\Delta k,\alpha}^\dagger |0\rangle \langle 0| c_{k,\alpha}. \quad (2.1.2)$$

In reciprocal space, the system Hamiltonian is defined by

$$\mathcal{H} = \sum_k c_{k,\alpha}^\dagger [h_k]^{\alpha\beta} c_{k,\beta}, \quad (2.1.3)$$

where the sum is over repeated indexes. Making use of $[h_k]^{\alpha\beta} = \sum_n [u_k^n]^\alpha \epsilon_{k,n} [(u_k^n)^*]^\beta$, one can write $\mathcal{H}$ in the band representation:

$$\begin{aligned}
\mathcal{H} &= \sum_{k,n} c_{k,\alpha}^\dagger [u_k^n]^\alpha \epsilon_{k,n} [(u_k^n)^*]^\beta c_{k,\beta} \\
&= \sum_{k,n} \left(\sum_{\alpha} [u_k^n]^\alpha c_{k,\alpha}^\dagger \right) \epsilon_{k,n} \left(\sum_{\beta} [(u_k^n)^*]^\beta c_{k,\beta} \right) \\
&= \sum_{k,n} \gamma_{k,n}^\dagger \epsilon_{k,n} \gamma_{k,n},
\end{aligned} \tag{2.1.4}$$

where $\gamma_{k,n}^\dagger = \sum_{\alpha} [u_k^n]^\alpha c_{k,\alpha}^\dagger$. The operator $\gamma_{k,n}^\dagger$ physically represents the creation of an electron in a band n with crystalline momentum k , furthermore, this basis fully diagonalizes the Hamiltonian of the system with spectra $\epsilon_{k,n}$. The projector onto occupied bands P^{occ} is defined by:

$$P^{\text{occ}} = \sum_{n=1}^{N_{\text{occ}}} \sum_k \gamma_{k,n}^\dagger |0\rangle \langle 0| \gamma_{k,n}. \tag{2.1.5}$$

To obtain the Wannier functions, we need to project the position operator $\hat{x}$ onto the occupied bands ($P^{\text{occ}} \hat{x} P^{\text{occ}}$) and proceed with its diagonalization. For this, we start by explicitly writing $P^{\text{occ}} \hat{x} P^{\text{occ}}$:

$$P^{\text{occ}} \hat{x} P^{\text{occ}} = \sum_{q,\alpha} \sum_{n,m=1}^{N_{\text{occ}}} \sum_{k,k'} \gamma_{k,n}^\dagger |0\rangle \langle 0| \gamma_{k,n} c_{q+\Delta k,\alpha}^\dagger |0\rangle \langle 0| c_{q,\alpha} \gamma_{k',m}^\dagger |0\rangle \langle 0| \gamma_{k',m}. \tag{2.1.6}$$

Substituting $\langle 0| \gamma_{k,n} c_{q+\Delta k,\alpha}^\dagger |0\rangle = [(u_k^n)^*]^\alpha \delta_{k,q+\Delta k}$ and $\langle 0| c_{q,\alpha} \gamma_{k',m}^\dagger |0\rangle = [u_{k'}^m]^\alpha \delta_{k',q}$ (see A.1) in equation 2.1.6 we have

$$\begin{aligned}
P^{\text{occ}} \hat{x} P^{\text{occ}} &= \sum_{q,\alpha} \sum_{n,m=1}^{N_{\text{occ}}} \sum_{k,k'} \gamma_{k,n}^\dagger |0\rangle [u_{k'}^m]^\alpha [(u_k^n)^*]^\alpha \delta_{k,q+\Delta k} \delta_{k',q} \langle 0| \gamma_{k',m} \\
&= \sum_{q,\alpha} \sum_{n,m=1}^{N_{\text{occ}}} \gamma_{q+\Delta k,n}^\dagger |0\rangle [u_q^m]^\alpha [(u_{q+\Delta k}^n)^*]^\alpha \langle 0| \gamma_{q,m} \\
&= \sum_{n,m=1}^{N_{\text{occ}}} \sum_k \gamma_{k+\Delta k,n}^\dagger |0\rangle \langle u_{k+\Delta k}^n | u_k^m \rangle \langle 0| \gamma_{k,m} \\
&= \sum_{n,m=1}^{N_{\text{occ}}} \sum_k \gamma_{k+\Delta k,n}^\dagger |0\rangle [G_{x,k}]^{n,m} \langle 0| \gamma_{k,m}.
\end{aligned} \tag{2.1.7}$$

To reach this result, the following relation was used $\langle u_k^n | u_q^m \rangle = \sum_{\alpha} [u_q^m]^\alpha [(u_k^n)^*]^\alpha \neq \delta_{k,q} \delta_{n,m}$ which is different from the usual orthogonality relation $\langle u_k^n | u_k^m \rangle = \delta_{n,m}$. $P^{\text{occ}} \hat{x} P^{\text{occ}}$ is a single particle operator that is fully defined by the matrix $[G_{x,k}]^{n,m} = \langle u_{k+\Delta k}^n | u_k^m \rangle$ which is only unitary in the thermodynamic limit, $\lim_{N \rightarrow \infty} G_{x,k} = F_{x,k}$. For discrete systems, one can make use of singular value decomposition (*SVD*) to write $G_{x,k} = U D V^\dagger$ so that we can define a unitary matrix $F_{x,k} \approx U V^\dagger \implies D \rightarrow \mathbb{I}$, as in the supplementary material of Ref. [49]. However, the matrix $G_{x,k}$ quickly becomes unitary, with $N \geq 50$ yielding a practically unitary matrix. In this manner, there is no need to perform an *SVD* decomposition

in practical cases. From this point on, it is assumed that L_x is big enough such that $G_{x,k}$ is unitary or that SVD was applied. The final form for the projected position operator is:

$$P^{\text{occ}} \hat{x} P^{\text{occ}} = \sum_{n,m=1}^{N_{\text{occ}}} \sum_k \gamma_{k+\Delta k,n}^\dagger |0\rangle [F_{x,k}]^{n,m} \langle 0| \gamma_{k,m}. \quad (2.1.8)$$

To diagonalize this operator, consider the following equation $(P^{\text{occ}} \hat{x} P^{\text{occ}}) |\psi^j\rangle = E^j |\psi^j\rangle$ which can be written in matrix form:

$$\begin{pmatrix} 0 & 0 & 0 & \dots & F_{k_N} \\ F_{k_1} & 0 & 0 & \dots & 0 \\ 0 & F_{k_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} v_{k_1} \\ v_{k_2} \\ v_{k_3} \\ \vdots \\ v_{k_N} \end{pmatrix}^j = E^j \begin{pmatrix} v_{k_1} \\ v_{k_2} \\ v_{k_3} \\ \vdots \\ v_{k_N} \end{pmatrix}^j, \quad (2.1.9)$$

where F_{k_i} are $N_{\text{occ}} \times N_{\text{occ}}$ matrices and v_{k_i} are vectors. The previous matrix equation can be rewritten as a system of N -coupled equations:

$$\begin{cases} F_{k_N} v_{k_N}^j = E^j v_{k_1}^j \\ F_{k_1} v_{k_1}^j = E^j v_{k_2}^j \\ \dots \\ F_{k_{N-1}} v_{k_{N-1}}^j = E^j v_{k_N}^j \end{cases}. \quad (2.1.10)$$

Iterating this set of equations one obtains:

$$\begin{aligned} F_{k_N} F_{k_{N-1}} (\dots) F_{k_2} F_{k_1} v_{k_1}^j &= (E^j)^N v_{k_1}^j \\ \mathcal{W}_{x,k} v_k^j &= (E^j)^N v_k^j. \end{aligned} \quad (2.1.11)$$

Thus, a new unitary operator is defined, the Wilson loop operator $(\mathcal{W}_{x,k})$ which sweeps the FBZ along the x direction. Since the matrices $F_{x,k}$ are unitary, so is the Wilson loop operator, implying that its eigenvalue problem can be written as:

$$\mathcal{W}_{x,k} |v_{x,k}^j\rangle = e^{2\pi i \nu_x^j} |v_{x,k}^j\rangle, \quad (2.1.12)$$

where the phases ν_x^j are defined mod 1. It is also clear that these phases do not depend on the starting k . However, the same cannot generally be stated about the corresponding eigenvectors $v_{x,k}^j$. From the Wilson loop operator phases, one can obtain the eigenvalues of the projected position operator, noting the following correspondence: $(E^j)^N = e^{2\pi i(\nu_x^j + m)} \implies E^j = e^{i\Delta k(\nu_x^j + R)^1}$. The phases ν_x^j are called the Wannier centers. Since these arguments have been derived using reciprocal space, assuming PBC, this is valid for each unit cell and is related to a bulk property of the system. In this manner,

¹ N is the number of crystalline momenta in the considered direction $N = L_x$ and since our objective is to apply this to 2D systems we make the substitution of m by R where R is a lattice vector $R = ma$ with $a = 1$.

the operator $P^{\text{occ}} \hat{x} P^{\text{occ}}$ diagonalizes as $(P^{\text{occ}} \hat{x} P^{\text{occ}}) |\psi_R^j\rangle = e^{i\Delta k(R+\nu_x^j)} |\psi_R^j\rangle$, where $|\psi_R^j\rangle$ are called the Wannier functions:

$$|\psi_R^j\rangle = \frac{1}{\sqrt{L_x}} \sum_{n=1}^{N_{\text{occ}}} \sum_k \gamma_{n,k}^\dagger |0\rangle [v_{x,k}^j]^n e^{-ikR} \quad (2.1.13)$$

with $j = 1, \dots, N_{\text{occ}}$. The Wannier functions are localized functions in real space that form an orthonormal basis of the Hamiltonian, i.e. $\langle \psi_{R_1}^i | \psi_{R_2}^j \rangle = \delta_{R_1, R_2} \delta_{i,j}$. As the Wannier centers ν_x^j represent the shifts of electrons with regard to the background positive charges inside the unit cells, the electronic contribution to polarization is proportional to the sum of the Wannier centers. Each individual electron that is shifted by ν_x^j provides a contribution proportional to ν_x^j thus the bulk polarization is:

$$p = e \sum_{j=1}^{N_{\text{occ}}} \nu_x^j \mod e. \quad (2.1.14)$$

Since ν_x^j are the phases of the Wilson loop operator, one can write:

$$p = -\frac{ie}{2\pi} \log(\det[\mathcal{W}_{x,k}]) \mod e. \quad (2.1.15)$$

Furthermore, in the thermodynamic limit, defining the Berry connection $[\mathcal{A}(k)]^{n,m} = -i \langle u_k^n | \partial_k u_k^m \rangle$ yields:

$$p = -\frac{ie}{2\pi} \log \left(\det \left[e^{-i \int_k^{k+2\pi} \mathcal{A}(k) dk} \right] \right) \mod e \quad (2.1.16)$$

$$= -\frac{e}{2\pi} \int_k^{k+2\pi} \text{Tr} \{ \mathcal{A}(k) \} dk \mod e, \quad (2.1.17)$$

which is the expression of polarization in the modern theory of polarization [66].

2.1.2 Polarization in 2D crystals

The formalism presented in 2.1.1 can be generalized for 2D crystals. Most of the algebraic and analytical arguments presented previously follow in the 2D case. However, one starts by noticing that the projected position operator now has an additional index k_y :

$$P^{\text{occ}} \hat{x} P^{\text{occ}} = \sum_{n,m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}} \gamma_{\mathbf{k}+\Delta k_x, n}^\dagger |0\rangle \langle u_{\mathbf{k}+\Delta k_x}^n | u_{\mathbf{k}}^m \rangle \langle 0 | \gamma_{\mathbf{k}, m}. \quad (2.1.18)$$

This operator is diagonal in k_y and therefore their eigenstates can be labeled by k_y . Each block of this matrix diagonalizes as in the 1D case. Thus, the Wannier functions are:

$$|\psi_{R_x, k_y}^j\rangle = \frac{1}{\sqrt{L_x}} \sum_{n=1}^{N_{\text{occ}}} \sum_{k_x} \gamma_{n, \mathbf{k}}^\dagger |0\rangle [v_{x, \mathbf{k}}^j]^n e^{-ik_x R_x}, \quad (2.1.19)$$

where $\langle \psi_{R_x, k_y}^i | \psi_{R'_x, k'_y}^j \rangle = \delta_{R_x, R'_x} \delta_{i,j} \delta_{k_y, k'_y}$. The Wilson loop operator is defined exactly in the same way. However, it also depends on k_y . Its eigenvalue equation becomes:

$$\mathcal{W}_{x,\mathbf{k}} \left| \nu_{x,\mathbf{k}}^j \right\rangle = e^{2\pi i \nu_x^j(k_y)} \left| \nu_{x,\mathbf{k}}^j \right\rangle. \quad (2.1.20)$$

Just as in the 1D case, the Wilson loop eigenvectors $\left| \nu_{x,\mathbf{k}}^j \right\rangle$ depend on the starting value of $\mathbf{k}$. However, its phases $\nu_x^j(k_y)$ now depend on k_y . The contribution to polarization follows in the same manner as in the 1D case, yielding:

$$p_x(k_y) = e \sum_j \nu_x^j(k_y) \quad (2.1.21)$$

$$p_x(k_y) = -\frac{ie}{2\pi} \log(\det[\mathcal{W}_{x,\mathbf{k}}]) \mod e. \quad (2.1.22)$$

To obtain the bulk polarization, we need to sum over all allowed k_y such that:

$$p_x = \frac{1}{L_y} \sum_{k_y} p_x(k_y) \quad (2.1.23)$$

2.1.3 Wannier Bands and Nested Wilson loop

Now that we know how to compute the bulk polarization of a 2D crystal, we turn our attention to higher-order bulk multipole moments, such as the quadrupole moment density. It has been shown that $\mathcal{W}_{x,\mathbf{k}} = e^{i\mathcal{H}_{\mathcal{W}_x}(k_y)}$ where $\mathcal{H}_{\mathcal{W}_x}$ is adiabatically connected to the physical boundary Hamiltonian [64]. It follows that the topological properties of $\mathcal{H}_{\mathcal{W}_x}$ are the same as the true boundary Hamiltonian. This is where the nested Wilson loop approach reveals its potential. We can, for instance, start by performing a regular Wilson loop along x and then perform a second Wilson loop over the Wannier bands. In this manner, the second Wilson loop characterizes boundary topology. As stated, a system with a bulk quadrupole moment q_{xy} has edge polarizations with $q_{xy} = p_x = p_y$. Classically, this can be done projecting the tensor q_{ij} onto each boundary.

All the calculations necessary to reach the end of this section are in A.2, following the work presented in [49, 67]. The phases $\nu_x^j(k_y)$ of the first Wilson loop define a new band structure adiabatically connected to that of the edge Hamiltonian, being defined in the BZ with $k_y = [-\pi, \pi[$. To have a nontrivial topological phase defined by a bulk quadrupole moment, one needs a boundary Hamiltonian with a gapped band structure, this way one defines the Wannier sectors ν_x^- and ν_x^+ that are the set of Wannier bands such that:

$$\begin{aligned} \nu_x^- &= \{ \nu_x^j(k_y) : \forall j \text{ } \nu_x^j(k_y) \text{ below the gap} \} \\ \nu_x^+ &= \{ \nu_x^j(k_y) : \forall j \text{ } \nu_x^j(k_y) \text{ above the gap} \}. \end{aligned}$$

With the band structure of the edge defined, the objective is to perform a second Wilson loop in the y direction. The reasoning is analogous to what was previously presented. We define the projector that spans the occupied Wannier sectors as:

$$P_{\nu_x} = \sum_{j=1}^{N_W} \sum_{R_x, k_y} \left| \psi_{R_x, k_y}^j \right\rangle \left\langle \psi_{R_x, k_y}^j \right| = \sum_{j=1}^{N_W} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}} \gamma_{n, \mathbf{k}}^\dagger |0\rangle \left[v_{x, \mathbf{k}}^j \right]^n \left[\left(v_{x, \mathbf{k}}^j \right)^* \right]^m \langle 0 | \gamma_{m, \mathbf{k}}, \quad (2.1.24)$$

where N_W is the number of occupied Wannier sectors. To study the topological properties of the boundary Hamiltonian, one needs to project the position operator $\hat{y}$ into the occupied Wannier sector ($P_{\nu_x} \hat{y} P_{\nu_x}$). The position operator $\hat{y}$ has an analogous expression to eq. 2.1.1. Thus, it takes the form:

$$\hat{y} = \sum_{\mathbf{k}, \alpha} c_{\mathbf{k}+\Delta k_y, \alpha}^\dagger |0\rangle \langle 0| c_{\mathbf{k}, \alpha}. \quad (2.1.25)$$

To simplify notation and calculations, the following definitions are used:

$$\left| \omega_{x, \mathbf{k}}^j \right\rangle = \sum_{n=1}^{N_{\text{occ}}} \left[v_{x, \mathbf{k}}^j \right]^n |u_{\mathbf{k}}^n\rangle \quad (2.1.26)$$

$$\left[F_{y, \mathbf{k}}^{\nu_x} \right]^{n, m} = \sum_{i, j=1}^{N_W} \left[v_{x, \mathbf{k}+\Delta k_y}^i \right]^n \left\langle \omega_{x, \mathbf{k}+\Delta k_y}^i | \omega_{x, \mathbf{k}}^j \right\rangle \left[\left(v_{x, \mathbf{k}}^j \right)^* \right]^m. \quad (2.1.27)$$

Then, $P_{\nu_x} \hat{y} P_{\nu_x}$ has the form:

$$P_{\nu_x} \hat{y} P_{\nu_x} = \sum_{n, m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}} \gamma_{n, \mathbf{k}+\Delta k_y}^\dagger |0\rangle \left[F_{y, \mathbf{k}}^{\nu_x} \right]^{n, m} \langle 0 | \gamma_{m, \mathbf{k}}. \quad (2.1.28)$$

Note that this operator is diagonal in k_x . To diagonalize it, one proceeds exactly the same way as presented in the previous section, which leads to the definition of the second Wilson loop:

$$\left[\mathcal{W}_{y, \mathbf{k}}^{\nu_x} \right]^{m, n} = \sum_{i, j=1}^{N_W} \left[v_{x, \mathbf{k}}^i \right]^m \left[\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x} \right]^{i, j} \left[\left(v_{x, \mathbf{k}}^j \right)^* \right]^n, \quad (2.1.29)$$

where $\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x} = \prod_{j=0}^{L_y} \tilde{F}_{y, \mathbf{k}+j\Delta k_x}^{\nu_x}$ is the Wilson loop performed in the y direction over the Wannier basis and $\left[\tilde{F}_{y, \mathbf{k}}^{\nu_x} \right]^{i, j} = \left\langle \omega_{x, \mathbf{k}+\Delta k_y}^i | \omega_{x, \mathbf{k}}^j \right\rangle$. In fact, we only need to work with $\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x}$ since it is connected by a unitary transformation to $\mathcal{W}_{y, \mathbf{k}}^{\nu_x}$ (we further discuss this in A.2). To compute the Wannier sector polarizations, i.e., the boundary polarization, we diagonalize the Wilson loop $\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x}$ such that it obeys the following eigenvalue equation:

$$\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x} \left| \tilde{\nu}_{y, \mathbf{k}}^{\nu_x, j} \right\rangle = e^{2\pi i \tilde{\nu}_{y, \mathbf{k}}^{\nu_x, j}(k_x)} \left| \tilde{\nu}_{y, \mathbf{k}}^{\nu_x, j} \right\rangle. \quad (2.1.30)$$

Then the boundary polarization contribution from each k_x is:

$$p_y^{\nu_x}(k_x) = -\frac{ei}{2\pi} \log \det \left[\tilde{\mathcal{W}}_{y, \mathbf{k}}^{\nu_x} \right] \mod e, \quad (2.1.31)$$

and the total polarization of the Wannier sector ν_x :

$$p_y^{\nu_x} = \frac{1}{N_x} \sum_{k_x} p_y^{\nu_x}(k_x). \quad (2.1.32)$$

Furthermore, in the thermodynamic limit, defining the Berry connection over the Wannier sector $\left[\tilde{\mathcal{A}}_{y,\mathbf{k}}^{\nu_x}\right]^{n,m} = -i \left\langle \omega_{x,\mathbf{k}}^n | \partial_{k_y} \omega_{x,\mathbf{k}}^m \right\rangle$ yields:

$$p_y^{\nu_x} = -\frac{e}{(2\pi)^2} \int_{\text{BZ}} \text{Tr} \left\{ \tilde{\mathcal{A}}_{y,\mathbf{k}}^{\nu_x} \right\} d^2\mathbf{k} \mod e. \quad (2.1.33)$$

Final Remarks

Until now, we have explored how Wilson loops emerge from the projected position operator and, consequently, how polarization is connected to these operators. For the reader not as versed in topology, the connection between Wilson loops and topological indexes might not be clear. The last Wilson loop defines a topological $\mathbb{Z}$ index of the boundary, the winding number (ν).

$$\nu = -\frac{i}{\pi} \log \det \left[\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x} \right] \quad (2.1.34)$$

The winding number effectively fixes the polarization ($p = \nu/2 \mod 1$). Furthermore, topologically, it counts the number of zero-energy boundary states per boundary that appear when the boundaries of the system are opened. In this manner, computing the winding number for each direction (ν_x and ν_y) tells us the total number of zero-energy boundary states² and thus defines bulk topology.

2.2 Real Space Multipole Operators

Wilson loops are an efficient way of calculating the topological properties of a system. However, its validity holds if certain conditions are met, such as translation invariance or the presence of a spectral gap. Moreover, Wilson loops are computationally more complex in the absence of translational symmetry and fail when reflection symmetries commute since there is no Wannier gap [49]. Another way to compute multipole moments in crystals is through their classical definition and, using Resta's argument, construct the quantum mechanical equivalent. Resta in Ref. [65] starts off with the intent of computing $\langle X \rangle$. As it turns out, $\langle X \rangle$ equals the total dipole moment of the system in units of e (electric charge):

$$\langle \hat{X} \rangle = \frac{L}{2\pi} \text{Im} \log \langle \Psi_0 | e^{i\frac{2\pi}{L} \sum_x x \hat{n}(x)} | \Psi_0 \rangle \mod L, \quad (2.2.1)$$

where $\hat{n}(x) = c_x^\dagger c_x$. One might be tempted to argue that $\langle \hat{X} \rangle = \int dx x n(x)$ is the correct definition. However, in a PBC system, the wave function obeys:

$$\psi(x_1, \dots, x_i, \dots, x_N) = \psi(x_1, \dots, x_i + L, \dots, x_N) \quad (2.2.2)$$

and thus $\langle \hat{X} \rangle$ is not invariant under translations. Under a translation of L , $\langle \hat{X} \rangle \rightarrow \langle \hat{X} \rangle + L$. Thus, in systems with Hilbert space defined by eq. 2.2.2 this operator is ill-defined. Using the proposed average

² $2(\nu_x + \nu_y)$ in 2D

value with the exponential makes $\langle \hat{X} \rangle$ invariant since the ground states are invariant under a translation of L and the exponential is defined mod L . In Refs. [68, 69] these arguments are generalized to obtain higher-order multipole moments such as the quadrupole moment density per unit cell. These are defined as:

$$\tilde{p}_x = \frac{1}{2\pi} \text{Im} \log \langle \Psi_0 | e^{2\pi i \sum_x \hat{p}_x} | \Psi_0 \rangle \quad \text{mod } 1 \quad (2.2.3)$$

$$\tilde{q}_{xy} = \frac{1}{2\pi} \text{Im} \log \langle \Psi_0 | e^{2\pi i \sum_{\mathbf{r}} \hat{q}_{xy}(\mathbf{r})} | \Psi_0 \rangle \quad \text{mod } 1, \quad (2.2.4)$$

where $\hat{p}_x = \frac{x\hat{n}(x)}{L_x}$, $\hat{q}_{xy}(\mathbf{r}) = \frac{xy\hat{n}(\mathbf{r})}{L_x L_y}$ and $|\Psi_0\rangle$ is the many-body ground state of the system. This approach full knowledge of the many body ground state of the system, since the exponential operators are many-body operators. The question that remains is how do we implement this method in a crystalline system. It is well known that $\langle \Psi_0 | \Psi_0 \rangle = \det(U_o^\dagger U_o)$ is a Slater determinant in the absence of interactions, where U_o in real space takes the form:

$$U_o = \begin{pmatrix} \varphi_{\mathbf{r}_1}^{(1)} & \varphi_{\mathbf{r}_1}^{(2)} & \dots & \varphi_{\mathbf{r}_1}^{(N_{occ})} \\ \varphi_{\mathbf{r}_2}^{(1)} & \varphi_{\mathbf{r}_2}^{(2)} & \dots & \varphi_{\mathbf{r}_2}^{(N_{occ})} \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\mathbf{r}_N}^{(1)} & \varphi_{\mathbf{r}_N}^{(2)} & \dots & \varphi_{\mathbf{r}_N}^{(N_{occ})} \end{pmatrix}, \quad (2.2.5)$$

with each column a single particle state. In the real space basis, $e^{2\pi i \sum_x \hat{p}_x}$ is very straightforward since it is diagonal, thus:

$$\langle x_1, x_2, \dots, x_N | e^{i \frac{2\pi}{L_x} \sum_x x \hat{n}(x)} | \Psi \rangle = e^{\frac{2\pi i}{L_x} (x_1 + x_2 + \dots + x_N)} \langle x_1, x_2, \dots, x_N | \mathbb{I} | \Psi \rangle = \langle x_1, x_2, \dots, x_N | \mathbb{I} | \tilde{\Psi} \rangle, \quad (2.2.6)$$

with $|\tilde{\Psi}\rangle = e^{i \frac{2\pi}{L_x} \sum_x x \hat{n}(x)} | \Psi \rangle$. In this manner, $e^{i \frac{2\pi}{L_x} \sum_x x \hat{n}(x)}$ can be interpreted as the matrix $D_1 = \text{diag} \{ e^{2\pi i x_j / L_x} \}_{j=1}^N$, which leads to $\langle \Psi_0 | e^{2\pi i \sum_x \hat{p}_x} | \Psi_0 \rangle = \langle \Psi_0 | \tilde{\Psi}_0 \rangle = \det(U_o^\dagger \tilde{U}_o)$, where $\tilde{U}_o$ is defined by $D_1 U_o$. The same argument can be used for the quadrupole moment in 2D. The only change that is required is the that $D_2 = \text{diag} \{ e^{2\pi i x_j y_j / (L_x L_y)} \}_{j=1}^N$. Following this, the multipole moments can be computed via:

$$\tilde{p}_x = \frac{1}{2\pi} \text{Im} \log \det(U_o^\dagger D_1 U_o) \quad \text{mod } 1 \quad (2.2.7)$$

$$\tilde{q}_{xy} = \frac{1}{2\pi} \text{Im} \log \det(U_o^\dagger D_2 U_o) \quad \text{mod } 1. \quad (2.2.8)$$

For the quadrupole moment, it is hard to reach large system sizes, since this method implies diagonalizing the single particle $\mathcal{H}$ that has the dimension of the Hilbert space $n_{\text{orb}} L_x L_y$. In Refs. [69, 70, 71] the authors argue that these definitions need corrections. Thus, the polarization and quadrupole moment are defined as:

$$p_x = \left(\tilde{p}_x - p_x^{(0)} \right) \mod 1 \quad (2.2.9)$$

$$q_{xy} = \left(\tilde{q}_{xy} - q_{xy}^{(0)} \right) \mod 1m \quad (2.2.10)$$

where $p_x^{(0)}$ and $q_{xy}^{(0)}$ correspond to the background positive charge contributions:

$$p_x^{(0)} = \sum_{j=1}^N \frac{x_j}{L} \mod 1 \quad (2.2.11)$$

$$q_{xy}^{(0)} = \frac{1}{2} \sum_{j=1}^N \frac{x_j y_j}{L_x L_y} \mod 1. \quad (2.2.12)$$

For the present case we will be focusing our attention on the BBH model, which is a 2D model with 4 orbitals per unit cell, and the SSH model, which has 2 orbitals per unit cell both at half filling $N = 2N_{occ}$. Thus, in these particular cases the background contributions are:

$$p_x^{(0)} = \frac{L_x+1}{2} \mod 1 \quad q_{xy}^{(0)} = \frac{(L_x+1)(L_y+1)}{2} \mod 1, \quad (2.2.13)$$

which yield an additional phase factor depending on the parity of L_x, L_y . An insulator at half filling that preserves chiral symmetry obeys $2q_{xy} = 0 \mod 1$. In Appendix B, we show that chiral symmetry is responsible for this quantization.

2.3 Localization Methods

2.3.1 Inverse Participation Ratio (IPR) and Scaling

A detailed characterization of localization properties is fundamental when studying condensed matter. A simple way of tackling this problem is through an analysis of the inverse participation ratio (IPR) and its behavior with system size. Consider a state $|\psi\rangle$, for a given basis $\{|\phi_n\rangle\}$ the IPR is defined as:

$$\text{IPR} = \frac{\sum_n |\langle \phi_n | \psi \rangle|^4}{\left(\sum_n |\langle \phi_n | \psi \rangle|^2 \right)^2}. \quad (2.3.1)$$

Any basis can be considered in IPR calculations. Nonetheless, in the present context, we are more interested in the real-space and k-space localization properties. States are distinguished according to three types of localization: extended, critical and localized. Consider a system with volume N . An extended state with a homogenous distribution has $|\langle \mathbf{r} | \psi \rangle|^2 = \frac{1}{N}$, such that $\text{IPR} = \frac{1}{N}$. On the other hand, for a fully localized state $|\langle \mathbf{r} | \psi \rangle|^2 = \delta_{\mathbf{r}, \mathbf{0}}$, which yields $\text{IPR} = 1$. So it is clear that the IPR has a dependency on system size, and thus in the thermodynamic limit, delocalized states have an IPR going to zero and localized states have their IPR remaining constant. With this in mind, we introduce the idea of scaling. The best way of concluding if a state is localized or extended with IPR is through the analysis of its dependency on system size, $N \propto L^D$, where D is the dimension of the system. In this manner, we

propose that $\text{IPR} = aL^{-D_2}$, such that:

$$\begin{cases} D_2 = D & \text{extended} \\ D_2 \in]0, D[& \text{critical} \\ D_2 = 0 & \text{localized} \end{cases}, \quad (2.3.2)$$

where D_2 is the fractal dimension. Numerically, in order to estimate D_2 the IPR is computed for a set of states on a given energy window for various L . Then a fit to the data is performed, estimating a and D_2 .

As stated, the calculation of the IPR can be done on any basis of our choice, always keeping in mind that the localization properties inferred from said IPR calculation are relative to the chosen basis. With this in mind, it is usually relevant to compute the IPR in reciprocal space, IPR_k . Here, one usually finds two different regimes. For localized states in k -space we are in a ballistic regime, while for extended states in k -space and in real space the system is in a diffusive regime. Due to the Heisenberg uncertainty principle, a given state $|\psi\rangle$ cannot be simultaneously localized in real and reciprocal space. Furthermore, since in the clean limit the solutions to the Schrödinger equation are Bloch waves with well-defined $\mathbf{k}$ (which are localized functions in reciprocal space), their IPR is compatible with that of an extended state.

2.3.2 Transfer Matrix Method (TMM)

Here TMM is presented [72, 73], which allows us to obtain the localization length of the electrons wave functions at a given energy E . Its implementation on 2D systems enables the classification of electronic states as localized, extended or critical. In this thesis, it is applied in the context of the study of the localization properties of the BBH model under disordered potentials, either to study gap edge properties or to cross-check gap and topological results. This method is of general implementation. Nonetheless, here we stick with the implementation in a square lattice geometry, that will be employed afterward.

For implementing this model in a 2D system, we start by defining a system with N_L and M unit cells along the longitudinal and transverse directions, respectively, keeping in mind that $N_L \gg M$. Its implementation on a square lattice with nearest neighbors (NN) hoppings is straight-forward. We choose the x direction as the transversal one and the y direction as the longitudinal one. A tight binding model with hoppings between NN unit cells has a tridiagonal form:

$$\mathcal{H} = \sum_{n=1}^{N_L} \sum_{i,j=1}^M \left(|n, i\rangle h_n^{ij} \langle n, j| + |n+1, i\rangle V_{n+1,n}^{ij} \langle n, j| + |n-1, i\rangle V_{n-1,n}^{ij} \langle n, j| \right), \quad (2.3.3)$$

where the state $|n, i\rangle$ belongs to the local site basis with i being the orbital index in the n -th strip and h_n^{ij} is the n -th stripe internal matrix elements including NN hoppings and onsite energies. To further simplify notation, notice that $\mathbf{h}_n$ represents the Hamiltonian of the n^{th} stripe and $\mathbf{V}_{n+1,n} = \mathbf{V}_{n-1,n}^\dagger = \mathbf{V}_n$ represent the couplings between consecutive stripes. All of these matrices have dimensions $n_{\text{orb}}M \times n_{\text{orb}}M$. In this manner, the Hamiltonian in matrix form is:

$$\mathcal{H} = \begin{pmatrix} \mathbf{h}_1 & \mathbf{V}_1^\dagger & 0 & 0 & 0 & \cdots & 0 \\ \mathbf{V}_1 & \mathbf{h}_2 & \mathbf{V}_2^\dagger & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{V}_2 & \mathbf{h}_3 & \mathbf{V}_3^\dagger & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{V}_3 & \mathbf{h}_4 & \mathbf{V}_4^\dagger & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{V}_{N_L-2} & \mathbf{h}_{N_L-1} & \mathbf{V}_{N_L-1}^\dagger \\ 0 & 0 & 0 & \cdots & 0 & \mathbf{V}_{N_L-1} & \mathbf{h}_{N_L} \end{pmatrix}. \quad (2.3.4)$$

Consider an eigenstate $|\psi\rangle$ of $\mathcal{H}$ with energy E . The eigenstates $|\psi\rangle$ can be expanded on a local site basis $|\psi\rangle = \sum_{n,i} \psi_n^i |n, i\rangle$, and thus:

$$\begin{aligned} \langle n, i | \mathcal{H} | \psi \rangle &= E \langle n, i | \psi \rangle \Leftrightarrow \sum_j V_{n,n+1}^{ij} \psi_{n+1}^j = \sum_j \left[(E\delta_{ij} - h_n^{ij}) \psi_n^j - V_{n,n-1}^{ij} \psi_{n-1}^j \right] \\ &\Leftrightarrow \mathbf{V}_{n,n+1} \boldsymbol{\psi}_{n+1} = (E\mathcal{I} - \mathbf{h}_n) \boldsymbol{\psi}_n - \mathbf{V}_{n,n-1} \boldsymbol{\psi}_{n-1}, \end{aligned} \quad (2.3.5)$$

where in the last step we have written the equation in matrix form. We can rewrite this equation:

$$\begin{aligned} \begin{bmatrix} \mathbf{V}_{n,n+1} & 0 \\ 0 & \mathbf{V}_{n,n+1} \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi}_{n+1} \\ \boldsymbol{\psi}_n \end{bmatrix} &= \begin{bmatrix} (E\mathcal{I} - \mathbf{h}_n) & -\mathbf{V}_{n,n-1} \\ \mathcal{I} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi}_n \\ \boldsymbol{\psi}_{n-1} \end{bmatrix} \Leftrightarrow \\ &\Leftrightarrow \begin{bmatrix} \boldsymbol{\psi}_{n+1} \\ \boldsymbol{\psi}_n \end{bmatrix} = \begin{bmatrix} \mathbf{V}_{n,n+1}^{-1} (E\mathcal{I} - \mathbf{h}_n) & -\mathbf{V}_{n,n+1}^{-1} \mathbf{V}_{n,n-1} \\ \mathcal{I} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi}_n \\ \boldsymbol{\psi}_{n-1} \end{bmatrix} \\ &\Leftrightarrow \begin{bmatrix} \boldsymbol{\psi}_{n+1} \\ \boldsymbol{\psi}_n \end{bmatrix} = \mathbf{T}_n \begin{bmatrix} \boldsymbol{\psi}_n \\ \boldsymbol{\psi}_{n-1} \end{bmatrix} \\ &\Leftrightarrow \begin{bmatrix} \boldsymbol{\psi}_{n+1} \\ \boldsymbol{\psi}_n \end{bmatrix} = \mathbf{M}_n \begin{bmatrix} \boldsymbol{\psi}_1 \\ \boldsymbol{\psi}_0 \end{bmatrix}, \end{aligned} \quad (2.3.6)$$

where $\mathbf{T}_n$ is the a $2n_{\text{orb}}M \times 2n_{\text{orb}}M$ matrix known as the transfer matrix of the system and $\mathbf{M}_n$ is the product of all the transfer matrices from $\mathbf{T}_n$ to $\mathbf{T}_1$. $\mathbf{M}_n$ satisfies the Oseledets theorem [74] which proves the existence of the limiting matrix $\boldsymbol{\Gamma}$, such that:

$$\boldsymbol{\Gamma} = \lim_{N_L \rightarrow \infty} \left(\mathbf{M}_{N_L} \mathbf{M}_{N_L}^\dagger \right)^{\frac{1}{2N_L}}. \quad (2.3.7)$$

This limiting matrix has eigenvalues e^{γ_i} , with $i \in \{1, 2, \dots, 2n_{\text{orb}}M\}$ and γ_i being the Lyapunov exponents of the matrix $\mathbf{M}_{N_L}$. If $|\nu_i\rangle$ is an eigenvector of $\boldsymbol{\Gamma}$, then Oseledets theorem implies that:

$$\lim_{N_L \rightarrow \infty} \frac{1}{N_L} \ln (|\langle \nu_i | \mathbf{M}_{N_L} | \nu_i \rangle|) = \gamma_i \quad (2.3.8)$$

These exponents control the exponential increase ($\gamma_i > 0$) or decrease ($\gamma_i < 0$) of the wave function along the longitudinal direction. The negative Lyapunov exponents should not contribute in the thermodynamic limit since they should quickly “kill” the wave function amplitudes. Thus, we are interested on studying

the positive exponents. For a given system size M , the Lyapunov positive exponents are the inverse of the localization lengths λ_M . The smallest γ_i corresponds to the biggest localization length, and thus the measured localization length of any given state is $\lambda_M = \min\{\gamma_i\}$. As usual, these types of studies are accompanied by scaling analysis, and TMM is no exception, such that the quantity of interest is $\Lambda_M = \lambda_M/M$. If Λ_M goes to zero as M increases, the states at the considered energy are localized; if Λ_M grows with M , the states are extended; and if Λ_M does not scale with M then the states are critical.

It appears we have all the tools to implement this method. However the nature of the Lyapunov exponents presents some caveats. If we take the product of $\mathbf{T}_n$ matrices N_L times, the ratio between the biggest and smallest Lyapunov exponents would quickly be of the order of machine precision (10^{-16}), and thus we would only be capable of computing the largest exponent. To surpass this, we can perform a $\mathbf{QR}$ decomposition of $\mathbf{M}_n$ each k products of $\mathbf{T}_n$, where $\mathbf{Q}$ is an unitary matrix ($\mathbf{Q}^{-1} = \mathbf{Q}^\dagger \implies \mathbf{Q}^\dagger \mathbf{Q} = \mathcal{I}$) and $\mathbf{R}$ is an upper triangular matrix. Taking these successive decompositions, one arrives at:

$$\begin{aligned} \mathbf{M}_{N_L} &= \prod_{i=1}^{N_L} \mathbf{T}_i = \left(\prod_{i=k+1}^{N_L} \mathbf{T}_i \right) \prod_{i=1}^k \mathbf{T}_i = \left(\prod_{i=k+1}^{N_L} \mathbf{T}_i \right) \mathbf{Q}^{(1)} \mathbf{R}^{(1)} = \left(\prod_{i=2k+1}^{N_L} \mathbf{T}_i \right) \left(\prod_{i=k+1}^{2k} \mathbf{T}_i \mathbf{Q}^{(1)} \right) \mathbf{R}^{(1)} \\ &= \left(\prod_{i=2k+1}^{N_L} \mathbf{T}_i \right) \mathbf{Q}^{(2)} \mathbf{R}^{(2)} \mathbf{R}^{(1)} = \dots = \mathbf{Q}^{(n)} \prod_{i=1}^n \mathbf{R}^{(i)} = \mathbf{Q}^{(n)} \tilde{\mathbf{R}}^{(n)}, \end{aligned} \quad (2.3.9)$$

where $n = \frac{N_L}{k}$ and $\tilde{\mathbf{R}}^{(n)} = \prod_{i=1}^n \mathbf{R}^{(i)}$. Assuming that the Lyapunov exponents are in ascending order $\gamma_1 < \gamma_2 < \dots < \gamma_{2n_{\text{orb}}M}$ and through equation 2.3.8 it can be shown:

$$\lim_{n \rightarrow \infty} \frac{1}{nk} \ln \left(\tilde{R}_{ll}^{(n)} \right) = \lim_{n \rightarrow \infty} \frac{1}{nk} \sum_{i=1}^n \ln \left(R_{ll}^{(i)} \right) = \gamma_{2n_{\text{orb}}M-l-1}. \quad (2.3.10)$$

In this manner, we only need to store the diagonal entries of $\mathbf{R}^{(n)}$ every time a $\mathbf{QR}$ decomposition is made to compute all the Lyapunov exponents and then select the smaller positive one. The choice of k needs to be tuned to each particular problem. For clean systems $k = 10$ is usually enough to not lose information on $\min\{\gamma_i\}$. However, for disordered systems, a smaller k might be needed³. The choice of N_L can be made taking into account the convergence of λ_M . For this, we introduce the coefficients c_i and d_i :

$$\begin{aligned} c_1^{(i)} &= \ln R_{ii}^{(1)} \\ c_j^{(i)} &= c_{j-1}^{(i)} + \ln R_{ii}^{(j)}, j \in \{2, \dots, n\} \\ d_1^{(1)} &= \left(\ln R_{ii}^{(1)} \right)^2 \\ d_j^{(i)} &= d_{j-1}^{(i)} + \left(\ln R_{ii}^{(j)} \right)^2, j \in \{2, \dots, n\}. \end{aligned} \quad (2.3.11)$$

The variance of random variables $\left\{ \ln R_{ii}^{(1)}, \dots, \ln R_{ii}^{(n)} \right\}$ is given by

³Usually $k = 2$ is enough.

$$\Delta_n^{(i)} = \sqrt{\frac{d_n^{(i)}}{n} - \left(\frac{c_n^{(i)}}{n}\right)^2}. \quad (2.3.12)$$

Since we are interested in studying the convergence of $\lambda_M^{-1} = \min\{\gamma_i\} = \frac{c_n}{nk}$ we can compute the relative error of λ_M^{-1} by using that the standard deviation of the average c_n/n is $\Delta_n/\sqrt{n}$, thus the relative error of λ_M^{-1} is:

$$\epsilon = \frac{\Delta_n \sqrt{n}}{c_n}. \quad (2.3.13)$$

Throughout this work, the the value for N_L is chosen to be a minimum, such that $\epsilon < 1\%$.

2.4 Spectral Methods

2.4.1 Kernel Polynomial Expansion (KPM) and the Density of States (DOS)

Here we explore a well known method initially presented and implemented in [75] to compute the time evolution operator $U(t, t_0)$. As it turns out, this method has applications in the computation of several important quantities, such as the DOS of a system. It is of particular interest since it is far more efficient than exact diagonalization, which allows us to consider systems closer to the thermodynamic limit, thus removing finite-size effects.

Chebyshev Polynomials

The main trick of this method is that one can expand any analytical function in terms a of an power series. We start by defining the Chebyshev polynomials $T_n(x)$:

$$T_n(x) = \cos(n \arccos(x)). \quad (2.4.1)$$

At first glance, it is evident that these polynomials are defined in a given domain $x \in [-1, 1]$. These polynomials obey the recursive relation:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad (2.4.2)$$

and follow the orthogonality condition

$$\int_{-1}^1 \frac{T_n(x)T_m(x)}{\pi\sqrt{1-x^2}} dx = \frac{1+\delta_{n,0}}{2} \delta_{n,m}. \quad (2.4.3)$$

In this manner, one can define any integrable function with $f :]-1, 1[\rightarrow \mathbb{R}$, as a series of Chebyshev polynomials:

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x). \quad (2.4.4)$$

To compute the coefficients a_n , we make use of 2.4.3 which yields:

$$a_n = \frac{2}{1 + \delta_{n,0}} \int_{-1}^1 \frac{dx}{\pi \sqrt{1-x^2}} T_n(x) f(x). \quad (2.4.5)$$

For practicality, the coefficients a_n can be rewritten at the cost of a new set of coefficients, yielding the following expression:

$$f(x) = \sum_{n=0}^{\infty} \frac{2\Delta_n}{1 + \delta_{n,0}} T_n(x) \quad (2.4.6)$$

$$\Delta_n = \int_{-1}^1 \frac{dx}{\pi \sqrt{1-x^2}} T_n(x) f(x). \quad (2.4.7)$$

With this in mind, for a given function $f : [-1, 1] \rightarrow \mathbb{R}$ it is enough to compute Δ_n to fully obtain its Chebyshev polynomial expansion.

Expansion of Dirac Delta in Chebyshev Series

Since our goal is to compute the DOS using KPM, we need to know the form of $\delta(x)$ in Chebyshev polynomials. For the Dirac delta function $\delta(x - \tilde{\epsilon})$, where $\tilde{\epsilon} \in [-1, 1]$, it follows:

$$\begin{aligned} \Delta_n &= \int_{-1}^1 \frac{dx}{\pi \sqrt{1-x^2}} T_n(x) \delta(x - \tilde{\epsilon}) \\ &= \frac{T_n(\tilde{\epsilon})}{\pi \sqrt{1-\tilde{\epsilon}^2}}. \end{aligned} \quad (2.4.8)$$

With 2.4.6 and 2.4.8 is trivial to conclude:

$$\delta(x - \tilde{\epsilon}) = \frac{1}{\pi \sqrt{1-\tilde{\epsilon}^2}} \left(1 + 2 \sum_{n=1}^{\infty} T_n(\tilde{\epsilon}) T_n(x) \right). \quad (2.4.9)$$

Chebyshev Polynomials and Operators

Functions of operators $f(A)$ are well-defined when the respective functions have a power series expansion. Using the recursive relation 2.4.2 it can be shown that $T_n(x)$ is indeed a polynomial, thus the operator $T_n(A)$ is well-defined and is trivial in the basis that diagonalizes A . Keeping in mind that the Chebyshev polynomials are only defined for $x \in]-1, 1[$, the eigenvalues of the operator A also need to fall within this interval. In this manner, the objective is to compute moments of the type:

$$\mu_m = \langle \psi | T_m(A) | \phi \rangle. \quad (2.4.10)$$

The first two moments are trivially defined using $T_0(x) = 1$ and $T_1(x) = x$

$$\mu_0 = \langle \psi | \phi \rangle \quad (2.4.11)$$

$$\mu_1 = \langle \psi | A | \phi \rangle. \quad (2.4.12)$$

We can then use the recursion relation 2.4.2 to compute the higher-order moments. Making use of the notation $|\phi_m\rangle = T_m(A)|\phi\rangle$, we can write:

$$|\phi_{m+1}\rangle = 2A|\phi_m\rangle - |\phi_{m-1}\rangle. \quad (2.4.13)$$

Taking the bra with the previous equation, one gets the recursion relation for the moments:

$$\mu_{m+1} = \langle\psi|2A|\phi_m\rangle - \mu_{m-1}. \quad (2.4.14)$$

The same approach is valid if we want to compute moments of the form $\mu_m^B = \langle\psi|BT_m(A)|\phi\rangle$. This can be tackled if we define $\langle\psi^B| = \langle\psi|B$ since $\mu_m^B = \langle\psi^B|T_m(A)|\phi\rangle$, which has the same form of the previously considered moments.

Stochastic Evaluation of the Trace

Before we are able to use this formalism to compute the DOS of a system, we still need an efficient way of calculating objects of the type $\text{Tr}[f(A)]$. As we know, we can expand the function f at the cost of a Chebyshev series and so using the linear property of the trace, we only need to know how to calculate $\text{Tr}[T_m(A)]$. Let $\{|\psi_i\rangle\}$ be the base in which A is represented. Then $\text{Tr}[T_m(A)] = \sum_i \langle\psi_i|T_m(A)|\psi_i\rangle$. This is a terrible approach to compute the trace since for each term in the Chebyshev series we will have to take the previous sum over all states $\{|\psi_i\rangle\}$, if A has dimension D , then this sum involves D moments $\langle\psi_i|T_m(A)|\psi_i\rangle$. There is a more efficient way of computing this trace, which starts by defining the following random vector:

$$|r\rangle = \sum_i \xi_i^r |\psi_i\rangle, \quad (2.4.15)$$

such that the coefficients ξ_i^r have the following properties:

$$\langle\xi_i^r\rangle = 0 \quad \langle\xi_i^r \xi_j^{r'}\rangle = \delta_{r,r'} \delta_{i,j} \quad (2.4.16)$$

The easiest way of defining ξ_i^r is by considering a phase that is uniformly distributed in the interval $\theta \in [0, 2\pi[$, and then taking the complex exponential $\xi_j^r = e^{i\theta}$. The trace of the operator can be estimated by taking averages over different initial random vectors:

$$\text{Tr}[T_m(A)] \approx \frac{1}{R} \sum_{r=0}^{R-1} \mu_m^r, \quad (2.4.17)$$

where $\mu_m^r = \langle r|T_m(A)|r\rangle$. Thus, one just needs to define a random starting vector and then apply the method explored previously to recursively compute the moments μ_m^r . The advantage of this method is that the required number of averages (R) is much smaller than the dimension (D) of the operator A , $R \ll D$. Often, setting $R = 10$ is more than enough to estimate the trace. Furthermore, the bigger the operator dimension D , the smaller the number of averages that are needed.

Density of States (DOS)

The DOS is defined as:

$$\rho(E) = \frac{1}{N} \sum_{n=0}^N \delta(E - \epsilon_n) \quad (2.4.18)$$

Where N is the dimension of the Hilbert space. We substitute the Dirac Delta by the Chebyshev series expansion 2.4.9. Since we need $E \in]-1, 1[$, a rescale of the system Hamiltonian is performed.

$$\tilde{H} = \frac{(H-b)}{\lambda} \quad \tilde{E} = \frac{(E-b)}{\lambda} \quad , \quad (2.4.19)$$

where we choose b and λ such that $\tilde{E} \in]-1, 1[$:

$$b = \frac{(E_{max} + E_{min})}{2} \quad \lambda = \frac{(E_{max} - E_{min})}{2 - \epsilon} \quad . \quad (2.4.20)$$

Scaling the energies and using $\delta(\lambda x) = \frac{1}{|\lambda|} \delta(x)$:

$$\begin{aligned} \rho(\tilde{E}) &= \frac{1}{N} \sum_{n=0}^N \delta(\lambda \tilde{E} + b - \lambda \tilde{E}_n - b) \\ &= \frac{1}{|\lambda|N} \text{Tr} \left[\delta(\tilde{E} - \tilde{H}) \right] \\ &\approx \frac{1}{|\lambda|N} \left(\frac{\Delta_0(\tilde{E})\mu_0}{2} + \sum_{m=1}^M \Delta_m(\tilde{E})\mu_m \right) , \end{aligned} \quad (2.4.21)$$

where $\Delta_m(\tilde{E}) = \frac{2T_m(\tilde{E})}{\pi\sqrt{1-\tilde{E}^2}}\omega_m^J$ and $\mu_m = \text{Tr} \left[T_m(\tilde{H}) \right]$ are computed using stochastic evaluation.

Numerically, we need to truncate the series to a finite number of M moments, in doing so, the so-called Gibbs oscillations appear around where the expanded function is discontinuous. To prevent these types of oscillations, a kernel (ω_m^J) is introduced in the definition of Δ_m . The Jackson Kernel is the common choice when computing the DOS, which broadens the Dirac deltas as Gaussian curves. Its definition is given below:

$$\omega_m^J = \frac{(M - m + 1) \cos\left(\frac{\pi m}{M+1}\right) + \sin\left(\frac{\pi m}{M+1}\right) \cot\left(\frac{\pi}{M+1}\right)}{M + 1} . \quad (2.4.22)$$

2.4.2 The Recursive method for computing the Local DOS (LDOS)

We have seen an efficient method to compute the DOS of a system using KPM. However there are other quantities of interest closely related to the DOS. An example is the LDOS. Here we present an efficient method to compute this quantity known as the recursive method [76, 77]. Let ϵ_n be an eigenvalue of $\mathcal{H}$ with eigenstate $|\phi_n\rangle$, then the LDOS $\rho(\mathbf{R}, E)$ in the local site basis $|\mathbf{R}, \alpha\rangle^4$ is:

⁴where α represents internal degrees of freedom such as orbital index

$$\rho(\mathbf{R}, \alpha, E) = \sum_n |\langle \mathbf{R}, \alpha | \phi_n \rangle|^2 \delta(E - \epsilon_n). \quad (2.4.23)$$

The Green's function is defined as usual by:

$$G(E) = (E\mathcal{I} - \mathcal{H})^{-1}, \quad (2.4.24)$$

and it contains information about the spectral properties of the system. A connection between the LDOS 2.4.23 and the local Green's function exists. We can compute the latter projecting the full Green's function 2.4.24 onto the local site basis $|\mathbf{R}, \alpha\rangle$, thus:

$$G(\mathbf{R}, \alpha, E) = \langle \mathbf{R}, \alpha | G(E) | \mathbf{R}, \alpha \rangle. \quad (2.4.25)$$

This quantity relates to the LDOS through

$$\rho(\mathbf{R}, \alpha, E) = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \text{Im} \{G(\mathbf{R}, \alpha, E + i\eta)\}. \quad (2.4.26)$$

One needs to compute $G(\mathbf{R}, \alpha, E)$ however, full inversion algorithms are inefficient for large enough systems. To obtain $G(\mathbf{R}, \alpha, E)$ we first need to define the Green's function matrix. To achieve this more efficiently, we employ a trick that will simplify our calculations further ahead. We start by computing a basis where $\mathcal{H}$ is tridiagonal, this can be done via Lanczos decomposition, as presented in appendix C.1, by setting the starting vector $|u_0\rangle = |\mathbf{R}, \alpha\rangle$, where $|\mathbf{R}, \alpha\rangle$ is the site at which we want to compute the LDOS. In the Jacobi basis ($|u_n\rangle$) the Green's function is:

$$G(E) = \begin{pmatrix} E - a_0 & -b_1 & 0 & \dots & 0 & 0 \\ -b_1 & E - a_1 & -b_2 & \dots & 0 & 0 \\ 0 & -b_2 & E - a_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & E - a_{N-2} & -b_{N-1} \\ 0 & 0 & 0 & \dots & -b_{N-1} & E - a_{N-1} \end{pmatrix}^{-1}. \quad (2.4.27)$$

Since we chose $|u_0\rangle = |\mathbf{R}, \alpha\rangle$ the local Green's function is $G(\mathbf{R}, \alpha, E) = \langle u_0 | G(E) | u_0 \rangle = G_0$ which clarifies the choice $|u_0\rangle = |\mathbf{R}, \alpha\rangle$. For each site, one needs to perform a Lanczos decomposition with a new starting vector. In appendix C.2 a recursive form of computing the matrix element G_{00} when the inverse matrix $E\mathcal{I} - \mathcal{H}$ is in Jacobi form is presented. This allows us to reach a continued fraction to compute $G_0 = G(\mathbf{R}, \alpha, E)$:

$$G_0 = \frac{1}{E - a_0 - b_1^2 \frac{1}{E - a_1 - b_2^2 \frac{1}{\ddots - b_{N-1}^2 \frac{1}{E - a_{N-1}}}}}, \quad (2.4.28)$$

where a_n and b_n are the coefficients obtained from Lanczos decomposition of the systems Hamiltonian $\mathcal{H}$. In practice, Lanczos decomposition cannot generally generate the full Hilbert space of our problem,

and for this reason, we can only compute a reduced amount of coefficients $0 < k < N$. In this manner, we truncate the continued fraction to the calculated coefficients. The LDOS in a UC $|\mathbf{R}\rangle$ is simply $\rho(\mathbf{R}, E) = \sum_{\alpha} \rho(\mathbf{R}, \alpha, E + i\eta)$ where the complex part approximates the delta Dirac function as a Lorentzian with width defined by η . The recursive method provides an efficient and fast way of computing the LDOS of a system.

2.5 Boundary Green's Function

Previously, we presented a way of computing bulk multipole moments, such as the bulk dipole and quadrupole moments. Although these are bulk properties, if we open the boundaries of the system, boundary states appear in the gap. Some of these states are topologically protected and are directly linked to these bulk quantities via bulk-boundary correspondence. There is interest in studying boundary properties, however an effective boundary Hamiltonian is needed $\mathcal{H}_{\text{Bound}}$. The boundary Green's function method [78] allows us to obtain $\mathcal{H}_{\text{Bound}}$ at a given energy.

The method yields a dimensional reduction approach of the system Hamiltonian. Just as in the case with TMM, one considers a transversal direction with PBC and size M and a longitudinal direction with OBC and size N_L . The transversal direction can be converted to reciprocal space via Fourier transform or can be left in real space representation which yields higher dimensional matrices. Let us assume that our TB Hamiltonian can be written in tridiagonal form.

$$\mathcal{H} = \sum_{n=1}^N \left[\psi_n^\dagger \mathbf{h}_n \psi_n + \psi_{n+1}^\dagger \mathbf{V}_n \psi_n + \psi_n^\dagger \mathbf{V}_n^\dagger \psi_{n+1} \right] \quad (2.5.1)$$

The Hilbert space dimension is $n_{\text{orb}} N_L M \times n_{\text{orb}} N_L M$. The matrix $\mathbf{V}_n$ is the matrix that couples consecutive transversal stripes of the system, while $\mathbf{h}_n$ is the Hamiltonian of the n th stripe. In matrix form, the Hamiltonian is tridiagonal:

$$\mathcal{H} = \begin{pmatrix} \mathbf{h}_1 & \mathbf{V}_1^\dagger & 0 & 0 & 0 & \cdots & 0 \\ \mathbf{V}_1 & \mathbf{h}_2 & \mathbf{V}_2^\dagger & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{V}_2 & \mathbf{h}_3 & \mathbf{V}_3^\dagger & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{V}_3 & \mathbf{h}_4 & \mathbf{V}_4^\dagger & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{V}_{N-2} & \mathbf{h}_{N-1} & \mathbf{V}_{N-1}^\dagger \\ 0 & 0 & 0 & \cdots & 0 & \mathbf{V}_{N-1} & \mathbf{h}_N \end{pmatrix}. \quad (2.5.2)$$

The Green function of the system is :

$$G(E) = (EI - \mathcal{H})^{-1}. \quad (2.5.3)$$

The boundary Green's function of the system is $G_N(E) = G_{NN}(E)$ which is the N th block of the full Green function of the system. Due to the simple Jacobi form of the Hamiltonian, one can take a blockwise matrix inversion analogous to C.2 to reach a Dyson equation along the longitudinal direction:

$$G_n(E) = \left(g_n^{-1} - V_{n-1} G_{n-1} V_{n-1}^\dagger \right)^{-1}, \quad (2.5.4)$$

where $g_n^{-1} = E\mathcal{I} - h_n$ is the Green's function of the n th stripe. This recursion can also be written as a continued fraction, as in eq. 2.4.28. Numerically, this equation converges to $G_N(E)$, and so we can iterate it for a given size N_L . In this manner, equation 2.5.4 should reach a fixed point defined by $G = (g^{-1} - VGV^\dagger)^{-1}$. This fixed point can be computed analytically for simple systems such as the SSH model by defining the β function, $\beta(G_n(E)) = G_n(E) - G_{n-1}(E)$ as in Ref. [78]. The zeros of the β function yield the fixed points and thus the boundary Green function. The derivative of the β function yields the stability of the given fixed point. After computing $G_N(E)$, the effective Hamiltonian of the boundary is trivially defined by:

$$\mathcal{H}_{\text{Bound}} = -(G_N(E = \epsilon_F))^{-1}, \quad (2.5.5)$$

where we have set the $E = \epsilon_F$ since we are interested in topological states that live at Fermi level. Nonetheless one can take E to be any energy.

2.6 Numerical Simulations on Quasi-Periodic Systems

Simulating incommensurate systems is more complex than simulating disordered ones. To this end, we explore some of the tricks and details relevant to having coherent and accurate results. For the sake of simplicity, throughout this chapter, we consider a 1D system with $a = 1$ and with the quasi-periodic potential of the form:

$$V_W = \frac{W}{2} \cos(2\pi\beta m + \phi_x), \quad (2.6.1)$$

where W is the strength of the potential, β the spatial frequency, m the unit cell index, and ϕ_x the phase shift. In general, for more complex quasi-periodic potentials, the arguments presented below should hold. These types of potentials can be taken to be onsite energies or hopping's modulation.

Choosing System Size (L)

The main purpose of a quasi-periodic modulation is to break translational invariance, which can only be achieved by choosing β to be an irrational number. For $\beta \in \mathbb{Q}$ the desired results is not achieved since, for any rational number $z = \frac{M}{N}$, a new unit cell of size N can be chosen, thus preserving translational invariance. These types of systems are labeled commensurate or periodic systems. We can achieve an incommensurate modulation by taking β to be any irrational number, and in this thesis one of the most common values in literature is used, the golden ratio, $\phi_{GR} = \frac{1+\sqrt{5}}{2}$. However, tackling this problem in finite systems goes beyond setting $\beta = \phi_{GR}$. To guarantee that the system remains incommensurate and in order to implement periodic boundary conditions without any boundary defect for any system size L , it is common to approximate ϕ_{GR} by a ratio of two co-prime numbers q, p . Luckily, there is a famous mathematical sequence whose ratio of consecutive numbers F_n and F_{n+1} approaches ϕ_{GR} monotonously⁵

⁵If this condition is not met, one might have defects when scaling analysis is performed, since when L is increased to reduce finite-size effects, the overall approximation of our incommensurate systems might worsen due to the ratio drifting

and whose any two consecutive pair of numbers, F_n and F_{n+1} , are co-prime. This is the Fibonacci sequence 2.1. To this end, we set $L = F_n$ and $\beta = F_{n+1}/F_n$ which avoids boundary defects and guarantees that the system remains incommensurate as we increase system size.

F_0	F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8	F_9	F_{10}	F_{11}	F_{12}	F_{13}	F_{14}	F_{15}	F_{16}	...
1	1	2	3	5	8	13	21	34	55	89	144	233	377	610	987	1597	...

Table 2.1: First 17 numbers of the Fibonacci sequence, each new number is obtained from the sum of the two that precede it.

Averaging over Phase Shifts

Nothing has been said regarding the potential phase shifts (ϕ_x). At first glance, the results should be dependent on any particular choice of ϕ_x , however, in the thermodynamic limit, the system should not depend on the choice of the phase shift. To motivate this statement, let us consider an infinite system with an observer in the middle of the lattice ($\mathbf{R} = \mathbf{0}$). For a given value of ϕ_x^0 , the observer sees a particular configuration of the potential. Now, changing $\phi_x^0 \rightarrow \phi_x^1$ the observer sees another configuration. We can translate the system (or the observer) to a new site, where he will see the initial configuration. In this manner, for a finite system with size L we average over phase shifts, but as the system approaches the thermodynamic limit, the dependence on ϕ_x vanishes. Thus, we choose ϕ_x to be uniformly distributed in the range $[0, 2\pi[$. Furthermore, for finite systems, extended states are not usually dependent on the choice of ϕ_x , while critical and localized states are more susceptible to local changes in the potential.

Averaging over Phase Twists

Beyond phase shifts, there is another quantity over which we can take averages: phase twists. To apply phase twists, the boundaries are periodically closed (as for periodic boundary conditions), but with an additional twist, such that:

$$\psi_\alpha(\mathbf{R} + L\mathbf{a}_i) = e^{i\theta_i} \psi_\alpha(\mathbf{R}), \quad (2.6.2)$$

where $\psi_\alpha(\mathbf{R}) = c_{\mathbf{R},\alpha}^\dagger |0\rangle$. To implement this in a tight binding system, we add the term $e^{i\theta_i}$ to the matrix elements at the boundary ($|n=0\rangle \langle n=L-1|$) which is equivalent to spreading this contribution over all intra-UC hopping as follows $t \rightarrow te^{i\theta_i/L_i}$. As it turns out, having the first or the latter is nothing more than choosing a particular gauge, with the latter being more intuitive. As the system approaches the thermodynamic limit, any dependence on phase twists should vanish due to $\lim_{L_i \rightarrow \infty} e^{i\theta_i/L_i} \rightarrow 1$. In contrast to phase shifts and for finite system sizes, extended and critical states are usually dependent on the choice of θ_i , while localized states remain unaffected. For these reasons, as in the previous case, we can also perform averages over phase twists by sampling θ_i from a uniform distribution defined in the interval $[0, 2\pi[$.

away from ϕ_{GR} .

Phase Twists and Spectral Gap

Not always taking averages over phase twists is to our advantage. Phase twists are slightly more tricky than phase shifts, especially when dealing with small system sizes and gap-dependent results. For a finite periodic system of size L , the allowed $\mathbf{k}$'s are $\mathbf{k}_i = \left(-\frac{\pi}{L} + \frac{2\pi}{L}n\right) \mathbf{b}_i$ with $n \in \mathbb{Z}$. Here, we have assumed that the FBZ is centered in the Γ point. Introducing phase twists leads to shifts in the allowed $\mathbf{k}$'s, such that if a twist θ_i is introduced then $\mathbf{k}_i = \left(-\frac{\pi}{L} + \frac{2\pi}{L}n + \frac{\theta_i}{L}\right) \mathbf{b}_i$.

For the sake of simplicity, consider a 1D TB system with a gap that closes at $k_x = 0$ (maximum of the valence band), and that our target computation is the calculation of the spectral gap via exact diagonalization (ED) of the Hamiltonian for a system with size L . If we set $k_n = 0$, then it follows $n = \frac{L}{2}$. Since $n \in \mathbb{Z}$, $n = \frac{L}{2}$ is valid only if L is even. However, for odd L , $k_n = 0$ is not an allowed crystalline momentum, such that performing ED of the Hamiltonian for and odd L , will lead to an overestimation of the spectral gap. This effect is particularly relevant for small L and for $|\partial_{k_x} \epsilon_{k_x}| \gg 1$. One way of tackling this problem is to consider bigger system sizes, since eventually $\frac{2\pi}{L}$ will be small enough that considering even or odd L is no longer relevant.

Due to the high computational cost of performing ED for large system sizes, another approach is required to tackle gap scaling in finite crystalline systems. We can add a twist that shifts all the allowed k_x 's in such a way that, for odd L , $k_n = 0$ is a possible value of crystalline momenta. This is achieved by considering $\theta_x = \pi$ for odd L while for even L we use regular periodic boundary conditions⁶. This trick is also relevant even if a direct calculation of the spectral gap is not being performed. Gap-dependent results as topological phases and TPT are sensible to gap closures, and thus for small systems, it is important to make an appropriate choice of phase twists even when evaluating system topology. With this in mind, throughout the main results of the thesis, it is always specified if averages over phase twists or a fixed twist were considered.

The previous argument holds when translational invariance is preserved, although it is not clear that in the absence of translational symmetry, using phase twists is advantageous. In fact, even for some disordered systems, phase twists solve spectral gap finite-size effects. Quasi-periodic systems in the low W regime maintain ballistic states at Fermi level, and so setting a non-zero twist can improve gap calculations, especially when the gap closes in a ballistic-ballistic transition. In contrast, regular uncorrelated disorder does not benefit from phase twists, since all of the electronic states are Anderson localized (for low-dimensional systems).

⁶which is the same as considering twists with $\theta_x = 0$

Chapter 3

Quasi-Periodic modulation and first-order Topology

Before tackling HOTIs it is logical that we first build up our intuition with a first-order topological insulator. To this end, we focus this chapter on the analysis of a Chern insulator under quasi-periodic modulation while maintaining brevity. This is original work that is available at arXiv [37].

3.1 Model

We consider a QBCP model in a square lattice with two orbitals per unit cell (UC), as in Ref. [79]. This model is defined by the following clean limit $\mathbf{k}$ -space Hamiltonian:

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}_{\mathbf{k}} \Psi_{\mathbf{k}}, \quad (3.1.1)$$

where $\Psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k},A}^\dagger, c_{\mathbf{k},B}^\dagger)$, with $c_{\mathbf{k},\alpha}^\dagger$ the creation operator of a state with crystal momentum $\mathbf{k}$ in the α orbital and

$$\mathcal{H}_{\mathbf{k}} = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (3.1.2)$$

with $\boldsymbol{\sigma}$ the vector of Pauli matrices and the vector $\mathbf{h}(\mathbf{k})$ given by

$$h_x = 2t_x \sin(k_x) \sin(k_y) \quad h_y = 1 + \frac{B+1}{2} (\cos(k_x) + \cos(k_y)) \quad h_z = 2t_z (\cos(k_x) - \cos(k_y)) . \quad (3.1.3)$$

Throughout this chapter, the hopping amplitudes are fixed to unity ($t_x = t_y = t = 1$), so that every physical observable with energy units comes in units of t .

For $h_y = 0$, the system is gapless with quadratic band crossing points at the Fermi level. In contrast with Dirac semimetals, QBCP systems exhibit a finite DOS at Fermi level ($\epsilon_F = 0$). Moreover, these new types of crossings display an interesting topological character since QBCP transport a total Chern number of 1, unlike Dirac cones, which transport a total Chern number of 1/2. The introduction of a non-zero h_y perturbation opens a gap and breaks time reversal symmetry, which are two ingredients

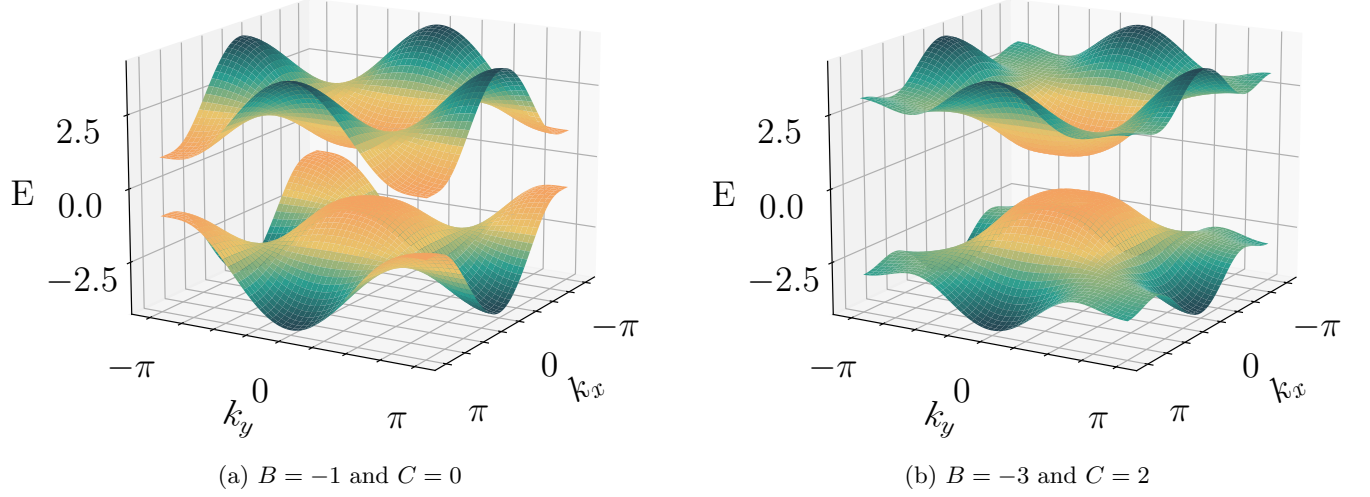


Figure 3.1: Band structure for different values of topological mass B .

needed for the emergence of Chern insulating phases. For this model, a single QBCP occurs at M for $B = 0$, and for $B = -2$ at Γ . These are the only values of B for which the system becomes gapless and where topological phase transitions between phases with $C = 2 \leftrightarrow C = 0$ ($B = -2$) and $C = 0 \leftrightarrow C = -2$ ($B = 0$) take place. For trivial phases ($C = 0$), quadratic band crossing points (QBCP in Fig. 3.1a) with symmetric berry curvatures (Fig. 3.2a) occur at $\Gamma = (0, 0)$ and $M = (\pm\pi, \pm\pi)$ points of the FBZ. When integrating over the entire FBZ, the symmetric contributions cancel each other out yielding $C = 0$, as shown in Fig. 3.2a¹. For topological phases such as $B = -3$, the QBCPs only appear at either the Γ or M points of the FBZ, as seen in Fig. 3.1b, which leads to $C = 2$ phases. This is justified by the fact that the Berry curvature is either positive or negative throughout the entire FBZ, with most of its weight concentrated around the QBCP, as seen in Fig. 3.2b.

To study the effect of quasi-disorder, which is our main focus, we consider the Aubry-André unidirectional potential given by the real-space Hamiltonian,

$$\mathcal{H}_W = \frac{W}{2} \sum_{\mathbf{R}, \alpha} \cos(2\pi\beta n) c_{\mathbf{R}, \alpha}^\dagger c_{\mathbf{R}, \alpha}, \quad (3.1.4)$$

where $\mathbf{R} = ma\hat{\mathbf{e}}_x + na\hat{\mathbf{e}}_y$ is a lattice vector and β is the potential frequency. In the thermodynamic limit, we choose β to be an irrational number in order to break translational invariance, in particular the golden ratio ($\beta = \phi_{\text{GR}} = (1 + \sqrt{5})/2$) as previously discussed. The potential in Eq. 3.1.4 maintains translation invariance along the x direction, and so one can perform the Fourier transform along this direction to obtain $\mathcal{H}_{k_x}$, an Hamiltonian diagonal in Bloch momentum k_x (see Appendix D).

¹ $B = -1$ is used as an example, in fact for $B \in]-2, 0[$ the system is in a trivial phase, however the band structure and the Berry curvature follows the same behavior.

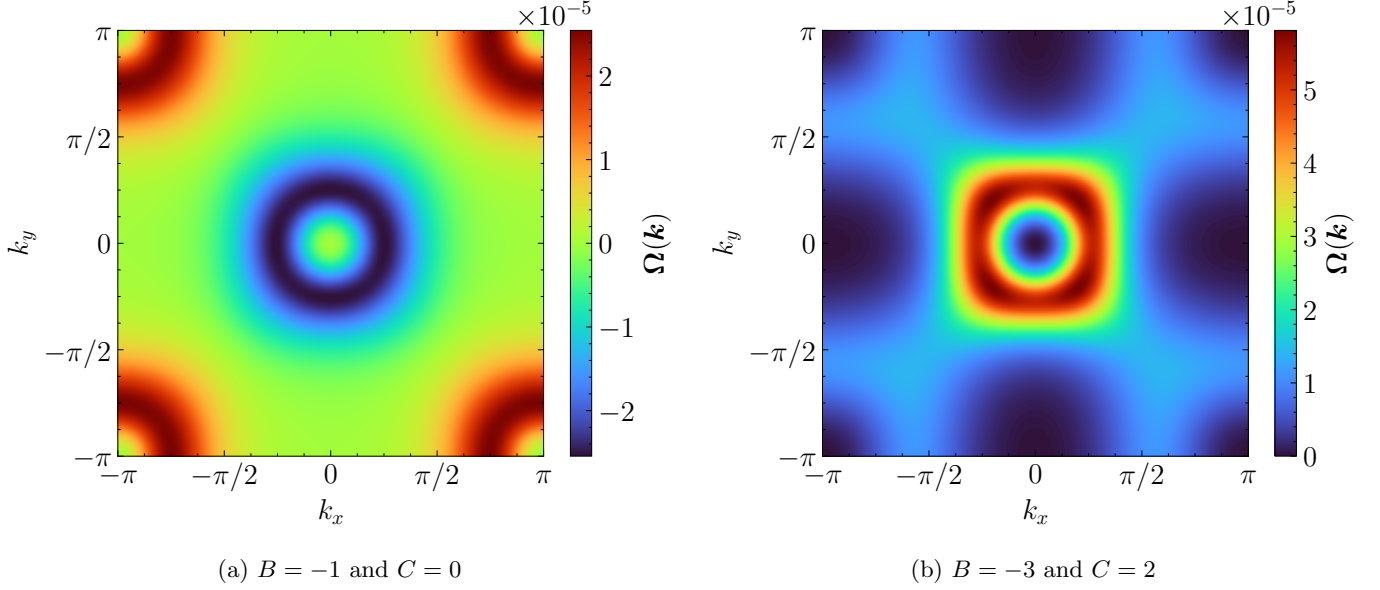


Figure 3.2: Berry curvature ($\Omega(\mathbf{k})$) for different values of topological mass B and $L = 1000$. The scale of the color maps differs between Fig. (a) and (b). In (a) the scale is symmetric, while in (b) the scale is definite and positive.

3.2 Results and Discussion

We start by characterizing the topological phase diagram, shown in Fig. 3.3(left) in the plane of topological mass B and intensity of the quasi-periodic potential W . The phase diagram was obtained for a system with 21×21 unit cells averaged over 20 random phase twists with twisted boundary conditions.

The clean limit presents topological phase transitions from $C = \pm 2$ to $C = 0$, with the gap closing at a QBCP ($B = \{-2, 0\}$). These transitions are robust for small W , still occurring at $B = \{-2, 0\}$. The observed behavior contrasts with the case of uncorrelated disorder, studied in Ref. [79], where it was shown that for infinitesimal disorder strength W , $C = \pm 1$ phases appear. In the present case of an incommensurate potential, $C = \pm 1$ phases only appear at large enough potential strengths, indicating a rather different phenomenology. Interestingly, along the lines of fixed $B = -2, 0$, where the QBCP occurs, we see the appearance of very small $C = \pm 1$ bubbles, indicated by the arrows in Fig. 3.3. If we keep increasing W , topological phase transitions occur into $C = \pm 1$ phases. These phases are not present in the clean limit, which shows that a quasi-periodic potential can induce topological phases of entirely new character. As we will see in the following chapters, the same is true about HOTIs. For large enough potential strength, all topological phases are suppressed, and a trivial phase is eventually reached. Unlike in the disordered case, where all the $C = \pm 1$ phases are gapless, there are both gapped and gapless $C = \pm 1$ phases separated by the black lines in Fig. 3.3.

Regarding spectral properties, we can see in Fig. 3.3(right) that the gap closes and reopens in most of the topological phase transitions. A small gapless region for strong disorder is present (wider blackish regions at high W). This greatly contrasts with the case of Anderson disorder, where the novel $C = \pm 1$ phases are always gapless.

Besides relevant topological properties, quasi-periodicity is far richer than Anderson disorder in regard

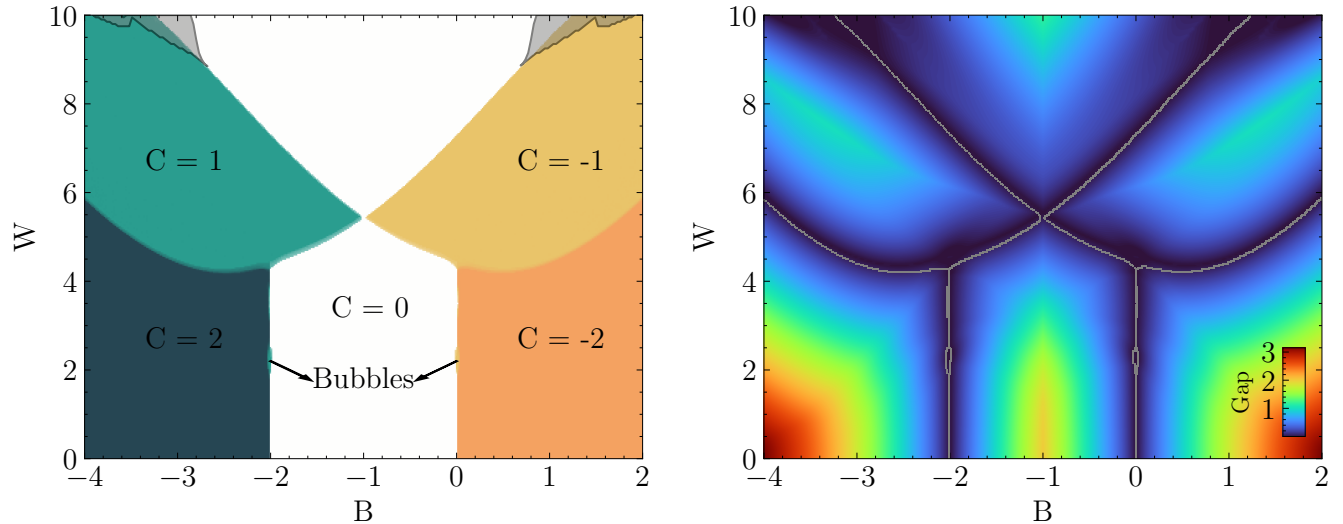


Figure 3.3: (left) Chern number as a function of B and W for a system size of $L = 21$ and 20 different twist realizations. The grayed-out areas are gapless. (right) Energy gap as a function of B and W for $L_y = 1597$. No twist realizations were considered. The gray lines represent the lines at which a topological phase transition occurs.

to localization phenomena. To this end, TMM is a powerful tool to characterize each of the observed phases. By sweeping the system at Fermi level ($E = 0$), we are able to catch gap opening and closing transitions since TMM captures a diverging localization length due to the delocalized bulk states whenever the gap closes, i.e., at TPT, as is evident from Fig. 3.4.

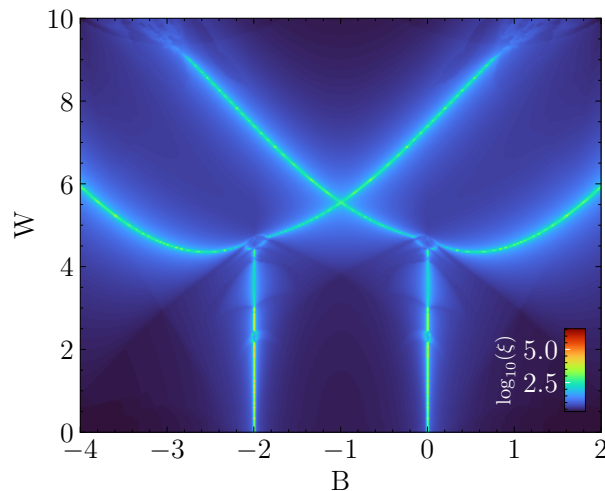


Figure 3.4: TMM results at Fermi level ($E = 0$) at the k_x where the gap closes. Obtained for a 1D system size of $N = 30000$ such that $\epsilon \approx 1\%$. The grid discretization is 300×300 .

The localization properties were also found to be very distinct from the disordered case at small W . In the presence of disorder, all the eigenstates are always localized, except for extended states that live on very narrow energy windows. This contrasts with the quasi-periodic case, where considerably large clusters of bulk states remain extended (top plots of Fig. 3.5). Furthermore, at large potential strengths, a

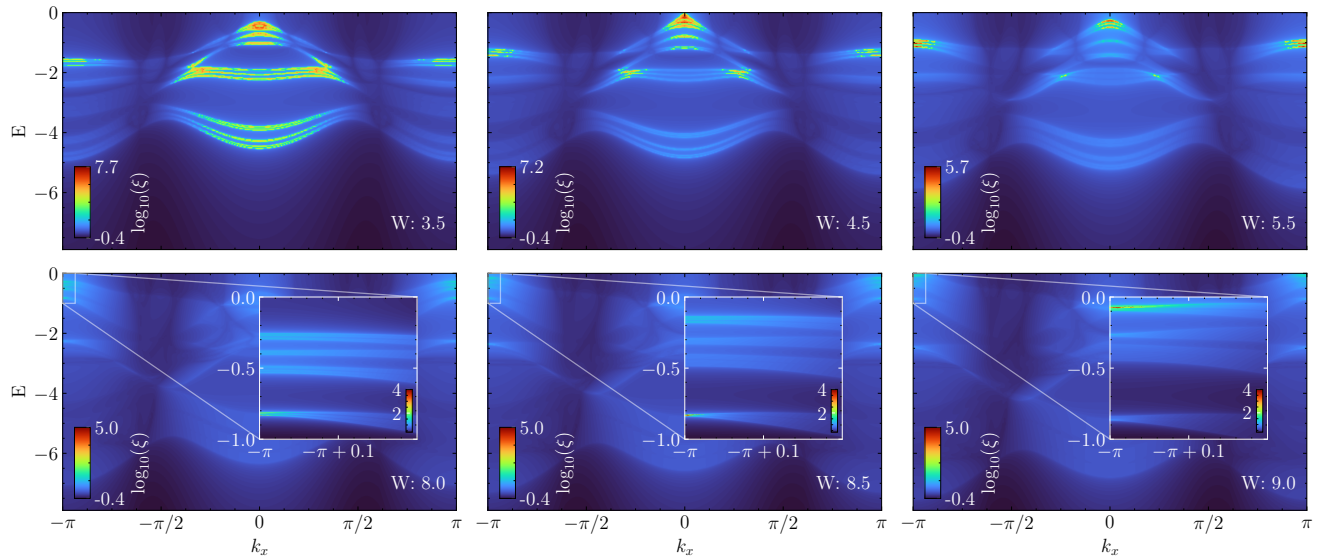


Figure 3.5: TMM bulk phase diagram at $B = -3$ for the entire range of the valence band, $E \in [-7, 0]$ and $k_x \in [-\pi, \pi]$. The insets follow the same procedure for a smaller region ($E \in [-1, 0]$ and $k_x \in [-\pi, -\pi + 0.2]$) with a grid discretization of 600×600 .

mechanism similar to the “levitation and annihilation” mechanism can be observed close to the transitions from the $C = \pm 1$ phases into the trivial phase. In fact, in this large potential limit, the $C = \pm 1$ phases can become gapless, with extended states only existing at very narrow energy windows (bottom plots of Fig. 3.5). After the topological transition into the trivial phase, all states become localized, as in the disordered case.

The topological and localization properties therefore show a mixture of features present in the homogeneous and disordered cases, as was also previously observed for quasi-periodic Chern insulators [?]. The small potential results are also in agreement with Ref. [80], where a different QBCP system was found to be robust to the application of a (in this case, fully two-dimensional) quasi-periodic potential.

Chapter 4

Benalcazar-Bernevig-Hughes (BBH) Model in 2 dimensions

In this chapter, we turn to the study of HOTIs by introducing the paradigmatic BBH model, that will be used extensively hereafter. Initially, we focus our attention on the clean limit as presented in Ref. [49] elaborating on its topological properties. Lastly, we dive into the disordered limit and study how a chiral symmetry-preserving disorder can induce novel topological quadrupole phases, as in Ref. [50].

4.1 Clean Limit

The BBH model is a 2D tight binding model with four orbitals per UC that describes spineless electrons in a square lattice, as seen in Fig. 4.1.

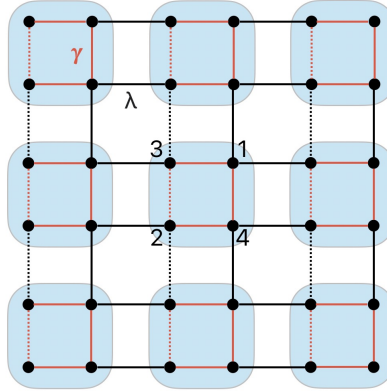


Figure 4.1: Tight binding scheme of the BBH model. The dotted “connections” are negative in relation to γ and λ .

The BBH model is defined by the following Bloch Hamiltonian:

$$\mathcal{H}_{\mathbf{k}} = [\gamma + \lambda \cos(k_x)] \Gamma_4 + \lambda \sin(k_x) \Gamma_3 + [\gamma + \lambda \cos(k_y)] \Gamma_2 + \lambda \sin(k_y) \Gamma_1 + \delta \Gamma_0, \quad (4.1.1)$$

where Γ are 4×4 matrices ($\Gamma_0 = \tau_3 \otimes \sigma_0$, $\Gamma_k = -\tau_2 \otimes \sigma_k$, $\Gamma_4 = \tau_1 \otimes \sigma_0$) that define the internal degrees of freedom within a unit cell. The matrixes τ_i and σ_i are Pauli matrixes. Throughout the rest of this thesis,

we set the lattice constants as the length scale of our problem ($a_x, a_y = 1$). The system has 4 energy bands ($E(\mathbf{k}) = \delta \pm \sqrt{2\lambda^2 + 2\gamma^2 + 2\lambda\gamma(\cos(k_x) + \cos(k_y))}$) each of which is twofold degenerate and preserves all the three discrete symmetries, C_4 and mirror symmetries $m_x = \tau_1 \otimes \sigma_3$, $m_y = \tau_1 \otimes \sigma_1$. The BBH model has its topological phase protected by several distinct symmetries, such as C_4 and mirror symmetries m_x, m_y , as well as chiral symmetry. In this manner, as long as one of these symmetries is enforced, topological quadrupole insulating phases can be observed. In Fig 4.2 the band structure is represented for different

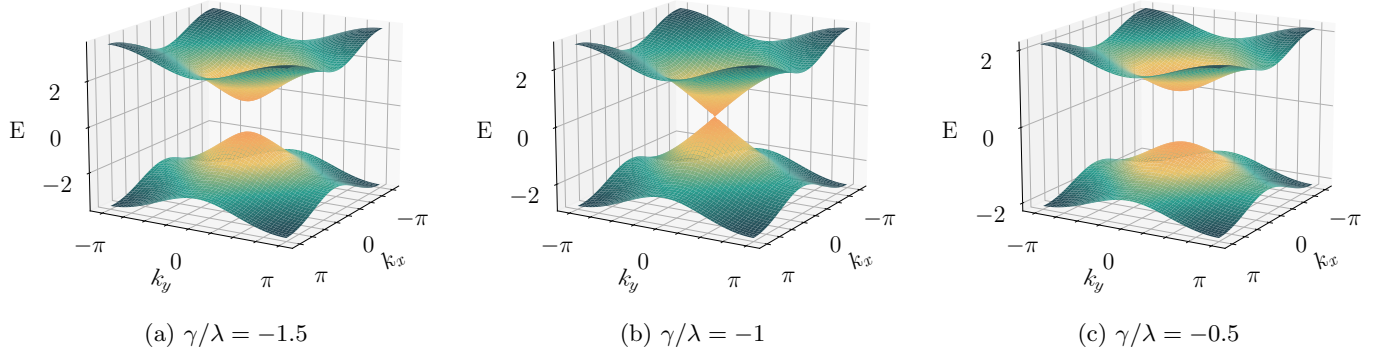


Figure 4.2: Band Structure of the 2D BBH model for different values of the hopping ratio γ/λ and with $\delta = 0$

values of the hopping ratio γ/λ . At $\gamma/\lambda = 1(-1)$ the system is a Dirac semimetal, with the gap closing at the $M(\Gamma)$ points of the FBZ. For $|\gamma/\lambda| > 1$ the system is in a gapped trivial insulating phase ($q_{xy} = 0$) and for $|\gamma/\lambda| < 1$ the system is in a gapped topological quadrupole insulating phase ($q_{xy} = 0.5$).

By bulk-boundary correspondence, opening the boundaries of the system leads to the appearance of boundary properties, thus, at the topological phase ($|\gamma/\lambda| < 1$), the BBH model displays zeroth-dimensional boundary states entitled corner states as depicted in Fig. 4.3(left) in red. These corner states give rise to localized fractional corner charges $Q_i = \pm 0.5$ where $i \in \{1, 2, 3, 4\}$ labels each corner and Q_i comes in units of elementary charge e , Fig. 4.3(right). Away from the topological regime, the trivial phase ($|\gamma/\lambda| > 1$) is defined by $q_{xy} = 0$, with an absence of zero-energy corner modes.

Regarding the electronic charge density, it displays a bulk homogeneous distribution $\rho_e(\mathbf{r}) = 2$ that is canceled by the contribution from the positive atomic charges. Therefore, integrating the total charge density over one of the corner regions yields a fractional corner charge $Q_i = \pm 0.5$. A small δ is considered to break the hybridization of the fourfold zero-energy corner states, and the inter unit cell hopping is chosen to be small ($\gamma = 10^{-3}$) in order to resolve the corner states in Dirac deltas. Furthermore, approaching the TPT by increasing γ leads to increasing localization length of the corner modes. For example, for $\gamma \approx 0.5$, the corner states span a few UC's around the corner. From this point on, we shall set $\lambda = 1$.

Topology and bulk-boundary correspondence on the BBH model

From a classical perspective, a canonical quadrupole moment is composed of two canceling dipoles and four corner charges. In fact, this perspective should hold whether the quadrupole moment has its origins in a perfect canonical structure or if it emerges from quantum behavior. These properties are observed in the quadrupole insulating (QI) topological phase of the BBH model ($|q_{xy}| = |p_i| = |Q_i| = 0.5$).

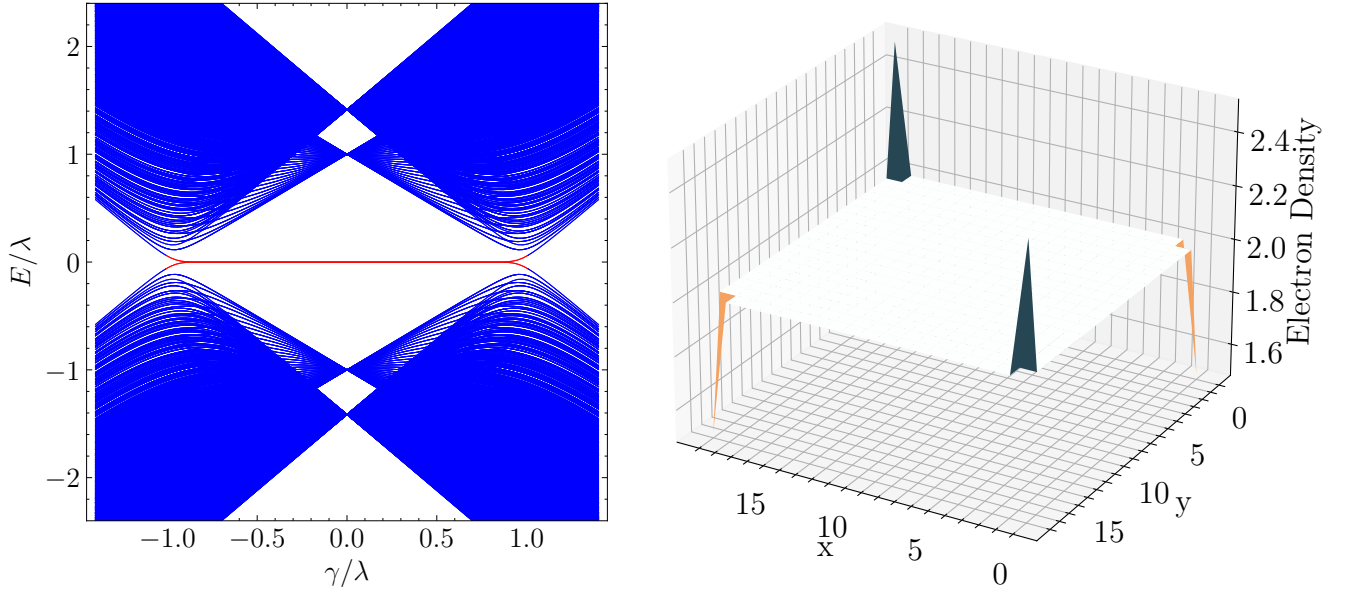


Figure 4.3: (left) Energy Spectrum as a function of γ/λ obtained by ED for a system with open boundaries and $L = 30$. The gap does not close properly at $|\gamma/\lambda| = 1$ due to finite-size effects. In red, the energy corner modes. (right) Electron charge density for $\gamma = \delta = 10^{-3}$.

This said, how can we characterize the topology of such types of topological insulators? For the particular case of the BBH model, the simplest way of computing the bulk quadrupole moment is via real-space methods, as in Sec. 2.2. However, there are more efficient ways of achieving the same result. The Nested Wilson loop (A.2) is one of these approaches, allowing us to compute both boundary polarizations and thus define a boundary invariant $P = 4|p_x p_y|$. We can take advantage of the hierarchy of nested topological insulators to characterize the topological properties of the bulk via the topological properties of the boundary. Apart from the nested Wilson loops that require the existence of translational invariance, there is an additional method capable of reaching the boundary. The boundary Green's function method tackled in Sec. 2.5 is a valid approach in reciprocal-space and in real-space, which makes it ideal to implement in disordered systems. With this method, the authors in Ref. [78] obtained the boundary Bloch Hamiltonian of the BBH model, given by:

$$\mathcal{H}_{\text{Bound}} = f_k \begin{pmatrix} 0 & \gamma + \lambda e^{-ik} \\ \gamma + \lambda e^{ik} & 0 \end{pmatrix}, \quad f_k = \frac{\lambda(\lambda + \alpha\gamma)}{\gamma^2 + \lambda^2 + 2\lambda\gamma \cos(k)}. \quad (4.1.2)$$

Aside from the pre-factor f_k , the Hamiltonian is identical to that of the SSH model and is defined for $|\gamma| \neq 1$.¹ Thus, it can be shown that $\mathcal{H}_{\text{Bound}}$ has the same topological properties as the SSH model. Let us prove the previous statement. Let $|u_k^{\text{SSH}}\rangle$ be a Bloch eigenstate of $\mathcal{H}_{\text{SSH}}(k)$ with energy ϵ_k^{SSH} that obeys the following eigenvalue equation:

$$\mathcal{H}_{\text{SSH}}(k) |u_k^{\text{SSH}}\rangle = \epsilon_k |u_k^{\text{SSH}}\rangle. \quad (4.1.3)$$

¹For $|\gamma| = 1$ the system is a metal, and the Green's function at zero-energy is not defined, which in turn leads to a non-defined boundary Green's function.

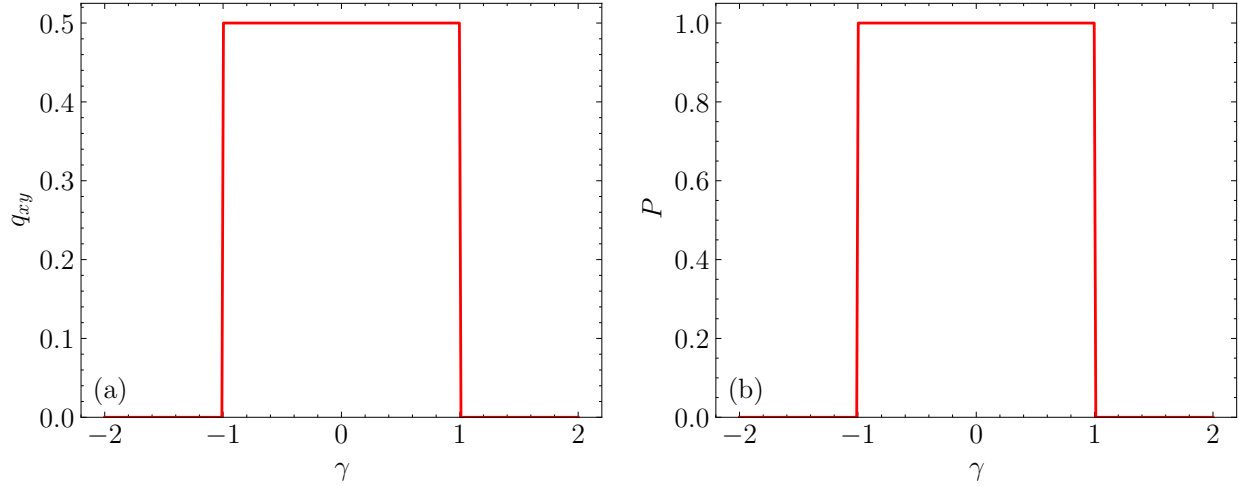


Figure 4.4: (a) q_{xy} as a function of the hopping γ computed via real-space methods for a system size of $L = 10$. (b) $P = 4 |p_x p_y|$ invariant computed via nested Wilson loops for a system size of $L = 10$.

The boundary Hamiltonian obtained analytically from the boundary Green's function is $\mathcal{H}_{\text{Bound}}(k) = f_k \mathcal{H}_{\text{SSH}}(k)$ implying that $[\mathcal{H}_{\text{Bound}}, \mathcal{H}_{\text{SSH}}] = 0$. In this manner, $|u_k^{\text{SSH}}\rangle$ is also an eigenvector of $\mathcal{H}_{\text{Bound}}(k)$ with energy $f_k \epsilon_k^{\text{SSH}}$. Since the Bloch wavefunctions remain unchanged and following the definition of topological indexes via Wilson loops as in Sec. 2.1.1, it is clear that the two models have the same topology. Going from reciprocal-space into real-space, the factor f_k , which is k dependent, introduces long range hopping's.

With either of those methods, we can compute the boundary polarizations p_x and p_y , thus defining the boundary invariant:

$$P = 4 |p_x p_y| = \begin{cases} 1 & q_{xy} = 0.5 \\ 0 & q_{xy} = 0 \end{cases}. \quad (4.1.4)$$

This characterization holds for the BBH model but care is needed since there is indication that topological phases can occur with $p_x = 0$, $p_y = 0.5$ and vice versa [81, 82], albeit we do not dwell such regimes.

To conclude this section, we make some finishing remarks. If our focus is on quadruple phases protected by crystalline symmetries, the nested Wilson loop approach and the traditional $\mathbb{Z}_2$ invariants computed by constructing the Pfaffian over high symmetry k -points (as in the Fu-Kane invariant, Ref. [83]) are possible invariants that define q_{xy} . However, since we are interested in disordered chiral QIs, these two approaches are not viable. The BBH model falls within the BDI (chiral orthogonal) symmetry class [13] which has no $\mathbb{Z}$ topological index in 2 dimensions. However, such classification might not hold for HOTIs since the tenfold way can only properly classify first-order topological insulators. More recently, it has been shown that chiral-symmetric HOTIs have well-defined topological invariants entitled multipole chiral numbers (MCNs), which are a generalization of the winding number to higher dimensions [84]. Furthermore, the authors show that phases with $q_{xy} = 0.5$ are always topological, while phases with $q_{xy} = 0$ might be topological or trivial. This said, a complete picture of the topology of chiral QIs can be accomplished not only by the characterization of the quadrupole moment using PBC but also by opening the boundaries, studying the number of corner states in each regime, and examining the

emergent boundary signatures. Overall, a chiral symmetric quadrupole topological phase is defined by a quadrupole moment quantized to 0 or 0.5 as long as zero-energy corner modes are present, and their number is divisible by the number of boundaries in the system (4 in 2D). Regarding the BBH model and the disordered variants considered in this thesis, the phases with $q_{xy} = 0$ are always trivial, and so we refrain from computing multipole chiral numbers. It follows that in such cases, the quadrupole moment acts as a topological invariant.

4.2 Chiral Disorder

In this section, we explore the work published in Ref. [50], where the authors study the effect of chiral disorder in the BBH model. We replicate some results from the paper in question, which allow us to test much of the methods we have introduced in Chapter 2, building up our intuition to later tackle quasi-periodicity. In the original paper, the authors study a model of their creation that is connected via a local transformation to the BBH model. The results that follow are for chiral disorder, and we use the BBH model as the underlying TB system. As we will see, applying chiral disorder to the BBH model yields identical results to the ones obtained by the authors of Ref. [50]. Before proceeding, let us note that most of the graphs display vertical dotted lines that mark phase transitions, with **dark blue** lines marking gap closures or openings and **gray** lines representing TPTs or localization transitions. These act as guidelines throughout the discussion that follows.

Disordered hopping

In order to preserve chiral symmetry, onsite Anderson disorder cannot be introduced into the system. With this in mind, the internal UC hoppings (γ) can be perturbed with Anderson disorder, ensuring that chiral symmetry is preserved. In this manner, we take:

$$\gamma \rightarrow \gamma + \frac{W}{2}\alpha_i, \quad (4.2.1)$$

where W is the disorder strength and α_i is sampled from a uniform distribution such that $\alpha_i \in [-1, 1]$ with $i \in \{1, 2, 3, 4\}$.

Main results

In Fig. 4.5(a), we show the quadrupole moment and the boundary invariant as a function of W and in Fig. 4.5(b), we show the spectral gap (ΔE) as a function of disorder strength W . For $W = 0$, the system is in a trivial phase that is robust to increasing disorder strength (I). Eventually, the gap closes and reopens at $W_c^{I \rightarrow II} \approx 2.1$. This behavior stands in stark contrast to Anderson disorder, which leads to the permanent closure of the spectral gap. Into phase II , the boundary invariant plateaus at 1, which is accompanied by the gap closing and reopening. Although the boundary invariant (P) quantizes to 1 in the topological phase (II), even for $L = 200$, it still suffers from finite-size effects. Regarding the quadrupole moment, it never quantizes, despite the clear scaling with increasing system size. As it turns out, the absence of quantization is a consequence of small system sizes. To tackle this, the authors perform a scaling analysis in these regions and conclude that, for big enough L , $q_{xy} \rightarrow 0.5$. Phase III is gapless but

topological. To this end, we refer to phase *II* and *III* as higher-order topological Anderson insulators (HOTAI).

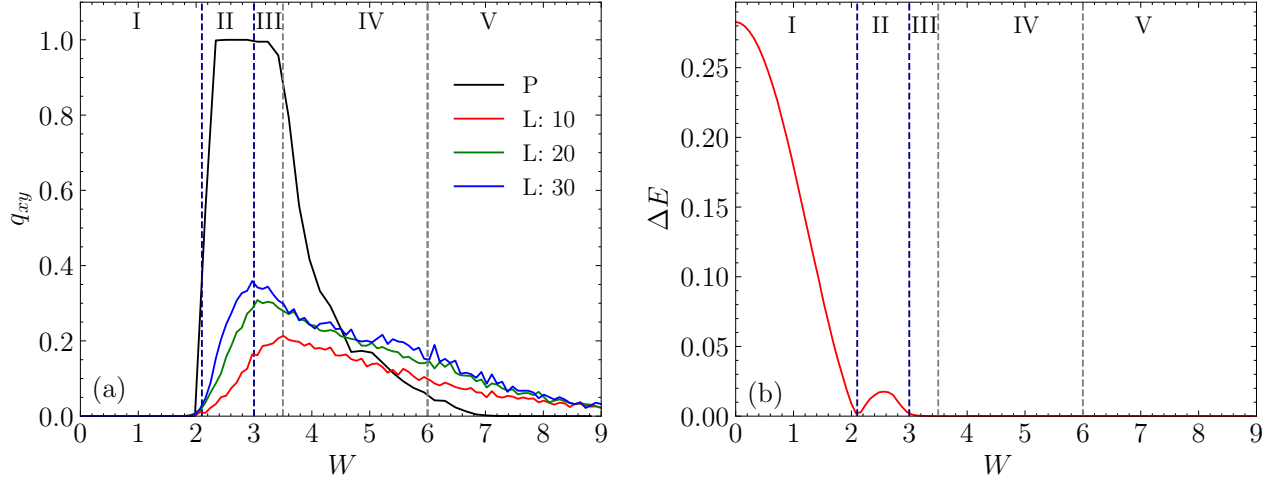


Figure 4.5: (a) q_{xy} and P as a function of W . The P invariant was computed for a system size of $L = 200$ and averaged over 200 disorder configurations. q_{xy} was obtained via real space methods, with 1000 disorder configurations for $\gamma = 1.1$, $L = 10$ and 20 while for $L = 30$ 500 configurations were considered. (b) Spectral gap (ΔE) as a function of W for $\gamma = 1.1$, $L = 200$ and averaged over 150 disorder configurations.

Further increasing disorder induces a TPT at $W_c^{III \rightarrow IV} \approx 3.5$, and the system reaches a Griffiths regime (phase *IV*), which displays “mixed topology”. Although for each disorder configuration the quadrupole moment and boundary invariant remain quantized, their average yields an intermediary value. At high W (phase *V*) the system exhibits the same phenomenology of an Anderson insulating phase.

Spectral Properties

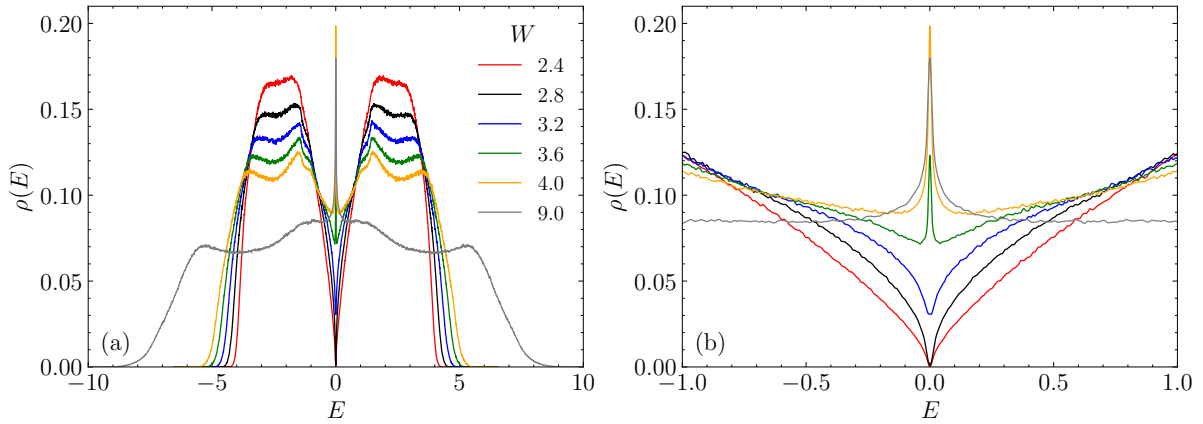


Figure 4.6: DOS as a function of E calculated through KPM for a system of size $L = 1000$, $M = 5000$ moments, $R = 10$ disorder and random vectors configurations for several values of disorder strength. (a) Full DOS. (b) Zoomed-in view around Fermi level.

Now we turn to the spectral properties under increasing W . In Fig. 4.6 we show the density of states ($\rho(E)$) as a function of E obtained via KPM for several values of disorder strength. Just as Anderson disorder, chiral disorder flattens and increases the bandwidth of the system. However, for certain values of W a singularity at $E = 0$ appears, which is later killed, further strengthening the disorder, as in Ref. [85].

To confirm that *II* and *III* are topological, alongside a quantized quadrupole moment, the system also needs to display zero-energy corner modes when the boundaries are opened. To this end, in Fig. 4.7 the local DOS at $E = 0$ computed for an open boundary system is plotted as a function of $\mathbf{r}$ for a W in each of the topological phases. For either of the phases, there is a clear spectral weight concentrated at the corner. Overall, the quantized quadrupole moment, boundary invariant, and the existence of corner modes at these particular phases are enough to conclude that phase *II* and *III* correspond to gapped and gapless HOTIs respectively.

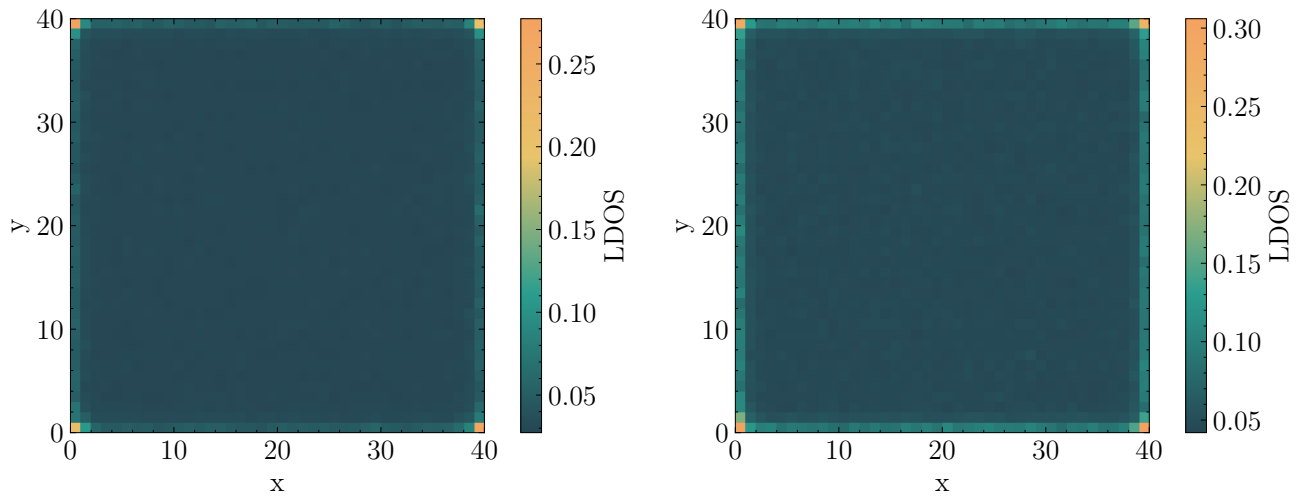


Figure 4.7: LDOS for $E = 0$ as a function of position $\mathbf{r} = (x, y)$ calculated using the recursive method for a system size $L = 40$. (left) $W = 2.6$ (phase *II*) and 500 disorder configurations. (right) $W = 3.4$ (phase *III*) and 1000 disorder configurations.

Localization Properties

We now turn to the study of the localization properties of each phase. Implementing TMM at the Fermi level is a powerful tool to tackle topological phase transitions and compute the localization length of eigenstates at the Fermi level, in gapless regimes. In gapped regions, TMM generates localized wave functions corresponding to evanescent waves that live in the gap. In Fig. 4.8, we plot the normalized localization length (ξ/M) at Fermi level ($E = 0$) as a function of W .

In the gapped phases *I* and *II*, TMM gives localized states. However, at the TPT, the normalized localization length diverges, indicating the existence of extended states at Fermi level. In phase *III*, which is gapless, the bulk Fermi level states are localized. This is relevant to ensure that a TPT does not occur, since localized states at the Fermi level can hybridize with the corner modes without inducing a TPT. Phase *IV* is a critical metal, which can be distinguished by the absence of scaling of ξ/M as M increases, implying that the localization length is always of the order of the system size. These types of critical metal regimes have been previously observed in systems with disordered hoppings [85, 86]. Eventually,

for high enough disorder, the typical AI phase is reached (V).

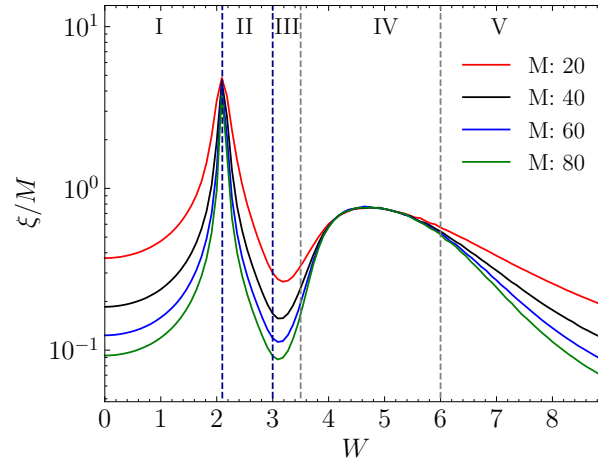


Figure 4.8: Normalized localization length (ξ/M) as a function of W at Fermi level, obtained with TMM for $\gamma = 1.1$ for different transversal sizes M . The size of the longitudinal direction N was chosen such that $\epsilon < 1\%$.

Chapter 5

Chiral Quasi-Periodic Quadrupole Insulator (QPQI)

Finally, we reach the main focus of this thesis. Until this point, we explored numerical and analytical methods we can employ to study single particle systems on a lattice, first-order and higher-order topologies, and introduced the BBH model and its disordered cousin. In this chapter, we perform a detailed study of a chiral QPQI model, starting with the topological properties, followed by spectral and localization properties, and finishing with boundary phenomenon and its connection to the observed bulk properties.

5.1 Model

At this point in the thesis, it should be clear that chiral symmetry is important to have a quantized quadrupole moment. With this in mind, an appropriate form of the potential needs to be chosen in order to break translational invariance while preserving chiral symmetry. This can be achieved by perturbing the internal UC hopping's (γ) with a quasi-periodic (QP) modulation while maintaining the intra-UC hopping's (λ) unchanged. Thus, in analogy to what was done in Chapter 3, we consider the BBH model with the following hopping modulation:

$$\gamma \rightarrow \gamma + \frac{W}{2} \cos(2\pi\beta m + \phi_x) \cos(2\pi\beta n + \phi_y), \quad (5.1.1)$$

where β is an approximant of ϕ_{GR} (the golden ratio), $\mathbf{R} = m\hat{\mathbf{e}}_x + n\hat{\mathbf{e}}_y$ is a lattice vector and ϕ_i are the phase shifts. Unlike the case of the QBCP Chern insulator, the QP potential is chosen to vary in both directions to fully break translational invariance. For generic $\phi = (\phi_x, \phi_y)$, the QP modulation breaks the mirror and C_4 crystalline symmetries. Therefore, this symmetry is broken for the finite-size systems that we study. Nonetheless, it should be recovered in the thermodynamic limit, when there should be no ϕ dependence of the bulk properties.

5.2 Main Results

In this section, we unveil the main results of this thesis, namely the phase diagram of the system on the (γ, W) plane, as shown in Fig. 5.1, where 5.1(a) is for the topological properties and 5.1(b) for the spectral properties. These plots allow for a general perspective of the phase diagram that enable us to focus on specific regions of interest. In this manner, in Fig. 5.1(a) the quadrupole moment and in Fig. 5.1(b) the bulk spectral gap phase diagrams.

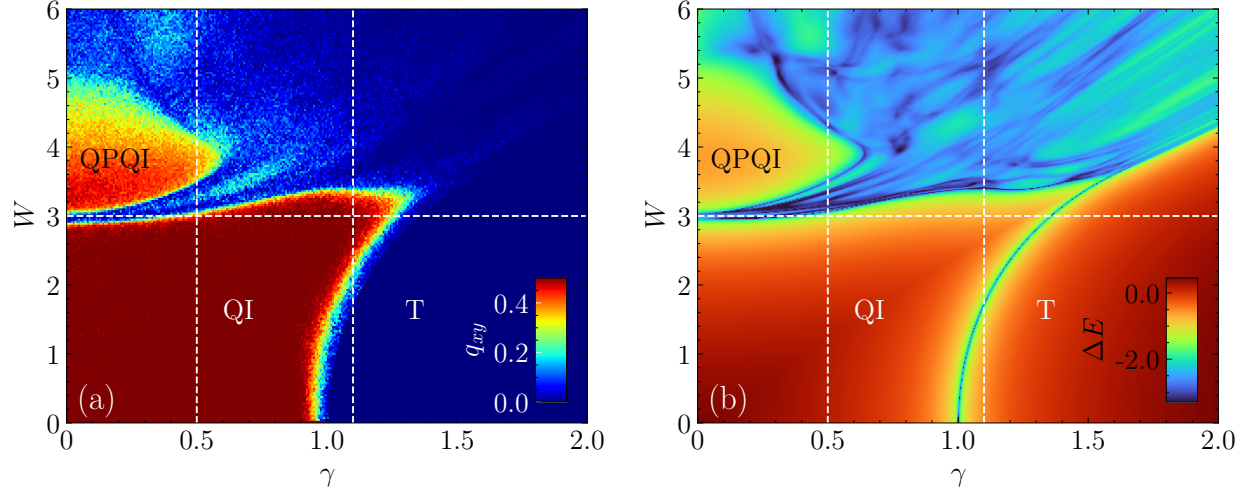


Figure 5.1: (a) Quadrupole moment (q_{xy}) in the (γ, W) plane, computed for a system size $L = 13$, with $\theta_i = \pi$ and averaged over 100 random phase shifts realizations. (b) The logarithm spectral gap ($\log_{10}(\Delta E)$) in the (γ, W) plane for a system size $L = 34$, with $\theta_i = 0$ and averaged over 50 realizations of phase shifts. A minimum value of the spectral gap was chosen ($\Delta E < 10^{-3}$) to highlight all the gapped and gapless phases appearing in the phase diagram. The dotted white lines are constant γ and W cuts for $\gamma = 0.5, 1.1$ and $W = 3$, respectively.

The clean limit quadrupole insulating (QI) and trivial (T) phases are robust to QP modulations. In the trivial regime, these modulations can induce a TPT into a QI phase adiabatically connected to the clean limit phase or remain trivial, while in the topological case, the QP modulations eventually induce a TPT into a gapless critical metal, blueish region in Fig. 5.1 between QI and QPQI phase. Further increasing the strength of the QP modulation leads to a novel reentrant topological regime, which we entitle quasi-periodic QI (QPQI). These phases exhibit the same boundary signatures as their clean limit counterparts, such as boundary polarizations ($p_x = p_y = 0.5$) and four-fold zero-energy corner modes that give rise to fractional corner charges. In these regimes, an intricate interplay between phase shift-dependent edge states and corner modes emerges, leading to behavior not observed in the QI phases, such as edge-corner hybridization. This behavior is unique to the QPQI phase. Overall, the observed TPT between various regimes occurs in gap closing or opening as seen in Fig. 5.1(b).

To thoroughly characterize each of the observed phases, two cuts along constant γ were characterized (depicted as vertical dotted white lines), with the intent of analyzing various electronic properties as W increased. In this manner, two distinct values of the hopping amplitude were selected such that multiple regions of the phase diagram were incorporated into the cuts. Furthermore, to study the robustness of each clean limit phase, we opted for $\gamma = 0.5(1.1)$, which for $W = 0$ corresponds to the topological (trivial)

insulating phase. Additionally, we also consider a constant W cut at $W = 3$ seen in Fig. 5.1 (depicted by a horizontal dotted white line). The results associated with this cut are in Appendix F and despite the gapless QPQI regime with localized states at Fermi level, no relevant regimes have been found.

5.3 Topological and Spectral Properties

As we know, topological phase transitions are usually associated with some gap mechanism, whether it be a gap closure as usually seen in clean systems or gap-edge localization transitions that induce a TPT as observed in topological Anderson insulators. Although gap closures are not a requirement for a TPT, they are still a good indicator that one has occurred, especially when the system has delocalized gap-edge states. To this end, in Fig. 5.2, the spectral gap (ΔE) is plotted as a function of W for each of the different starting phases. The spectral gap was obtained via ED and estimated as $\Delta E = 2\epsilon^+$, where ϵ^+ is

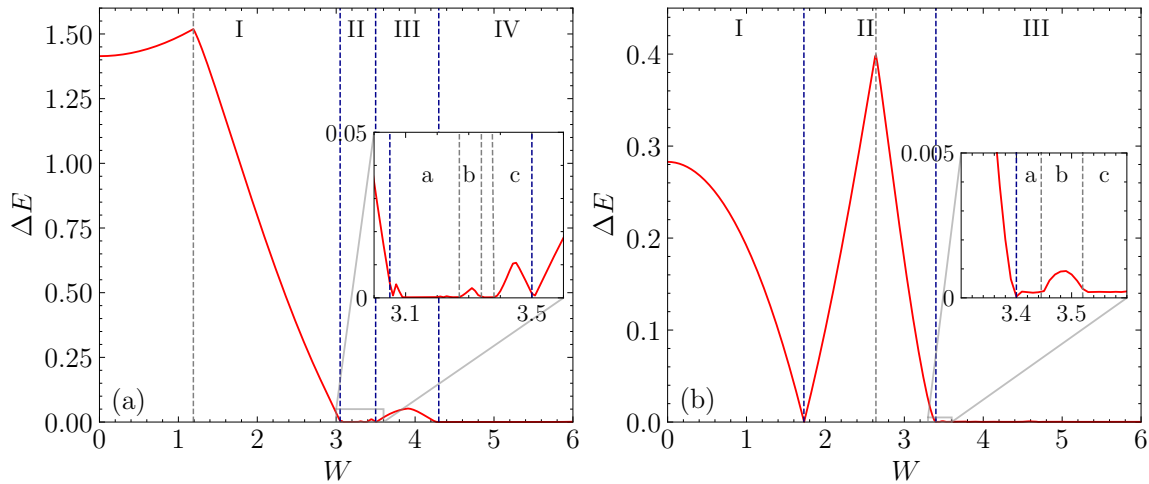


Figure 5.2: Spectral gap (ΔE) as a function of W computed for an even system size $L = 144 \implies \theta_i = 0$ and averaged over 50 phase shifts realizations. (a) $\gamma = 0.5$. (b) $\gamma = 1.1$.

the positive eigenvalue closest to zero. The dotted [dark blue](#) lines mark gap closures or openings and thus a change of region per example, $I \rightarrow II$. As per the dotted [gray](#) lines, they mark level crossings, which will be clearer when we tackle localization properties. From start to finish of our analysis, the dotted lines act as a visual guide throughout the discussion that follows. The calculation of ΔE was performed for an even system size. However, the results can be identically duplicated for odd L if we add a phase twist $\theta_i = \pi$ in both directions. Furthermore, no error bars are plotted since the curves $\Delta E \pm 2\sigma$ are over-imposed with the main plot, indicating that the bulk spectral gap has no dependence on phase shifts.

In Fig. 5.3 the quadrupole moment (q_{xy}) and the boundary invariant (P) are plotted as a function of the quasi-periodic potential strength (W). All the results discussed in this chapter revolve around these two cuts, and so they will be mentioned throughout this discussion.

The quadrupole moment was computed for several system sizes via the multipole operators. Since some of the sizes are odd, a twist of π was fixed in each direction in order to have a well-defined gap closure¹. The boundary invariant (P) was obtained via the boundary Green's function method followed

¹If we perform the calculation of q_{xy} for a big enough odd value of L the twist will play no part in resolving the TPT.

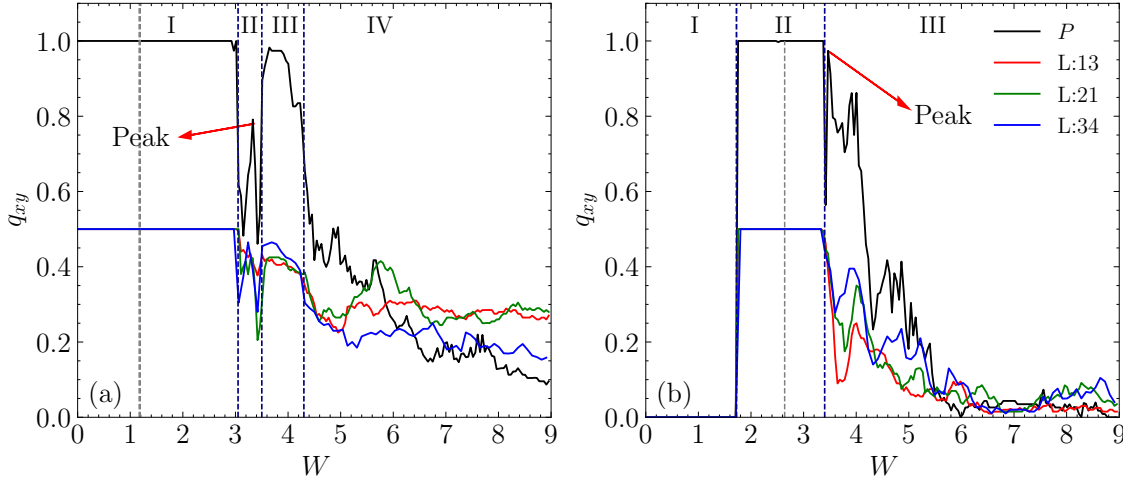


Figure 5.3: q_{xy} and P as a function of W . The P invariant was computed for a system size of $L = 610$ with 115 averages over phase shifts. q_{xy} was obtained via real-space methods with 100 averages over phase shifts. For even L , $\theta_x = \theta_y = 0$; for odd L $\theta_x = \theta_y = \pi$. (a) $\gamma = 0.5$. (b) $\gamma = 1.1$.

by the multipole operator for polarization, with $\theta_i = 0$ in both directions² since we take L to be even.

Discussion - Starting Topological The results obtained by increasing W , starting at a topological phase, are shown in Fig. 5.3(a) and 5.2(a). For $\gamma = 0.5$ and $W = 0$ the system is in a topological phase. Both the quadrupole moment and the boundary invariant are quantized, respectively, to 0.5 or 1 for each realization of phase shifts. This quantization remains with increasing W , leading us to conclude that the QI phase (I) is robust to QP modulations. Eventually, at $W_c^{I \rightarrow II} \approx 3.05$, the gap closes and a TPT occurs into a critical metal phase (IIa, see inset of Fig. 5.2) which we motivate below after tackling localization properties. Reaching IIb, the gap reopens into a topological regime (IIb) with both the P and $q_{xy}^{L=34}$ invariants exhibiting a sharp peak in the region, as indicated in Fig. 5.3(a). The fact that these peaks approach 1(0.5) with increasing system size while the value of P ($q_{xy}^{L=34}$) in IIa and IIc go to zero, hint that IIb is a quadrupole insulating phase. Additionally, because this is a very narrow W window and the gap is small ($\Delta E \approx 10^{-3}$), we attribute the lack of quantization of either invariants to finite-size effects. Further increasing W induces a trivial insulating phase (IIc) before another quadrupole insulating regime is reached (III) that suffers from the same finite-size effects of IIb. Since both IIb and III are gapped, the proof presented in Appendix B holds, and in the thermodynamic limit q_{xy} and P should quantize to 0.5 and 1 respectively. In this manner, quasi-periodic modulations can induce a novel type of SOTI phases which we entitle QPQI phases³. Towards the strong W limit, the gap closes ($W_c^{III \rightarrow IV} \approx 4.3$) and the system reaches a gapless trivial phase (IV) with a finite, although not quantized, quadrupole moment ($q_{xy} \neq 0$). For each individual phase shift realization $q_{xy}(P)$ remain quantized to either 0 or 0.5(1), however, its average yields a finite intermediary value, indicating a trivial regime. One might be tempted to use chiral symmetry to argue that this region is either trivial or topological. However, due to

²The open boundary is only considered in the longitudinal direction. Along the transversal direction, the boundaries are periodically closed since the considered system size is even. Although a twist can be added, for such large system sizes, they should play no part in resolving gap closures and thus TPTs.

³Quasi-Periodic Quadrupole Insulator

the gapless nature of the system, its ground state is ill-defined due to the high degeneracy of zero-energy states, which in turn leads to a non-quantized quadrupole moment. In spite of this, since both invariants scale down to zero as the system size increased, phase *IV* is trivial.

Discussion - Starting Trivial For $\gamma = 1.1$ and $W = 0$ the system is in a gapped trivial phase, which is stable to the application of a QP modulation (*I*). Increasing W induces a TPT into a gapped QI phase (*II*) with the gap closing and reopening at $W_c^{I \rightarrow II} \approx 1.73$. Furthermore, the gap reaches its maximum, with a level crossing between energy levels in the gap edge occurring at $W \approx 2.64$ (dotted gray line). Away from the QI phase, the gap closes ($W_c^{II \rightarrow III} \approx 3.4$) and reopens in *IIIb* with a sharp peak in P that almost quantizes to 1 as seen in Fig. 5.3(b). Just as in the previous case ($\gamma = 0.5$), we attribute the lack of quantization of the boundary invariant to finite-size effects, classifying *IIIb* as QPQI phase. Eventually, at the high W regime, the system undergoes a TPT into a gapless trivial regime (*IIIc*).

Around $W \approx 4$, peaks can be observed in the P invariant and q_{xy} , with the latter approaching 0.5 with increasing system size. Bulk gap calculations (Fig. 5.2) indicate a gapless regime with localized states at the gap-edge ($D_2 \rightarrow 0$ as seen in Fig. 5.9), however, we cannot conclude that these regions are topological due to finite-size effects.

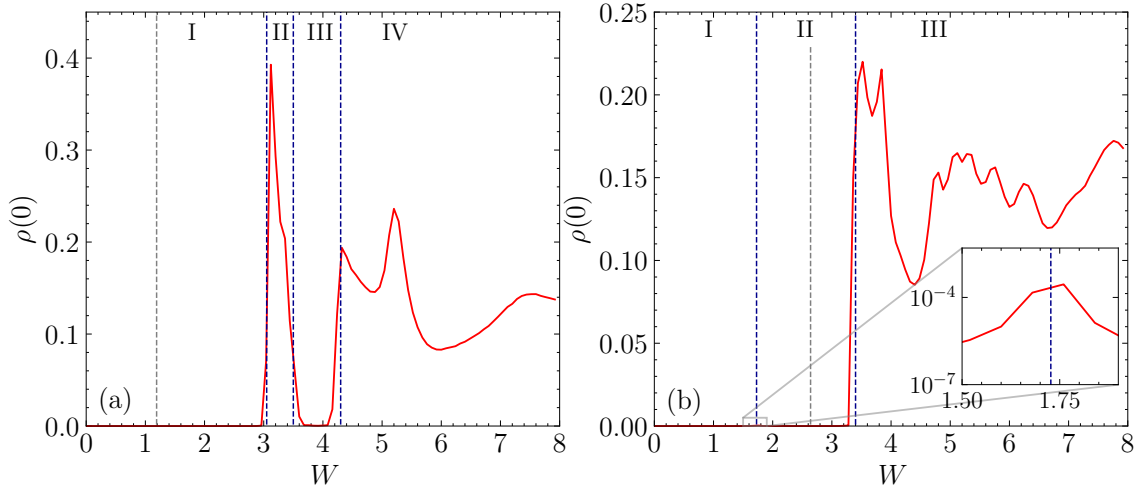


Figure 5.4: The DOS at zero-energy ($\rho(0)$) as a function of W . The following KPM parameters were used: $L = 987$, $M = 5000$, $R = 10$. (a) $\gamma = 0.5$. (b) $\gamma = 1.1$.

Density of States In Fig. 5.4, we plot the DOS at $E = 0$ as a function of W with the intent of verifying the results of the spectral gap presented in Fig. 5.2. In gapped regions $\rho(0) \approx 0$,⁴ while in gapless regions, the system should have a finite DOS (excluding the possibility of a semimetal). All gapless phases (*II* and *IV* for $\gamma = 0.5$ and *III* for $\gamma = 1.1$) display a finite DOS at Fermi level. Furthermore, at the transition $I \rightarrow II$ ($\gamma = 1.1$) the gap closes and reopens at a critical QP potential strength ($W_c^{I \rightarrow II} \approx 1.73$), which is signaled by a small increase of $\rho(0)$ around it, as shown in Fig. 5.4(b-inset). The Jackson kernel broadens the Dirac delta as a Gaussian with spread $\sigma \propto 1/M$. For this reason, it was not possible to reach enough resolution to capture the gapped *I*b and *I*c phases that are filled by the tails of the Gaussian. The same

⁴It might not be zero since, in gapped regions, the DOS scales to zero with the number of Chebyshev moments M .

occurs for $\gamma = 1.1$ in phase *IIIb*. These narrow phases are only expected to be resolved for larger system sizes and number of moments.

Away from the Fermi level, the effects of QP modulations on the energy spectrum contrast with the effects of onsite or chiral disorder. As per the latter, disorder tends to smooth the DOS, quickly killing singularities, increasing bandwidth and closing gaps. Furthermore, for high enough W , regular disorder transforms the DOS into a homogeneous distribution with width W . To explore the effects of quasi-periodicity, we compute the DOS with KPM using the Jackson kernel. In Fig. 5.5 the clean limit DOS is plotted as a function of E for the two cases ($\gamma = 0.5$ and $\gamma = 1.1$).

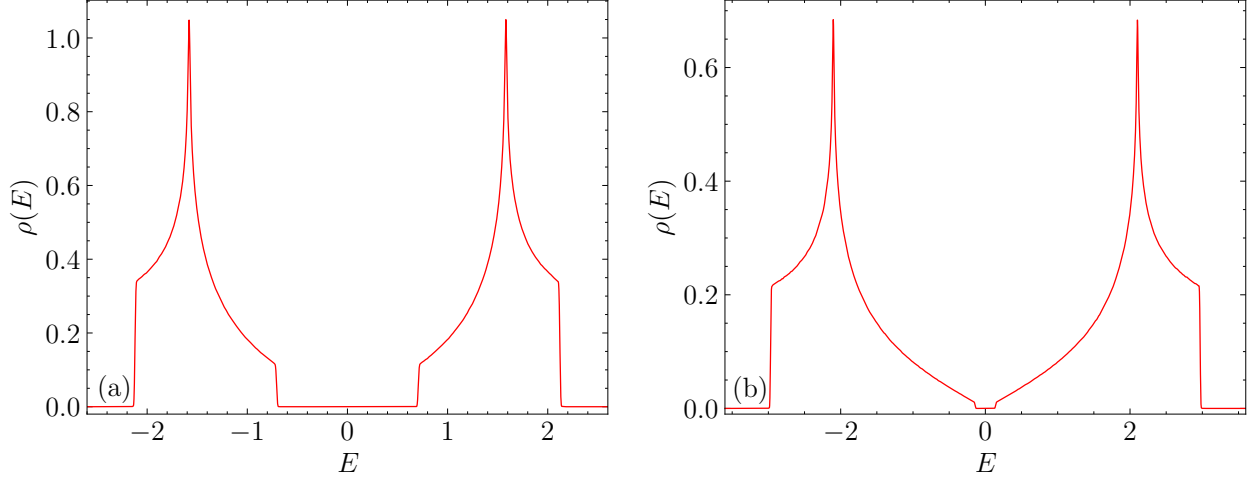


Figure 5.5: Clean limit DOS as a function of E . The following KPM parameters were used: $L = 987$, $M = 4000$, $R = 10$ (a) $\gamma = 0.5$. (b) $\gamma = 1.1$.

To complete our study, we show in Fig. 5.6 the evolution of $\rho(E)$ under increasing W for $\gamma = 1.1$. The QP potential induces mid-bulk gaps even for small W . For higher W , all the gaps are killed, with the bandwidth of the system growing monotonously with W . The same behavior can be observed for $\gamma = 0.5$ (Fig. F.1).

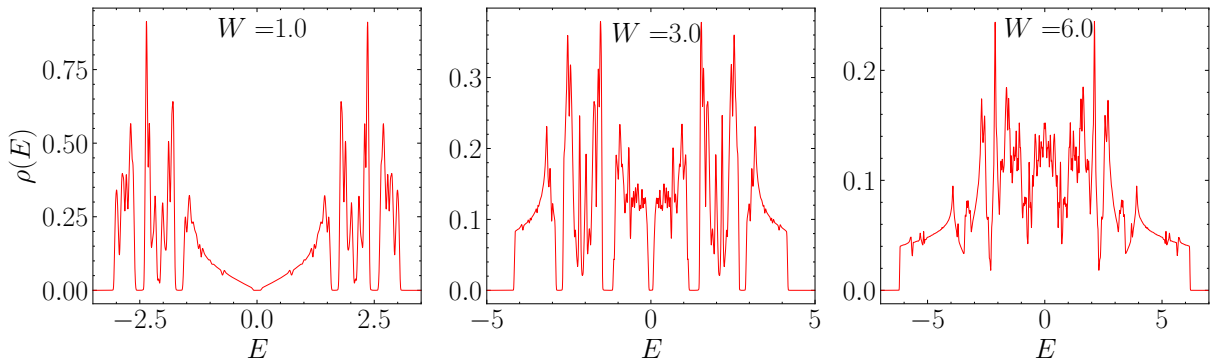


Figure 5.6: DOS as a function of E for $\gamma = 1.1$ and different values of quasi-periodic potential strength (W). The following KPM parameters were used: $L = 987$, $M = 2000$, $R = 10$.

Overall, the effects of a QP modulation on the energy spectra of the system is independent of the

starting phase. Furthermore, these types of modulations (whether they are chiral or onsite) tend to induce bulk gaps and sometimes even spectral gaps that remain well into a strong W regime. This phenomenology is common in quasi-periodic systems and can be observed in the notorious Aubry-André model [27] and in the QBCP Chern insulator with QP modulations discussed in Chapter 3.

5.4 Localization properties

In this section, we turn our attention to localization properties. In Fig. 5.7, we plot the normalized localization length (ξ/M) at Fermi level ($E = 0$), obtained using TMM. In regions with a larger gap, it is clear that ξ/M scales down to zero, since TMM captures localized evanescent wave solutions of the Schrödinger equation. At gapless regions, or regions with small gaps, the results are noisier, and in some cases, sufficiently larger system sizes would be needed to understand whether ξ/M converges with M , showing critical behavior, or if it decreases with M signaling gapless localized states. This will become more clear from the eigenstate analysis based in exact diagonalization that we carry out below.

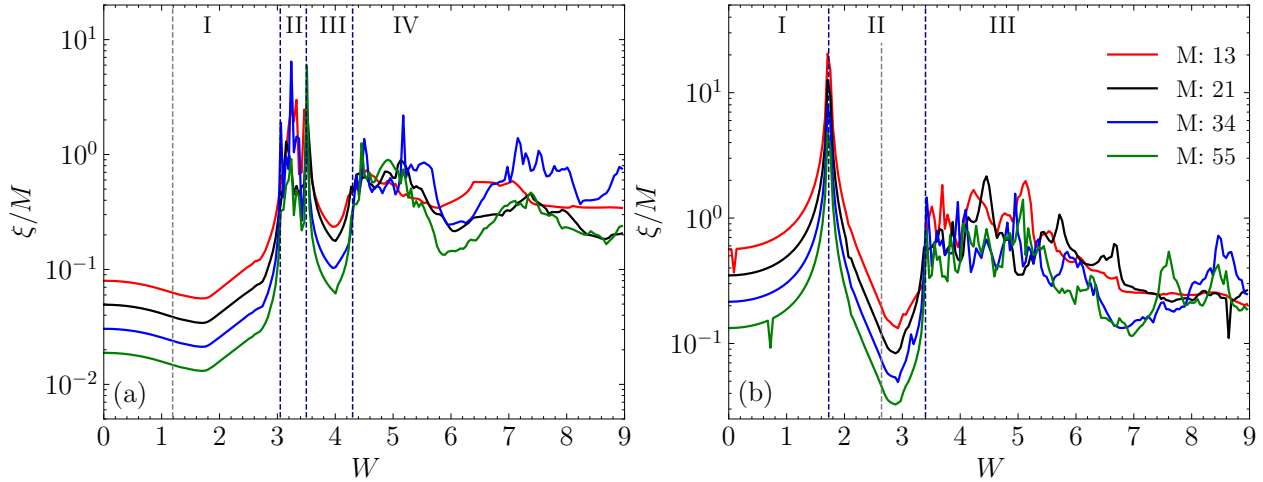


Figure 5.7: TMM at Fermi level ($E = 0$) for several transversal system sizes (M). For odd M we add a twists of $\theta_M = \pi$. The size of the longitudinal direction was chosen such that the relative error $\epsilon < 1\%$. (a) $\gamma = 0.5$. (b) $\gamma = 1.1$.

Below, we characterize the localization properties of the eigenstates with energies closer to $E = 0$. In the gapped phases, these correspond to eigenstates at the gap edge that are not captured by the TMM at Fermi level. In Fig. 5.8, we plot the average IPR and IPR_k of the 8 eigenstates closer to the Fermi level as a function of W . Whenever a gap closure occurs, TMM and IPR calculations are in agreement, as we discuss below.

We also plot the fractal dimensions D_2 and D_2^k in Fig. 5.9 estimated with the calculations of IPR and IPR_k respectively.

Discussion - Starting Topological For $\gamma = 0.5$, in the gapped phase I , the eigenstates at the gap edge start off ballistic, as seen in Fig. 5.9, $D_2 \rightarrow 2$ and $D_2^k \rightarrow 0$. They undergo a ballistic $\rightarrow$ localized ($D_2 \rightarrow 0$ and $D_2^k \rightarrow 2$) transition at $W \approx 1.19$ (gray line) further ascertaining that a level crossing between

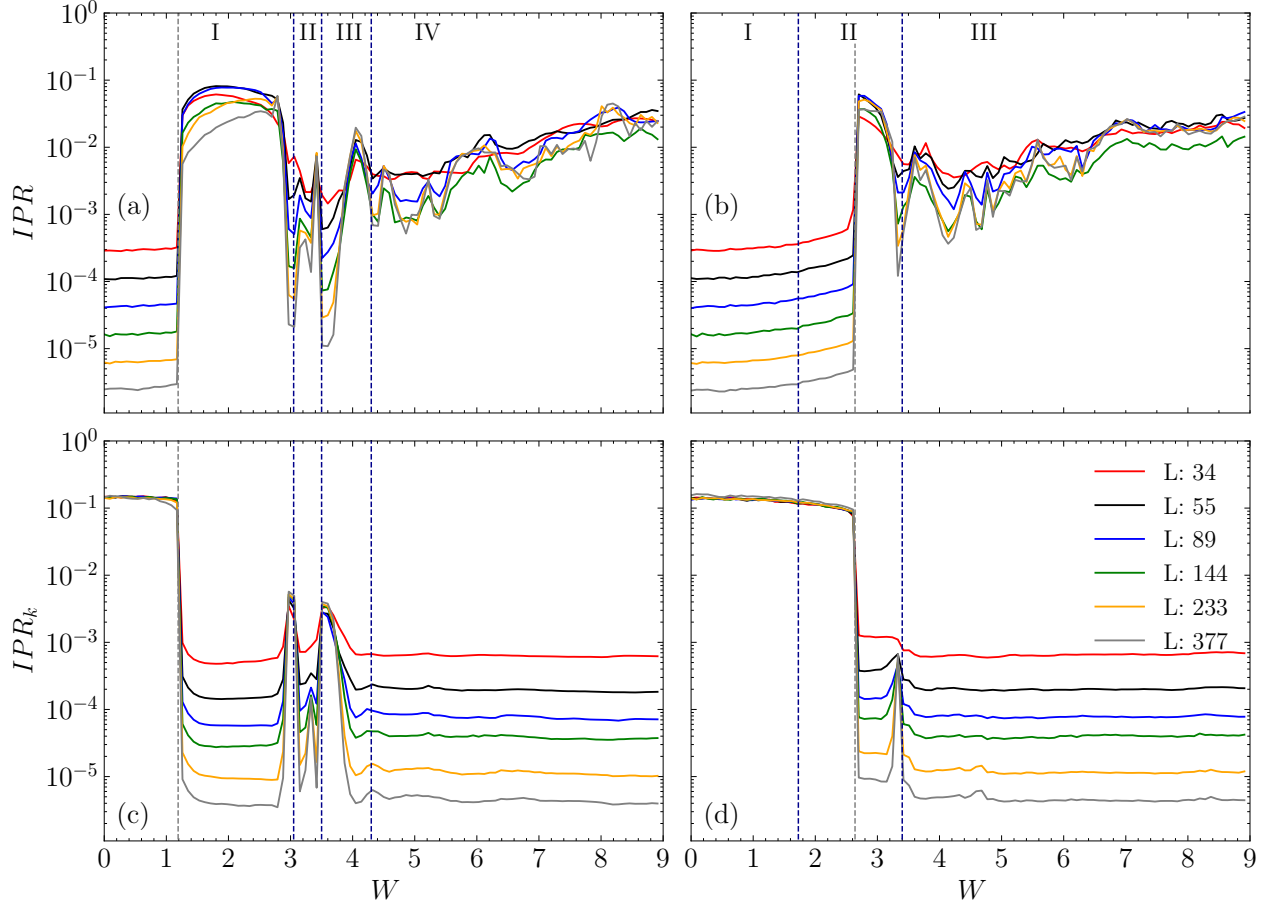


Figure 5.8: IPR (a,b) and IPR_k (c,d) calculations for different system sizes obtained with exact diagonalization methods. The IPR and IPR_k are averaged over 100 phase twists, shifts and over the first 8 eigenstates with energies closest to $E = 0$. (a,c) $\gamma = 0.5$. (b,d) $\gamma = 1.1$.

gap edge states occurs. This transition is not captured by the TMM since the system remains gapped. At the TPT ($I \rightarrow II$) the gap-edge states are ballistic, however, these states quickly turn critical, as seen by $D_2 \approx 1$, indicating that the gapless critical metal regime is reached (IIa). The normalized localization length (ξ/M) obtained via TMM, does not diverge at the transition. Instead, it goes to a constant value (see Fig. 5.7(a)), in agreement with the critical metal regime. In the QPQI phase (IIb), the gap-edge states remain critical, localizing for the IIc phase. In these latter regimes, TMM fails to capture such narrow behavior, due to the lack of discretization in TMM calculations. At the transition from $II \rightarrow III$, IPR , IPR_k (Fig. 5.8) and D_2 (Fig. 5.9) indicate a ballistic regime, with the gap-edge states undergoing a ballistic-localized transition halfway through phase III .

Phase IV is of difficult classification with any of the methods at our disposal. At the transition $III \rightarrow IV$ the IPR results suggest that the eigenstates are critical.

After this transition, TMM and IPR results are noisy, however, considering the fractal dimension computed with the last three system sizes, D_2 approaches zero, indicating that the system has reached an Anderson insulating phase ($D_2 \rightarrow 0$).

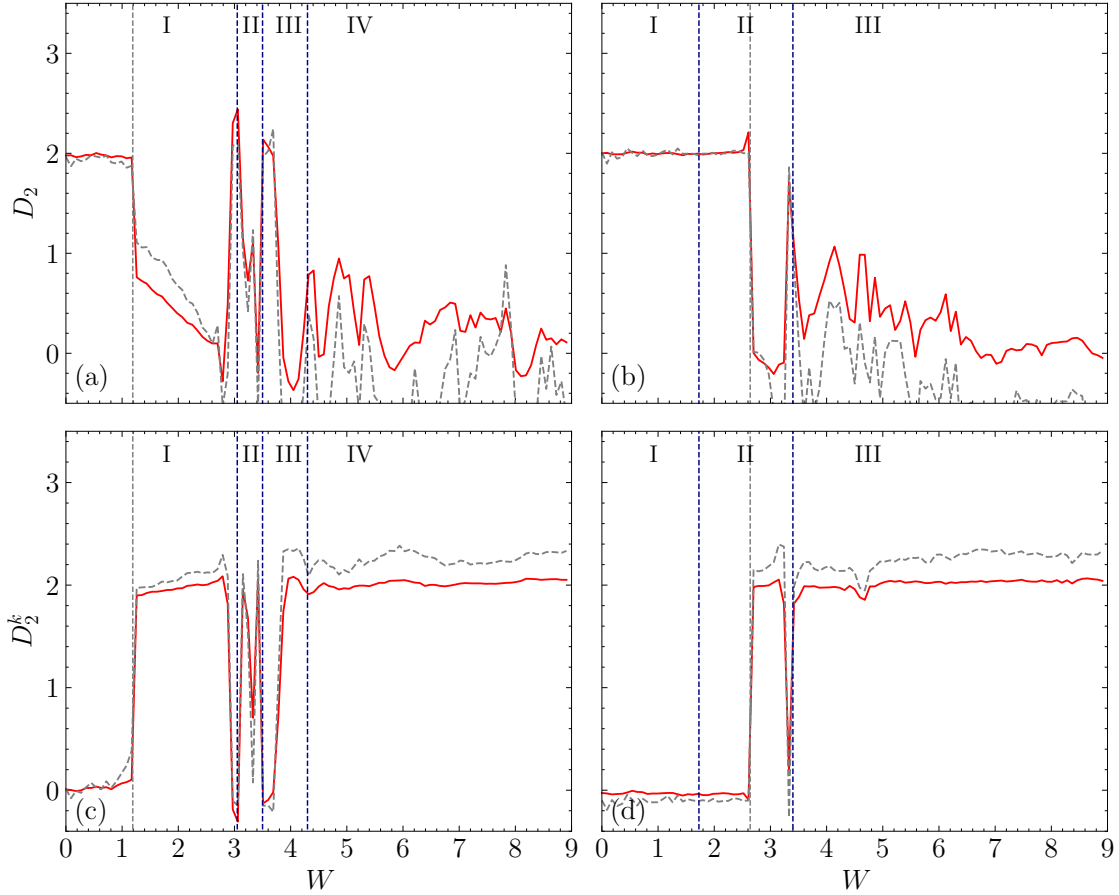


Figure 5.9: D_2 (a,b) and D_2^k (c,d) calculations for different system sizes obtained from the IPR and IPR_k results respectively. (a,c) $\gamma = 0.5$. (b,d) $\gamma = 1.1$. The red curves were estimated making a fit in log – log scale for all $L = \{34, 55, 89, 144, 233, 377\}$, while the dotted gray lines were obtained only considering the biggest three system sizes $L = \{144, 233, 377\}$.

Discussion - Starting Trivial Starting at the trivial phase with $\gamma = 1.1$, the gap edge eigenstates are ballistic within phase *I* and remain ballistic even after the transition into phase *II* ($D_2 \rightarrow 2$ and $D_2^k \rightarrow 0$, see Fig. 5.9). At the TPT ($I \rightarrow II$), a gap closing and reopening topological transition with ballistic gap edge states occurs, as in the absence of quasi-periodicity, which explains why this particular gap closure is highly dependent on the choice of twists, especially for small system sizes [87]. As in the previous case, the ballistic regime is maintained until the level crossing between ballistic and localized gap edge levels occurs (gray line) where we observe the gap-edge states sharply localize ($D_2 \rightarrow 0$). For higher W slightly before the gap closing at $W_c^{II \rightarrow III} \approx 3.4$, gap edge states delocalize and then become critical at the transition ($D_2 \approx 1.2$). The results for the final phase (*III*) are similar to phase *IV* of the previous cut, leading us to conclude that an Anderson insulating regime is reached.

5.5 Opening the Boundaries

Until now, we have spent much of our time on calculations involving periodic or twisted boundary conditions. However, a full characterization of these phases is not complete without considering an open

boundary system.

As it was discussed, an important hallmark of topological quadrupole insulators is that quadrupole phases defined by $q_{xy} = 0.5$ have zero-energy corner modes that give rise to fractional corner charges in open boundary systems. In this manner, a study of boundary signatures for each of the observed phases is important in order to have a complete and detailed picture of the chiral QPQI. Before proceeding, we introduce a simple yet powerful quantity, the corner occupation probability (P_{occ}) defined as

$$P_{occ} = \sum_{\mathbf{R} \in \text{corner}} \sum_{\alpha=1}^4 |\psi_n^\alpha(\mathbf{R})|^2, \quad (5.5.1)$$

where $\psi_n^\alpha(\mathbf{R})$ represent the α^{th} orbital at site $\mathbf{R}$ of the eigenstate with energy E_n . For the calculations that follow, we average out P_{occ} of the four eigenstates closest to the Fermi level. On one hand, in a QI phase zero-energy corner modes occur thus $P_{occ} \approx 1$, on the other hand, for a trivial phase, no corner modes exist such that $P_{occ} < 1$. Since the corner states display a localization length dependent on W and γ we compute P_{occ} over an $l \times l$ region which we assume to be the corner, i.e. we restrict the sum in Eq. 5.5.1 to that region. Therefore, l is effectively an estimation of the localization length of the corner modes. In Fig. 5.10(a-b) the P_{occ} as a function of W is shown for several sizes of the corner (l). In Fig. 5.10(c-d) we show the averaged corner charge $\bar{Q} = \sum_i |Q_i|$ as a function of W , obtained from $Q_i = \sum_{\mathbf{R} \in \text{corner}} \rho(\mathbf{R})$, where $\rho(\mathbf{R}) = 2 - \sum_{n \in \text{occ.}} \sum_{\alpha=1}^4 |\psi_n^\alpha(\mathbf{R})|^2$ is the charge density. The first and second terms arise from the atomic positive charges and from the electronic density, respectively. Unlike the computations for P_{occ} the system is partitioned into four quadrants, each of the size of a quarter of the system. Then, the corner charge is computed by integrating $\rho(\mathbf{R})$ over each of the quadrants. In quadrupole insulating phases $\bar{Q} = 0.5$.

Discussion - Starting Topological For $\gamma = 0.5$, P_{occ} has perfect plateaus at 1 for every considered l , indicating the existence of highly localized corner states ($\xi_l < 10$ where ξ_l is the localization length of the corner modes). Similarly, the corner charge also quantizes at $\bar{Q} = 0.5$ throughout the topological phase. In phase *II*, the critical metal (*IIa*) and trivial insulator (*IIc*) display a finite, yet significantly smaller P_{occ} , that arises from contributions of edge or bulk states (below we will provide a detailed discussion on edge states). The same is observed regarding the corner charge. In the narrow topological regime observed (*IIb*), P_{occ} sharply peaks, scaling closer to 1 as seen in Fig. 5.10(a). Despite this, the peak does not properly quantize to 1 for the studied l , that we attribute to the large localization length of the corner modes $\xi_l > 30$, which is expected due to the very small gap in this phase. A peak can also be observed in the corner charge for $L = 55$ as seen in Fig. 5.10(c), albeit smaller due to the considerably smaller system size. Regarding phase *III*, P_{occ} has a noisy plateau that scales to 1 as l increases, indicating again that the corner states display a larger localization length than the maximum considered corner ($l = 30$). The corner charge also scales to 0.5 with increasing size, further ascertaining that *III* is indeed topological, with corner modes characterized by a large localization length.

Finally, as expected, phase *IV* has a small P_{occ} . However, we also see a growth with increasing corner/system size. This increase is explained by the gapless nature of this phase. As l increases, more and more bulk spectral weight falls within the considered $l \times l$ corner, leading to a visible increase in P_{occ} . Regarding the corner charge, although there are no quantized corner charges, for some realizations

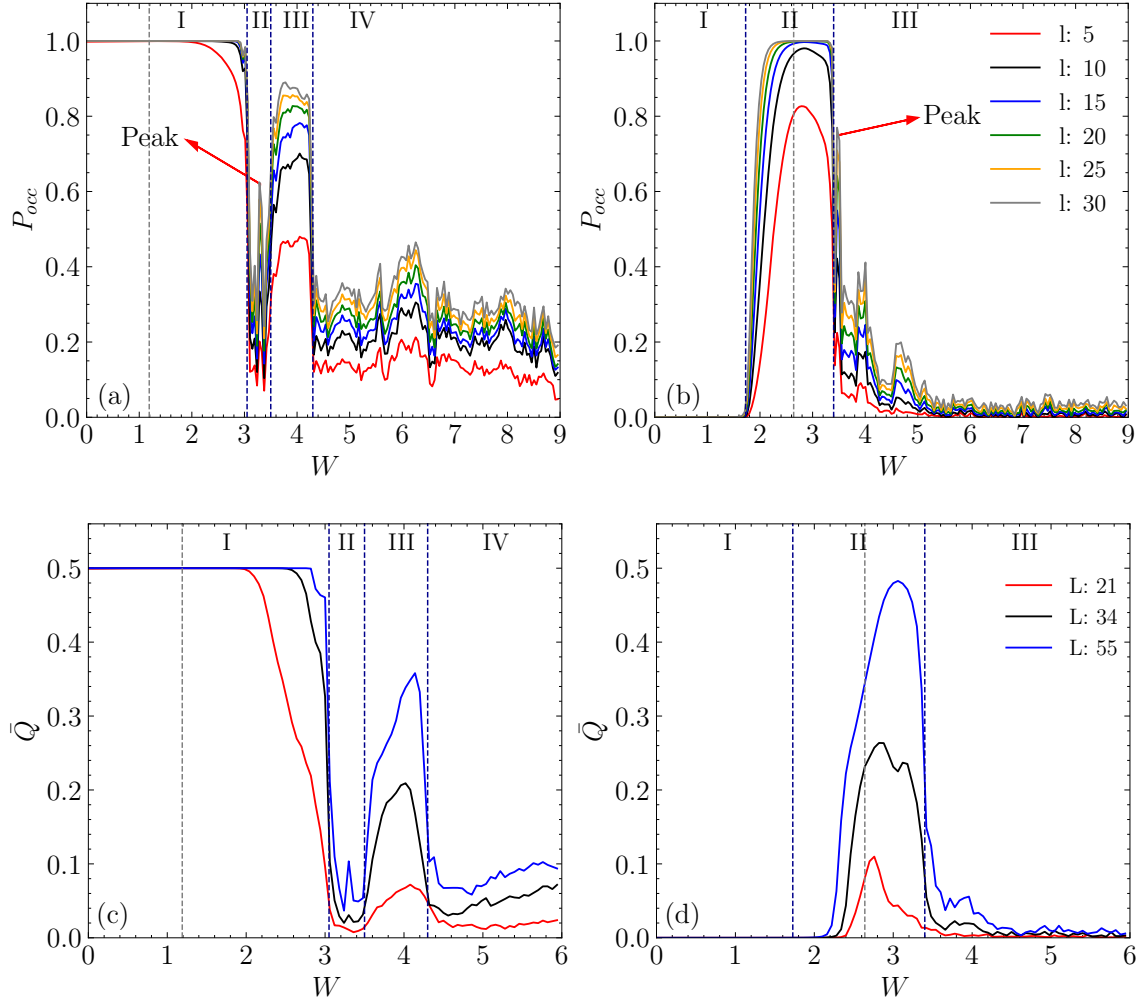


Figure 5.10: (a-b) Corner occupation probability (P_{occ}) as a function of W for the first 2 zero-energy states. The results were obtained for a system size of $L = 377$ and averaged over 200 phase shifts. (c-d) Corner charge ($\bar{Q}$) as a function of W for several system sizes and averaged over 100 phase shifts and over the 4 corners. A small $\delta = 10^{-5}$ was used in both cases to split the degeneracy of the four-fold corner modes. (a,c) $\gamma = 0.5$. (b,d) $\gamma = 1.1$.

of phase shifts the charge density displays fluctuations which leads to finite contributions to the corner charge. This occurs due to the breaking of chiral symmetry by the small δ introduced to lift the degeneracy of the corner modes. Overall, the P_{occ} and $\bar{Q}$ of each phase agrees well with the topological phase diagram.

Discussion - Starting Trivial For $\gamma = 1.1$ both trivial phases *I* and *IIIc* exhibit $P_{occ} = 0$, as seen in Fig. 5.10(b). For phase *II* the corner occupation probability, though initially suffers from finite-size effects, eventually reaches 1. Its dependence on l after the TPT ($I \rightarrow II$) indicates a diverging localization length of the corner states as the critical point is approached. Deeper into the QI phase, the corner modes become more localized. This is exactly the same behavior observed around the TPT of the clean BBH model. Regarding *IIIb*, P_{occ} has a small peak in this region as indicated in Fig. 5.10(b), however, the corner charge calculations do not have enough resolution to catch these narrow topological regimes. Regarding the corner charge, it displays scaling with increasing system size. Nonetheless, a plateau cannot be seen

even for the largest considered size $L = 55$. Looking at P_{occ} in phase *II*, it is clear that for a system size $L = 377$ considering the corner to be a 30×30 square is not enough to measure all the weight of the corner state since they display a localization length $\xi_l > 30$. Therefore, simulating a system of size $L = 55$,⁵ leads to the hybridization of the corner modes, which in turn leads to a non-quantized corner charge. In Appendix E some remarks are made regarding corner mode hybridization, its relation to finite-size effects, and consequently to non-quantized corner charges, as seen in phase *II* with $\gamma = 1.1$.

Density of States Another quantity worth exploring is the ratio of open boundary DOS (ρ_{OBC}) and periodic boundary DOS (ρ_{PBC}). Specifically, for the same system, we compute the DOS with open boundary conditions (ρ_{OBC}), then with periodic boundary conditions (ρ_{PBC}) and proceed to define the ratio ρ_{OBC}/ρ_{PBC} . In regions where there are no boundary states, we expect $\rho_{OBC}/\rho_{PBC} \approx 1$,⁶ however, in gapped regions where boundary states can live, we expect $\rho_{OBC}/\rho_{PBC} \gg 1$. In Fig. 5.11 we show the ratio ρ_{OBC}/ρ_{PBC} for $\gamma = 1.1$ as a function of E . As expected, in gapped regions (grayed-out zones) we have $\rho_{OBC}/\rho_{PBC} \gg 1$.

Overall, $\rho_{OBC}/\rho_{PBC} \gg 1$ in gapped regions (grayed-out zones), furthermore, for values of W in the topological phases ($W = 2.0$ and $W = 3.0$ in phase *II*) spectral weight at Fermi level ($E = 0$) is observed, indicating the existence of topological corner modes. For high W , all the bulk gaps eventually close, leading to $\rho_{OBC}/\rho_{PBC} \rightarrow 1$. The exact same behavior can be seen for $\gamma = 0.5$ in Fig. F.2 in Appendix F.

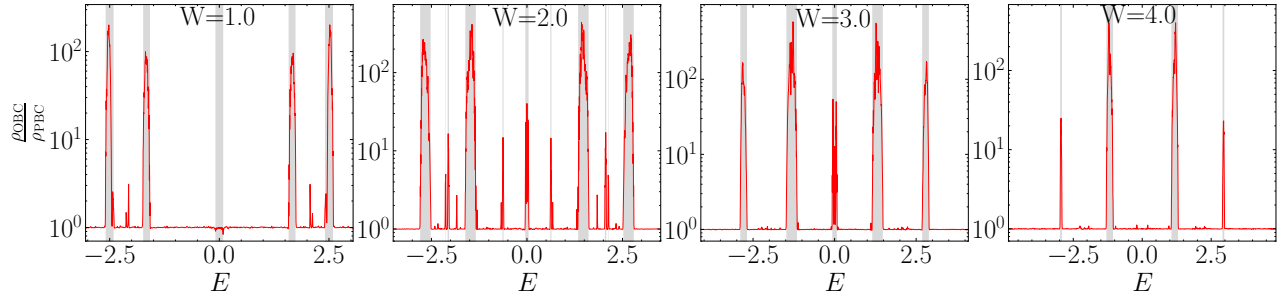


Figure 5.11: Ratio of open boundary DOS (ρ_{OBC}) and periodic boundaries DOS (ρ_{PBC}) as a function of energy for W in different phases and $\gamma = 1.1$. The grayed-out regions are bulk gaps opened by the QP modulation and were estimated by setting a threshold for the PBC DOS ($\rho_{PBC} < 10^{-3}$). The following KPM parameters were used: $L = 987$, $M = 5000$, $R = 10$.

Properties of QPQI phases Until now, a proper characterization of the QPQI phases has not been provided. In the paragraphs that follow, we aim to fully define these quasi-periodic-induced regime. We start with their definition: a QPQI phase is a topological quadrupole insulating phase that is not adiabatically connected to any of the clean limit phases⁷ while displaying a quasi-periodic induced bulk-spectral gap⁸.

⁵Notice that for $\xi_l > 30$, the localization length of the corner state is of the order of the linear size of the entire system.

⁶For big enough system sizes.

⁷Two phases are adiabatically connected if there is at least one continuous path connecting both phases, throughout which the bulk spectral gap remains open.

⁸Or is gapless but displays localized states at the Fermi level, as discussed in Appendix F in relation to the constant W cut).

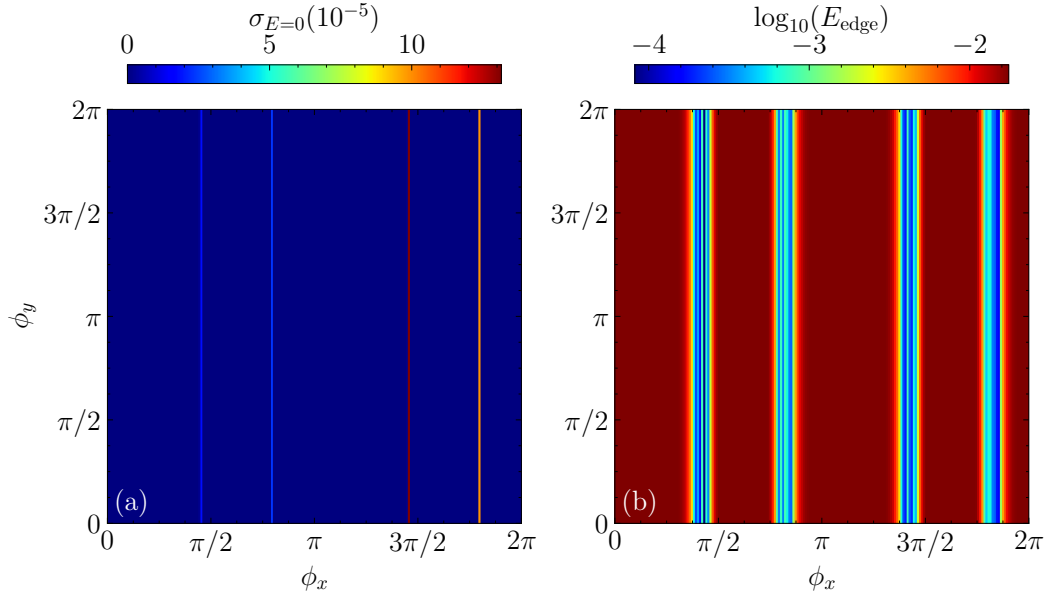


Figure 5.12: (a) Standard deviation ($\sigma_{E=0}$) of the energies of the corner modes as a function of the phase shifts (ϕ_x, ϕ_y). (b) Logarithm of edge state energy ($\log_{10}(E_{edge})$) as a function of the phase shifts (ϕ_x, ϕ_y). Results obtained for $W = 3$, $\gamma = 0.5$ for a system size $L = 233$.

We have found that quasi-periodic-induced gapped phases usually display edge states that disperse with the phase shifts. This phenomenon is common in QP systems and can be observed in the Aubry-André model. As ϕ changes, the energy of the edge states can move closer or even cross the Fermi level. This phenomenon is particularly relevant in topological regimes since the edge states can hybridize with zero-energy topological modes, thus pulling them away from zero-energy. We expect that when such crossing occurs, the system behaves as in the trivial regime, displaying $P = 0$. Furthermore, P_{occ} is also impacted since the corner modes are hybridized with edge states that exhibit spectral weight outside the corners.

In order to check the existence of edge states and study edge-corner hybridization, we resort to exact diagonalization of the open boundary system Hamiltonian, calculating the 6 eigenvalues closest to Fermi level. Assuming we choose a point of the phase diagram that resides in a SOTI phase, out of the 6 energies, 4 correspond to zero-energy corner modes, with the remaining two corresponding to the edge states with energy closest to Fermi level. We then proceed to compute the standard deviation of the corner modes energy ($\sigma_{E=0} = \sqrt{\frac{1}{N} \sum_i E_i^2}$) and the energy of the edge state closest to the Fermi level (E_{edge}). In this manner, when the edge states energy approaches the Fermi level ($E_{edge} \rightarrow 0$) a peak should be seen in $\sigma_{E=0}$, indicating that the corner modes have hybridized with the edge states. Before tackling QPQI phases that display complex dynamics, we consider a simpler case. In Fig. 5.3(a), just before the TPT from $I \rightarrow II$, a small dip can be seen in the P invariant ($W \approx 3$ and $\gamma \approx 0.5$), suggesting that some dependence on the phase shifts might exist. In this manner, in Fig. 5.12 we show the density plots of $\sigma_{E=0}$ (a) and E_{edge} (b) in the (ϕ_x, ϕ_y) plane. Four lines of constant ϕ_x can be observed where $\sigma_{E=0} > 0$ for $E_{edge} \rightarrow 0$, indicating that the corner modes hybridized away from zero energy (see Fig. 5.14). Moreover, not all four corner modes hybridize with the edge states. In fact, only two of them move away from zero-energy while also demonstrating signs of hybridization, prompting us to distinguish the four corner

states. We attribute the term “Inner Corner Modes” to the two corner modes that remain at $E = 0$ and “Outer Corner Modes” to the remaining corner states that move away from zero energy.

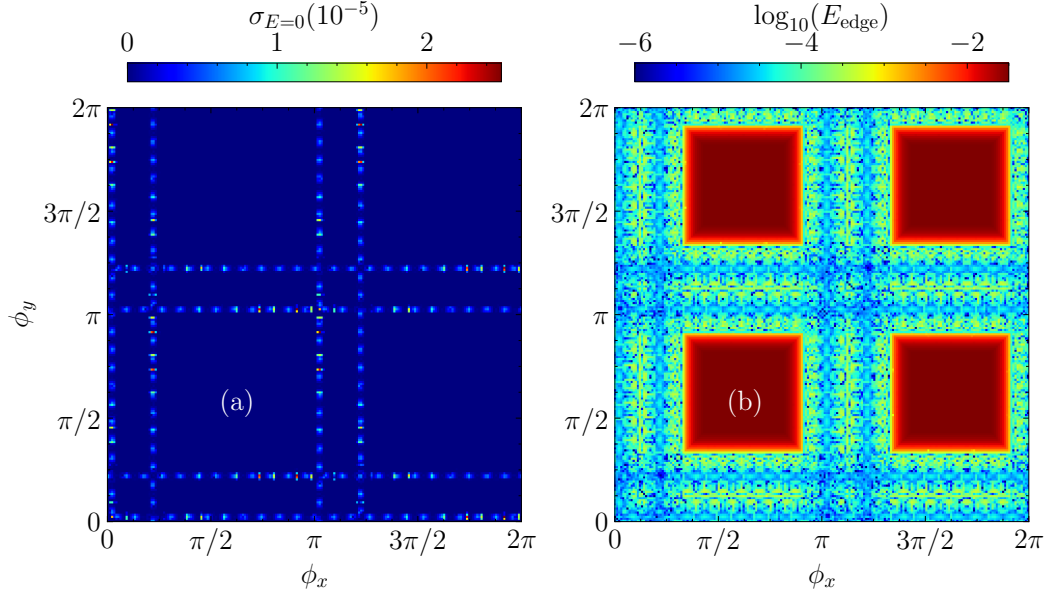


Figure 5.13: (a) Standard deviation ($\sigma_{E=0}$) of the energies of the corner modes as a function of the phase shifts (ϕ_x, ϕ_y) . (b) Logarithm of edge state energy ($\log_{10}(E_{edge})$) as a function of the phase shifts (ϕ_x, ϕ_y) . Results obtained for $W = 3.8$ and $\gamma = 0.2$ in the QPQI phase for a system size $L = 377$.

A distinct feature of QPQI phases is their much stronger dependence on phase shifts. In Fig. 5.13 we show $\sigma_{E=0}$ and $E_{edge} \rightarrow 0$ for the choice of parameters $\gamma = 0.2$ and $W = 3.8$, well inside the QPQI phase. Just as before, regions with $\sigma_{E=0} > 0$ are correlated to regions where $E_{edge} \rightarrow 0$. Furthermore, increasing system size confines these regions to singular points (for smaller system sizes, see Appendix F). This behavior suggests that as these regions collapse to singular points, all the quantities of relevance (P, P_{occ} and q_{xy}) quantize to their respective values, since these points will have no statistical importance.

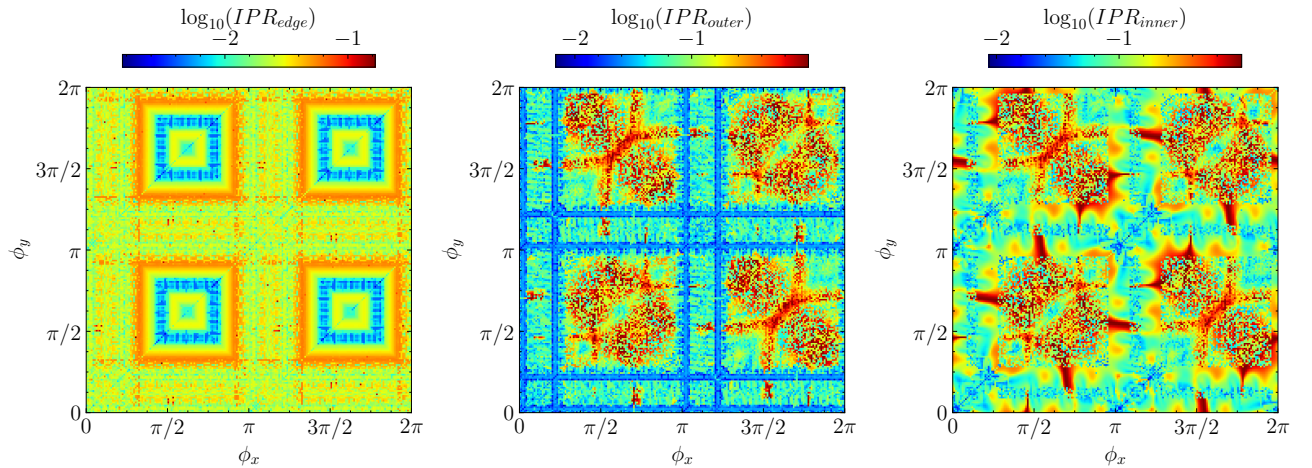


Figure 5.14: IPR of the edge, outer and inner states plotted from left to right respectively for $L = 377$.

As $E_{edge} \rightarrow 0$ we expect the localization length of the corner modes to increase as the states hybridize.

In Fig. 5.14, we plot the IPR of the edge and corner states for $L = 377$. As discussed previously, only one of the pairs of corner modes hybridizes, which can be seen by the clear pattern emerging in the middle plot of Fig. 5.14 corresponding to the IPR of the outer corner states. As the edge states cross the Fermi energy, the IPR of the outer corner modes decreases, indicating that the localization length increases. Although, IPR alone is not enough to conclude about the localization length of a state, for fully delocalized states $IPR \approx \frac{1}{N}$, thus for the considered system size ($L = 377$), $IPR \approx 10^{-5}$. Therefore, an IPR of the order of 10^{-2} is a good indication that the corner modes remain localized throughout the (ϕ_x, ϕ_y) plane.

Overall, QPQI phases exhibit a strong correlation between the localization length of the corner modes and the edge gap (which is ϕ dependent). As the edge states energy approach the Fermi level, they localize, moving towards the corners, thus hybridizing with the corner modes. The hybridization “pulls” the outer corner modes away from zero-energy while increasing their localization length. In the QI regime, the corner modes display oscillating localization length with varying phase shifts, however, to a far lesser degree than in the QPQI phases. Furthermore, unlike the QPQI regimes, there is no apparent correlation between the localization length of the corner modes and the energy of the edge states, suggesting that the oscillations on the localization length have a different origin than corner-edge hybridization.

Chapter 6

Conclusion and Outlook

Throughout this thesis, we sought to study and characterize the effects of a quasi-periodic modulation on the prototypical BBH model for higher-order topology.

In Chapter 2 we have explored several methods to tackle topological systems, starting with the introduction of the nested Wilson loop approach by demonstrating its connection with the diagonalization of the projected position operator. Furthermore, we related their spectra to bulk and boundary topology with the introduction of the winding number, which in turn defines the bulk electronic polarization. We have also explored generalizations of Resta's formula to higher-order multipole moments that are needed for the characterization of quadrupole insulators, showing that these multipole moments are quantized by chiral symmetry. Since our main goal was to study systems lacking translational invariance, we introduced several methods that allow us to study spectral (KPM and recursive method), localization (TMM and *IPR*) and boundary properties (Green's functions) via real-space approaches.

Before tackling higher-order topological insulators, we study a Chern insulator under the effect of a 1D quasi-periodic onsite potential in Chapter 3, where it was demonstrated that Chern insulating phases ($C = \pm 2$) are robust to quasi-periodic modulations while eventually a gap closing and opening in Dirac cone transition occurs. This induces a topological phase transition into a gapped $C = \pm 1$ phase characterized by several extended bulk states. These results greatly contrast to those obtained for Anderson disorder, where it has been shown that the gap closes before the topological phase transitions and that the entire spectra is Anderson localized, but for a few punctual critical states that carry all the topology [79]. Overall, QP topological systems are phenomenologically different from their disordered cousins. With this analysis, we built up our intuition to tackle higher-order quasi-periodic topological systems.

In Chapter 4, we started off with the introduction of the BBH model and its overall properties. Later the effects of chiral symmetry preserving disorder was considered on the BBH model, where it was shown that chiral disorder induces a topological phase transition into a phase with quantized quadrupole moment ($q_{xy} = 0.5$), quantized boundary polarizations ($p_x = p_y = 0.5$) and zero-energy corner modes. This SOTI phase is initially gapped, with a smaller gapless region appearing. Thus, two distinct phases were found which the authors in Ref. [50] entitled gapped and gapless HOTAI. This behavior is identical to the one observed in first-order TAIs. Eventually the system undergoes a transition into a critical metal with mixed topological properties, the Griffiths regime. For high enough disorder, the entire spectrum

localizes, and the system reaches an Anderson insulating phase.

In Chapter 5 we reached the main focus of this thesis, where the properties of the BBH model under chiral quasi-periodic modulations were studied. We performed a detailed study of the system, characterizing most of the relevant phases observed in the phase diagram. Overall, clean limit topological phases (QI) are shown to be robust to the application of such type of modulations. Furthermore, quasi-periodic modulations can induce transitions into QPQI phases. Although these phases are defined by a quantized quadrupole moment ($|q_{xy}| = 0.5$), quantized boundary polarizations ($|p_x| = |p_y| = 0.5$) and zero-energy corner modes, just like the regular QI regimes, these newly found QPQI phases display far richer localization properties and dynamics, like corner-edge hybridization, gapped and gapless regimes, and are not adiabatically connected to regular QI phases. For low modulation strength, ballistic-ballistic transitions occur and even transitions with critical states at Fermi level are observed. In the range of W comparable to where the Griffiths regime is observed for the disordered case, the same mixed topology emerges, however, with localized states at Fermi level. For high modulation strength, the system reaches an Anderson Insulating phase. Furthermore, all the observed SOTI phases exhibit zero-energy corner modes that give rise to quantized fractional corner charges.

Unfortunately, this thesis does not answer all the questions, with some work left to be done. Reaching bigger system sizes will be an instrumental tool in better defining some of the observed phases, especially the QPQI regimes. Furthermore, a characterization of each phase with the multipole chiral numbers might paint a more illuminating picture in the mixed regimes. Regarding boundary properties, we have encountered an interesting dynamics involving the phase shift and the energy of the edge states that separates the QI phases from the QPQI regimes. Certainly, further studying this interplay between quasi-periodic topology and chiral SOTI phases is of interest in the present state of quasi-periodicity and HOTIs. Moreover, a perturbative approach via self-consistent Born approximation would be welcomed to better understand the mechanism behind the TPT from $I \rightarrow II$ at $\gamma = 1.1$, which we suspect to be in the common hopping renormalization mechanism. Last but not least, it would be interesting to find signatures of the corner-edge dynamics that could be used in possible cold atom experiments to detect QPQI phases.

Appendix A

Wilson Loops - Supplementary Calculations

A.1 $\langle 0 | \gamma_{k,n} c_{q+\Delta k, \alpha}^\dagger | 0 \rangle$ and $\langle 0 | c_{q, \alpha} \gamma_{k', m}^\dagger | 0 \rangle$ correlators

Here we calculate the correlators:

$$\langle 0 | \gamma_{k,n} c_{q+\Delta k, \alpha}^\dagger | 0 \rangle \quad (\text{A.1.1})$$

$$\langle 0 | c_{q, \alpha} \gamma_{k', m}^\dagger | 0 \rangle. \quad (\text{A.1.2})$$

For the first one (A.1.1):

$$\begin{aligned} \langle 0 | \gamma_{k,n} c_{q+\Delta k, \alpha}^\dagger | 0 \rangle &= \\ &= \sum_{\beta} [(u_k^n)^*]^\beta \langle 0 | c_{k, \beta} c_{q+\Delta k, \alpha}^\dagger | 0 \rangle \\ &= \sum_{\beta} [(u_k^n)^*]^\beta \delta_{\alpha, \beta} \delta_{k, q+\Delta k} \\ &= [(u_k^n)^*]^\alpha \delta_{k, q+\Delta k}. \end{aligned} \quad (\text{A.1.3})$$

For the second one (A.1.2) the calculation is analogous:

$$\begin{aligned} \langle 0 | c_{q, \alpha} \gamma_{k', m}^\dagger | 0 \rangle &= \\ &= \sum_{\beta} [u_{k'}^m]^\beta \langle 0 | c_{q, \alpha} c_{k', \beta}^\dagger | 0 \rangle \\ &= \sum_{\beta} [u_{k'}^m]^\beta \delta_{\alpha, \beta} \delta_{k', q} \\ &= [u_{k'}^m]^\alpha \delta_{k', q}. \end{aligned} \quad (\text{A.1.4})$$

A.2 Polarization of Wannier Sectors

The phases $\nu_x^j(k_y)$ of the first Wilson loop define a new band structure of the edge, they are defined in the BZ with $k_y = [-\pi, \pi[$. To have a non-trivial topological phase defined by a bulk quadrupole moment, one needs a boundary Hamiltonian with a gapped band structure. This way, one defines the Wannier sectors ν_x^- and ν_x^+ that are the set of Wannier bands.

$$\begin{aligned}\nu_x^- &= \{\nu_x^j(k_y) : \forall j \text{ } \nu_x^j(k_y) \text{ below the gap}\} \\ \nu_x^+ &= \{\nu_x^j(k_y) : \forall j \text{ } \nu_x^j(k_y) \text{ above the gap}\}\end{aligned}$$

With the band structure of the edge defined, the objective is to perform a second Wilson loop in the y direction. The projector that spans the occupied Wannier sectors is given by:

$$\begin{aligned}P_{\nu_x} &= \sum_{j=1}^{N_W} \sum_{R_x, k_y} |\psi_{R_x, k_y}^j\rangle \langle \psi_{R_x, k_y}^j| \\ &= \frac{1}{N_x} \sum_{j=1}^{N_W} \sum_{R_x, k_y} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{k_x, k'_x} \gamma_{n, [k_x, k_y]}^\dagger |0\rangle \left[v_{x, [k_x, k_y]}^j \right]^n e^{-ik_x R_x} \langle 0 | \gamma_{m, [k'_x, k_y]} \left[\left(v_{x, [k'_x, k_y]}^j \right)^* \right]^m e^{ik'_x R_x} \\ &= \sum_{j=1}^{N_W} \sum_{k_y} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{k_x, k'_x} \gamma_{n, [k_x, k_y]}^\dagger |0\rangle \left[v_{x, [k_x, k_y]}^j \right]^n \langle 0 | \gamma_{m, [k'_x, k_y]} \left[\left(v_{x, [k'_x, k_y]}^j \right)^* \right]^m \frac{1}{N_x} \sum_{R_x} e^{-i(k_x - k'_x) R_x} \\ &= \sum_{j=1}^{N_W} \sum_{k_y} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{k_x, k'_x} \gamma_{n, [k_x, k_y]}^\dagger |0\rangle \left[v_{x, [k_x, k_y]}^j \right]^n \langle 0 | \gamma_{m, [k'_x, k_y]} \left[\left(v_{x, [k'_x, k_y]}^j \right)^* \right]^m \delta_{k_x, k'_x} \\ &= \sum_{j=1}^{N_W} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}} \gamma_{n, \mathbf{k}}^\dagger |0\rangle \left[v_{x, \mathbf{k}}^j \right]^n \left[\left(v_{x, \mathbf{k}}^j \right)^* \right]^m \langle 0 | \gamma_{m, \mathbf{k}}.\end{aligned}\tag{A.2.1}$$

Now one needs to project the position operator $\hat{y}$ into the occupied Wannier sector ($P_{\nu_x} \hat{y} P_{\nu_x}$). The position operator $\hat{y}$ has an analogous expression to eq. 2.1.1 in reciprocal-space, its form is:

$$\hat{y} = \sum_{\mathbf{k}, \alpha} c_{\mathbf{k}+\Delta k_y, \alpha}^\dagger |0\rangle \langle 0| c_{\mathbf{k}, \alpha}.$$

The projected position operator takes the form:

$$\begin{aligned}P_{\nu_x} \hat{y} P_{\nu_x} &= \sum_{i, j=1}^{N_W} \sum_{n, m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}, \mathbf{k}'} \sum_{\mathbf{q}} \gamma_{n, \mathbf{k}}^\dagger |0\rangle \left[v_{x, \mathbf{k}}^i \right]^n \left[\left(v_{x, \mathbf{k}}^i \right)^* \right]^m \langle 0 | \gamma_{m, \mathbf{k}} c_{\mathbf{q}+\Delta k_y, \alpha}^\dagger |0\rangle \\ &\quad \langle 0 | c_{\mathbf{q}, \alpha} \gamma_{n', \mathbf{k}'}^\dagger |0\rangle \left[v_{x, \mathbf{k}'}^j \right]^{n'} \left[\left(v_{x, \mathbf{k}'}^j \right)^* \right]^{m'} \langle 0 | \gamma_{m', \mathbf{k}'}.\end{aligned}\tag{A.2.2}$$

Substituting the results deduced previously for the correlators A.1:

$$\begin{aligned}
P_{\nu_x} \hat{y} P_{\nu_x} &= \sum_{i,j=1}^{N_W} \sum_{\substack{n,m=1 \\ n',m'=1}}^{N_{\text{occ}}} \sum_{\mathbf{k}, \mathbf{k}'} \sum_{\alpha} \gamma_{n,\mathbf{k}}^{\dagger} |0\rangle [v_{x,\mathbf{k}}^i]^n \left[(v_{x,\mathbf{k}}^i)^* \right]^m [(u_{\mathbf{k}}^m)^*]^{\alpha} [u_{\mathbf{k}'}^{n'}]^{\alpha} \delta_{\mathbf{k}, \mathbf{q} + \Delta k_y} \\
&\quad \delta_{\mathbf{k}', \mathbf{q}} [v_{x,\mathbf{k}'}^j]^{n'} \left[(v_{x,\mathbf{k}'}^j)^* \right]^{m'} \langle 0 | \gamma_{m', \mathbf{k}'}, \\
P_{\nu_x} \hat{y} P_{\nu_x} &= \sum_{i,j=1}^{N_W} \sum_{\substack{n,m=1 \\ n',m'=1}}^{N_{\text{occ}}} \sum_{\mathbf{q}, \alpha} \gamma_{n, \mathbf{q} + \Delta k_y}^{\dagger} |0\rangle [v_{x, \mathbf{q} + \Delta k_y}^i]^n \left[(v_{x, \mathbf{q} + \Delta k_y}^i)^* \right]^m \left[(u_{\mathbf{q} + \Delta k_y}^m)^* \right]^{\alpha} [u_{\mathbf{q}}^{n'}]^{\alpha} \\
&\quad [v_{x, \mathbf{q}}^j]^{n'} \left[(v_{x, \mathbf{q}}^j)^* \right]^{m'} \langle 0 | \gamma_{m', \mathbf{q}}, \\
P_{\nu_x} \hat{y} P_{\nu_x} &= \sum_{i,j=1}^{N_W} \sum_{\substack{n,m=1 \\ n',m'=1}}^{N_{\text{occ}}} \sum_{\mathbf{q}} \gamma_{n, \mathbf{q} + \Delta k_y}^{\dagger} |0\rangle [v_{x, \mathbf{q} + \Delta k_y}^i]^n \left(\sum_{n', m'=1}^{N_{\text{occ}}} \langle u_{\mathbf{q} + \Delta k_y}^m | \left[(v_{x, \mathbf{q} + \Delta k_y}^i)^* \right]^m [v_{x, \mathbf{q}}^j]^{n'} | u_{\mathbf{q}}^{n'} \rangle \right) \\
&\quad \left[(v_{x, \mathbf{q}}^j)^* \right]^{m'} \langle 0 | \gamma_{m', \mathbf{q}}. \quad (\text{A.2.3})
\end{aligned}$$

To simplify notation and calculations the following definitions are used:

$$|\omega_{x,\mathbf{k}}^j\rangle = \sum_{n=1}^{N_{\text{occ}}} [v_{x,\mathbf{k}}^j]^n |u_{\mathbf{k}}^n\rangle \quad (\text{A.2.4})$$

$$[F_{y,\mathbf{k}}^{\nu_x}]^{n,m} = \sum_{i,j=1}^{N_W} [v_{x,\mathbf{k} + \Delta k_y}^i]^n \langle \omega_{x,\mathbf{k} + \Delta k_y}^i | \omega_{x,\mathbf{k}}^j \rangle \left[(v_{x,\mathbf{k}}^j)^* \right]^m. \quad (\text{A.2.5})$$

Substituting these definitions in eq. A.2.3 we get:

$$P_{\nu_x} \hat{y} P_{\nu_x} = \sum_{n,m=1}^{N_{\text{occ}}} \sum_{\mathbf{k}} \gamma_{n, \mathbf{k} + \Delta k_y}^{\dagger} |0\rangle [F_{y,\mathbf{k}}^{\nu_x}]^{n,m} \langle 0 | \gamma_{m, \mathbf{k}}. \quad (\text{A.2.6})$$

Note that this operator is diagonal in k_x . To diagonalize the operator let us consider the following eigenvectors equation $P_{\nu_x} \hat{y} P_{\nu_x} |\psi^j\rangle = E^j |\psi^j\rangle$ which in matrix form for each k_x reduces to (for simplicity in notation the k_x index is hidden):

$$\begin{pmatrix} 0 & 0 & 0 & \dots & F_{y,k_N}^{\nu_x} \\ F_{y,k_1}^{\nu_x} & 0 & 0 & \dots & 0 \\ 0 & F_{y,k_2}^{\nu_x} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} \nu_{y,k_1} \\ \nu_{y,k_2} \\ \nu_{y,k_3} \\ \vdots \\ \nu_{y,k_N} \end{pmatrix}^j = E^j \begin{pmatrix} \nu_{y,k_1} \\ \nu_{y,k_2} \\ \nu_{y,k_3} \\ \vdots \\ \nu_{y,k_N} \end{pmatrix}^j, \quad (\text{A.2.7})$$

where $F_{y,k_i}^{\nu_x}$ are $N_{\text{occ}} \times N_{\text{occ}}$ matrices. This eigenvalue problem can be rewritten has a set of N equations:

$$\begin{cases} F_{y,k_N}^{\nu_x} \nu_{y,k_N}^j = E^j \nu_{y,k_1}^j \\ F_{y,k_1}^{\nu_x} \nu_{y,k_1}^j = E^j \nu_{y,k_2}^j \\ F_{y,k_2}^{\nu_x} \nu_{y,k_2}^j = E^j \nu_{y,k_3}^j \\ \dots \\ F_{y,k_{N-1}}^{\nu_x} \nu_{y,k_{N-1}}^j = E^j \nu_{y,k_N}^j \end{cases}, \quad (\text{A.2.8})$$

which fully defines

$$\begin{aligned} F_{y,k_N}^{\nu_x} F_{y,k_{N-1}}^{\nu_x} (\dots) F_{y,k_2}^{\nu_x} F_{y,k_1}^{\nu_x} \nu_{y,k_1}^j &= (E^j)^N \nu_{y,k_1}^j \\ \mathcal{W}_{y,\mathbf{k}}^{\nu_x} \nu_{y,\mathbf{k}}^j &= (E^j)^N \nu_{y,\mathbf{k}}^j. \end{aligned} \quad (\text{A.2.9})$$

One can now write explicitly the Wilson loop operator as a product of matrices $F_{y,\mathbf{k}}^{\nu_x}$ and then expand them using eq. A.2.5.

$$\begin{aligned} \mathcal{W}_{y,\mathbf{k}}^{\nu_x} &= \prod_{i=0}^{N_y} F_{y,\mathbf{k}+i\Delta k_y}^{\nu_x} \\ &= \left(\prod_{i=2}^{N_y} F_{y,\mathbf{k}+i\Delta k_y}^{\nu_x} \right) F_{y,k_2}^{\nu_x} F_{y,k_1}^{\nu_x} \\ [\mathcal{W}_{y,\mathbf{k}}^{\nu_x}]^{m,n} &= \sum_{l,l'} U_{m,l} [F_{y,k_2}^{\nu_x}]_{l,l'} [F_{y,k_1}^{\nu_x}]_{l',n} \\ &= \sum_{l,l'=1}^{N_{\text{occ}}} \sum_{\substack{i,j=1 \\ i',j'=1}}^{N_W} U_{m,l} [v_{x,k_3}^i]^l \langle \omega_{x,k_3}^i | \omega_{x,k_2}^j \rangle \left[(v_{x,k_2}^j)^* \right]^{l'} [v_{x,k_2}^{i'}]^{l'} \langle \omega_{x,k_2}^{i'} | \omega_{x,k_1}^{j'} \rangle \left[(v_{x,k_1}^{j'})^* \right]^n \\ &= \sum_{l=1}^{N_{\text{occ}}} \sum_{\substack{i,j=1 \\ i',j'=1}}^{N_W} U_{m,l} [v_{x,k_3}^i]^l \langle \omega_{x,k_3}^i | \omega_{x,k_2}^j \rangle \delta_{j,i'} \langle \omega_{x,k_2}^{i'} | \omega_{x,k_1}^{j'} \rangle \left[(v_{x,k_1}^{j'})^* \right]^n \\ &= \sum_{l=1}^{N_{\text{occ}}} \sum_{\substack{i,j=1 \\ j'=1}}^{N_W} U_{m,l} [v_{x,k_3}^i]^l \langle \omega_{x,k_3}^i | \omega_{x,k_2}^j \rangle \langle \omega_{x,k_2}^j | \omega_{x,k_1}^{j'} \rangle \left[(v_{x,k_1}^{j'})^* \right]^n \end{aligned} \quad (\text{A.2.10})$$

Iterating this procedure until there are no $F_{y,\mathbf{k}}^{\nu_x}$ left in the product yields:

$$[\mathcal{W}_{y,\mathbf{k}}^{\nu_x}]^{m,n} = \sum_{i,j=1}^{N_W} [v_{x,\mathbf{k}}^i]^m [\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x}]^{i,j} \left[(v_{x,k_1}^j)^* \right]^n, \quad (\text{A.2.11})$$

where $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x} = \prod_{j=0}^{L_y} \tilde{F}_{y,\mathbf{k}+j\Delta k_x}^{\nu_x}$ is the Wilson loop performed in the y direction over the Wannier basis and $[\tilde{F}_{y,\mathbf{k}}^{\nu_x}]^{i,j} = \langle \omega_{x,\mathbf{k}+\Delta k_y}^i | \omega_{x,\mathbf{k}}^j \rangle$. As it turns out, it suffices to work with $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x}$. To diagonalize the operator

$P_{\nu_x} \hat{y} P_{\nu_x}$ we need to diagonalize the Wilson loop operator defined in the occupied bands subspace $\mathcal{W}_{y,\mathbf{k}}^{\nu_x}$. The relevant information should come from the Wilson loop defined in the Wannier sector subspace $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x}$. In fact these two Wilson loop operators are connected via a unitary transformation U defined as an $N_{\text{occ}} \times N_W$ matrix:

$$U = \begin{pmatrix} | & | & | & | \\ v_{x,\mathbf{k}}^1 & v_{x,\mathbf{k}}^2 & \dots & v_{x,\mathbf{k}}^{N_W} \\ | & | & | & | \\ | & | & | & | \end{pmatrix} \quad (\text{A.2.12})$$

The transformation U maps the Wilson loop $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x}$ onto the occupied bands subspace, and obeys:

$$UU^\dagger = I_{N_{\text{occ}} \times N_{\text{occ}}} \quad (\text{A.2.13})$$

$$U^\dagger U = I_{N_W \times N_W}. \quad (\text{A.2.14})$$

Thus, one can write $\mathcal{W}_{y,\mathbf{k}}^{\nu_x} = U \tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x} U^\dagger$ and $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x} = U^\dagger \mathcal{W}_{y,\mathbf{k}}^{\nu_x} U$, which follows from the unitary conditions of U . Assuming that $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x} |\tilde{v}_{y,\mathbf{k}}^{\nu_x,j}\rangle = e^{2\pi i \tilde{\nu}_y^{\nu_x,j}(k_x)} |\tilde{v}_{y,\mathbf{k}}^{\nu_x,j}\rangle$, it can be shown that from the N_W eigenvectors and eigenvalues of $\tilde{\mathcal{W}}_{y,\mathbf{k}}^{\nu_x}$, half of the eigenvalues and eigenvectors of $\mathcal{W}_{y,\mathbf{k}}^{\nu_x}$ are defined with $|v_{y,\mathbf{k}}^{\nu_x,j}\rangle = U |\tilde{v}_{y,\mathbf{k}}^{\nu_x,j}\rangle$.

With the Wilson loop phases, one can now compute the boundary polarization:

$$p_y^{\nu_x}(k_x) = e \sum_j \tilde{\nu}_y^{\nu_x,j}(k_x), \quad (\text{A.2.15})$$

and the total polarization of the Wannier sector ν_x is:

$$p_y^{\nu_x} = \frac{1}{N_x} \sum_{k_x} p_y^{\nu_x}(k_x). \quad (\text{A.2.16})$$

Under certain symmetries constrains $p_y^{\nu_x}(k_x)$ does not depend on k_x and thus the sum is redundant.

Appendix B

Chiral Symmetry and Bulk Multipole Moments

Here we present a proof that shows that the quadrupole moment $q_{xy} = \left(\tilde{q}_{xy} - q_{xy}^{(0)} \right) \bmod 1$ is quantized to 0 or 0.5 when a half-filled system preserves chiral symmetry. This proof is available in [50]. The quadrupole moment is:

$$\tilde{q}_{xy} = \frac{1}{2\pi} \text{Im det} \left(U_o^\dagger D U_o \right), \quad (\text{B.0.1})$$

where U_o is the matrix whose columns are the occupied eigenstates, which corresponds to half the states at half filling. Now considering a model with chiral symmetry such that $\Pi \mathcal{H} \Pi^\dagger = -\mathcal{H} \implies \{\mathcal{H}, \Pi\} = 0$, one can construct the unoccupied eigenstates via the chiral symmetry operator Π , such that if $|\psi_n^o\rangle$ is an occupied eigenstate with energy E_n then $\Pi |\psi_n^o\rangle$ is an unoccupied eigenstate with energy $-E_n$. The unoccupied states matrix is $U_u = \Pi U_o$.

$$\begin{aligned} \tilde{q}_{xy}^u &= \frac{1}{2\pi} \text{Im det} \left(U_u^\dagger D U_u \right) \\ &= \frac{1}{2\pi} \text{Im det} \left(U_o^\dagger \Pi^\dagger D \Pi U_o \right) \end{aligned} \quad (\text{B.0.2})$$

Clearly D commutes with the chiral symmetry transformation Π since both matrixes are diagonal, i.e., $[D, \Pi] = 0$, and so

$$\tilde{q}_{xy}^u = \frac{1}{2\pi} \text{Im det} \left(U_o^\dagger D U_o \right) = \tilde{q}_{xy}. \quad (\text{B.0.3})$$

The bulk quadrupole moment is defined by

$$q_{xy} = \left(\tilde{q}_{xy} - q_{xy}^{(0)} \right) \bmod 1, \quad (\text{B.0.4})$$

where $q_{xy}^{(0)}$ is the contribution from the background static positive charges. We want to prove that $q_{xy} + q_{xy}^u = 0 \bmod 1$ which is equivalent to $\tilde{q}_{xy} + \tilde{q}_{xy}^u - 2q_{xy}^{(0)} = 0 \bmod 1$. We start by defining $U_t = (U_o, U_u)$ which is the unitary transformation that diagonalizes the Hamiltonian of the system. It is clear that:

$$\begin{aligned}
2q_{xy}^{(0)} &= \sum_{j=1}^{n_a} \frac{x_j y_j}{L_x L_y} \\
&= \frac{1}{2\pi} \text{Im} \log \det(D) \mod 1 \\
&= \frac{1}{2\pi} \text{Im} \log \det(U_t^\dagger D U_t) \mod 1,
\end{aligned} \tag{B.0.5}$$

where the last step follows from the unitarity of U_t , so $\det(U_t^\dagger D U_t) = \det(U_t^\dagger) \det(D) \det(U_t) = \det(D)$. Now the objective is to write $2q_{xy}^{(0)}$ at the cost of the electronic contributions to the quadrupole moment:

$$\text{Im} \log \det(U_t^\dagger D U_t) = \text{Im} \log \det \begin{pmatrix} U_o^\dagger D U_o & U_o^\dagger D U_u \\ U_u^\dagger D U_o & U_u^\dagger D U_u \end{pmatrix}. \tag{B.0.6}$$

Let M be a 2×2 block matrix of the form $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. If A is invertible, the following algebraic identity holds:

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A) \det(D - C A^{-1} B). \tag{B.0.7}$$

Making the due correspondences yields $C A^{-1} = U_u^\dagger D U_o (U_o^\dagger D U_o)^{-1} = U_u^\dagger D U_o U_o^{-1} D^{-1} (U_o^\dagger)^{-1}$. Although U_o is a $n_a \times n_c$ matrix, its inverse is still-defined, U_o^{-1} is the pseudo-inverse of U_o such that the definition of inverse holds, i.e. $U_o^{-1} U_o = I_{n_c \times n_c}$, in fact, $U_o^{-1} = U_o^\dagger$, which follows from the orthogonality relations of the eigenbasis of $\mathcal{H}$. The pseudo-inverse is tricky in the sense that $U_o^{-1} U_o \neq U_o U_o^{-1} = I_{n_a \times n_a}$. Keeping this in mind, it follows:

$$\begin{aligned}
U_u^\dagger D U_o U_o^{-1} D^{-1} (U_o^\dagger)^{-1} &= U_u^\dagger D D^{-1} U_o \\
&= U_u^\dagger U_o \\
&= 0,
\end{aligned} \tag{B.0.8}$$

where we have used the orthogonality of the occupied and unoccupied subspaces. We then obtain:

$$\begin{aligned}
\text{Im} \log \det \begin{pmatrix} U_o^\dagger D U_o & U_o^\dagger D U_u \\ U_u^\dagger D U_o & U_u^\dagger D U_u \end{pmatrix} \mod 2\pi &= \text{Im} \log \left\{ \det(U_o^\dagger D U_o) \det(U_u^\dagger D U_u) \right\} \mod 2\pi \\
&= \text{Im} \log \det(U_o^\dagger D U_o) + \text{Im} \log \det(U_u^\dagger D U_u) \mod 2\pi \\
&= \frac{1}{2\pi} \text{Im} \log \det(U_o^\dagger D U_o) + \frac{1}{2\pi} \text{Im} \log \det(U_u^\dagger D U_u) \mod 1,
\end{aligned} \tag{B.0.9}$$

which leads to:

$$\begin{aligned}
2\pi \left(\tilde{q}_{xy} + \tilde{q}_{xy}^u - 2q_{xy}^{(0)} \right) &= \text{Im} \log \det \left(U_o^\dagger D U_o \right) + \text{Im} \log \det \left(U_u^\dagger D U_u \right) - \\
&\quad - \text{Im} \log \det \left(U_o^\dagger D U_o \right) - \text{Im} \log \det \left(U_u^\dagger D U_u \right) \mod 2\pi = 0 \mod 2\pi. \quad (\text{B.0.10})
\end{aligned}$$

We have $q_{xy} + q_{xy}^u = 0 \mod 1$ using $q_{xy} = q_{xy}^u$ one concludes $2q_{xy} = 0 \mod 1$, namely, q_{xy} is quantized to 0 or 0.5. In this manner, the quadrupole moment is quantized by chiral symmetry in half-filling insulators. An analogous approach can be made regarding any of the remaining multipole operators, concluding each time that chiral symmetry also quantizes the bulk polarization and bulk octupole moment density at half-filling insulators.

Appendix C

Tridiagonal Matrices

When considering TB systems, it is common to have a Hamiltonian that is tridiagonal, in fact, for several of the employed methods, the tridiagonal form has been exploited to our advantage. It is only natural that we delve into some properties of such matrices.

C.1 Lanczos Decomposition

We start by presenting an algorithm that, from a general hermitian matrix A in some basis $\{|\phi_n\rangle\}$, can generate a new basis $\{|u_n\rangle\}$ in which A is tridiagonal (Lanczos algorithm [88]). In Jacobi form, A can be written as:

$$A = \begin{pmatrix} a_0 & b_1 & 0 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & 0 & \dots \\ 0 & 0 & b_3 & a_3 & b_4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (\text{C.1.1})$$

The first big advantage of an hermitian matrix in Jacobi form is that we can store the entire matrix with two vectors, one that stores the coefficients a_n and another that stores the coefficients b_n . Knowing these coefficients fully defines A . In the tridiagonal orthonormal basis $\{|u_n\rangle\}$, the following equation holds:

$$A|u_n\rangle = a_n|u_n\rangle + b_n|u_{n-1}\rangle + b_{n+1}|u_{n+1}\rangle. \quad (\text{C.1.2})$$

The way to generate the new basis and the coefficients is as follows:

1. We choose an arbitrary normalized state $|u_0\rangle$ which defines $a_0 = \langle u_0|A|u_0\rangle$
2. We obtain $|\tilde{u}_1\rangle$ by acting with A on $|u_0\rangle$ and removing the leftover projection $|u_0\rangle$ i.e. $|\tilde{u}_1\rangle = A|u_0\rangle - a_0|u_0\rangle$
3. Now we normalize $|\tilde{u}_1\rangle$. With C.1.2 we get $\langle \tilde{u}_1|\tilde{u}_1\rangle = |b_1|^2$ thus, $|u_1\rangle = \frac{1}{b_1}|\tilde{u}_1\rangle$
4. We keep iterating this method

- (a) $a_n = \langle u_n | A | u_n \rangle$
- (b) $|\tilde{u}_{n+1}\rangle = \mathcal{H} | u_n \rangle - a_n | u_n \rangle - b_{n-1} | u_{n-1} \rangle$
- (c) $|b_{n+1}|^2 = \langle \tilde{u}_{n+1} | \tilde{u}_{n+1} \rangle$
- (d) $|u_{n+1}\rangle = \frac{1}{b_{n+1}} |\tilde{u}_{n+1}\rangle$

Generally, we choose $|u_0\rangle$ which has at least one caveat: we might not be able to generate the entirety of the Hilbert space of A , and thus, for a general $|u_0\rangle$, we might be confined to a subspace of A . Luckily, for most applications, we can truncate the Lanczos method to a reduced number of terms.

C.2 Inverting Tridiagonal Matrices

Another relevant operation where Jacobi form simplifies the calculations is when we want to obtain a given entrance of the inverse of a tridiagonal matrix. Let us assume A has the form in C.1.1. The objective is to compute $(A^{-1})_{00}$, but first let us see how to invert a matrix. The inverse of A is defined as:

$$A^{-1} = \frac{\text{Adj}\{A\}}{\det\{A\}}, \quad (\text{C.2.1})$$

where $\text{Adj}\{A\}$ is the adjoint matrix of A , which is simply the transpose of the cofactor matrix C : $\text{Adj}\{A\} = C^T$. In turn, the cofactor matrix is defined by

$$C_{ij} = (-1)^{i+j} M_{ij}, \quad (\text{C.2.2})$$

where M_{ij} is the determinant of the matrix obtained by removing the i^{th} row and j^{th} column of A . In this manner, setting $G = A^{-1}$, we have that

$$G_{00} = G_0 = \frac{M_{00}}{\det\{A\}}. \quad (\text{C.2.3})$$

To compute $\det\{A\}$, we make a Laplace expansion of A along the zeroth row, arriving at:

$$\det\{A\} = a_0 M_{0,0} - b_1 M_{0,1} \quad (\text{C.2.4})$$

Defining the following determinants of sub-matrices of A

$$D_n = \det \begin{pmatrix} a_n & b_{n+1} & 0 & 0 & 0 & \dots \\ b_{n+1} & a_{n+1} & b_{n+2} & 0 & 0 & \dots \\ 0 & b_{n+2} & a_{n+2} & b_{n+3} & 0 & \dots \\ 0 & 0 & b_{n+3} & a_{n+3} & b_{n+4} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (\text{C.2.5})$$

it is clear that $M_{00} = D_1$ and $M_{01} = b_1 D_2$, where we employed another Laplace expansion along the first column of M_{01} . We then reach

$$G_{00} = \frac{1}{a_0 - b_1^2 \frac{D_2}{D_1}}. \quad (\text{C.2.6})$$

The ratio $\frac{D_2}{D_1}$ is nothing more than $(A^{(1)})_{00}^{-1} = G_{00}^{(1)} = G_1$, which is the first element of the inverse of the sub-matrix of A

$$A^{(1)} = \begin{pmatrix} a_1 & b_2 & 0 & 0 & 0 & \dots \\ b_2 & a_2 & b_3 & 0 & 0 & \dots \\ 0 & b_3 & a_3 & b_4 & 0 & \dots \\ 0 & 0 & b_4 & a_4 & b_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (\text{C.2.7})$$

I hope that now is clear that the tridiagonal form leads to an iterative equation that allows us to compute G_0 at the cost of sub-matrices of A which yields a continued fraction equation

$$G_0 = \frac{1}{a_0 - b_1^2 \frac{1}{a_1 - b_2^2 \frac{1}{\ddots - b_{N-1}^2 \frac{1}{a_{N-1}}}}}, \quad (\text{C.2.8})$$

or in recursive form

$$G_n = \frac{1}{a_n - b_{n+1}^2 G_{n+1}} \quad (\text{C.2.9})$$

$$G_{N-1} = \frac{1}{a_{N-1}}. \quad (\text{C.2.10})$$

This iterative approach is particularly relevant when we are dealing with Green's functions and need to compute a specific entry or block of a Green's function. We can usually truncate this method to a number of coefficients smaller than $N - 1$. This greatly improves the numerical efficiency since we do not need (and generally cannot) generate the full basis $\{|u_n\rangle\}$. This approach is valid if the objective is to compute $(A^{-1})_{N-1, N-1}$. In this case, the procedure is just applied backwards. For block tridiagonal matrices, the generalization is analogous. One just needs to trade the coefficients for the respective matrices and be careful with the order of matrix multiplication.

Appendix D

k_x -dependent Model

In this section, we present the k_x -dependent Hamiltonian for the quasi-periodic QBCP model. We start from the Hamiltonian written in the real space basis and take plane wave solutions along the invariant direction x . Since we are reducing our problem to an effective 1D model $\mathcal{H}(k_x)$, we can reach sizes far closer to the thermodynamic limit. This transformation comes with some caveats, since to have the full picture of the 2D system, we need to consider the entire FBZ along the invariant direction, and so when computing gaps, for example, one needs to know exactly at which k_x the gap closes. The real-space Hamiltonian is:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_B + \mathcal{H}_{1D} \quad (\text{D.0.1})$$

Where each term is defined by:

$$\begin{aligned} \mathcal{H}_0 = \sum_{\mathbf{R}} \{ & t_z (|\mathbf{R} \pm a\hat{e}_x, A\rangle \langle \mathbf{R}, A| - |\mathbf{R} \pm a\hat{e}_y, A\rangle \langle \mathbf{R}, A|) - \\ & - t_z (|\mathbf{R} \pm a\hat{e}_x, B\rangle \langle \mathbf{R}, B| + |\mathbf{R} \pm a\hat{e}_y, B\rangle \langle \mathbf{R}, B|) + \\ & + \frac{t_x}{2} (|\mathbf{R} \pm a\hat{e}_x \pm a\hat{e}_y, A\rangle \langle \mathbf{R}, B| - |\mathbf{R} \pm a\hat{e}_x \mp a\hat{e}_y, A\rangle \langle \mathbf{R}, B|) + \\ & + \frac{t_x}{2} (|\mathbf{R} \pm a\hat{e}_x \pm a\hat{e}_y, B\rangle \langle \mathbf{R}, A| - |\mathbf{R} \pm a\hat{e}_x \mp a\hat{e}_y, B\rangle \langle \mathbf{R}, A|) \}, \quad (\text{D.0.2}) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_B = \sum_{\mathbf{R}} \{ & i (|\mathbf{R}, B\rangle \langle \mathbf{R}, A| - |\mathbf{R}, A\rangle \langle \mathbf{R}, B|) \\ & - i \frac{B+1}{4} (|\mathbf{R} \pm a\hat{e}_x, A\rangle \langle \mathbf{R}, B| + |\mathbf{R} \pm a\hat{e}_y, A\rangle \langle \mathbf{R}, B|) \\ & + i \frac{B+1}{4} (|\mathbf{R}, B\rangle \langle \mathbf{R} \pm a\hat{e}_x, A| + |\mathbf{R}, B\rangle \langle \mathbf{R} \pm a\hat{e}_y, A|) \}, \quad (\text{D.0.3}) \end{aligned}$$

$$\mathcal{H}_{1D} = \frac{W}{2} \sum_{\mathbf{R}} \cos(2\pi\beta na) \{ |\mathbf{R}, A\rangle \langle \mathbf{R}, A| + |\mathbf{R}, B\rangle \langle \mathbf{R}, B| \}. \quad (\text{D.0.4})$$

We can now make a change of basis along the invariant direction, using $|m, \alpha\rangle = \frac{1}{\sqrt{L_x}} \sum_{k_x} e^{-ik_x m a} |k_x, \alpha\rangle$, and obtain the 1D hamiltonian $\mathcal{H} = \sum_{k_x} \mathcal{H}(k_x) |k_x\rangle\langle k_x|$:

$$\mathcal{H}(k_x) = \mathcal{H}_0(k_x) + \mathcal{H}_B(k_x) + \mathcal{H}_{1D}(k_x), \quad (\text{D.0.5})$$

where:

$$\begin{aligned} \mathcal{H}_0(k_x) = & \sum_n \{ t_z (2 \cos(k_x a) |n, A\rangle\langle n, A| - |n \pm 1, A\rangle\langle n, A|) + \\ & + t_z (-2 \cos(k_x a) |n, B\rangle\langle n, B| + |n \pm 1, B\rangle\langle n, B|) + \\ & + it_x \sin(k_x a) (|n+1, A\rangle\langle n, B| - |n-1, A\rangle\langle n, B|) + \\ & + it_x \sin(k_x a) (|n+1, B\rangle\langle n, A| - |n-1, B\rangle\langle n, A|) \}, \end{aligned} \quad (\text{D.0.6})$$

$$\begin{aligned} \mathcal{H}_B(k_x) = & \sum_n \{ i (|n, B\rangle\langle n, A| - |n, A\rangle\langle n, B|) - \\ & - i \frac{B+1}{4} (2 \cos(k_x a) |n, A\rangle\langle n, B| + |n \pm 1, A\rangle\langle n, B|) + \\ & + i \frac{B+1}{4} (2 \cos(k_x a) |n, B\rangle\langle n, A| + |n, B\rangle\langle n \pm 1, A|) \}, \end{aligned} \quad (\text{D.0.7})$$

$$\mathcal{H}_{1D}(k_x) = \frac{W}{2} \sum_n \cos(2\pi a \beta n) \{ |n, A\rangle\langle n, A| + |n, B\rangle\langle n, B| \}. \quad (\text{D.0.8})$$

Appendix E

Corner Mode Hybridization

As we have seen, computations of the corner charge for phase *II* at $\gamma = 1.1$ do not yield a quantized value, despite its scaling with system size. In this appendix, we argue that the lack of quantization of the corner charge is due to corner mode hybridization, brought up by finite-size effects. In Fig. E.1 the probability density ($|\psi(\mathbf{R})|^2$) of the 6 eigenstates closer to Fermi level for $\gamma = 1.1$ and $W = 2.2$ are shown. We consider $\delta = 10^{-7}$ to split the degeneracy of the fourfold corner modes, thus, for ED calculations, two corner modes are shifted towards negative energies $E = -\delta$ and the remaining two are shifted towards positive energies $E = \delta$. Moreover, each of the pairs have their corner modes living in opposite corners to each other. Therefore, in a half-filled system the two opposite occupied corner modes give rise to an excess of charge in the corresponding corners ($\bar{Q} = 0.5$) while the unoccupied corner modes lead to a deficit of charge in the corresponding corners ($\bar{Q} = -0.5$).

In Fig. E.1(a) ($L = 89$) the four middle states are localized in the corners, however, their energies do not come in pairs and the two modes with negative energy do not live in opposite corners. In fact, each eigenstate has spectral weight in three of the four corners, suggesting that they hybridize with each other. This is also seen in the energies of each of the corner modes. Although the spectrum remains symmetric due to particle hole symmetry, as indicated in Fig. E.1, there are “outer” corner modes with $E \approx 10^{-4}$ and “inner” corner modes with $E \approx 10^{-5}$, which indicates that they hybridize away from zero-energy (in this case $E = \pm\delta$). Furthermore, in Refs. [84, 89], the authors argue that for chiral QI, each corner mode has a well-defined chiral charge ($\Pi|\psi\rangle = \pm|\psi\rangle$)¹ and so when two corner modes with different corner charges hybridize, their energy moves away from zero-energy, which is the observed behavior. This hybridization occurs when the localization length of the corner modes is of the order of the system size ($\xi_l \approx L$), leading to the corner modes decaying into the bulk thus “feeling the influence” of their neighbors. This is exactly the observed behavior. Considering larger system sizes, as in Fig. E.1(b), further localizes each mode in its respective corner, impeding corner mode hybridization and consequently leading to a quantized corner charge. The observed hybridization is dependent on the random phase shifts realization, with some realizations leading to lower hybridization and so to a well-defined corner charge, while other realizations lead to higher hybridization between the corner modes and thus to non-quantized corner charges.

¹Which is the same as stating that each corner mode lives in only one sub-lattice.

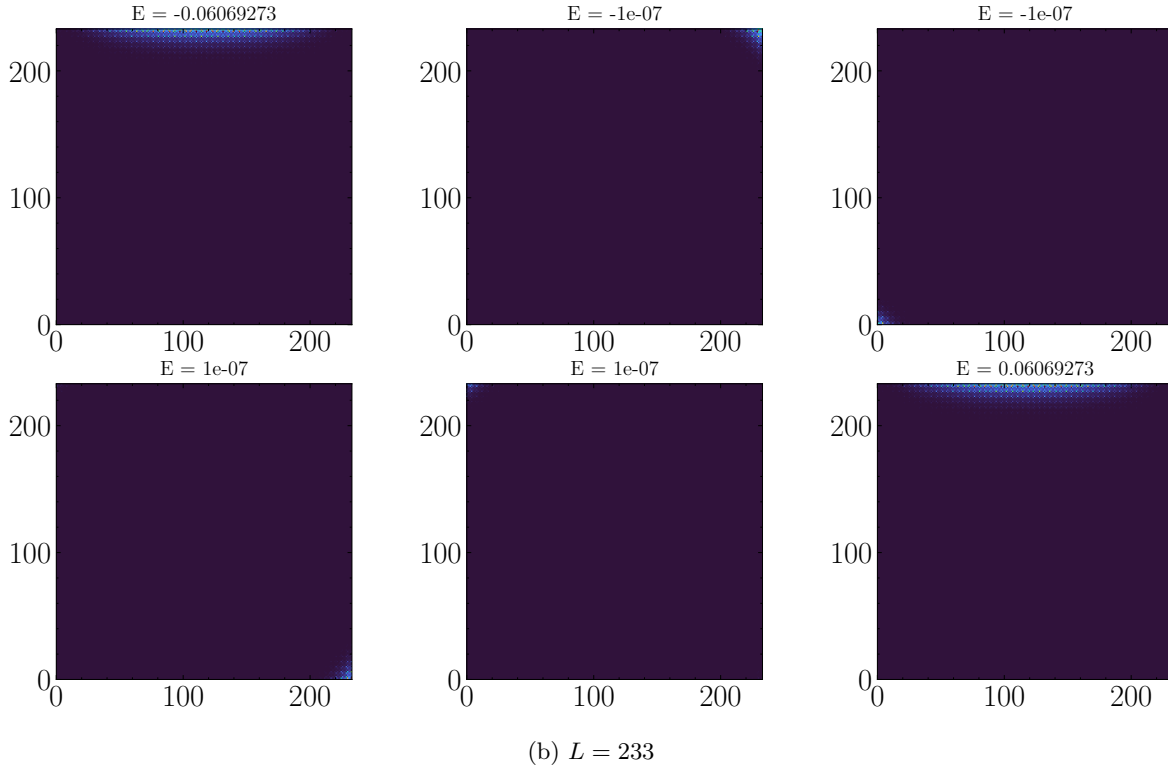
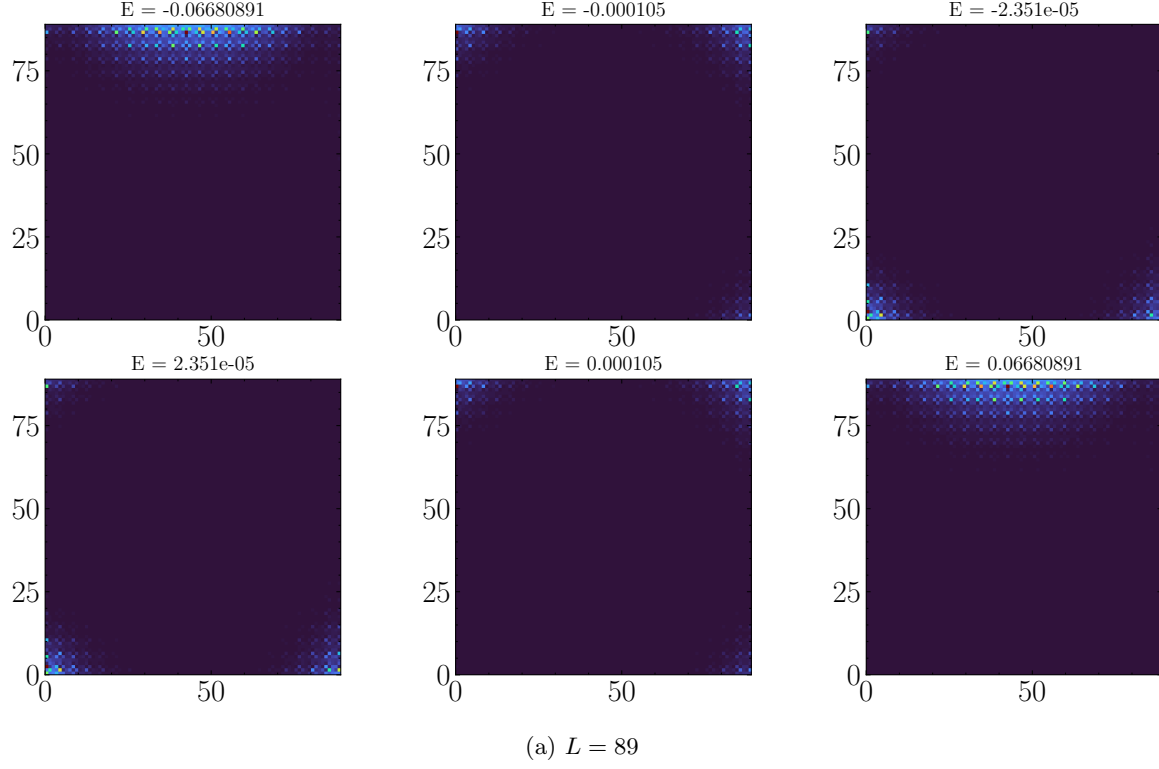


Figure E.1: Probability density ($|\psi(\mathbf{R})|^2$) of the 6 eigenstates around Fermi level for $\gamma = 1.1, W = 2.2$ (phase II in Fig. 5.3) for one realization of random shifts and with $\delta = 10^{-7}$ to split the degeneracy of the four-fold corner modes. Each sub-figure is a different system size, increasing from top to bottom.

Appendix F

Complementary Results

Here we complement the results of Chapter 5 with additional plots. In Fig. F.1 and Fig. F.2 we provide similar plots as those in Fig. 5.6 and Fig. 5.11, respectively, but for $\gamma = 0.5$.

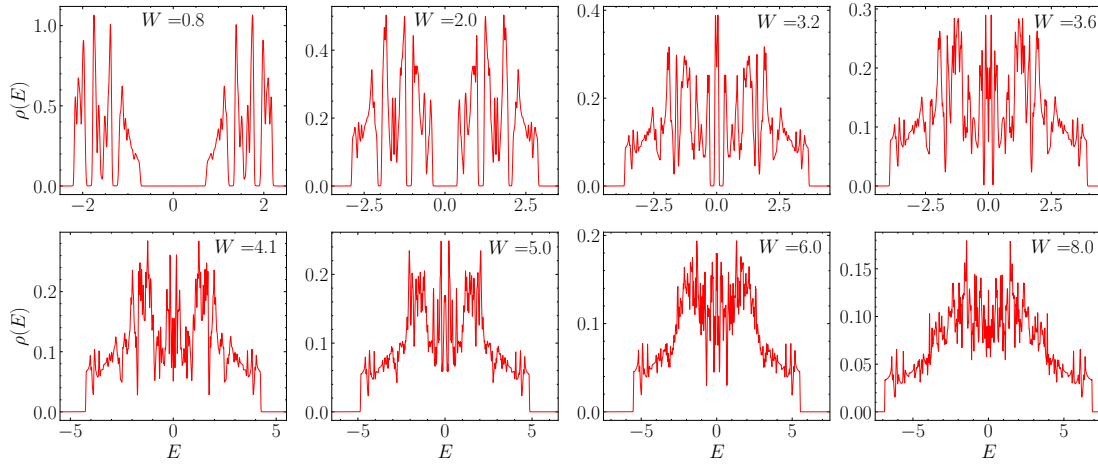


Figure F.1: DOS as a function of energy (E) for $\gamma = 0.5$ and different values of quasi-periodic potential strength (W). The following parameters were used in the KPM: system size $L = 987$, number of Chebyshev momenta $M = 2000$ and number of averages over traces and phase shifts $R = 10$.

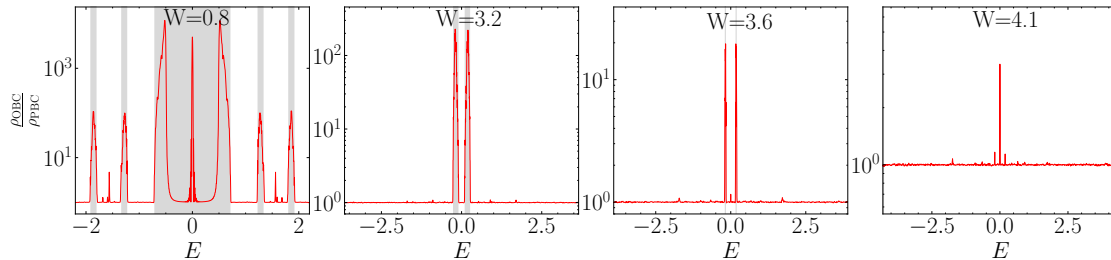


Figure F.2: Ratio of open boundary DOS and periodic boundaries DOS as a function of energy for W in different phases and $\gamma = 0.5$. The grayed out regions are bulk gaps opened by the QP modulation. The following KPM parameters were utilized: $L = 987$, $M = 5000$, $R = 10$.

Constant W Cut

In the main text, we have focused our analysis in two constant γ cuts. However, a constant W cut was also performed, as seen in Fig. 5.1. We plot several quantities as a function of hopping strength (γ), such as the quadrupole moment and boundary invariant (a), the bulk spectral gap (b), fractal dimensions (c-d), corner occupation probability (e), and the corner charge (f).

The most interesting result is regarding phase *I* which is a gapless QPQI phase. Although this regime is gapless, the states at Fermi level are localized, which allows for the existence of localized topological corner modes at zero energy. Despite the topological nature of this regime, P_{occ} does not quantize since the numerical ED of the system Hamiltonian yields linear combinations of localized corner modes and localized bulk states that live at zero energy. Phase *II* displays several trivial gapped regimes with either a localized or critical gap edge. From phase *II* to *III* the gap closes in a ballistic gap-edge into a gapped QI phase with well quantized q_{xy} and P . Regarding the corner occupation probability, it plateaus for most of phase *III*, however, at around $\gamma \approx 0.5$, it displays two dips that are associated with corner edge hybridization, which we further discuss in Appendix. F. Furthermore, if we consider the constant $\gamma = 0.5$ cut and set $W = 3$ (end of phase *I*, Fig. 5.3(a)), a small dip can also be observed in the P invariant, in P_{occ} and in $\bar{Q}$. Phase *IV* is a band gap trivial insulator. Overall, the results of this analysis agree with the previous results. However, we have found the existence of a gapless QPQI phase which has not been seen thus far. This topological gapless regime is phenomenologically similar to the gapless HOTAI phase found in Ref. [50].

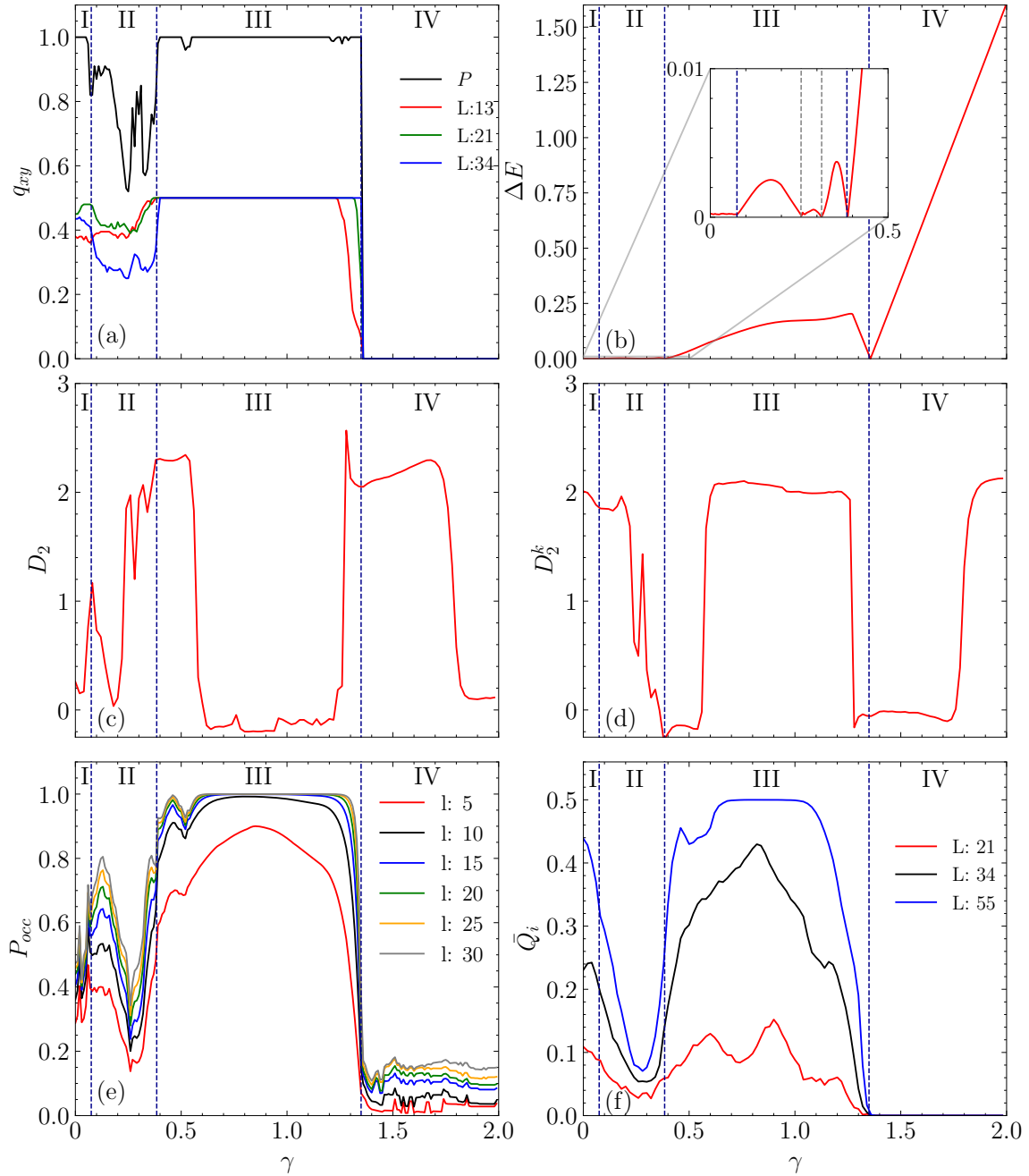


Figure F.3: (a) q_{xy} and P as a function of W . The P invariant was computed for a system size of $L = 610$ with 100 averages over phase shifts. q_{xy} was obtained via real space methods with 100 averages over phase shifts. For even L , $\theta_x = \theta_y = 0$; for odd L $\theta_x = \theta_y = 0$. (b) Spectral gap as a function of W computed for an even system size $L = 144 \implies \theta_i = 0$ and averaged over 50 phase shifts realizations. (c-d) Fractal dimension averaged out over 100 phase twists, shifts and over the first 8 eigenstates with energies closest to $E = 0$. (e) Corner occupation probability (P_{occ}) as a function of W for the first 2 zero-energy states. The results were obtained for a system size of $L = 377$ and averaged over 100 phase shifts. (f) Corner charge ($\bar{Q}$) as a function of W for several system sizes and averaged over 100 phase shifts and over the 4 corners. (e-f) $1/\delta = 10^{-5}$.

Corner-Edge Hybridization

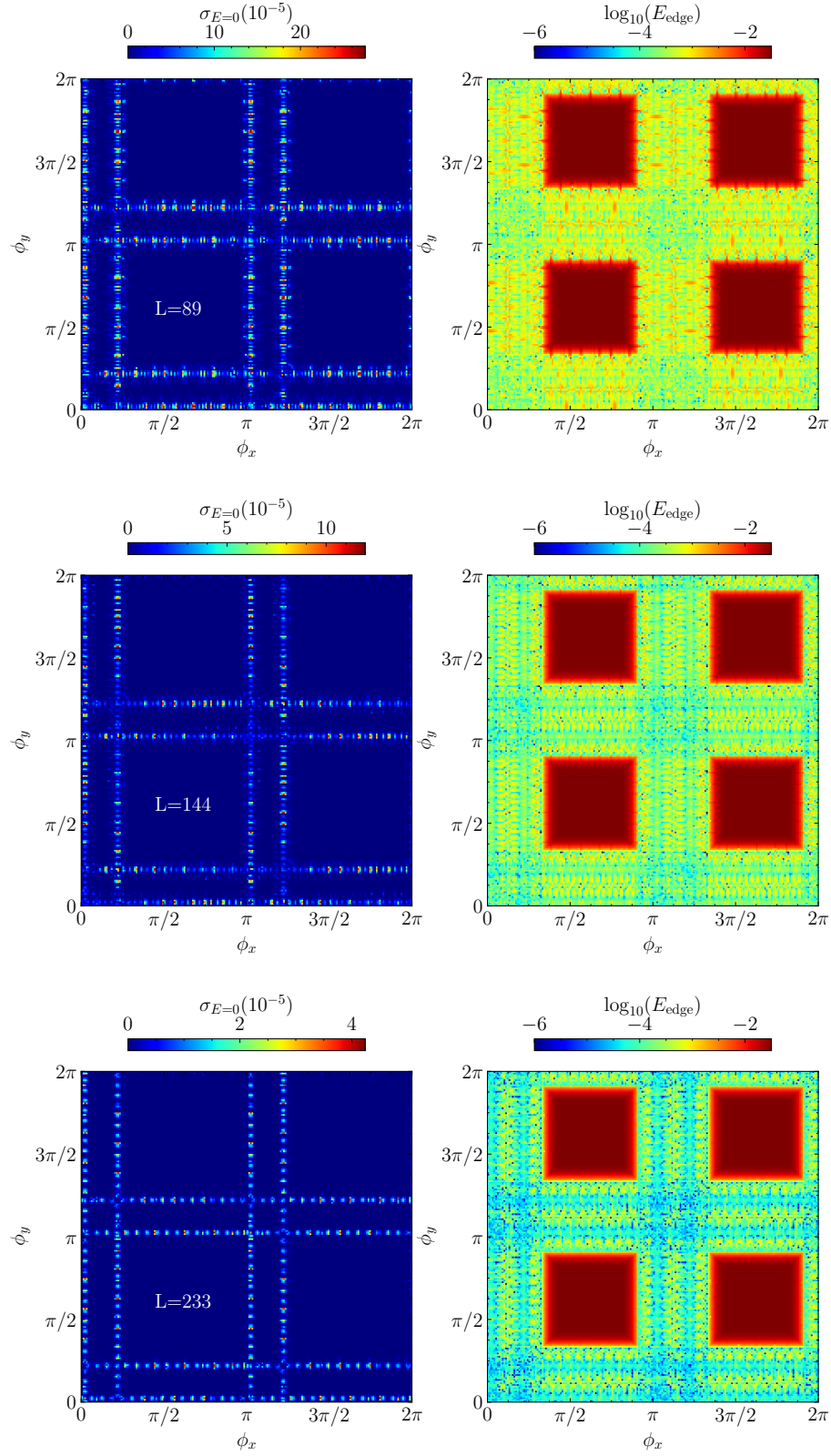


Figure F.4: Standard deviation ($\sigma_{E=0}$) of the energies of the corner modes as a function of the phase shifts (ϕ_x, ϕ_y) and logarithm of edge state energy ($\log_{10}(E_{edge})$) as a function of the phase shifts (ϕ_x, ϕ_y) . Results obtained for $W = 3.8$ and $\gamma = 0.2$ in the QPQI phase for system sizes $L = \{89, 144, 233\}$ as indicated.

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