

On Exponentially Localized Wannier Functions in
Non-Periodic Insulators

by

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Dissertation submitted in partial fulfillment of the
requirements for the degree of Doctor of Philosophy
in the Department of Mathematics
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ABSTRACT

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Abstract

Exponentially localized Wannier functions (ELWFs) are an orthogonal basis for the low energy states of a material consisting of functions which decay exponentially quickly in space. When a material is insulating and periodic, conditions which guarantee the existence of ELWFs in dimensions one, two, and three are well-known and methods for constructing ELWFs numerically are well-developed. In this dissertation, we consider the case where the material is insulating but not necessarily periodic and develop an algorithm for calculating ELWFs.

In Chapter 3, we propose an optimization-free algorithm for constructing Wannier functions in both periodic and non-periodic insulating systems. In this chapter, we rigorously prove that under the assumption of “uniform spectral gaps”, a technical assumption we introduce, that our algorithm constructs ELWFs.

While the uniform spectral gaps assumption is not always met in practice, in Chapter 4, we prove that for a wide class of systems (both periodic and non-periodic) it is always possible to modify our algorithm so that the uniform spectral gaps assumption holds. As a consequence of this result, we conclude that for both periodic and non-periodic systems our algorithm can construct ELWFs whenever they exist.

The results in this dissertation open the door for extending the theory of topological insulators, a recently discovered class of materials, to fully non-periodic systems.

Acknowledgements

First and foremost I would like to thank my advisor Jianfeng Lu for all of his support during my time at Duke. I am extremely grateful to Jianfeng for his great patience in helping me grow as an applied mathematician. I would also like to thank Alex Watson for working with me these past three years. While we didn't always see eye to eye, I believe I am a better researcher because of my interactions with Alex.

I would like to thank Robert Calderbank, Henry Pfister, and Xiuyuan Cheng for being a part of my dissertation committee.

I would also like to thank all of the people who have been a part of my life while I've been at Duke. I would particularly like to thank my D33 roommates, Matthew Beckett and William Duncan for being my friends these past six years; they made my life at Duke much brighter. I'd also like to thank my F3C roommate, Sven Hirsch, for inviting me to live with him this past year. I would also like to thank my "math friends", Orsola Capovilla-Searle, Yu Cao, Josh Cruz, Ryan Gunderson, Didong Li, John Malik, Erika Ordog, Thomas Tran, Do Tran, and Zhe Wang, as well as my "Gross friends", Sarah Brandsen, Cheng Cheng, Yi Feng, Mengke Lian, Panchali Nag, Matthias Sachs, Deborshee Sen, Shan Shan, Rob Ravier, and Narayanan Rengaswamy.

I have been lucky to have most of my graduate career funded without teaching obligations. For this, I would like to thank the Duke Graduate School, the National Science Foundation, and the Duke Math Department. I would particularly like to thank Professor Colleen Robles and Shawn MacDuff for ensuring that my sixth year at Duke was fully funded.

Finally, I would like to thank my parents, Margretta Diemer and Bradley Stubbs, for being a constant source of support for me throughout my life.

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Chapter 1

Introduction

1.1 Overview

Over the past century, quantum mechanics has been shown to be a powerful tool for modeling physical systems on the atomic and subatomic scales. While quantum mechanics has been extremely useful in understanding real world experiments, numerically modeling large quantum systems remains a significant computational challenge due in part to their inherent high dimensionality. As a first step to decreasing the computational complexity of simulating large quantum systems, many algorithms begin by reducing the computation space from a high dimensional Hilbert space to a smaller subspace of physically relevant quantum states. Once this subspace is chosen, to perform calculations we must make a choice of basis for this subspace. Not all bases are equally well suited for computation however. When we are interested in studying local observables of a material (such as polarization or magnetization) bases which are *well localized in space* allow for sparse representations of these observables which drastically speeds up calculations.

In this dissertation, we consider insulating electronic systems in two dimension whose dynamics are described by an effective single-particle Hamiltonian, H . For such a system, the subspace of physically relevant states is defined by an orthogonal projection P , called the Fermi projection. When the Hamiltonian is periodic, that is H commutes with a group of translations, a natural choice of localized basis for the Fermi projection is given by the *Wannier functions*. For periodic insulating systems in two dimensions, there has been much work on understanding when a basis of exponentially localized Wannier functions exist and how to calculate them in practice.

The main contribution of this dissertation is to propose and prove the correctness of an algorithm for calculating exponentially localized bases for the Fermi projection in *both* periodic and non-periodic insulators. Since our algorithm produces Wannier functions in the periodic case, we refer to the results of our algorithm as generalized Wannier functions. Furthermore, as a consequence of our proof of correctness, we also establish sufficient conditions for when an exponentially localized basis for the Fermi projection exist in non-periodic systems.

The remainder of this chapter is organized as follow: In Section 1.2, we give details of how Wannier functions arise as part of electron structure calculations and the role the Wannier functions play in the study of topological phases of matter. In Section 1.3, we will review the basics of Bloch theory and the standard construction of Wannier functions in periodic systems. Next, in Section 1.4 we will give an overview of the previous work on the theory of Wannier functions.

1.2 Wannier Functions in Context

1.2.1 Kohn-Sham Density Functional Theory

Kohn-Sham density functional theory (KSDFFT) is the most widely used technique for solving electron structure calculations today and in practice KSDFFT achieves the best compromise between accuracy and efficiency [HK64, KS65].

The starting point of KSDFFT is the many-body Schrödinger equation. Typically, when modeling a molecular system, we have nuclei (composed of protons and neutrons) and electrons. Since nuclei are much heavier than the electrons, we can often assume that the nuclei are essentially stationary as compared to the electrons; this assumption is known as the Born-Oppenheimer approximation. For a system with N electrons under the Born-Oppenheimer approximation, the many-body Schrödinger equation without spin is defined by the following Hamiltonian which acts on suitable

functions on \mathbb{R}^{3N} :

$$H = -\frac{1}{2} \sum_{i=1}^N \Delta_{\mathbf{x}_i} + \sum_{i=1}^N V_{ext}(\mathbf{x}_i) + V_{ee}(\mathbf{x}_1, \dots, \mathbf{x}_N). \quad (1.1)$$

In the above equation $\{\mathbf{x}_i\}_{i=1}^N \subseteq \mathbb{R}^3$, $\Delta_{\mathbf{x}_i}$ denotes the Laplacian with respect to \mathbf{x}_i , V_{ext} denotes the external potential induced by nuclei, and V_{ee} denotes the electron-electron interactions.

Even under the Born-Oppenheimer approximation, the many-body Schrödinger operator (1.1) is a differential operator on $3N$ -dimensional space. Even for relatively small systems (say $N \approx 100$), attempting to solve any problem involving (1.1) directly is intractable due to the curse of dimensionality.

The first key idea underlying KSDFIT is Hohenberg-Kohn theorem, which allows us to mitigate the curse of dimensionality. To state the Hohenberg-Kohn theorem, we must first define the notion of an electron density function

Definition 1. Given any function $\Psi : \mathbb{R}^{3N} \rightarrow \mathbb{R}$ where $\int |\Psi|^2 = 1$, the *electron density* corresponding to Ψ is defined as follows:

$$\rho(\mathbf{x}) := N \int |\Psi(x, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N.$$

Next, let Ψ_0 be the ground state of a Hamiltonian H as in Equation (1.1) (i.e. Ψ_0 is the eigenvector of (1.1) with smallest eigenvalue). Furthermore, let ρ_0 be the electron density corresponding to Ψ_0 . The Hohenberg-Kohn theorem states that the mapping $\rho_0 \mapsto H$ is injective up to an additive constant¹. Since any quantum system is completely determined by its Hamiltonian, the injectiveness of this map implies that *any* property of the system can be derived as a function of the ground state density ρ_0 . Hence, the overall goal of KSDFIT is to calculate the ground state density, ρ_0 .

¹That is if H_1 and H_2 are two Hamiltonians with the same ground state density ρ_0 , then $H_1 - H_2 =$ (constant). Such a constant simply shifts the spectrum of H and hence does not change the physically relevant properties of H .

By definition, ρ_0 minimizes an energy functional $E[\cdot]$. For a general interacting inhomogeneous electronic system, we can write the energy functional for this system as follows [HK64]:

$$E[\rho] = \int V_{ext}(\mathbf{x})\rho(\mathbf{x}) d\mathbf{x} + \frac{1}{2} \int \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} + G[\rho]. \quad (1.2)$$

In this equation, the first term comes from the nuclei-electron interactions and the second term comes from the electron-electron interactions. The functional in the final term, $G[\cdot]$, is correction term to the energy which is defined through Hohenberg-Kohn theorem. The second key idea underlying KSDFT is to approximate the functional $G[\cdot]$ as a sum of two terms:

$$G[\rho] := E_K[\rho] + E_{xc}[\rho]$$

where $E_K[\rho]$ is the energy of N non-interacting electrons and $E_{xc}[\rho]$ is known as the “exchange correlation”. Philosophically, writing the functional $G[\rho]$ in this way imposes the ansatz that the system can be modeled as N non-interacting electrons with some correction. Using this approximation for $G[\rho]$, via the Euler-Lagrange equation, we can translate minimizing the energy in (1.2) to finding the N lowest eigenpairs $\{(\varepsilon_i, \psi_i)\}_{i=1}^N$ of the following eigenequation

$$\left(-\frac{1}{2}\Delta + V_{\text{eff}}[\rho]\right) \psi_i = \varepsilon_i \psi_i \quad (1.3)$$

where $\rho = \sum_{i=1}^N |\psi_i|^2$.

The effective potential, $V_{\text{eff}}[\rho]$, written above has an explicit formula which incorporates the nuclei-electron interactions, the electron-electron interactions, and the exchange correlation. Notice that (1.3) depends on the electron density ρ which in turn depends on the collection $\{\psi_i\}_{i=1}^N$. In practice, (1.3) is solved iteratively until convergence is reached.

Connection with this Dissertation

In this dissertation, we consider Hamiltonians of the form

$$H = (i\nabla + A)^2 + V \tag{1.4}$$

where both A and V satisfy some regularity assumptions (see Assumption 1). Note that if we take $A \equiv 0$, then we obtain a Hamiltonian which is of the same form as the one considered in (1.3). The function A represents the effects of a magnetic field and a Hamiltonian of the form (1.4) can be derived as part of KSDFT by repeating the argument from the previous section with the addition of a magnetic field.

Let us assume that we have found the lowest N eigenstates of Equation (1.3) with the above Hamiltonian self-consistently. The main results of this dissertation are concerned with finding a new basis for this low lying eigenspace which decays quickly in space. A well-localized basis can drastically speed up calculations when we are interested in studying local observables of a material.

1.2.2 Topological Insulators

One important concept in the study of materials is that of different states of matter (i.e. solid, liquid, gas, etc.). Oftentimes, transitions between the different states of matter are controlled by continuous parameters such as temperature or pressure. In the early 1980s, it was found that there are also phase transitions which are controlled by parameters which take on discrete values. In particular, work by Thouless, Kohmoto, Nightingale, and den Nijs showed that the properties of a certain materials can be connected to topological invariants [TKNdN82]. Such systems are said to exhibit “topological order”.

One class of systems with topological order are known as “topological insulators”. Unlike normal insulators, which impede the flow of electric current, topological insulators act as insulators in their interior but conduct electricity with minimal resistance along their surface [KM05]. This ability to conduct electricity with low resistance

has led to great interest for their application in low-power electronic devices. Furthermore, recently topological insulators have been experimentally realized [Moo10].

Connection with this Dissertation

Most previous work on topological insulators has considered systems which are periodic or close to periodic. In these works, periodicity plays a central role in building the connection between properties of the material and topology. As we will see in Section 1.3, in periodic systems, the existence of exponentially localized Wannier functions is completely determined by whether the material in question is topological or not.

In this dissertation, we define an algorithm for constructing exponentially localized Wannier functions in both periodic and non-periodic system and prove sufficient conditions for when this algorithm succeeds in constructing exponentially localized Wannier functions. Because of the correspondence between exponentially localized Wannier functions and topological invariants in periodic systems, we conjecture that our algorithm can be used as part of extending the theory of topological insulators to both periodic and non-periodic systems. This extension is of great practical interest because most real world materials are not periodic.

1.3 Bloch Theory and Wannier Functions

In this section, we will review the basics of the Bloch theory and Wannier functions. While we will only make use of this theory in Appendix A.4, it will be useful to review these results to make the connection with previous work more clear. To clearly illustrate the ideas behind the standard construction of the Wannier functions, we will consider a simple system in two dimensions.

We begin by defining a translation operators T_X and T_Y so that for any function

$f : \mathbb{R}^2 \rightarrow \mathbb{C}$,

$$T_X f(x_1, x_2) = f(x_1 + 1, x_2) \quad T_Y f(x_1, x_2) = f(x_1, x_2 + 1).$$

Next, we will consider the following Hamiltonian densely defined on $L^2(\mathbb{R}^2)$:

$$H = -\Delta + V \tag{1.5}$$

where $V \in L^\infty(\mathbb{R}^2)$ and V is 1-periodic in both variables (i.e. $T_X V = T_Y V = V$). Under this assumption on H , standard results show that H is an essentially self-adjoint operator densely defined on $L^2(\mathbb{R}^2)$ and that H is bounded below [RS75a]. Hence the spectral theorem applies and H has purely real spectrum.

Our second assumption on H is that it describes an insulator. Mathematically, this translates to assuming there exists a scalar $E_F \in \mathbb{R}$, called the Fermi energy, such that E_F is not in the spectrum of H . Under this assumption, the Fermi projection, P , is defined as the projector onto the span on eigenvectors with eigenvalues less than E_F (or more precisely, the spectral projector associated with the set $\sigma(H) \cap (-\infty, E_F]$).

Since the Laplacian is translation invariant and V is periodic, it is easy to check that if H is as in Equation (1.5) then $[H, T_X] = [H, T_Y] = 0$. Therefore, we should expect to be able to find a simultaneous basis of eigenfunctions of H , T_X , and T_Y . This result is known as Bloch's theorem and the basis of simultaneous eigenfunctions is known as a Bloch basis [AM76]. Formally, we denote the Bloch basis by $\{\psi_{n,\mathbf{k}}\}$ where $\mathbf{k} = (k_1, k_2) \in [-\pi, \pi)^2$ and $n \in \mathbb{N}$ and we have that

$$\begin{aligned} H\psi_{n,\mathbf{k}} &= E_{n,\mathbf{k}}\psi_{n,\mathbf{k}} \\ T_X\psi_{n,\mathbf{k}} &= e^{ik_1}\psi_{n,\mathbf{k}} \\ T_Y\psi_{n,\mathbf{k}} &= e^{ik_2}\psi_{n,\mathbf{k}} \end{aligned} \tag{1.6}$$

The eigenvalues for $E_{n,\mathbf{k}}$ are ordered so that for each $\mathbf{k} \in [-\pi, \pi)^2$:

$$E_{1,\mathbf{k}} \leq E_{2,\mathbf{k}} \leq E_{3,\mathbf{k}} \leq \dots$$

In the physics literature, the eigenvalue $E_{n,\mathbf{k}}$ is known as the energy and the variables $\mathbf{k} = (k_1, k_2)$, corresponding to the phases in Equation (1.6), are known as the crystal quasi-momenta.

Because of the assumption that E_F is not in the spectrum of H and the fact that $n \in \mathbb{N}$, we can find some N , called the band number, so that for all $\mathbf{k} \in [-\pi, \pi]^2$, $E_{N,\mathbf{k}} < E_F < E_{N+1,\mathbf{k}}$. Hence, by definition of the projector P , we have that:

$$\text{range}(P) = \text{span}(\{\psi_{n,\mathbf{k}}(x) : 1 \leq n \leq N, \mathbf{k} \in [-\pi, \pi]^2\}).$$

While we can use the Bloch basis as a basis for $\text{range}(P)$, using the definition of T_X, T_Y we see that Equation (1.6) implies that $\psi_{n,\mathbf{k}}(x_1 + 1, x_2 + 1) = e^{i(k_1 + k_2)} \psi_{n,\mathbf{k}}(x)$ so the functions $\psi_{n,\mathbf{k}}$ do not decay as $|\mathbf{x}| \rightarrow \infty$.

To transform the Bloch functions to a basis which quickly decays in space, Wannier [Wan37] proposed taking the inverse Fourier transform of the Bloch basis in the crystal quasi-momentum as follows:

$$w_{n,\mathbf{R}}(x) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{-i\mathbf{k} \cdot \mathbf{R}} \psi_{n,\mathbf{k}}(x) d\mathbf{k}. \quad (1.7)$$

The collection of functions $\{w_{n,\mathbf{R}}\}$ are known as a basis of Wannier functions. Importantly, the functions $\{w_{n,\mathbf{R}}\}$ as defined in Equation (1.7) are not the only possible basis of Wannier functions. Since eigenfunctions of H are only defined up to a choice of complex phase we could alternatively define the Wannier functions in Equation (1.7) by making the substitution:

$$\psi_{n,\mathbf{k}}(x) \mapsto e^{i\lambda_{n,\mathbf{k}}} \psi_{n,\mathbf{k}}(x) \quad \text{where} \quad \lambda_{n,\mathbf{k}} \in \mathbb{R} \quad (1.8)$$

More generally, for a system with N bands, this degeneracy is defined by a collection of $N \times N$ unitary matrices $\{U^{(\mathbf{k})}\}_{\mathbf{k} \in [-\pi, \pi]^2}$ and substituting the following expression into Equation (1.7):

$$\psi_{n,\mathbf{k}}(x) \mapsto \sum_m U_{n,m}^{(\mathbf{k})} \psi_{m,\mathbf{k}}(x), \quad (1.9)$$

The mapping in Equation (1.9) is known as a “gauge transformation” and an instance of the matrices $\{U^{(\mathbf{k})}\}_{\mathbf{k} \in [-\pi, \pi]^2}$ is known as “choice of gauge”. By changing

the choice of gauge, one can change whether the corresponding Wannier functions are localized in space or not. In particular, since Wannier functions are defined by an inverse Fourier transform in the crystal quasi-momentum \mathbf{k} , if we can choose a gauge $\{U^{(\mathbf{k})}\}_{\mathbf{k}\in[-\pi,\pi]^2}$ so that the functions in Equation (1.9) are analytic and periodic in \mathbf{k} then one can show that the resulting Wannier functions decay exponentially quickly in space [MPPT18, Appendix A].

In pioneering work, Kohn [Koh59] proved that for inversion-symmetric crystals in one dimension with an isolated band ($N = 1$) there always exists a choice of gauge so that the corresponding Wannier functions decay exponentially fast in space. Since this work by Kohn, there have been many works which have studied exponentially localized Wannier functions from this perspective.

1.4 Previous Work on Exponentially Localized Wannier Functions

In this section, we review of some previous work on the study of exponentially localized Wannier functions (ELWFs) both theoretical existence results (Section 1.4.1) and numerical techniques (Section 1.4.2).

1.4.1 Theoretical Results

Inspired by Kohn’s result on ELWFs, there have been much research devoted to understanding when ELWFs exist by analyzing different choices of gauge. As a result of these efforts, it is now well understood that for periodic insulators in dimension one, two, and three the existence of ELWFs is tied to the vanishing of certain topological invariants. We give a quick review of these theoretical results

- In one spatial dimension, a basis of ELWFs for Fermi projection of an insulating crystalline material always exists [Clo64, DC64, Nen83, HS88, Nen91].

- In two dimensions, the same result holds if and only if the Chern number, a topological invariant associated with the Fermi projector, vanishes [BPC⁺07, Pan07, MPPT18].
- In three dimensions, the result holds as long as three “Chern-like” numbers all vanish [BPC⁺07, Pan07, MPPT18].
- In two or three dimensions, if a system satisfies time reversal symmetry then the Chern number vanishes and hence a basis of ELWFs always exist [BPC⁺07].

To complement these results which connect ELWFs and topology, in [MPPT18] the authors were able to show that for periodic systems in two dimensions that the Chern number vanishes if and only if there exists a basis of Wannier functions with finite second moment (and similarly in three dimensions). This result, combined with the previous results connecting ELWFs to the Chern number, forms the basis of the localization-topology correspondence or *localization dichotomy*. More formally stated we have the following theorem:

Theorem 1 (The Localization Dichotomy, adapted from [MPPT18]). *Suppose that H is a Hamiltonian densely defined on $L^2(\mathbb{R}^2)$ of the form*

$$H = (i\nabla + A)^2 + V$$

which is insulating and satisfies a regularity assumption (for example, Assumptions 1 and 2 are sufficient). Then the following are equivalent:

- 1) *There exists a choice of gauge corresponding to a basis of Wannier functions $\{w_{n,\mathbf{R}}\}$ which has finite second moment. That is there exists a constant $C < \infty$ such that for all (n, \mathbf{R}) :*

$$\int_{\mathbb{R}^2} |\mathbf{x} - \mathbf{R}|^2 |w_{n,\mathbf{R}}(\mathbf{x})|^2 dx \leq C$$

- 2) *The Chern number for the projector P vanishes.*

3) *There exists a choice of gauge corresponding to a basis of Wannier functions $\{\tilde{w}_{n,\mathbf{R}}\}$ which is exponentially localized. That is there exists a constant $C' < \infty$ and a constant $\gamma > 0$ such that for all (n, \mathbf{R}) :*

$$\int_{\mathbb{R}^2} e^{2\gamma|\mathbf{x}-\mathbf{R}|} |\tilde{w}_{n,\mathbf{R}}(\mathbf{x})|^2 dx \leq C'$$

The fact that the existence of an well localized basis is tied to the Chern number (a topological invariant) has led materials with non-zero Chern number to be called *topological insulators*.

1.4.2 Numerical Results

In addition to their theoretical significance, Wannier functions have proved to be an important tool for numerical simulations. In particular, Wannier functions are used to understand the nature of chemical bonds, calculate polarization in materials, and construct accurate model Hamiltonians (discrete approximations to continuum Hamiltonians) [MSV03]. Due to the many practical uses for well localized Wannier functions, there have been a number of works which have proposed techniques for constructing well localized Wannier functions in both periodic and non-periodic systems. These methods can be roughly classified into two classes: those which use gauge optimization and those which do not. Note that gauge optimization techniques can only be used in periodic systems.

With regards to gauge optimization based approaches, as discussed in Section 1.4.1 for periodic systems, once the Bloch functions are chosen, calculating a basis of Wannier functions is equivalent making a choice of gauge $\{U^{(\mathbf{k})}\}$. In a highly influential work, Marzari and Vanderbilt proposed optimizing the gauge so that the corresponding Wannier functions have variance which is as small as possible [MV97]. In the mathematical physics community, this objective function (minimizing the variance of the Wannier functions) has been dubbed the Marzari-Vanderbilt functional. Since this initial work, the original ideas of Marzari-Vanderbilt functional minimiza-

tion have been greatly expanded and implemented into highly optimized software packages such as `Wannier90` [PVA⁺20]. Furthermore, in certain cases, it has been shown that the minimizers of the Marzari-Vanderbilt functional exist and these minimizers correspond to exponentially localized Wannier functions [PP13]. Outside of gauge optimization-based approaches, a number of other works have looked at constructing a good choice of gauge algorithmically [CLPS17, CHN16, CMT17, CM17, FMP16a, FMP16b].

Much less work has been done on algorithms which do not use gauge optimization. A typical approach is to mimic the Marzari-Vanderbilt approach by choosing an appropriate cost functional and performing an optimization routine to construct well localized Wannier functions (see [MCY20, SMY20] for some recent examples of this approach). There also have been propositions to generate localized Wannier function by using tools from numerical linear algebra (i.e. rank revealing QR factorizations) [DLY15, DLY17].

Chapter 2

Notation and Assumptions

2.1 Notation and Conventions

We begin by fixing some notations. Vectors in \mathbb{R}^d will be denoted by bold face with their components denoted by subscripts. For example, $\mathbf{v} = (v_1, v_2, v_3, \dots, v_d) \in \mathbb{R}^d$. For any $\mathbf{v} \in \mathbb{R}^d$, we use $|\cdot|$ to denote its Euclidean norm. That is

$$|\mathbf{v}| := \left(\sum_{i=1}^d v_i^2 \right)^{1/2}$$

For any $f : \mathbb{R}^2 \rightarrow \mathbb{C}$, we will use $\|f\|$ to denote the L^2 -norm of f defined as follows:

$$\|f\| := \left(\int_{\mathbb{R}^2} |f(\mathbf{x})|^2 d\mathbf{x} \right)^{1/2}.$$

Similarly, for any linear operator we will use $\|A\|$ to denote the induced norm when we view A as a mapping $L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^2)$. That is,

$$\|A\| := \sup_{\substack{f \in L^2(\mathbb{R}^2) \\ f \neq 0}} \frac{\|Af\|}{\|f\|}.$$

We define the L^∞ -norm of a function $f : \mathbb{R}^2 \rightarrow \mathbb{C}$ as follows

$$\|f\|_{L^\infty} := \inf \{C \geq 0 : |f(x)| \leq C \text{ almost everywhere}\}.$$

Given two sets $A, B \subseteq \mathbb{R}$ we define their diameter and distance as follows:

$$\text{diam}(A) := \sup\{|a_1 - a_2| : a_1, a_2 \in A\}$$

$$\text{dist}(A, B) := \inf\{|a - b| : a \in A, b \in B\}$$

For any contour in the complex plane, \mathcal{C} , we will use $\ell(\mathcal{C})$ to denote the length of \mathcal{C} .

2.1.1 Exponentially Tilted Operators

Given a point $(a, b) \in \mathbb{R}^2$, and a non-negative constant $\gamma \geq 0$, we define an exponential growth operator, $B_{\gamma,(a,b)}$, by

$$B_{\gamma,(a,b)} := \exp\left(\gamma\sqrt{1 + (X - a)^2 + (Y - b)^2}\right) = e^{\gamma|(X-a, Y-b, 1)|}.$$

where X and Y are the standard position operators are defined as follows:

$$Xf(\mathbf{x}) = x_1f(\mathbf{x}) \quad Yf(\mathbf{x}) = x_2f(\mathbf{x}).$$

Given a linear operator A , we define

$$A_{\gamma,(a,b)} := B_{\gamma,(a,b)}AB_{\gamma,(a,b)}^{-1}. \quad (2.1)$$

We refer to $A_{\gamma,(a,b)}$ as “exponentially-tilted” relative to A . We will often prove estimates where we use the notation (2.1) but omit the point (a, b) . In this case the estimate should be understood as uniform in the choice of point (a, b) . As a note, per our convention, when $\gamma = 0$, $A_{\gamma,(a,b)} = A$. Throughout this paper, we will assume that the Fermi projector P is fixed to be the spectral projector onto σ_0 for H satisfying Assumptions 1 and 2. For this projection we also define the operators Q , P_γ , Q_γ :

$$\begin{aligned} Q &:= I - P \\ P_\gamma &:= B_{\gamma,(a,b)}PB_{\gamma,(a,b)}^{-1} \\ Q_\gamma &:= B_{\gamma,(a,b)}QB_{\gamma,(a,b)}^{-1} = I - P_\gamma \end{aligned}$$

where we have used our convention for exponentially tilted operators defined above.

Observe that

$$P_\gamma^2 = \left(B_{\gamma,(a,b)}PB_{\gamma,(a,b)}^{-1}\right)\left(B_{\gamma,(a,b)}PB_{\gamma,(a,b)}^{-1}\right) = B_{\gamma,(a,b)}P^2B_{\gamma,(a,b)}^{-1} = P_\gamma$$

so P_γ is also a projection. Similarly, it can be checked that Q_γ is also a projection.

2.2 Assumptions

Now that we've setup our notations, we can move on to formally state our assumptions. With regards to our proofs, the assumptions on H are mostly used to establish some decay estimates on the Fermi projector P . We state these decay estimates in Section 2.2.1 and formally prove these estimates in Appendix A.1.

Assumption 1 (Regularity on H). *Throughout this dissertation, we will assume that the Hamiltonian H takes the following form*

$$H = (i\nabla + A)^2 + V$$

where $A \in L^\infty(\mathbb{R}^2; \mathbb{R}^2)$, $\operatorname{div}(A) \in L^\infty(\mathbb{R}^2; \mathbb{R})$, and $V \in L^\infty(\mathbb{R}^2; \mathbb{R})$.

Remark 2.2.1. Following the analysis given in [MMP20], we expect that our regularity assumptions can be relaxed to $A \in L^4(\mathbb{R}^2; \mathbb{R}^2)$, $\operatorname{div}(A) \in L^2_{\text{loc}}(\mathbb{R}^2)$, and $V \in L^2_{\text{uloc}}(\mathbb{R}^2)$. We assume that A , $\operatorname{div}(A)$, and V are all L^∞ to simplify the analysis. For more details on the role of these assumptions see Remark 2.2.5.

Using standard techniques it is easy to verify that Assumption 1 implies H is essentially self-adjoint on $L^2(\mathbb{R}^2)$ [RS75a]. Our second assumption on H concerns its spectrum:

Assumption 2 (H has a spectral island). *We suppose that H has a spectral island. That is we can decompose the spectrum of H as $\sigma(H) = \sigma_0 \cup \sigma_1$ where $\operatorname{dist}(\sigma_0, \sigma_1) > 0$ and $\operatorname{diam}(\sigma_0) < \infty$.*

Assumption 2 slightly generalizes the assumption that H is insulating that we discussed in the Chapter 1.

2.2.1 Decay Estimates on P

As mentioned previously, a key part underlying our proofs in this dissertation are some operator norm estimates on the projector P . At a high level, these estimates

quantify the statement “ P is exponentially localized” in a technical sense. The most fundamental of these estimates is the following bound. There exists a $C > 0$ such that for all γ sufficiently small

$$\|P_\gamma\| \leq C.$$

This bound is best understood when the system is a finite matrix. For any $\lambda = (\lambda_x, \lambda_y)$ and $\mu = (\mu_x, \mu_y)$, we can find vectors v_λ and v_μ which are simultaneous eigenvectors of X and Y so that

$$\begin{aligned} Xv_\lambda &= \lambda_x v_\lambda & Yv_\lambda &= \lambda_y v_\lambda \\ Xv_\mu &= \mu_x v_\mu & Yv_\mu &= \mu_y v_\mu \end{aligned}$$

By the definition of the spectral norm, we have that

$$\begin{aligned} \|P_\gamma\| &\leq C \\ \implies |\langle v_\mu, B_{\gamma,(a,b)} P B_{\gamma,(a,b)}^{-1} v_\lambda \rangle| &\leq C \\ \implies e^{\gamma|(\mu_x - a, \mu_y - b, 1)|} e^{-\gamma|(\lambda_x - a, \lambda_y - b, 1)|} |\langle v_\mu, P v_\lambda \rangle| &\leq C \\ \implies |\langle v_\mu, P v_\lambda \rangle| &\leq C e^{-\gamma(|(\mu_x - a, \mu_y - b, 1)| - |(\lambda_x - a, \lambda_y - b, 1)|)} \\ \implies |\langle v_\mu, P v_\lambda \rangle| &\leq C' e^{-\gamma \sqrt{1 + (\mu_x - \lambda_x)^2 + (\mu_y - \lambda_y)^2}} \end{aligned}$$

where in the last line we have set $(a, b) = (\lambda_x, \lambda_y)$. From this calculation, we see that in the position basis, the off diagonal entries of P decay exponentially quickly.

Formally, our proof requires the following technical estimates which we verify are true for any Hamiltonian satisfying Assumptions 1 and 2 (see Lemma 2.2.3):

Assumption 3 (Decay Estimates for P). *We say that the orthogonal projector P satisfies decay estimates, if there exist finite, positive constants $(\gamma^*, C_1, C_2, C_3, C_4, C_5)$ such that for all $0 \leq \gamma \leq \gamma^*$ and any $\lambda \in \mathbb{R}$ we have the following operator norm bounds:*

$$(i) \quad \|P_\gamma - P\| \leq C_1 \gamma$$

$$(ii) \quad (a) \quad \|[P, X]\| \leq C_2$$

- (b) $\|[P, Y]\| \leq C_2$
- (iii) (a) $\|[P_\gamma - P, X]\| \leq C_3\gamma$
- (b) $\|[P_\gamma - P, Y]\| \leq C_3\gamma$
- (iv) $\|[P, \langle X - \lambda \rangle^{1/2}]\| \leq C_4$
- (v) (a) $\|\langle X - \lambda \rangle^{1/2}[P, X]\langle X - \lambda \rangle^{-1/2}\| \leq C_5.$
- (b) $\|\langle X - \lambda \rangle^{1/2}[P, Y]\langle X - \lambda \rangle^{-1/2}\| \leq C_5.$

Assuming that P satisfies the bounds in Assumption 3, it is straightforward to verify the following additional bounds (which we make use of in our proofs) also hold:

Corollary 2.2.2. *If P satisfies decay estimates (Assumption 3), then P also satisfies the following estimates for all $\gamma \geq 0$ sufficiently small (including $\gamma = 0$):*

- (i) $\|P_\gamma\|, \|Q_\gamma\| = O(1)$
- (ii) $\|P_\gamma X Q_\gamma\|, \|Q_\gamma X P_\gamma\|, \|P_\gamma Y Q_\gamma\|, \|Q_\gamma Y P_\gamma\| = O(1)$
- (iii) $\|[P_\gamma, X]\|, \|[P_\gamma, Y]\| = O(1)$
- (iv) $\|P_\gamma X Q_\gamma - P X Q\|, \|Q_\gamma X P_\gamma - Q X P\| = O(\gamma)$
- (v) $\|\langle X - \lambda \rangle^{1/2} P Y Q \langle X - \lambda \rangle^{-1/2}\|, \|\langle X - \lambda \rangle^{1/2} P X Q \langle X - \lambda \rangle^{-1/2}\| = O(1)$
- (vi) $\|\langle X - \lambda \rangle^{1/2} Q Y P \langle X - \lambda \rangle^{-1/2}\|, \|\langle X - \lambda \rangle^{1/2} Q X P \langle X - \lambda \rangle^{-1/2}\| = O(1)$

Proof. We will show that Assumption 3 implies

$$\|\langle X - \lambda \rangle^{1/2} P Y Q \langle X - \lambda \rangle^{-1/2}\| = O(1).$$

The remaining parts of the corollary follow by similar techniques, and will be omitted.

We calculate

$$\begin{aligned}
& \langle X - \lambda \rangle^{1/2} P Y Q \langle X - \lambda \rangle^{-1/2} \\
&= \langle X - \lambda \rangle^{1/2} P [Y, Q] \langle X - \lambda \rangle^{-1/2} \\
&= \langle X - \lambda \rangle^{1/2} P \langle X - \lambda \rangle^{-1/2} \langle X - \lambda \rangle^{1/2} [Y, Q] \langle X - \lambda \rangle^{-1/2} \\
&= -\langle X - \lambda \rangle^{1/2} P \langle X - \lambda \rangle^{-1/2} \langle X - \lambda \rangle^{1/2} [Y, P] \langle X - \lambda \rangle^{-1/2}
\end{aligned}$$

Hence

$$\begin{aligned}
& \| \langle X - \lambda \rangle^{1/2} P Y Q \langle X - \lambda \rangle^{-1/2} \| \\
&\leq \| \langle X - \lambda \rangle^{1/2} P \langle X - \lambda \rangle^{-1/2} \| \| \langle X - \lambda \rangle^{1/2} [Y, P] \langle X - \lambda \rangle^{-1/2} \| \\
&\leq \| [\langle X - \lambda \rangle^{1/2}, P] \langle X - \lambda \rangle^{-1/2} + P \| \| \langle X - \lambda \rangle^{1/2} [Y, P] \langle X - \lambda \rangle^{-1/2} \| \\
&\leq (\| [\langle X - \lambda \rangle^{1/2}, P] \| + 1) \| \langle X - \lambda \rangle^{1/2} [Y, P] \langle X - \lambda \rangle^{-1/2} \|
\end{aligned}$$

which is bounded due to Assumption 3(iv,v). \square

Importantly, the spectral projectors for Hamiltonians H satisfying Assumptions 1 and 2 also satisfy our decay estimates:

Lemma 2.2.3. *Suppose that H is a Hamiltonian satisfying Assumptions 1 and 2. If P is a spectral projector onto σ_0 , then P satisfies decay estimates (Assumption 3).*

Proof. See Appendix A.1. \square

Remark 2.2.4. If one can establish the projector P has an exponentially decaying kernel in the sense that there exists finite, positive constants (C, γ) such that:

$$|P(\mathbf{x}, \mathbf{x}')| \leq C e^{-\gamma |\mathbf{x} - \mathbf{x}'|}$$

then it is easy to verify Assumption 3 is true (cf. [MMP20]).

Remark 2.2.5. The main proofs in this work only rely on the specific properties of the Hamiltonian H in two places

1. Establishing that P satisfies decay estimates as in Assumption 3.
2. A compactness result. In particular our techniques require that the operator $f(H + i)^{-1}$ is compact for any $f \in C_c^\infty(\mathbb{R}^2)$.

If one can establish these two facts, then all the subsequent results follow. While we focus on continuum systems in this dissertation, since operator norm estimates are still well defined in discrete systems, our results can be easily extended to $L^2(\mathbb{Z}^2)$ as well as finite systems.

Chapter 3

Projected Position Operators and Localization

3.1 Introduction

In Chapter 1, we reviewed the theory behind Wannier functions in periodic materials and we have seen that the existence of exponentially localized Wannier functions (ELWFs) is tied to whether the Chern number associated to the Fermi projection vanishes or not (see Theorem 1). In periodic systems, the key technical tool for making the connection between localization and topology is the Fourier transform or more generally the Bloch-Floquet transform. The Bloch-Floquet transform however cannot be used in non-periodic systems and therefore it is unknown whether a similar localization dichotomy holds for non-periodic systems. There have been a number of works which have extended the localization dichotomy to non-periodic systems which are “close” to periodic systems by using perturbation or continuity-type arguments [KO73, NN93, Koh59, Nen91, GK93, RK74, EL11].

In this chapter, we discuss a general approach for calculating ELWFs in fully non-periodic systems by using *projected position operators*, that is operators of the form $\tilde{P}\tilde{X}\tilde{P}$ where \tilde{P} is an orthogonal projection and \tilde{X} is an essentially self-adjoint operator densely defined on $L^2(\mathbb{R}^2)$. Unlike previous results which rely on relating the non-periodic system of interest to a periodic system, the results in the chapter directly apply to any system regardless of underlying symmetries.

The remainder of this chapter is structured as follows. In Section 3.2, we will review the series of works by Kivelson [Kiv82], Niu [Niu91], and Nenciu-Nenciu

This chapter is prepared based on [SWL20a].

[NN98] which rigorously shows for a wide class of one dimensional, insulating systems, the eigenfunctions of PXP form an orthonormal, exponentially localized basis for range (P). In Section 3.3, we will discuss our extension of the work of Kivelson, Niu, and Nenciu-Nenciu to two dimensions. In particular, in this section we will prove the correctness of an algorithm for constructing ELWFs in non-periodic systems in two dimensions based on diagonalizing projected position operators. Since systems in two dimensions can have topological obstructions, the proof of correctness for our algorithm requires that we assume the operator PXP has “uniform spectral gaps”. As we will show directly in Appendix A.4, assuming PXP has uniform spectral gaps prohibits the existence of topological obstructions and therefore our results are in accordance with previously known theory. In Section 3.4, we will show how our algorithm can be generalized to three dimensions and higher. Finally, in Section 3.5 we will numerically demonstrate the effectiveness of our algorithm on the Haldane model (see Section 3.5 for the definition of the Haldane model).

3.2 Projected Position Operators in One Dimension

In one dimension, the eigenfunctions of projected position operator PXP was first proposed as a means to define non-periodic Wannier functions by Kivelson in [Kiv82]. On an intuitive level, the eigenfunctions of the position operator X are delta functions and so diagonalizing PXP can be thought of as constructing the ‘best approximation to a delta function from functions from range (P). To support his proposal, Kivelson showed that the exponentially localized Wannier functions constructed by Kohn in [Koh59] are in fact eigenfunctions of PXP . After the work by Kivelson, Niu [Niu91] argued heuristically that the eigenfunctions of PXP should decay faster than any polynomial. Finally, Nenciu-Nenciu [NN98] was able to rigorously prove that for a wide class of systems the eigenfunctions of PXP are exponentially localized. We will

now give a sketch the proof of Nenciu-Nenciu.

To fix ideas, consider the Hilbert space $L^2(\mathbb{R})$ and let H be a Hamiltonian of the form:

$$H = -\Delta + V(x) \quad V \in L^\infty(\mathbb{R}). \quad (3.1)$$

Under these assumptions, it can be shown that H is essentially self-adjoint and hence the spectral theorem applies [RS75a]. As in Section 1.3, we will assume that the spectrum of H has a gap at E_F , the Fermi energy, and will let P denote the spectral projection onto the states with energy less than E_F .

Due to the fact that H is a local operator and the fact that H has an energy gap at E_F , it can be shown using tools from Combes-Thomas-Agmon theory [CT73] in an L^2 -sense the “off-diagonal” entries of P decay exponentially quickly. In the case when P admits an integral kernel, these L^2 estimates roughly say that there exist finite, positive constants (C, γ) such that:

$$|P(\mathbf{x}, \mathbf{x}')| \leq C e^{-\gamma|\mathbf{x}-\mathbf{x}'|}.$$

Using the exponential decay of P , Nenciu-Nenciu first show that PXP is well-defined on the domain $\mathcal{D}(X) \cap \text{range}(P)$, and extends to an unbounded self-adjoint operator $\text{range}(P) \rightarrow \text{range}(P)$. Using properties of the resolvent $(H + i)^{-1}$ along with the fact that X^{-1} tends to zero as $X \rightarrow \infty$, Nenciu-Nenciu then show that $(PXP + i)^{-1}$ is compact and hence PXP only has real, discrete eigenvalues. Hence, the spectral theorem implies that the eigenfunctions of PXP form an orthonormal basis of $\text{range}(P)$. Therefore to complete the proof of their main result, it only remain to prove that the eigenfunctions of PXP exponentially decay. This can be verified by a direct calculation from the eigenequation $PXPf = \lambda f$ which again relies on exponential decay of P .

3.3 Projected Position Operators in Two Dimensions

3.3.1 Introduction

In two dimensions, diagonalizing PXP does not result in a basis of functions which are exponentially localized in both the X and Y simultaneously. In some numerical tests on a finite system, we found that the eigenfunction of PXP are typically localized along lines of the form $X = (\text{constant})$ (see Figure 3.3) and hence are not localized in both X and Y . More fundamentally, since X^{-1} only decays in one direction, generally PXP does not have compact resolvent in two dimensions and so PXP may not have any L^2 -eigenfunctions.

3.3.2 The Uniform Spectral Gaps Assumption

Considering the relationship between topology and ELWFs in two dimensions (Theorem 1), to generalize the approach of Kivelson, Niu, and Nenciu-Nenciu we must make an additional assumption which somehow prohibits topological obstructions. In this work, we assume that PXP has *uniform spectral gaps*, a notion we make precise in Assumption 4. The assumption is most clearly understood by considering numerical example. In Figure 3.1, we plot the sorted eigenvalues of PXP of the Haldane model [Hal88] in topological and non-topological phase.

In Figure 3.1, we can see that in the non-topological case the eigenvalues of PXP can be separated into discrete steps whereas in the topological case the eigenvalues are essentially continuous. Informally speaking, we say that PXP has uniform spectral gaps if its spectrum can be written as disjoint union of sets $\{\sigma_j\}$ which are separated by some minimum distance. It can be shown that in two dimensions, PXP is essentially self-adjoint, hence we can define a collection orthogonal projectors $\{P_j\}$ where P_j projects onto the span of the eigenvector with eigenvalue from σ_j . We will

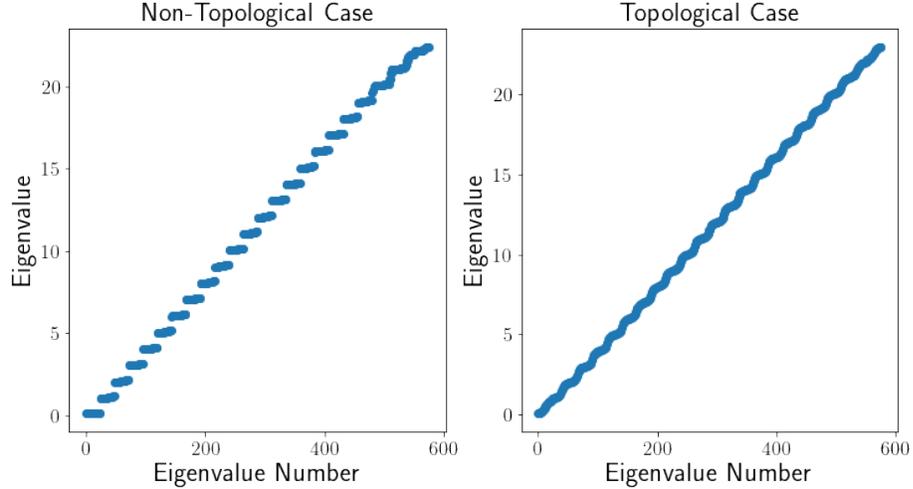


Figure 3.1: Detail from plot of the sorted non-zero eigenvalues of PXP where P is the Fermi projection and X is the lattice position operator $[X\psi]_{m,n} = [m\psi]_{m,n}$ for the Haldane model on a 24×24 lattice with periodic boundary conditions. Parameters for the Haldane model are defined in Section 3.5.1. The left plot corresponds to a non-topological phase (Chern = 0) with parameters $(t, t', v, \phi) = (1, 0, 1, 0)$. The right plot corresponds to topological phase (Chern = 1) with parameters $(t, t', v, \phi) = (1, \frac{1}{4}, 1, \frac{\pi}{2})$. In the non-topological phase, the spectrum of PXP shows clear gaps, while in the topological phase, the spectrum does not have clear gaps.

now give a sketch for how assuming PXP having uniform spectral gaps allows one to construct a ELWFs.

Proof Sketch

If we assume that PXP has uniform spectral gaps then we can reduce the original problem of finding an exponentially-localized basis of $\text{range}(P)$ to the problem of finding exponentially-localized bases of the collection of subspaces $\text{range}(P_j)$, where P_j denotes the spectral projection onto each separated component of the spectrum of PXP . Crucially, one can prove that

1. The projectors P_j are exponentially localized, and

2. Functions from $\text{range}(P_j)$ are quasi-one dimensional. That is, they are concentrated along lines of the form $X = \eta_j$, where η_j is a constant depending on P_j .

Using these properties, we can apply a modified version of the argument from Nenciu-Nenciu's work to each $\text{range}(P_j)$ in turn, and thereby build up a generalized Wannier basis of all of $\text{range}(P)$.

Towards these ends, we consider the family of operators $P_j Y P_j$, where Y is a position operator acting in a non-parallel direction to X . Using the exponential decay of P_j , we prove that each $P_j Y P_j$ is well-defined on the domain $\mathcal{D}(Y)$, and extends to unbounded self-adjoint operators on all of $L^2(\mathbb{R}^2)$. Since Y^{-1} decays in the Y direction and functions from $\text{range}(P_j)$ are concentrated along lines of the form $X = (\text{constant})$, we can extend Nenciu-Nenciu's analysis to show that each $P_j Y P_j$ has compact resolvent and hence only real, discrete eigenvalues. We finally prove that the eigenfunctions of $P_j Y P_j$ exponentially decay by a direct calculation from the eigenequation $P_j Y P_j f = \lambda f$, again using exponential decay of P_j . It now follows immediately that the union of the set of eigenfunctions of each of the $P_j Y P_j$ operators forms an exponentially localized basis of $\text{range}(P)$.

By using this argument, the main result we will prove in this chapter is the following:

Theorem 2. *Suppose that H is a Hamiltonian satisfying Assumptions 1 and 2 and P is the projector associated with σ_0 . Then, if PXP has uniform spectral gaps, there exist functions $\{\psi_{j,m}\}_{(j,m) \in \mathcal{J} \times \mathcal{M}}$ and points $\{(a_j, b_m)\}_{(j,m) \in \mathcal{J} \times \mathcal{M}} \in \mathbb{R}^2$ such that*

1. *The collection $\{\psi_{j,m}\}_{(j,m) \in \mathcal{J} \times \mathcal{M}}$ is an orthonormal basis of $\text{range}(P)$.*
2. *Each $\psi_{j,m}$ is exponentially localized at $(a_{j,m}, b_{j,m})$ in the sense that*

$$\int_{\mathbb{R}^2} e^{2\gamma\sqrt{1+(x-a_{j,m})^2+(y-b_{j,m})^2}} |\psi_{j,m}(x, y)|^2 dx dy \leq C, \quad (3.2)$$

where (C, γ) denote finite positive constants which are independent of j and m .

3. The set of $\{\psi_{j,m}\}_{(j,m)\in\mathcal{J}\times\mathcal{M}}$ are the set of eigenfunctions of the operators $P_j Y P_j$, where P_j are the band projectors defined by Definition 2.

Here \mathcal{J} and \mathcal{M} are the countable sets which index the projectors P_j and the eigenfunctions of $P_j Y P_j$ respectively.

3.3.3 Proof of Theorem 2

We begin by presenting the general outline of the proof of Theorem 2 assuming the correctness of a number of lemmas. We will then prove these lemmas in the subsequent sections (Sections 3.3.4, 3.3.5, and 3.3.6). Key to our proofs are a number of operator norm estimates on the Fermi projector P (Assumption 3) and the projectors P_j . The projectors P_j are formally defined in Definition 2 and the required estimates for P_j are proven in Appendix A.2.

Since H is essentially self-adjoint, by the spectral theorem there exists an orthogonal projector P associated with σ_0 . Because of Assumption 1 on H , by the Riesz projection formula we can find a contour \mathcal{C} in the complex plane enclosing σ_0 so that:

$$P = \frac{1}{2\pi i} \int_{\mathcal{C}} (\lambda - H)^{-1} d\lambda. \quad (3.3)$$

Furthermore, we may choose \mathcal{C} so that \mathcal{C} has finite length and

$$\sup_{\lambda \in \mathcal{C}} \|(\lambda - H)^{-1}\| < \infty.$$

Recall, we define two-dimensional position operators X and Y with respect to a choice of two-dimensional non-parallel axes by

$$Xf(x_1, x_2) = x_1 f(x_1, x_2), \text{ and } Yf(x, y) = x_2 f(x_1, x_2), \quad (3.4)$$

We now claim the following Lemma:

Lemma 3.3.1. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Then the operator PXP is well-defined on $\mathcal{D}(X)$ and essentially self-adjoint.*

We prove Lemma 3.3.1 in Section 3.3.4. Lemma 3.3.1 generalizes part (i) of Theorem 1 of Nenciu-Nenciu [NN98] to two dimensions. The proof is essentially identical, relying only on the exponential localization of P (Assumption 3).

We are now in a position to give our precise assumption on PXP . When it holds, we say that PXP has *uniform spectral gaps*.

Assumption 4 (Uniform Spectral Gaps). *We assume there exist constants (d, D) such that:*

1. *There exists a countable set, \mathcal{J} , such that:*

$$\sigma(PXP) = \bigcup_{j \in \mathcal{J}} \sigma_j.$$

2. *The distance between σ_j, σ_k ($j \neq k$) is uniformly lower bounded:*

$$d := \min_{j \neq k} \left(\text{dist}(\sigma_j, \sigma_k) \right) > 0.$$

3. *The diameter of each σ_j is uniformly bounded:*

$$D := \max_{j \in \mathcal{J}} \left(\text{diam}(\sigma_j) \right) < \infty.$$

If PXP has uniform spectral gaps in the sense of Assumption 4, we can define spectral projections associated with each subset $\{\sigma_j\}_{j \in \mathcal{J}}$ of $\sigma(PXP)$. We will refer to these projections as *band projectors*. Note that our use of “band” in this context should not be confused with its use in the context of Bloch eigenvalue bands of periodic operators.

Definition 2 (Band projectors). When PXP has uniform spectral gaps with constants (d, D) and decomposition $\{\sigma_j\}_{j \in \mathcal{J}}$ in the sense of Assumption 4, for each $j \in \mathcal{J}$ we let

$$P_j := P \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - PXP)^{-1} d\lambda \right) P, \quad (3.5)$$

where \mathcal{C}_j encloses σ_j and satisfies

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - PXP)^{-1}\| \leq Cd^{-1} \text{ and } \ell(\mathcal{C}_j) \leq C'(D + d) \quad (3.6)$$

for some absolute constants C, C' independent of j . In particular, P_j is an orthogonal projection onto the spectral subspace associated with σ_j .

Note that the existence of a contour \mathcal{C}_j satisfying (3.6) is clearly guaranteed by the uniform spectral gap assumption (Assumption 4).

The addition of P in the definition (3.5) of the band projectors, P_j , is to ensure that $\text{range}(P_j) \subseteq \text{range}(P)$. This is necessary to avoid the trivial null space of PXP consisting of functions in the null space of P . Since P commutes with PXP , we have that

$$P_j = \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - PXP)^{-1} d\lambda \right) P.$$

Our aim is to apply the Kivelson-Nenciu-Nenciu construction to each of the projections $\text{range}(P_j)$. We start with the following Lemma:

Lemma 3.3.2. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that PXP satisfies the uniform spectral gap assumption (Assumption 4). Let P_j , with $j \in \mathcal{J}$, be the band projectors as in Definition 2, and let Y be as in Equation (3.4). Then the operators $P_j Y P_j$ are each well-defined on the domain $\mathcal{D}(Y)$ and extend to unbounded, self-adjoint operators on $L^2(\mathbb{R}^2)$.*

We prove Lemma 3.3.2 in Section 3.3.4. The proof is very similar to the proof of Lemma 3.3.1, except that it relies on exponential localization of each P_j , proved in Appendix A.2.

We now claim that each of the operators $P_j Y P_j$ has compact resolvent:

Lemma 3.3.3. *Suppose that H is a Hamiltonian satisfying Assumptions 1 and 2 and P is the projector associated with σ_0 . Suppose further that PXP satisfies the uniform spectral gap assumption (Assumption 4). Let P_j , with $j \in \mathcal{J}$, be the band*

projectors as in Definition 2, and let Y be as in Equation (3.4). Then each of the operators $P_j Y P_j$ has compact resolvent.

We prove Lemma 3.3.3 in Section 3.3.5. Lemma 3.3.3 generalizes part (ii) of Theorem 1 of [NN98] to two dimensions (we sketch the generalization to higher dimensions in Section 3.4). The generalization is non-trivial since the decay induced by Y alone is not sufficient for the resolvent of $P_j Y P_j$ to be compact. To prove compactness, we make use of the fact that functions in each subspace $\text{range}(P_j)$ decay with respect to X .

Our final lemma states that eigenfunctions of the operators $P_j Y P_j$ are exponentially localized:

Lemma 3.3.4. *Let $P_j Y P_j$, $j \in \mathcal{J}$, be as in Lemma 3.3.2. Then there exists a $\gamma'' > 0$, independent of j , such that if $\psi \in \text{range}(P_j)$ and $P_j Y P_j \psi = \eta' \psi$, then for all $\eta \in \sigma_j$*

$$\int e^{2\gamma'' \sqrt{1+(x-\eta)^2+(y-\eta')^2}} |\psi(x, y)|^2 dx dy \leq 16e^{\gamma'' \sqrt{1+2b^2}}.$$

Here b is a finite positive constant (independent of j and ψ) which depends only on the collection $\{P_j\}_{j \in \mathcal{J}}$.

We prove Lemma 3.3.4 in Section 3.3.6. Lemma 3.3.4 generalizes part (iii) of Theorem 1 of Nenciu-Nenciu [NN98] to two dimensions (we sketch the generalization to higher dimensions in Section 3.4). Although the proof of Lemma 3.3.4 has a similar structure to that of [NN98], our proof involves technical innovations which are necessary to (1) generalize their proof to two dimensions and higher (2) give a proof which does not refer to the original Hamiltonian H , requiring only operator norm estimates on the projectors P_j . We are now in a position to state our main result in full detail.

Theorem 1. *Suppose that H is a Hamiltonian satisfying Assumptions 1 and 2 and P is the projector associated with σ_0 . Suppose further that PXP satisfies the uniform spectral gaps assumption (Assumption 4). Then there exist functions $\{\psi_{j,m}\}_{(j,m) \in \mathcal{J} \times \mathcal{M}}$ and points $\{(a_j, b_m)\}_{(j,m) \in \mathcal{J} \times \mathcal{M}} \in \mathbb{R}^2$ such that*

1. The collection $\{\psi_{j,m}\}_{(j,m) \in \mathcal{J} \times \mathcal{M}}$ is an orthonormal basis of $\text{range}(P)$.
2. Each $\psi_{j,m}, (j, m) \in \mathcal{J} \times \mathcal{M}$ is exponentially localized in the sense that

$$\int_{\mathbb{R}^2} e^{2\gamma\sqrt{1+(x-a_{j,m})^2+(y-b_{j,m})^2}} |\psi_{j,m}(x, y)|^2 dx dy \leq C, \quad (3.7)$$

where (C, γ) denote finite positive constants which are independent of j and m .

3. The set of $\{\psi_{j,m}\}_{(j,m) \in \mathcal{J} \times \mathcal{M}}$ are the set of eigenfunctions of the operators $P_j Y P_j$, where P_j are the band projectors defined by Definition 2.

Here \mathcal{J} and \mathcal{M} are the countable sets which index the band projectors as in Definition 2 and the eigenfunctions of $P_j Y P_j$ for fixed j , respectively.

Proof. The proof follows immediately from Lemmas 3.3.1, 3.3.2, 3.3.3, and 3.3.4 and the spectral theorem for self-adjoint operators. For each $(j, m) \in \mathcal{J} \times \mathcal{M}$, we define the points $(a_{j,m}, b_{j,m})$ by the (η, η') appearing in Lemma 3.3.4, i.e. $a_{j,m}$ can be taken as any $\eta \in \sigma_j$, while $b_{j,m}$ is the associated eigenvalue of $\psi_{j,m}$ considered as an eigenfunction of $P_j Y P_j$. \square

3.3.4 Proof that PXP and $P_j Y P_j$ are essentially self-adjoint (Proofs of Lemmas 3.3.1 and 3.3.2)

The proofs that PXP and $P_j Y P_j$ are essentially self-adjoint in two dimensions are almost exactly the same and they both use the same argument as given in [NN98]. Because the proofs are so similar, we will first prove that PXP is essentially self-adjoint and then note the changes which need to be made to prove that $P_j Y P_j$ is essentially self-adjoint.

Proof of essential self-adjointness of PXP

To prove PXP is well-defined on $\mathcal{D}(X)$ and essentially self-adjoint we two norm estimates for the projector P . We recall our notation for exponentially tilted operators

given in Section 2.1. Given a point $(a, b) \in \mathbb{R}^2$ and a non-negative constant $\gamma \geq 0$, we define an exponential growth operator by

$$B_{\gamma,(a,b)} := \exp\left(\gamma\sqrt{1 + (X - a)^2 + (Y - b)^2}\right).$$

Given an operator A , we can then define an “exponentially-tilted” version of A as

$$A_{\gamma,(a,b)} := B_{\gamma,(a,b)}AB_{\gamma,(a,b)}^{-1}. \quad (3.8)$$

We will often prove estimates where we use the notation (3.8) but omit the point (a, b) . In this case the estimate should be understood as uniform in of the choice of point (a, b) . As a note, when $\gamma = 0$, $A_{\gamma,(a,b)} = A$.

Using this notation, we recall some estimates from our decay estimates on P (Assumption 3). In particular, there exist finite, positive constants (C, C') such that:

$$\|P_\gamma\| \leq C \quad (3.9)$$

$$\|[P, X]\| \leq C' \quad (3.10)$$

With these estimates in hand, we can now prove that PXP is essentially self-adjoint.

Since X is essentially self-adjoint, we know that for all $\mu > 0$, $(X \pm i\mu)^{-1}$ is well defined and $\|(X \pm i\mu)^{-1}\| \leq \mu^{-1}$. Therefore, since P is a projection,

$$(PXP \pm i\mu)P(X \pm i\mu)^{-1}P = P(X \pm i\mu)P(X \pm i\mu)^{-1}P,$$

where both sides of this equation are well-defined using Equation (3.9). Commuting $(X \pm i\mu)$ and P now gives

$$\begin{aligned} (PXP \pm i\mu)P(X \pm i\mu)^{-1}P &= P(X \pm i\mu)P(X \pm i\mu)^{-1}P \\ &= P + P[X, P](X \pm i\mu)^{-1}P \\ &= P(I + P[X, P](X \pm i\mu)^{-1}P). \end{aligned} \quad (3.11)$$

Since $\|[X, P]\| \leq C' < \infty$ (Equation (3.10)), we can pick $\mu > 2\|[X, P]\|$ to conclude that

$$\|P[X, P](X \pm i\mu)^{-1}P\| \leq \frac{1}{2}.$$

Therefore, we may invert $I + P[X, P](X \pm i\mu)^{-1}P$ in Equation (3.11) to get

$$(PXP \pm i\mu)P(X \pm i\mu)^{-1}P \left(I + P[X, P](X \pm i\mu)^{-1}P \right)^{-1} = P.$$

Hence, $(PXP \pm i\mu)$ is surjective on $\text{range}(P)$. Since PXP acts trivially on $\text{range}(P)^\perp$ and $\mu > 0$ we can therefore conclude that $(PXP \pm i\mu)$ is surjective on its domain. Hence by the fundamental criterion of self-adjointness (see [RS72, Chapter VIII]), PXP is essentially self-adjoint.

Proof of essential self-adjointness of $P_j Y P_j$

In this section, we require analogous estimates on P_j as we required on P in Section 3.3.4.

Lemma 3.3.5. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that PXP satisfies the uniform gap assumption (Assumption 4). For each $j \in \mathcal{J}$, let P_j denote the band projectors defined in Definition 2. Then there exist finite, positive constants (C, K_2'', γ_0) such that for all $0 \leq \gamma \leq \gamma_0$, each P_j satisfies*

$$\|P_{j,\gamma}\| \leq C \tag{3.12}$$

$$\|[P_j, Y]\| \leq K_2'' \tag{3.13}$$

Proof. Given in Appendix A.2. □

We can now prove essential self-adjointness of $P_j Y P_j$ where $j \in \mathcal{J}$ by an identical calculation to that given in Section 3.3.4.

Using Equation (3.12), the operator

$$(P_j Y P_j \pm i\tilde{\mu})P_j(Y \pm i\tilde{\mu})^{-1}P_j$$

is well-defined for all $\tilde{\mu} > 0$. Since $\|[P_j, Y]\|$ is bounded (Equation (3.13)), we can choose $\tilde{\mu} > 2\|[P_j, Y]\|$ and repeat the same steps as in Section 3.3.4 to get that

$$(P_j Y P_j \pm i\tilde{\mu})P_j(Y \pm i\tilde{\mu})^{-1}P_j \left(I + P_j[Y, P_j](Y \pm i\tilde{\mu})^{-1}P_j \right)^{-1} = P_j \tag{3.14}$$

which shows that $P_j Y P_j \pm i\tilde{\mu}$ is surjective on $\text{range} P_j$ and we are done.

3.3.5 Proof that $P_j Y P_j$ has compact resolvent (Proof of Lemma 3.3.3)

In this section, in addition to Lemmas 3.3.5, we require the following additional estimate on P_j :

Lemma 3.3.6. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that PXP satisfies the uniform gap assumption (Assumption 4). For each $j \in \mathcal{J}$, let P_j denote the band projectors defined by Definition 2. Then, for any $\eta \in \sigma_j$, the operator $(X - \eta)P_j$ is bounded, i.e.*

$$\|(X - \eta)P_j\| \leq K_3''$$

where K_3'' is a positive constant independent of j .

Proof. Given in Appendix A.2. □

For the proof of Lemma 3.3.3, we will start by continuing the main calculation of Section 3.3.4. We used Equation (3.12) and (3.13) to derive Equation (3.14), which we restate here:

$$(P_j Y P_j \pm i\tilde{\mu})P_j(Y \pm i\tilde{\mu})^{-1}P_j \left(I + P_j[Y, P_j](Y \pm i\tilde{\mu})^{-1}P_j \right)^{-1} = P_j.$$

Since $P_j Y P_j$ is essentially self-adjoint on $\text{range}(P_j)$ we may invert $(P_j Y P_j \pm i\tilde{\mu})$ for $\tilde{\mu} > 0$ to get:

$$P_j(Y \pm i\tilde{\mu})^{-1}P_j \left(I + P_j[Y, P_j](Y \pm i\tilde{\mu})^{-1}P_j \right)^{-1} = (P_j Y P_j \pm i\tilde{\mu})^{-1}P_j.$$

Since the product of a compact operator and a bounded operator is compact, it follows that to show that $(P_j Y P_j \pm i\tilde{\mu})^{-1}$ is compact on $\text{range}(P_j)$ it is enough to show that $P_j(Y \pm i\tilde{\mu})^{-1}P_j$ is compact.

Let $\eta \in \sigma_j$, i.e. as in Lemma 3.3.6. Taking $P_j(Y \pm i\tilde{\mu})^{-1}P_j$ and inserting $(X - \eta + i)^{-1}(X - \eta + i)$ and $(-\Delta + 1)(-\Delta + 1)^{-1}$ gives:

$$\begin{aligned} & P_j(Y \pm i\tilde{\mu})^{-1}P_j \\ &= \left[P_j(-\Delta + 1) \right] \left[(-\Delta + 1)^{-1}(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \right] \left[(X - \eta + i)P_j \right]. \end{aligned} \quad (3.15)$$

We will prove Lemma 3.3.3 by proving that the first and last term of Equation (3.15) are bounded and the middle term is compact.

Proofs that first and last terms of (3.15) are bounded

The last term of (3.15) is bounded by Lemma 3.3.6:

$$\begin{aligned} \|(X - \eta + i)P_j\| &\leq \|(X - \eta)P_j\| + 1 \\ &\leq K_3'' + 1. \end{aligned}$$

As for the first term, since P_j is a spectral projection of PXP , we have

$$\|P_j(-\Delta + 1)\| = \|P_jP(-\Delta + 1)\| \leq \|P(-\Delta + 1)\| \leq \|P\Delta\| + 1. \quad (3.16)$$

It remains only to bound $P\Delta$. We will prove that ΔP is bounded, from which boundedness of $P\Delta$ follows immediately from duality. Recall that P is defined through the Riesz projection formula (3.3). Since the contour \mathcal{C} appearing in (3.3) has finite length and Δ and P are both self-adjoint, (3.16) will follow immediately if we can show

$$\sup_{\lambda \in \mathcal{C}} \|\Delta(\lambda - H)^{-1}\| < \infty. \quad (3.17)$$

To prove this bound we will essentially use the same technique used to prove [CFKS09, Proposition 1.3]. Let ϕ be arbitrary. Then for $\lambda \in \mathcal{C}$, $(\lambda - H)^{-1}\phi \in \mathcal{D}(\Delta)$. By Lemma A.1.2 it follows that

$$\begin{aligned} \|\Delta(\lambda - H)^{-1}\phi\| &\leq a\|H(\lambda - H)^{-1}\phi\| + b\|(\lambda - H)^{-1}\phi\| \\ &= a\|(\lambda - H)(\lambda - H)^{-1}\phi - \lambda(\lambda - H)^{-1}\phi\| + b\|(\lambda - H)^{-1}\phi\| \\ &\leq a\|\phi\| + (a|\lambda| + b)\|(\lambda - H)^{-1}\phi\|. \end{aligned}$$

The bound (3.17) then immediately follows using the Riesz projection formula along with the fact that \mathcal{C} has finite length.

Proof that middle term of (3.15) is compact

It remains only to prove that the middle term

$$(-\Delta + 1)^{-1}(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \quad (3.18)$$

is a compact operator. We will do so by proving it is the limit of compact operators in the operator norm topology. To this end, let χ_N denote a cutoff function

$$\chi_N(x, y) := \begin{cases} 1 & \text{if } |x| \leq N \text{ and } |y| \leq N \\ 0 & \text{otherwise.} \end{cases}$$

We can rewrite (3.18) using χ_N as

$$\begin{aligned} & (-\Delta + 1)^{-1}\chi_N(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \\ & + (-\Delta + 1)^{-1}(1 - \chi_N)(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \end{aligned} \quad (3.19)$$

We first note that since X^{-1} and Y^{-1} decay as $|X|, |Y| \rightarrow \infty$, for all N sufficiently large the second term is $O(N^{-1})$ in operator norm. Therefore,

$$\begin{aligned} \lim_{N \rightarrow \infty} (-\Delta + 1)^{-1}\chi_N(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \\ = (-\Delta + 1)^{-1}(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1} \end{aligned}$$

in the operator norm topology. It remains to prove that the first term in (3.19) is compact for each N . Since $(Y \pm i\tilde{\mu})^{-1}(X - \eta + i)^{-1}$ is bounded, it suffices to prove that

$$(-\Delta + 1)^{-1}\chi_N \quad (3.20)$$

is compact for each N .

We will prove (3.20) is compact by showing it is Hilbert-Schmidt by showing that its integral kernel is in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$. We start by defining, for real and positive z , the “modified Bessel function” $K_0(z)$ through the integral

$$K_0(z) := \int_0^\infty t^{-1} \exp\left(-\frac{z^2}{4t} - t\right) dt,$$

(see (10.32.10) of [OLBC10]). Note that $K_0(z)$ has a logarithmic singularity at the origin and decays exponentially in z . The integral kernel of $(-\Delta + 1)^{-1}$ in two dimensions can be computed explicitly as (see [LL97, Section 6.23]),

$$\frac{1}{2\pi} K_0 \left(\sqrt{(x-x')^2 + (y-y')^2} \right).$$

Hence (3.20) is an integral operator with kernel

$$K(x, y, x', y') := K_0 \left(\sqrt{(x-x')^2 + (y-y')^2} \right) \chi_N(x', y').$$

Integrating $K(x, y, x', y')$ we have

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} |K(x, y, x', y')|^2 dx dy dx' dy' = \frac{1}{4\pi^2} \int_{\mathbb{R}} \int_{\mathbb{R}} \left(|\tilde{K}_0|^2 * \chi_N \right) (x, y) dx dy,$$

where

$$\tilde{K}_0(x, y) := K_0 \left(\sqrt{x^2 + y^2} \right).$$

Hence we are done if we can show $|\tilde{K}_0|^2 * \chi_N(x, y) \in L^1(\mathbb{R}^2)$. By Young's convolution inequality, this holds as long as $\chi_N(x, y)$ and $|\tilde{K}_0(x, y)|^2$ are both in $L^1(\mathbb{R}^2)$. The first statement is obvious, while the second follows immediately when we change to polar coordinates (r, θ) where $x = r \cos \theta$ and $y = r \sin \theta$:

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \left| K_0 \left(\sqrt{x^2 + y^2} \right) \right|^2 dx dy = 2\pi \int_0^\infty |K_0(r)|^2 r dr,$$

and use exponential decay of $K_0(z)$.

3.3.6 Eigenfunctions of $P_j Y P_j$ are exponentially localized (Proof of Lemma 3.3.4)

In this section, we will need somewhat stronger bounds on P_j than in Section 3.3.5. Let us recall that we define the exponential growth operator, $B_{\gamma, (a, b)}$, for any $(a, b) \in \mathbb{R}^2$ and any $\gamma \geq 0$:

$$B_{\gamma, (a, b)} = \exp \left(\gamma \sqrt{1 + (X - a)^2 + (Y - b)^2} \right).$$

Since most of the steps in our proof are independent of the choice of (a, b) , we will suppress this subscript and simply write B_γ . Recall that for any $\gamma \geq 0$ we define

$$P_{j,\gamma} := B_\gamma P_j B_\gamma^{-1}.$$

With these notations, the following lemma states the bounds on P_j we require which are proved in Appendix A.2.

Lemma 3.3.7. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that PXP satisfies the uniform gap assumption (Assumption 4). For each $j \in \mathcal{J}$, let P_j denote the band projectors associated with the separated components σ_j of $\sigma(PXP)$ defined by Definition 2. Then there exist finite, positive constants $(\gamma'', K_1'', K_2'', K_3'')$, independent of j , such that for all $\gamma \leq \gamma''$*

1. $\|P_{j,\gamma} - P_j\| \leq K_1'' \gamma$
2. $\|[P_{j,\gamma}, Y]\| \leq K_2''$
3. For all $\eta \in \sigma_j$:

$$\|(X - \eta)P_{j,\gamma}\| \leq K_3'' \text{ and } \|P_{j,\gamma}(X - \eta)\| \leq K_3''.$$

Proof. Given in Appendix A.2. □

With these estimates in hand, we are now ready to prove Lemma 3.3.4. The overall strategy, which follows Nenciu-Nenciu [NN98], is to manipulate the eigenvalue equation $P_j Y P_j v = \eta' v$ into the form

$$v = \mathcal{L}v \tag{3.21}$$

for some operator \mathcal{L} , multiply both sides of (3.21) by $B_{\gamma,(a,b)}$ for some (a, b) , and then use properties of \mathcal{L} to deduce that the left-hand side is bounded. Our proof differs from Nenciu-Nenciu [NN98] in important details.

Suppose that $P_j Y P_j$ has an eigenvector v with eigenvalue η' and $v \in \text{range}(P_j)$. Since $v \in \text{range}(P_j)$ we have that

$$P_j Y P_j v = \eta' v \iff P_j Y P_j v = \eta' P_j v \iff P_j(Y - \eta')P_j v = 0.$$

Now for any operator O such that $v \in \mathcal{D}(P_j O P_j)$, adding $i P_j O P_j v$ to both sides of the above equation gives

$$P_j(Y - \eta' + iO)P_j v = i P_j O P_j v. \quad (3.22)$$

The main difference between our proof and the proof of Nenciu-Nenciu lies in the choice of the operator O . For now, let's suppose that we have chosen O so that $(Y - \eta' + iO)$ is invertible and multiply both sides of Equation (3.22) by $(Y - \eta' + iO)^{-1}$ to get

$$(Y - \eta' + iO)^{-1} P_j (Y - \eta' + iO) P_j v = i (Y - \eta' + iO)^{-1} P_j O P_j v. \quad (3.23)$$

We can simplify the left hand side of Equation (3.23) by commuting P_j and $(Y - \eta' + iO)$ as follows

$$\begin{aligned} & (Y - \eta' + iO)^{-1} P_j (Y - \eta' + iO) P_j \\ &= P_j + (Y - \eta' + iO)^{-1} [P_j, Y - \eta' + iO] P_j \\ &= \left(I + (Y - \eta' + iO)^{-1} ([P_j, Y] + i[P_j, O]) \right) P_j. \end{aligned}$$

Therefore, we can write Equation (3.23) as follows

$$\left(I + (Y - \eta' + iO)^{-1} ([P_j, Y] + i[P_j, O]) \right) P_j v = i (Y - \eta' + iO)^{-1} P_j O P_j v.$$

To reduce the number of terms in the next steps, let's define

$$A := (Y - \eta' + iO)^{-1} ([P_j, Y] + i[P_j, O]).$$

With this definition and using that $v \in \text{range}(P_j)$ we have that

$$(I + A)v = i(Y - \eta' + iO)^{-1} P_j O v. \quad (3.24)$$

For the next step of the proof, we will want to show that the $(I + A)$ has bounded inverse. To do this, by Neumann series, it is enough to show that

$$\|A\| = \|(Y - \eta' + iO)^{-1}([P_j, Y] + i[P_j, O])\| \leq \frac{3}{4}. \quad (3.25)$$

For Equation (3.25) to hold, we require a particular choice of the operator O which differs from the choice made in Nenciu-Nenciu [NN98]. We require that O satisfies the following properties:

1. O commutes with B_γ .
2. O contains a cutoff in both the X and Y directions.
3. $(Y - \eta' + iO)$ is invertible.

For our proof, we let $b > 0$ be a constant to be chosen later and set O to be the following operator:

$$O = b\Pi_{[\eta-b, \eta+b]}^X \Pi_{[\eta'-b, \eta'+b]}^Y + |X - \eta| \quad (3.26)$$

where Π_I^X (resp. Π_I^Y) is a spectral projection for X (resp. Y) onto the interval I and $|X - \eta|$ is the polar decomposition of $X - \eta$ defined by $|X - \eta| := \sqrt{(X - \eta)^2}$.

Before continuing we make three important observations about this choice for O :

1. Since X and Y commute and are essentially self-adjoint, the operator $\Pi_{[\eta-b, \eta+b]}^X \Pi_{[\eta'-b, \eta'+b]}^Y$ is an orthogonal projector.
2. Due to the properties of the polar decomposition [RS72] and our bounds on P_j we know that for all γ sufficiently small both $\|P_{j,\gamma}|X - \eta|\|$ and $\||X - \eta|P_{j,\gamma}\|$ are bounded¹.

¹The polar decomposition gives that there exist partial isometries U and V such that $|X - \eta| = U(X - \eta)$ and $X - \eta = (X - \eta)V$ and so

$$\begin{aligned} \||X - \eta|P_{j,\gamma}\| &= \|U(X - \eta)P_{j,\gamma}\| \leq \|(X - \eta)P_{j,\gamma}\| \\ \|P_{j,\gamma}|X - \eta|\| &= \|P_{j,\gamma}(X - \eta)V\| \leq \|P_{j,\gamma}(X - \eta)\| \end{aligned}$$

3. For all $b > 0$, $\|(Y - \eta' + iO)^{-1}\| \leq b^{-1}$.

In what follows, we will abbreviate $\Pi := \Pi_{[\eta-b, \eta+b]}^X \Pi_{[\eta'-b, \eta'+b]}^Y$.

The key trick which allows us to show that $\|A\| \leq \frac{3}{4}$ is the following lemma (see [WD08, Corollary 8] for an independent proof, see also [Kit07]):

Lemma 3.3.8. *Let B, C be two bounded operators. If B is positive semidefinite then*

$$\|[B, C]\| \leq \|B\| \|C\|.$$

If both B and C are positive semidefinite then

$$\|[B, C]\| \leq \frac{1}{2} \|B\| \|C\|.$$

Proof. Suppose that B is positive semidefinite and define $\tilde{B} := B - \frac{1}{2}\|B\|I$. Since B is a positive semidefinite operator its spectrum lies in the range $[0, \|B\|]$. Therefore, the spectrum of \tilde{B} lies in the range $[-\frac{1}{2}\|B\|, \frac{1}{2}\|B\|]$ and hence $\|\tilde{B}\| = \frac{1}{2}\|B\|$. Since the identity commutes with every operator we have

$$\|[B, C]\| = \|\tilde{B}, C\| = \|\tilde{B}C - C\tilde{B}\| \leq 2\|\tilde{B}\| \|C\| = \|B\| \|C\|.$$

If C is also positive semidefinite then we can repeat the same argument using $\tilde{C} := C - \frac{1}{2}\|C\|I$ as well to get $\|[B, C]\| \leq \frac{1}{2}\|B\| \|C\|$. \square

We can now prove that, for b sufficiently large, $\|A\| \leq \frac{3}{4}$. The following calculations are clear:

$$\begin{aligned} \|A\| &= \|(Y - \lambda + iO)^{-1}[P_j, Y + iO]\| \\ &\leq \|(Y - \lambda + iO)^{-1}\| \left(\|[P_j, Y]\| + \|[P_j, O]\| \right) \\ &\leq b^{-1} \left(\|[P_j, Y]\| + b\|[P_j, \Pi]\| + \|[P_j, |X - \eta|]\| \right) \\ &\leq \|[P_j, \Pi]\| + b^{-1} \left(\|[P_j, Y]\| + \|P_j|X - \eta|\| + \||X - \eta|P_j\| \right). \end{aligned}$$

Since P_j and Π are both orthogonal projectors we can apply Lemma 3.3.8 to conclude that $\|[P_j, \Pi]\| \leq \frac{1}{2}$. It now follows that

$$\|A\| \leq \frac{1}{2} + b^{-1} \left(\|[P_j, Y]\| + \|P_j|X - \eta|\| + \||X - \eta|P_j\| \right),$$

and if we choose b so that

$$b > 4 \left(\| [P_j, Y] \| + \| P_j |X - \eta| \| + \| |X - \eta| P_j \| \right),$$

we have that

$$\|A\| \leq \frac{3}{4}.$$

Note that because of our estimates from Lemma 3.3.7 we know that we can choose b so that $b < \infty$.

Returning to Equation (3.24), we now know that we can invert $(I + A)$ and get

$$\begin{aligned} (I + A)v &= i(Y - \eta' + iO)^{-1} P_j O v \\ v &= i(I + A)^{-1} (Y - \eta' + iO)^{-1} P_j O v \end{aligned} \tag{3.27}$$

To reduce the number of terms in the next steps, let's define

$$C := (I + A)^{-1} (Y - \eta' + iO)^{-1}.$$

With this definition Equation (3.27) becomes

$$v = iC P_j O v.$$

Recalling that we chose $O := b\Pi + |X - \eta|$, we have that

$$\begin{aligned} v &= iC P_j O v \\ &= iC P_j (b\Pi + |X - \eta|) v \\ &= ibC P_j \Pi v + iC P_j |X - \eta| v \\ (I - iC P_j |X - \eta|) v &= ibC P_j \Pi v. \end{aligned} \tag{3.28}$$

Similar to before, we would like to invert the operator $(I - iC P_j |X - \eta|)$. Recall that if

$$b > 4 \left(\| [P_j, Y] \| + \| P_j |X - \eta| \| + \| |X - \eta| P_j \| \right),$$

then $\|A\| \leq \frac{3}{4}$ so we have that

$$\begin{aligned}\|C\| &= \|(I + A)^{-1}(Y - \eta' + iO)^{-1}\| \\ &\leq \|(I + A)^{-1}\| \|(Y - \eta' + iO)^{-1}\| \\ &\leq 4b^{-1}.\end{aligned}$$

Therefore,

$$\|iCP_j|X - \eta|\| \leq 4b^{-1}\|P_j|X - \eta|\|.$$

Since we have chosen $b > 4\|P_j|X - \eta|\|$, the operator $(I - iCP_j|X - \eta|)$ is invertible.

Using this fact allows us to rewrite Equation (3.28) as

$$v = ib(I - iCP_j|X - \eta|)^{-1}CP_j\Pi v. \quad (3.29)$$

After all of these algebraic steps, we have been able to derive an expression for v as the product of a bounded operator and a cutoff function. The final step in this argument will be to multiply both sides of Equation (3.29) by the exponential growth operator B_γ and show that the result is bounded. The inclusion of the cutoff function is what makes it possible to control this multiplication because $B_\gamma\Pi$ is bounded.

At least formally, we can multiply both sides of Equation (3.29) by B_γ and insert copies of $B_\gamma^{-1}B_\gamma$ to get

$$\begin{aligned}B_\gamma v &= ibB_\gamma(I - iCP_j|X - \eta|)^{-1}CP_j\Pi v \\ &= ibB_\gamma(I - iCP_j|X - \eta|)^{-1}(B_\gamma^{-1}B_\gamma)C(B_\gamma^{-1}B_\gamma)P_j(B_\gamma^{-1}B_\gamma)\Pi v \\ &= ib\left[(I - iC_\gamma P_{j,\gamma}|X - \eta|)^{-1}\right]\left[C_\gamma P_{j,\gamma}\right]\left[B_\gamma\Pi\right]v,\end{aligned}$$

where we have used our convention for exponentially tilted operators $P_{j,\gamma} := B_\gamma P_j B_\gamma^{-1}$ and similarly for C . We will now show each of the bracketed terms are bounded.

The easiest term to bound is the last term, $B_\gamma\Pi$. Let's recall the definition of B_γ :

$$B_{\gamma,(a,b)} = \exp\left(\gamma\sqrt{1 + (X - a)^2 + (Y - b)^2}\right).$$

While we have ignored the center point (a, b) thus far in the argument, here we will explicitly choose $(a, b) = (\eta, \eta')$. Since $\Pi = \Pi_{[\eta-b, \eta+b]}^X \Pi_{[\eta'-b, \eta'+b]}^Y$ we clearly have:

$$\|B_{\gamma, (\eta, \eta')} \Pi\| \leq e^{\gamma\sqrt{1+2b^2}}.$$

To show that the first two terms are bounded we will show that, for γ sufficiently small, $\|C_\gamma\| = O(b^{-1})$. Once we show this, the second term, $C_\gamma P_{j, \gamma}$, is clearly bounded and we may pick b sufficiently large so that the first term is also bounded.

By definition, we have:

$$\begin{aligned} C_\gamma &= B_\gamma (I + A)^{-1} (Y - \eta' + iO)^{-1} B_\gamma^{-1} \\ &= B_\gamma \left(I + (Y - \eta' + iO)^{-1} [P_j, Y + iO] \right)^{-1} (Y - \eta' + iO)^{-1} B_\gamma^{-1} \\ &= \left(I + (Y - \eta' + iO)^{-1} [P_{j, \gamma}, Y + iO] \right)^{-1} (Y - \eta' + iO)^{-1}. \end{aligned}$$

For the above calculations to make sense, it suffices to show that

$$\|(Y - \eta' + iO)^{-1} [P_{j, \gamma}, Y + iO]\| \leq \frac{3}{4}.$$

Since $\|P_{j, \gamma} - P_j\| \leq K_1'' \gamma$ we have that:

$$\begin{aligned} &\|(Y - \eta' + iO)^{-1} [P_{j, \gamma}, Y + iO]\| \\ &\leq \|(Y - \eta' + iO)^{-1}\| \left(\| [P_{j, \gamma}, Y] \| + b \| [P_{j, \gamma}, \Pi] \| + \| [P_{j, \gamma}, |X - \eta|] \| \right) \\ &\leq b^{-1} \left(\| [P_{j, \gamma}, Y] \| + b \| [P_{j, \gamma} - P + P, \Pi] \| + \| [P_{j, \gamma}, |X - \eta|] \| \right) \\ &\leq b^{-1} \left(\| [P_{j, \gamma}, Y] \| + b \| [P_{j, \gamma} - P, \Pi] \| + b \| [P, \Pi] \| + \| [P_{j, \gamma}, |X - \eta|] \| \right) \\ &\leq b^{-1} \left(\frac{1}{2} b + b \| P_{j, \gamma} - P \| + \| [P_{j, \gamma}, Y] \| + \| P_{j, \gamma} |X - \eta| \| + \| |X - \eta| P_{j, \gamma} \| \right) \\ &\leq \frac{1}{2} + K_1'' \gamma + b^{-1} \left(\| [P_{j, \gamma}, Y] \| + \| P_{j, \gamma} |X - \eta| \| + \| |X - \eta| P_{j, \gamma} \| \right). \end{aligned}$$

Therefore, if we pick $\gamma \leq (8K_1'')^{-1}$ and

$$b \geq 8 \left(\| [P_{j, \gamma}, Y] \| + \| P_{j, \gamma} |X - \eta| \| + \| |X - \eta| P_{j, \gamma} \| \right),$$

we have that

$$\|P_{j, \gamma} (Y - \eta' + iO)^{-1} [P_{j, \gamma}, Y + iO]\| \leq \frac{3}{4}.$$

Therefore, for these choices of b and γ we have that:

$$\begin{aligned}\|C_\gamma\| &\leq \left\| \left(I + P_{j,\gamma}(Y - \eta' + iO)^{-1}[P_{j,\gamma}, Y + iO] \right)^{-1} \right\| \|(Y - \eta' + iO)^{-1}\| \\ &\leq 4b^{-1}.\end{aligned}$$

Now recall the original equation we wanted to bound:

$$B_\gamma v = i \left[(I - iC_\gamma P_{j,\gamma} |X - \eta|)^{-1} \right] \left[bC_\gamma P_{j,\gamma} \right] \left[B_\gamma \Pi \right] v.$$

Since $b \geq 8\|P_{j,\gamma}|X - \eta|\|$ we have that

$$\|C_\gamma P_{j,\gamma} |X - \eta|\| \leq 4b^{-1}\|P_{j,\gamma}|X - \eta|\| \leq \frac{1}{2}.$$

Therefore,

$$\|(I - iC_\gamma P_{j,\gamma} |X - \eta|)^{-1}\| \leq 2,$$

so combining all of our bounds together gives:

$$\begin{aligned}\|B_{\gamma,(\eta,\eta')}v\| &\leq \left[2 \right] \left[4(1 + K_2''\gamma) \right] \left[e^{\gamma\sqrt{1+2b^2}} \right] \\ &\leq 16e^{\gamma\sqrt{1+2b^2}},\end{aligned}$$

so long as

$$\begin{aligned}\gamma &\leq (8K_2'')^{-1} \\ b &\geq 8 \left(\| [P_{j,\gamma}, Y] \| + \| P_{j,\gamma} |X - \eta| \| + \| |X - \eta| P_{j,\gamma} \| \right).\end{aligned}$$

This proves Lemma 3.3.4, completing the proof of Theorem 2.

3.4 Extension to Higher Dimensions

The proof of Theorem 2 generalizes to arbitrarily high dimensions under appropriate generalizations of the uniform spectral gaps assumption (Assumption 4) by an inductive procedure. We will explain in detail the necessary additional assumptions and adjustments of our argument for the proof in three dimensions, from which the necessary assumptions and adjustments in higher dimensions are obvious.

Assume regularity and spectral gap assumptions analogous to Assumptions 1 and 2 hold and consider position operators X , Y , and Z acting on $L^2(\mathbb{R}^3)$ along directions corresponding to a three-dimensional basis. Let P be the Fermi projection, and consider the operator PXP . Assume PXP has uniform spectral gaps in the sense of Assumption 4, and let P_j denote spectral projections onto each of the separated components of the spectrum of PXP . Now assume the operators P_jYP_j also have uniform spectral gaps in the sense of Assumption 4, and let $P_{j,k}$ denote spectral projections onto each of the separated components of the spectrum of P_jYP_j . By analogous reasoning to the two dimensional case, functions in $\text{range}(P_{j,k})$ are quasi-one dimensional in the sense that they decay away from lines $X = c_1$, $Y = c_2$ for constants c_1, c_2 . We therefore claim that the set of eigenfunctions of the operator $P_{j,k}ZP_{j,k}$ will form an exponentially localized basis of $\text{range}(P_{j,k})$ for each j, k , and that the union of all of these eigenfunctions over j and k will form an exponentially-localized basis of $\text{range}(P)$.

To make the above sketch rigorous, there are a few important steps in the proof which must be checked. We will discuss each step in turn.

Proving bounds on $P_{j,k}$

First, we must check that we can prove operator bounds on $P_{j,k}$ which are analogous to the operator bounds we prove in Appendices A.1 and A.2. To see that this is possible, note that when we proved bounds on P_j in Appendix A.2, we only required our decay estimates on P (Assumption 3). It follows that under a uniform gap assumption on P_jYP_j we can prove an analog to Lemma on $P_{j,k}$ by a similar calculation using only the estimates from Appendix A.2 on P_j .

Proving $P_{j,k}ZP_{j,k}$ has compact resolvent

To prove $P_{j,k}ZP_{j,k}$ has compact resolvent, mimicking the calculations preceding (3.15), it is sufficient to prove that $P_{j,k}(Z + i\tilde{\mu})^{-1}P_{j,k}$ is compact for each j, k . We

will first show how a naïve generalization of the proof that $P_j Y P_j$ is compact in two dimensions fails, and then present a correct generalization. Just as in equation (3.15), we can write

$$\begin{aligned}
P_{j,k}(Z \pm i\tilde{\mu})^{-1}P_{j,k} &= [P_{j,k}(-\Delta + 1)] \\
&\times [(-\Delta + 1)^{-1}(Z \pm i\tilde{\mu})^{-1}(X - \eta_j + i)^{-1}(Y - \eta_k + i)^{-1}] \\
&\times [(Y - \eta_k + i)(X - \eta_j + i)P_{j,k}]
\end{aligned} \tag{3.30}$$

where $\eta_j \in \sigma_j$, where σ_j is the j th separated component of $\sigma(PXP)$, and $\eta_k \in \sigma_{j,k}$, where σ_k is the k th separated component of $\sigma(P_j Y P_j)$. To prove $P_{j,k}(Z + i\tilde{\mu})^{-1}P_{j,k}$ is compact, we must prove that the first and third terms in (3.30) are bounded, while the second is compact. That the second term is compact and the first term is bounded follow from essentially the same arguments as given in Section 3.3.5. Unfortunately, it is unclear if the last term

$$(Y - \eta_k + i)(X - \eta_j + i)P_{j,k}$$

is bounded. The trick is to write, instead of (3.30),

$$\begin{aligned}
P_{j,k}(Z \pm i\tilde{\mu})^{-1}P_{j,k} &= [P_{j,k}(-\Delta + 1)] \\
&\times [(-\Delta + 1)^{-1}(Z \pm i\tilde{\mu})^{-1}(X - \eta_j + i)^{-1/2}(Y - \eta_k + i)^{-1/2}] \\
&\times [(Y - \eta_k + i)^{1/2}(X - \eta_j + i)^{1/2}P_{j,k}].
\end{aligned} \tag{3.31}$$

That the first term of (3.31) is bounded is clear. That the second term of (3.31) is compact follows from an almost identical argument as given in Section 3.3.5. We now show that the third term of (3.31) is bounded. Note that if $f \notin \text{range}(P_{j,k})$ then the operator acting on f is clearly bounded. So let $f \in \text{range}(P_{j,k})$. Then using the fact that the geometric mean is bounded by the arithmetic mean, we have that

$$\begin{aligned}
&\|(Y - \eta_k + i)^{1/2}(X - \eta_j + i)^{1/2}P_{j,k}f\|^2 \\
&\leq \frac{1}{2} (\|(Y - \eta_k + i)P_{j,k}f\|^2 + \|(X - \eta_j + i)P_{j,k}f\|^2).
\end{aligned}$$

The first term is bounded since $P_{j,k}$ is the projection onto a bounded subset of the spectrum of $P_j Y P_j$ (by the same proof as that of Lemma 3.3.6). The second term is bounded since $P_{j,k} = P_j P_{j,k}$ and $(X + \eta_j + i)P_j$ is bounded since P_j is the projection onto a bounded subset of the spectrum of PXP (Lemma 3.3.6).

Proving exponential localization of eigenfunctions of $P_{j,k} Z P_{j,k}$

The generalization of the proof of Lemma 3.3.4 to three dimensions is straightforward once we prove operator norm bounds on $P_{j,k}$ analogous to the operator norm bounds proved in Appendix A.2 on P_j . The only modification necessary is that in three dimensions the choice of the operator O (Equation (3.26)) must be changed to

$$O = b \Pi_{[\eta_j - b, \eta_j + b]}^X \Pi_{[\eta_{j,k} - b, \eta_{j,k} + b]}^Y \Pi_{[\eta_{j,k,l} - b, \eta_{j,k,l} + b]}^Z + |X - \eta_j| + |Y - \eta_{j,k}|,$$

where $\eta_j \in \sigma_j$, the j th component of $\sigma(PXP)$, $\eta_{j,k} \in \sigma_{j,k}$, the k th component of $\sigma(P_j Y P_j)$, and $\eta_{j,k,l}$ denotes the l th eigenvalue of $P_{j,k} Z P_{j,k}$.

3.5 Numerical Results

In this section we present results of implementing the numerical scheme suggested by Theorem 2 for generating exponentially localized generalized Wannier functions. The scheme is as follows:

1. Choose position operators X and Y acting in orthogonal directions.
2. Compute the Fermi projector P by diagonalizing the Hamiltonian H .
3. Diagonalize the operator PXP , and inspect $\sigma(PXP)$ for clusters of eigenvalues separated from other eigenvalues by spectral gaps.
4. Form band projectors P_j onto each cluster of eigenvalues.
5. Diagonalize the operators $P_j Y P_j$ to obtain exponentially localized eigenvectors which span the Fermi projection.

As numerically, one can only deal with a finite system, it is necessary to clarify two points compared with the infinite case.

First, note that any vector in a finite system is trivially exponentially-decaying by taking $C > 0$ sufficiently large and $\gamma > 0$ sufficiently small in (3.2). It is necessary to clarify, therefore, that the algorithm presented above yields exponentially-decaying eigenvectors with $C > 0$ and $\gamma > 0$ which are *independent of system size*. In this sense, our algorithm yields a non-trivial result.

Second, in finite systems, all operators have purely discrete spectrum and hence there will be a spectral gap between *any* pair of eigenvalues. However, to obtain localized eigenvectors it is not enough to simply form band projectors for each eigenvalue of PXP alone. Hence the clarification in the algorithm that we must form band projectors from clusters of nearby eigenvalues separated from the remainder of the spectrum by clear spectral gaps. This point is clarified by our rigorous analysis in the following sections, where we show that the localization of the generalized Wannier functions produced by our scheme is related to the minimal gap between the bands of $\sigma(PXP)$ (see Section 3.3.6).

We choose to test our scheme on the Haldane model [Hal88] at half-filling, a simple two-dimensional model whose Fermi projection, in the crystalline setting, may or may not have non-zero Chern number depending on model parameters. For this reason, the Haldane model is a natural model for investigating the connection between gaps of PXP and topological triviality of P in the case where the material is periodic. Historically, the Haldane model was the first model of a Chern insulator: a material exhibiting quantized Hall response without net magnetic flux through the material. We now briefly recap the essential features of this model.

3.5.1 The Haldane Model

The Haldane model describes electrons in the tight-binding limit hopping on a honeycomb lattice. In addition to real nearest-neighbor hopping terms, the model allows

for a real on-site potential difference between the A and B sites of the lattice, and for *complex* next-nearest-neighbor hopping terms which break time-reversal symmetry without introducing net magnetic flux.

In the crystalline case, the action of the Haldane tight-binding Hamiltonian acting on wave-functions $\psi \in l^2(\mathbb{Z}^2; \mathbb{C}^2)$ is:

$$\begin{aligned}
\begin{bmatrix} (H\psi)_{m,n}^A \\ (H\psi)_{m,n}^B \end{bmatrix} &= v \begin{bmatrix} \psi_{m,n}^A \\ -\psi_{m,n}^B \end{bmatrix} + t \begin{bmatrix} \psi_{m,n}^B + \psi_{m,n-1}^B + \psi_{m-1,n}^B \\ \psi_{m,n}^A + \psi_{m+1,n}^A + \psi_{m,n+1}^A \end{bmatrix} \\
&+ t' e^{i\phi} \begin{bmatrix} \psi_{m,n+1}^A + \psi_{m-1,n}^A + \psi_{m+1,n-1}^A \\ \psi_{m,n-1}^B + \psi_{m+1,n}^B + \psi_{m-1,n+1}^B \end{bmatrix} \\
&+ t' e^{-i\phi} \begin{bmatrix} \psi_{m,n-1}^A + \psi_{m+1,n}^A + \psi_{m-1,n+1}^A \\ \psi_{m,n+1}^B + \psi_{m-1,n}^B + \psi_{m+1,n-1}^B \end{bmatrix}.
\end{aligned} \tag{3.32}$$

Here, t, v, t' , and ϕ are real parameters expressing the magnitude of nearest-neighbor hopping, the magnitude of on-site potential difference, the magnitude of complex next-nearest neighbor hopping, and the complex argument of the nearest-neighbor hopping, respectively.

By definition, at half-filling the Fermi level is at 0. An explicit calculation using Bloch theory [Hal88] (see also [FC13]) shows that H has a spectral gap (and hence describes an insulator) at 0 whenever

$$v \neq \pm 3\sqrt{3}t' \sin \phi.$$

Further calculation shows that the Fermi projection has a non-trivial Chern number (equal to 1 or -1) whenever

$$|v| < 3\sqrt{3}|t' \sin \phi|. \tag{3.33}$$

In this case, exponentially-localized Wannier functions do not exist [MPPT18, MMMP19].

Whenever the parameters t, v, t', ϕ are such that (3.33) holds, we say the Haldane model is in its *topological phase*.

For some of our experiments, we add a perturbation to the Hamiltonian (3.32) which models disorder. We replace the on-site potential v in (3.32) by a spatially varying on-site potential $v + \eta(m, n)$, where $\eta(m, n)$ is drawn for each m, n from independent Gaussian distributions with mean 0 and variance σ^2 :

$$\eta(m, n) \sim \mathcal{N}(0, \sigma^2) \text{ for each } m, n. \quad (3.34)$$

We refer to this kind of disorder as “onsite” disorder. Assuming H (3.32) has a spectral gap with $\sigma^2 = 0$ (i.e. without disorder), then for sufficiently small σ^2 , the spectral gap will persist almost surely and our method can be applied.

To implement our method, we have to make a choice of position operators on the space $l^2(\mathbb{Z}^2; \mathbb{C}^2)$. The simplest choice is to define X and Y consistently with the crystal lattice by:

$$\begin{bmatrix} (X\psi)_{m,n}^A \\ (X\psi)_{m,n}^B \end{bmatrix} = \begin{bmatrix} m\psi_{m,n}^A \\ m\psi_{m,n}^B \end{bmatrix} \quad \begin{bmatrix} (Y\psi)_{m,n}^A \\ (Y\psi)_{m,n}^B \end{bmatrix} = \begin{bmatrix} n\psi_{m,n}^A \\ n\psi_{m,n}^B \end{bmatrix}.$$

We refer to this choice of X and Y as the standard position operators. A couple of remarks are in order. First, note that X and Y do not distinguish between A and B sites. Second, the crystal lattice vectors are not orthogonal hence eigenvalues of X and Y do not represent coordinates with respect to orthogonal axes. Since the lattice vectors are linearly independent our method can nonetheless be applied.

3.5.2 Parameters for numerical tests and further remarks

For our numerical tests, we consider the Haldane model just described truncated to a 24×24 lattice under the following conditions:

- Dirichlet boundary conditions with standard position operators, without disorder (Section 3.5.3).
- Dirichlet boundary conditions with standard position operators, with weak disorder which does not close the spectral gap of H (Section 3.5.4).

- Dirichlet boundary conditions with standard position operators, with strong disorder (Section 3.5.5). Note that in this case the spectral gap assumption on H is no longer valid; though P will still be exponentially localized due to the Anderson localization.
- Dirichlet boundary conditions with non-standard (rotated) position operators, without disorder (Section 3.5.6).
- Periodic boundary conditions with standard position operators, without disorder. We consider parameter values such that the system is in a non-topological phase and values such that the system is in a topological phase (Sections 3.5.7 and 3.5.8).

Note that we do not consider any examples with Dirichlet boundary conditions in the topological phase. This is because H does not have a spectral gap in this case due to edge states.

In each case we will display plots of the generalized Wannier functions generated by our algorithm. Specifically, given a generalized Wannier functions $\psi \in l^2(\{1, \dots, 24\}^2; \mathbb{C}^2)$, we will plot the following matrix in a 3D surface plot:

$$\begin{bmatrix} \sqrt{|\psi_{1,1}^A|^2 + |\psi_{1,1}^B|^2} & \sqrt{|\psi_{1,2}^A|^2 + |\psi_{1,2}^B|^2} & \cdots & \sqrt{|\psi_{1,24}^A|^2 + |\psi_{1,24}^B|^2} \\ \sqrt{|\psi_{2,1}^A|^2 + |\psi_{2,1}^B|^2} & \sqrt{|\psi_{2,2}^A|^2 + |\psi_{2,2}^B|^2} & \cdots & \sqrt{|\psi_{2,24}^A|^2 + |\psi_{2,24}^B|^2} \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{|\psi_{24,1}^A|^2 + |\psi_{24,1}^B|^2} & \sqrt{|\psi_{24,2}^A|^2 + |\psi_{24,2}^B|^2} & \cdots & \sqrt{|\psi_{24,24}^A|^2 + |\psi_{24,24}^B|^2} \end{bmatrix}. \quad (3.35)$$

To make the exponential decay of ψ as clear as possible, we will also show 2D plots of the elementwise logarithm of this matrix.

We remark that while our theoretical results hold equally well in the both periodic and non-periodic cases for infinite systems, we find for finite systems our algorithm

works better for systems with Dirichlet boundary conditions. This is not entirely surprising given that the position operators X and Y do not respect periodic boundary conditions. It is possible that a better choice (see [Res98, Zak00, VmcFdAaMB⁺19] for potentially related ideas) would improve the results in the case of periodic boundary conditions.

3.5.3 Dirichlet Boundary Conditions using Standard Position Operators

We consider the Haldane model with Dirichlet boundary conditions and parameters $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$, which correspond to the non-topological phase. For this choice of parameters the Hamiltonian H has a gap of ~ 1.006 . We plot the eigenvalues of PXP in Figure 3.2, where we see $\sigma(PXP)$ shows clear gaps. We plot the eigenvectors of PXP in Figure 3.3. We see that these eigenvectors are concentrated along lines $x = c$ for constants c . We finally plot the eigenfunctions of $P_j Y P_j$, which are localized with respect to x and y , for a few different values of j in Figure 3.4.

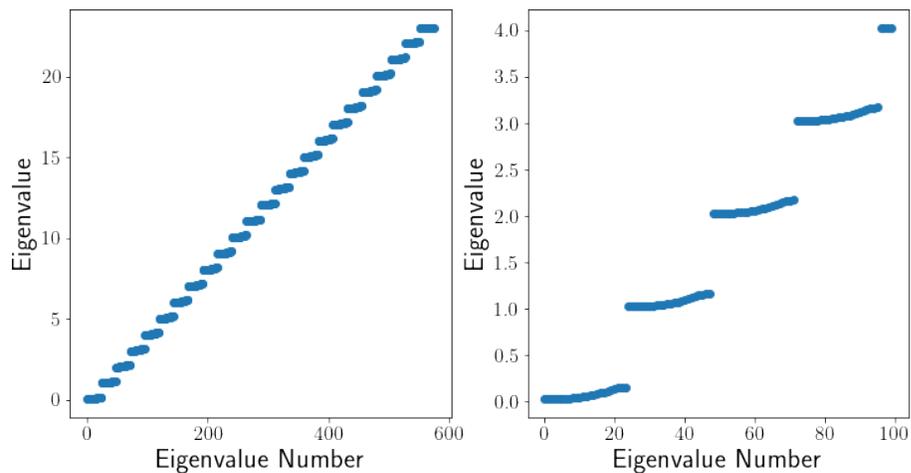


Figure 3.2: Plot of sorted non-zero eigenvalues of PXP where P is the Fermi projection and X is the lattice position operator for the Haldane model on 24×24 system with Dirichlet boundary conditions. Entire spectrum (left) and first 100 eigenvalues (right). Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. The spectrum shows clear gaps.

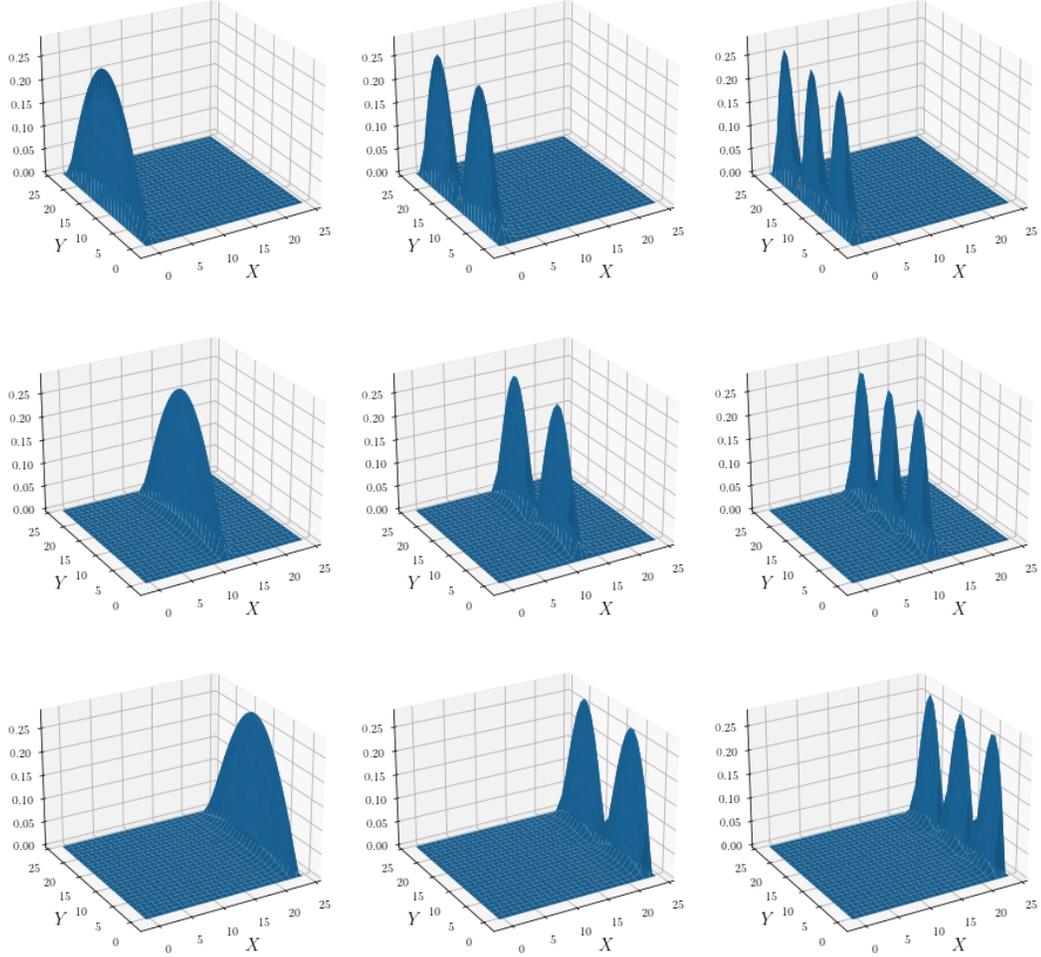


Figure 3.3: Plot of eigenfunctions of the operator PXP where P is the Fermi projection and X is the lattice position operator for the Haldane model on 24×24 system with Dirichlet boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. Each eigenvector of PXP is localized along a line $x = c$ for some constant c .

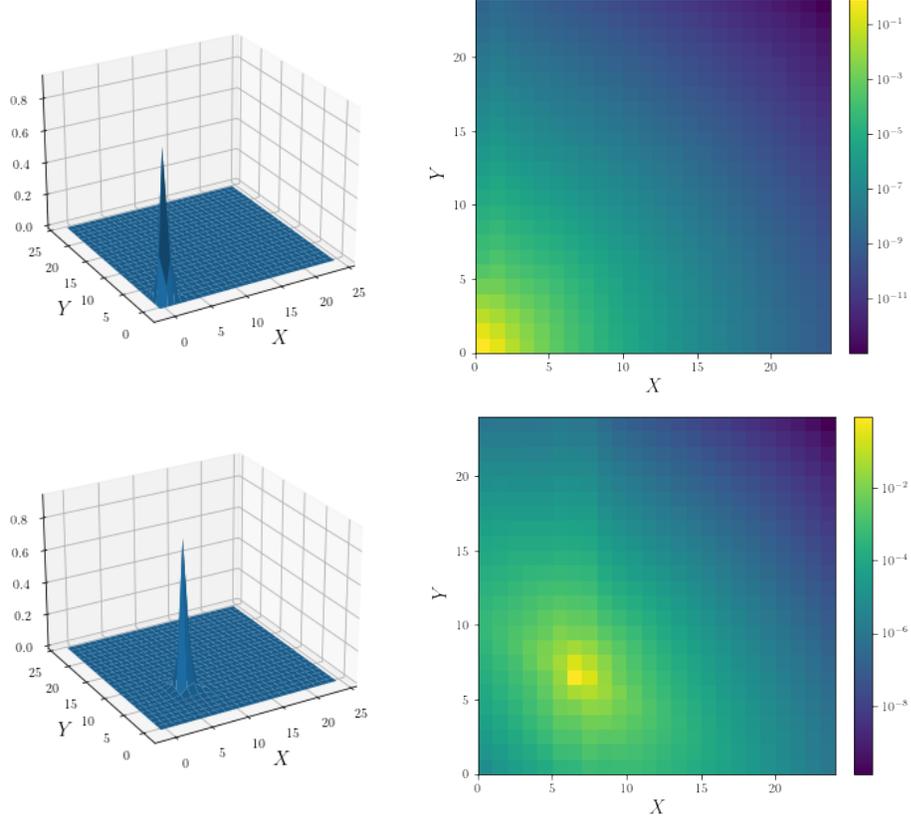


Figure 3.4: Plot of eigenfunctions of the operator $P_j Y P_j$ for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for PXP , P is the Fermi projection, and X, Y are the lattice position operators. The projection P comes from the Haldane model on 24×24 system with Dirichlet boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. Top row is a 3D surface plot of the matrix from Equation (3.35), bottom row is 2D log plot of the top row. Each eigenfunction shows clear exponential localization in line with our theoretical results.

3.5.4 Dirichlet Boundary Conditions with Weak Disorder

We now consider a case where translational symmetry is broken even away from the edge of the material. Starting with the same parameters as in Section 3.5.3, we add onsite disorder as in (3.34), with $\sigma^2 = \frac{1}{4}$. We plot results for a realization of the onsite disorder such that H has a clear gap $\sim .253$. We find that the eigenvalues of PXP show clear gaps despite the disorder, see Figure 3.5. We can therefore form projectors P_j , and the operators P_jYP_j . We plot the eigenfunctions of P_jYP_j in Figure 3.6. We observe that they are again exponentially localized, just as in the case without disorder (Figure 3.4), in line with our theoretical results.

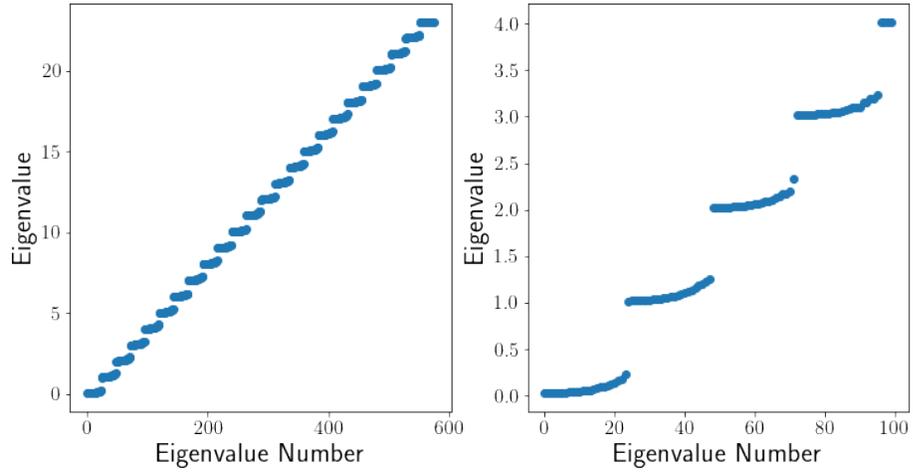


Figure 3.5: Plot of sorted non-zero eigenvalues of PXP where P is the Fermi projection and X is the lattice position operator for the Haldane model on 24×24 system with Dirichlet boundary conditions. Entire spectrum (left) and first 100 eigenvalues (right). Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$, with onsite disorder drawn from a mean zero normal distribution with variance $\frac{1}{4}$. Despite the disorder, the spectrum still shows clear gaps.

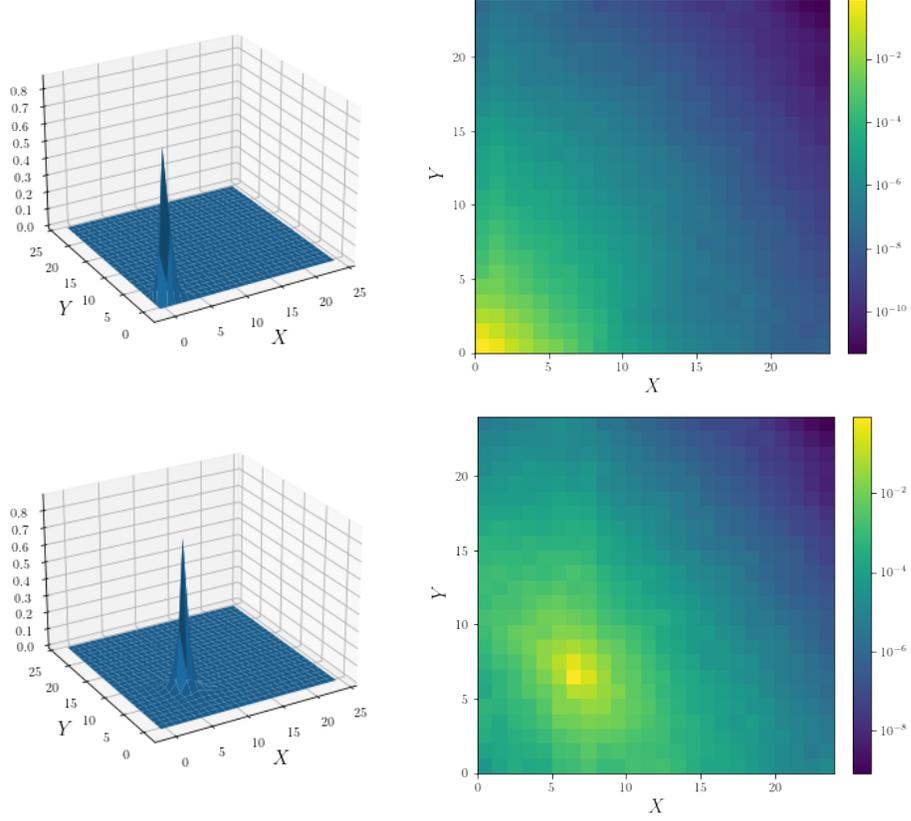


Figure 3.6: Plot of eigenfunctions of the operator $P_j Y P_j$ for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for PXP , P is the Fermi projection, and X , Y are the lattice position operators. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$, with onsite disorder drawn from a mean zero normal distribution with variance $\frac{1}{4}$. Top row is a 3D surface plot of the matrix from Equation (3.35), bottom row is 2D log plot of the top row. Despite the disorder, our algorithm yields exponentially-localized generalized Wannier functions.

3.5.5 Dirichlet Boundary Conditions with Strong Disorder

We consider the same setup as the previous section, but with disorder strong enough ($\sigma^2 = 100$) to close the gap of H (for the results shown in Figure 3.7, the gap of $H \approx .07$). Although our results do not directly apply to this case, the eigenfunctions of H are themselves localized because of Anderson localization [And58]. It is therefore plausible that PXP may have gaps and that the eigenfunctions of P_jYP_j are localized nonetheless.

We plot the non-zero eigenvalues in PXP in Figure 3.7. We find that $\sigma(PXP)$ shows clear gaps, and hence we may define projectors P_j and operators P_jYP_j .

We observe that the eigenfunctions of P_jYP_j are well localized. In Figure 3.8, we plot the eigenfunctions of H in order of increasing energy value and plot an eigenfunction of P_jYP_j which has the same center. We observe that as the energy level increases, the corresponding eigenfunction of H becomes less localized. In comparison, the eigenfunctions of P_jYP_j have similar rates of decay for all values of $j \in \mathcal{J}$.

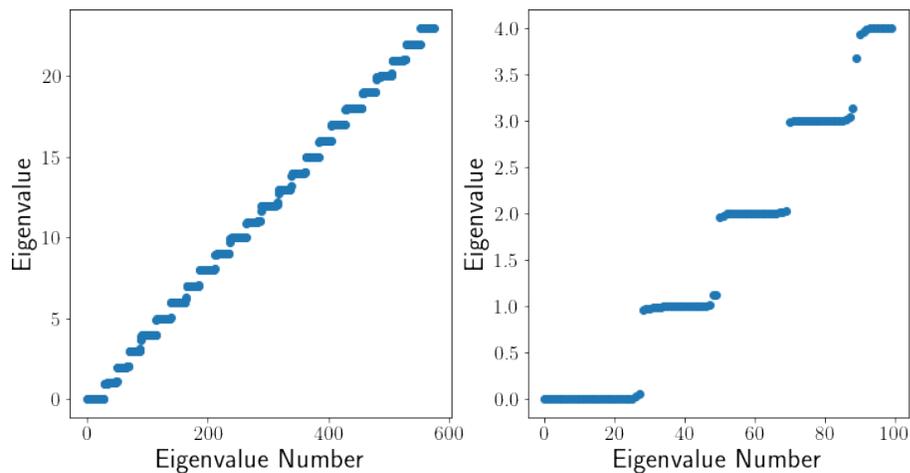


Figure 3.7: Plot of sorted non-zero eigenvalues of PXP where P is the Fermi projection and X is the lattice position operator for the Haldane model on 24×24 system with Dirichlet boundary conditions. Entire spectrum (left) and first 100 eigenvalues (right). Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$, with disorder is drawn from a mean zero normal distribution with variance 100.

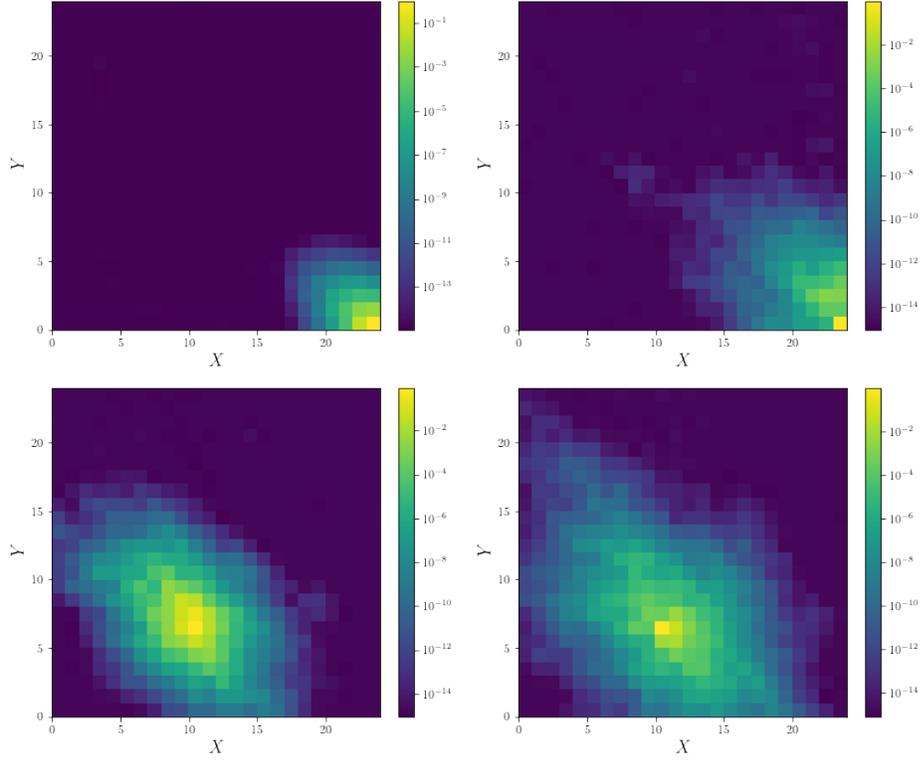


Figure 3.8: Plot of eigenfunctions of H (left) and $P_j Y P_j$ (right) for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for PXP , P is the Fermi projection, and X , Y are the lattice position operators. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$, while onsite disorder is drawn from a mean zero normal distribution with variance 100. The eigenfunctions of H are sorted in order of increasing energy (top \rightarrow low energy, bottom \rightarrow high energy) and eigenfunctions of $P_j Y P_j$ were chosen to have the same center as the corresponding H eigenfunction.

3.5.6 Dirichlet Boundary Conditions using Rotated Position Operators

We now consider how our results change when we choose to work with different two-dimensional position operators (equivalently, different two-dimensional axes). Note that, although our proofs are independent of any particular choice of position operators, we cannot rule out the possibility that the uniform spectral gap assumption on PXP (Assumption 4) holds only for particular choices. We also expect that different choices of position operators will yield different exponentially-localized generalized Wannier functions.

We consider the same Haldane model with Dirichlet boundary conditions but without disorder as in Section 3.5.3, and introduce rotated position operators

$$\tilde{X} := \frac{X - Y}{\sqrt{2}}, \quad \tilde{Y} := \frac{X + Y}{\sqrt{2}}. \quad (3.36)$$

The eigenvalues of $P\tilde{X}P$ are shown in Figures 3.9. We find that, just like the eigenvalues of PXP in Figure 3.2, the spectrum shows clear gaps. The eigenfunctions of $P\tilde{X}P$ are shown in Figure 3.10. They are clearly localized along lines $x + y = c$ for constant c . Since $P\tilde{X}P$ has gaps (Figure 3.9), we can define the band projectors P_j as before. The eigenfunctions of $P_j\tilde{Y}P_j$ are shown in Figure 3.11 and clearly exponentially decay similarly to those in Figure 3.4.

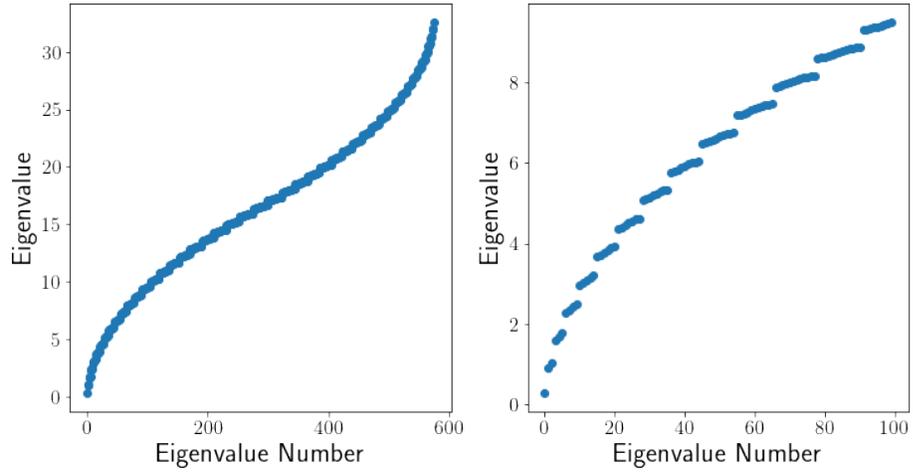


Figure 3.9: Plot of sorted non-zero eigenvalues of $P\tilde{X}P$ where P is the Fermi projection and \tilde{X} is the lattice position operator rotated by 45° (see Equation (3.36)) for the Haldane model on 24×24 system with Dirichlet boundary conditions. Entire spectrum (left) and first 100 eigenvalues (right). Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. Full non-zero spectrum (left), zoom-in for the first 100 eigenvalues (right). The spectrum shows clear gaps.

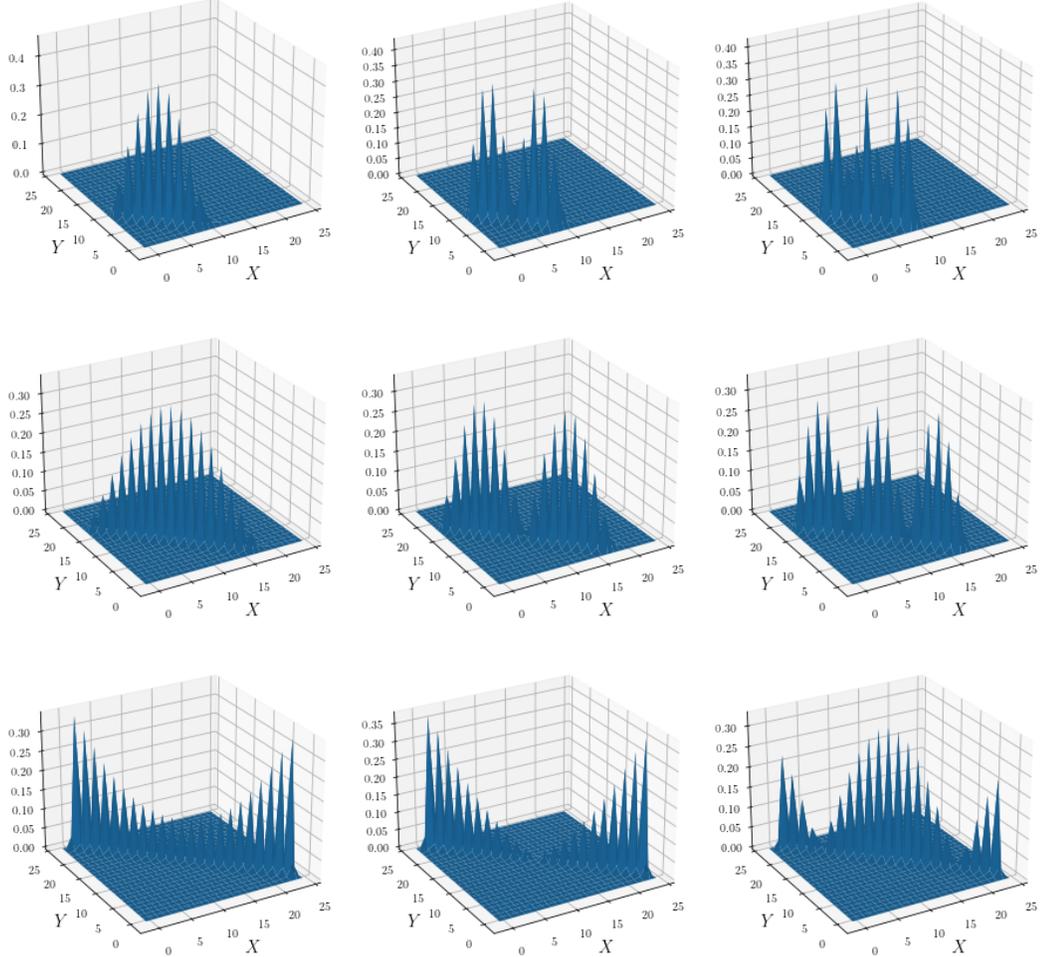


Figure 3.10: Plot of eigenfunctions of the operator $P\tilde{X}P$ where P is the Fermi projection and \tilde{X} is the rotated lattice position operator for the Haldane model on 24×24 system with Dirichlet boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. Each eigenfunction is localized along a line $x + y = c$ for some constant c .

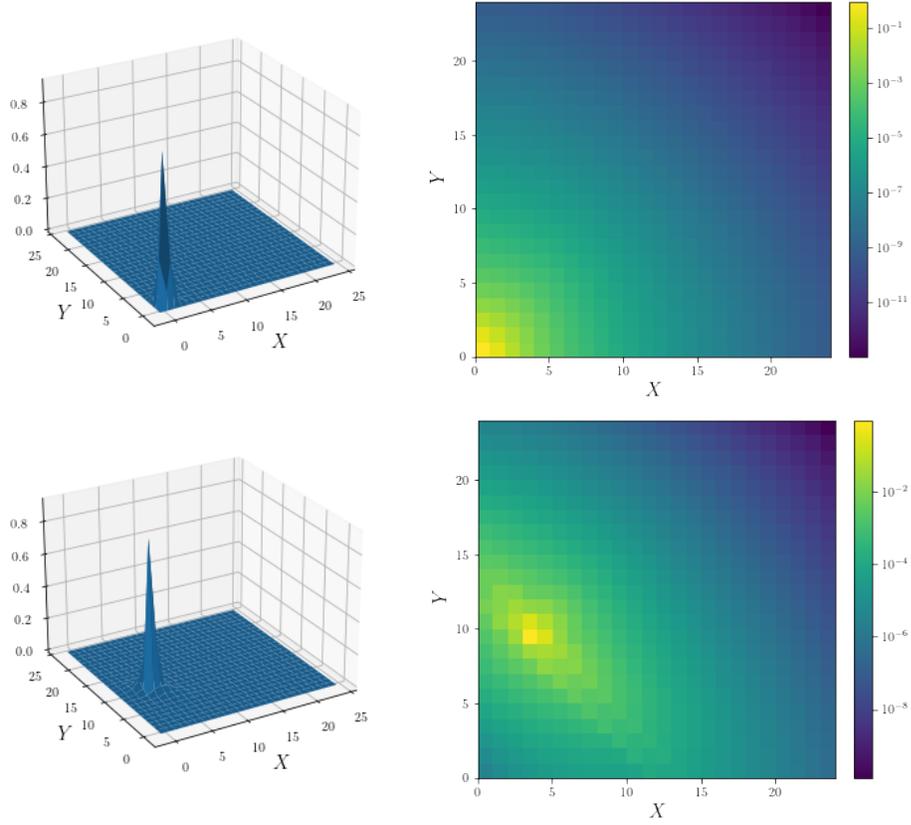


Figure 3.11: Plot of eigenfunctions of the operator $P_j \tilde{Y} P_j$ for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for $P \tilde{X} P$, P is the Fermi projection, and \tilde{X} , \tilde{Y} are the rotated lattice position operators (see Equation (3.36)). The projection P comes from the Haldane model on 24×24 system with Dirichlet boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, \frac{1}{10}, 1, \frac{\pi}{2})$. Top row is a 3D surface plot of the matrix from Equation (3.35), bottom row is 2D log plot of the top row.

3.5.7 Periodic Boundary Conditions, Topological versus Non Topological

We prove in Appendix A.4 (Theorem 6) that for an infinite periodic system, whenever PXP has uniform spectral gaps, the Chern number must vanish. In this section we provide numerical evidence that the uniform spectral gap assumption is actually equivalent to the Chern number vanishing in the case of the Haldane model by forming the Fermi projector P from the Haldane Hamiltonian with periodic boundary conditions and numerically computing the spectrum of PXP for different values of the Haldane model parameters. Our results are shown in Figure 3.12. For additional insight into these figures, see the proof of Theorem 6 and, in particular, Figure A.1.

We find that for model parameters such that the model is in a non-topological phase, $\sigma(PXP)$ shows clear gaps. For model parameters such that the model is in a topological phase, every gap of $\sigma(PXP)$ closes. This conclusion holds even when we choose model parameters such that the spectral gap of H is approximately equal in either case (≈ 2).

Note that in the case where every gap of $\sigma(PXP)$ closes, our construction is technically well defined since the spectrum of PXP is bounded on a finite domain. On the other hand, it is totally ineffective because we can only define one band projector P_j , which equals P . Hence the eigenfunctions of P_jYP_j in this case are the eigenfunctions of PYP , which do not decay in x .

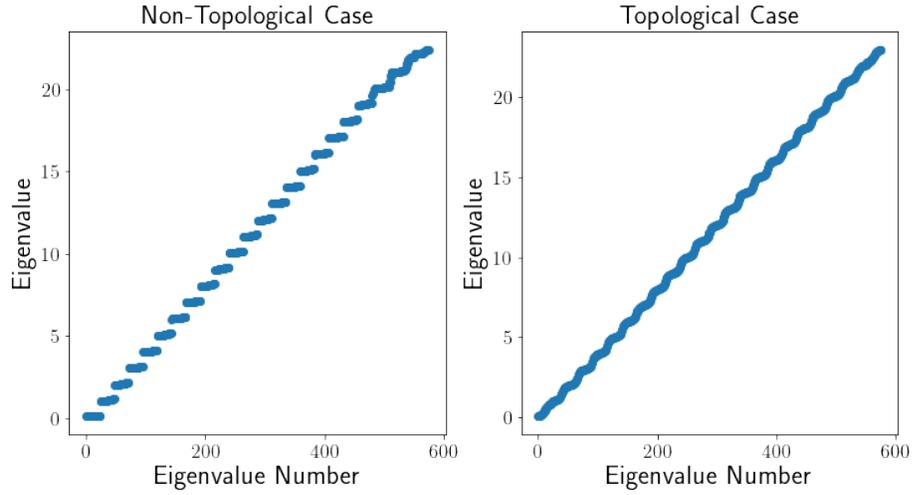


Figure 3.12: Plot of sorted non-zero eigenvalues of PXP where P is the Fermi projection and X is the lattice position operator for the Haldane model on 24×24 system with periodic boundary conditions. The left plot corresponds to parameters $(t, t', v, \phi) = (1, 0, 1, \frac{\pi}{2})$ (non-topological phase) and the right plot corresponds to parameters $(t, t', v, \phi) = (1, \frac{1}{4}, 0, \frac{\pi}{2})$ (topological phase). The gap in H for both non-topological and topological phase is ≈ 2 .

3.5.8 Periodic Boundary Conditions, Standard Position Operators

In this section we implement our algorithm in the non-topological phase of Haldane with periodic boundary conditions, when $\sigma(PXP)$ shows clear gaps (Figure 3.12). Note that when we take periodic boundary conditions the last three bands of PXP appear to merge together. Since this does not occur in the case of Dirichlet boundary conditions (see Figure 3.2), we conjecture that this behavior is because the operator X does not respect translation symmetry with respect to x .

Despite this, our theory still applies since we can enclose the last three bands by a single contour when we define the collection $\{P_j\}_{j \in \mathcal{J}}$. For all bands but the last one, we find the eigenfunctions of $P_j Y P_j$ are exponentially localized like before. These results are shown in Figure 3.13. For the last band, we find that instead of the eigenfunctions of $P_j Y P_j$ being localized along a single line $x = c$ for constant c , they are somewhat spread across an interval of x values: see Figure 3.14.

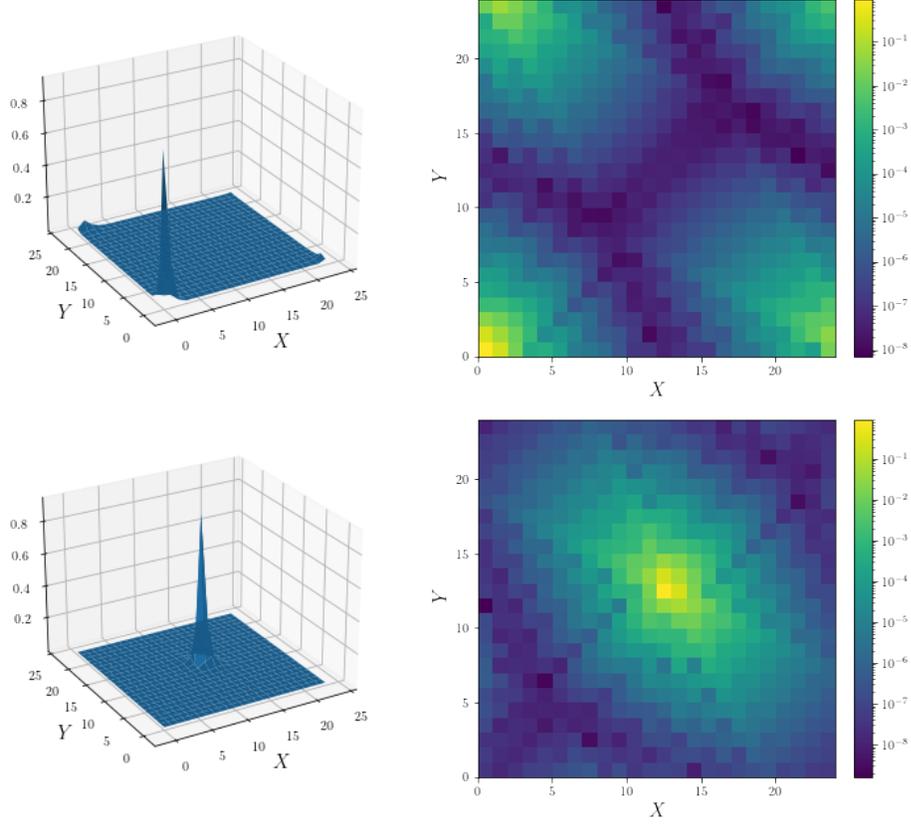


Figure 3.13: Plot of eigenfunctions of the operator $P_j Y P_j$ for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for PXP , P is the Fermi projection, and X, Y are the lattice position operators. The projection P comes from the Haldane model on 24×24 system with periodic boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, 0, 1, \frac{\pi}{2})$. Top row is a 3D surface plot of the matrix from Equation (3.35), bottom row is 2D log plot of the top row. For these figures we avoid the P_j where a few bands of the spectrum of PXP have clumped together (see Figure 3.12).

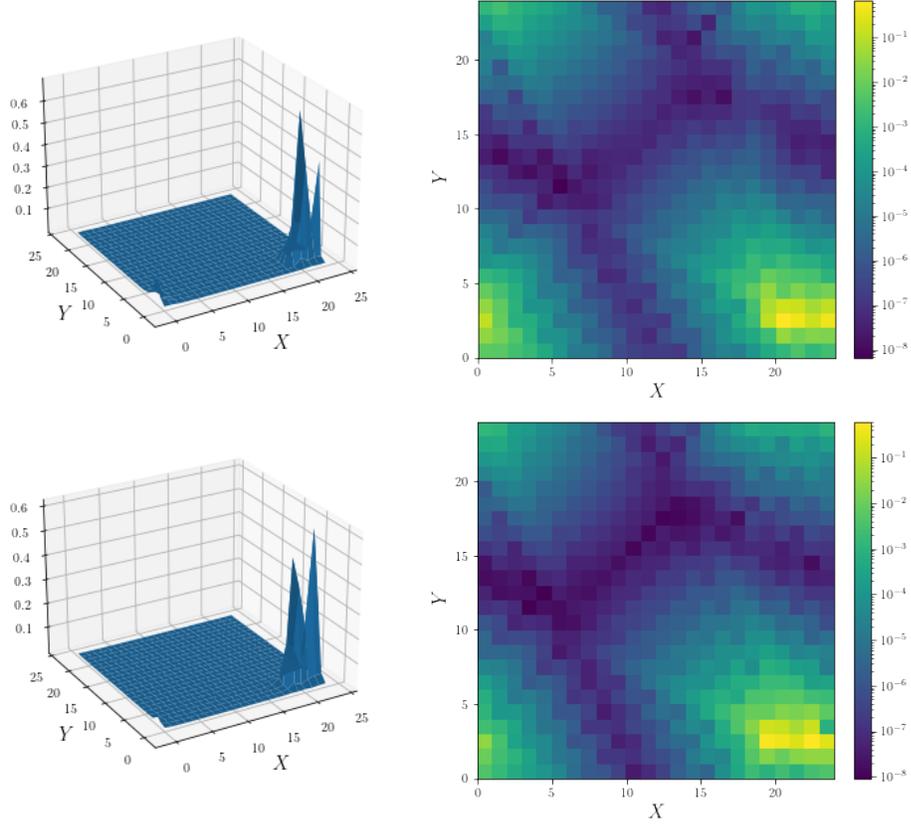


Figure 3.14: Plot of eigenfunctions of the operator $P_j Y P_j$ for different values of j where $\{P_j\}_{j \in \mathcal{J}}$ are the band projectors for PXP , P is the Fermi projection, and X, Y are the lattice position operators. The projection P comes from the Haldane model on 24×24 system with Dirichlet boundary conditions. Parameters chosen are $(t, t', v, \phi) = (1, 0, 1, \frac{\pi}{2})$. Top row is a 3D surface plot of the matrix from Equation (3.35), bottom row is 2D log plot of the top row. For these figures we consider the P_j where a few bands of the spectrum of PXP have clumped together (see Figure 3.12). Note that the generalized Wannier function generated by our method in this case has a relatively large spread in x relative to those plotted in Figure 3.13.

Chapter 4

A Weak Localization Dichotomy in Non-Periodic Insulators

4.1 Introduction

In Chapter 3, we have introduced and proved the correctness of an algorithm for constructing ELWFs. A key element of this proof was the notion of “uniform spectral gaps” (Assumption 4). By assuming that PXP has uniform spectral gaps we were able to construct a collection of orthogonal projectors $\{P_j\}_{j \in \mathcal{J}}$ (Definition 2), prove important estimates for this collection of projectors (Appendix A.2), and show that the eigenfunctions of P_jYP_j are exponentially localized (Lemma 3.3.4).

Due to the importance of uniform spectral gaps to our argument in Chapter 3, a natural question is “When does PXP have uniform spectral gaps?”. Since we know that PXP having uniform spectral gaps implies that $\text{range}(P)$ admits an exponentially localized basis due to Theorem 2, a more nuanced question is “If $\text{range}(P)$ admits an exponentially localized basis does PXP have uniform spectral gaps?”. The short answer to this question is no, but the complete story is more complicated.

We will discuss an important class of examples which show that $\text{range}(P)$ admitting an exponentially localized basis does not imply PXP has uniform spectral gaps in Section 4.1.1. Despite this class of counter examples, the technical machinery developed in Chapter 3 is quite robust and in Section 4.1.2 we will discuss how we can modify the algorithm presented in Chapter 3 to ensure that “ PXP ” always has uniform spectral gaps whenever $\text{range}(P)$ admits a basis with sufficiently fast decay.

This chapter is prepared based on [LS21].

This leads into the main result of this chapter: a weaker version of the localization dichotomy for non-periodic systems (Theorem 5).

4.1.1 A Counter Example to the Necessity of PXP having Uniform Spectral Gaps

As mentioned in Section 1.4.1, an important class of periodic insulators which always admit a basis of ELWFs are those which satisfy time reversal symmetry. A further subclass of time reversal symmetric systems are those which satisfy fermionic time reversal symmetry defined which we now define.

Definition 3. We say a Hamiltonian H satisfies *fermionic time reversal symmetry* if there exists an antiunitary operator¹ Θ satisfying the condition $\Theta^2 = -1$ such that $[\Theta, H] = 0$.

As a consequence of this definition, if a system satisfies fermionic time reversal symmetry, then the Fermi projector P also commutes with the time reversal operator Θ (i.e. $[\Theta, P] = 0$). For systems of physical interest, the time reversal operator, Θ , also commutes with the standard position operators X and Y (i.e. $[\Theta, X] = [\Theta, Y] = 0$).

Given a system which satisfies time reversal symmetry, a natural question is whether we can find a well localized basis for $\text{range}(P)$ which also satisfies time reversal symmetry. More specifically, we would like to find an orthonormal basis for $\text{range}(P)$ which is closed under the action of Θ up to a phase factor. Similar to the Chern number, which vanishes if and only if $\text{range}(P)$ admits a basis of ELWFs, whether $\text{range}(P)$ admits a well localized basis which satisfies time reversal symmetry is related to a topological invariant known as the \mathbb{Z}_2 invariant. In particular, we have the following theorem:

¹An operator Θ is antiunitary if it satisfies the relation $\langle \Theta w, \Theta v \rangle = \overline{\langle w, v \rangle} = \langle v, w \rangle$ for all $w, v \in \mathcal{H}$ where \mathcal{H} is a Hilbert space.

Theorem 3 (adapted from [FMP16b]). *Suppose that H satisfies Assumptions 1 and 2. Suppose further that H is periodic and satisfies fermionic time reversal symmetry. Then there exists a basis for ELWFs for $\text{range}(P)$ which satisfies time reversal symmetry if and only if the \mathbb{Z}_2 invariant is zero.*

As discussed in Chapter 1, interest in topological insulators has exploded over the fifteen years and there is much more which can be said about the physical properties of systems with non-zero \mathbb{Z}_2 invariant. We leave fully exploring the connection between our work and topology to future work. For the purposes of this dissertation, the example of systems with fermionic time reversal symmetry and non-zero \mathbb{Z}_2 invariant shows that there exist operators P and Θ such that:

1. $\text{range}(P)$ admits an exponentially localized orthonormal basis.
2. P commutes with Θ .
3. The position operators X and Y commute with Θ .
4. Any basis of ELWFs for $\text{range}(P)$ cannot satisfy time reversal symmetry.

Because of these four properties, it can be shown that for systems with fermionic time reversal symmetry and non-zero \mathbb{Z}_2 invariant, it is impossible for PXP to have uniform spectral gaps. The argument is as follows.

Towards a contradiction suppose that PXP has uniform spectral gaps. Since both P and X commute with Θ , we conclude that $[\Theta, PXP] = 0$. Since by assumption PXP has uniform spectral gaps, we can define the projectors P_j and using the Riesz projection formula for P_j (Equation (3.5)) and it follows that $[\Theta, P_j] = 0$. Hence, since Y also commutes with Θ , we conclude that $[\Theta, P_j Y P_j] = 0$. This is a contradiction however, since we have proven that the eigenfunctions of $P_j Y P_j$ are exponentially localized and if $P_j Y P_j$ commutes with Θ then its eigenfunctions can be chosen to satisfy time reversal symmetry. Therefore, despite the fact that $\text{range}(P)$ admits a basis of ELWFs, PXP cannot have uniform spectral gaps.

We note that a similar argument has been outlined by Vanderbilt and coauthors under the name the Wannier charge centers (WCCs) [SV11b, SV11a, TGV14, GAY⁺17, WZS⁺18]. In these works, the authors consider the eigenvalues of PXP and show that the \mathbb{Z}_2 invariant (and later the Chern number) can be connected to these eigenvalues in the periodic case.

4.1.2 Constructing a Choice of Position Operator

Combining various lemmas together, the result proven in Chapter 3 is the following:

Theorem 4 (Restatement of Lemmas 3.3.2, 3.3.3, 3.3.4 with technical bounds). *Suppose that P is the spectral projector onto σ_0 for a Hamiltonian satisfying Assumptions 1 and 2. Suppose further that there exists a collection of orthogonal projectors $\{P_j\}_{j \in \mathcal{J}}$ and finite, positive constants $(\gamma^*, K_1'', K_2'', K_3'')$ such that for all $0 \leq \gamma \leq \gamma^*$:*

1. *The projectors $\{P_j\}_{j \in \mathcal{J}}$ decompose $\text{range}(P)$ into orthogonal subspaces in the sense that*

$$(a) \sum_{j \in \mathcal{J}} P_j = P.$$

$$(b) P_j P_k = \begin{cases} P_j, & j = k; \\ 0, & j \neq k. \end{cases}$$

2. *Each P_j is exponentially localized in the sense that*

$$(a) \|P_{j,\gamma} - P_j\| \leq K_1'' \gamma,$$

$$(b) \|[P_{j,\gamma}, Y]\| \leq K_2''.$$

3. *Each P_j is concentrated along a line of the form $x = \xi_j$ in the sense that for each P_j there exists a $\xi_j \in \mathbb{R}$ such that:*

$$\|(X - \xi_j)P_{j,\gamma}\| \leq K_3'' \quad \text{and} \quad \|P_{j,\gamma}(X - \xi_j)\| \leq K_3''.$$

Then the following is true for each $j \in \mathcal{J}$:

1. The operator $P_j Y P_j$ is essentially self-adjoint (Lemma 3.3.2).
2. The operator $P_j Y P_j$ has discrete spectrum (Lemma 3.3.3)
3. There exists finite, positive constants $(C, \tilde{\gamma})$, independent of j , such that if $\psi \in \text{range}(P_j)$ and $P_j Y P_j \psi = \eta \psi$, then

$$\int e^{2\tilde{\gamma}\sqrt{1+(x-\xi_j)^2+(y-\eta)^2}} |\psi(x, y)|^2 dx dy \leq C.$$

Therefore by the spectral theorem, the collection of all eigenfunctions of the operators $\{P_j Y P_j\}_{j \in \mathcal{J}}$ form a complete, exponentially localized, orthogonal basis for $\text{range}(P)$ (Lemma 3.3.4).

An important point of Theorem 4 is that it *only* makes assumptions about a collection of orthogonal projections $\{P_j\}_{j \in \mathcal{J}}$. These orthogonal projections could be spectral projectors of the operator PXP but this is not strictly necessary. The main result of this chapter is to show that if there exists an orthogonal basis for $\text{range}(P)$ with sufficiently fast algebraic decay, then it is possible to construct an essentially self-adjoint operator \hat{X} such that:

1. \hat{X} is close to the true position operator X .
2. \hat{X} is exponentially localized.
3. The operator $P\hat{X}P$ has uniform spectral gaps.

Using these properties, it can be shown that the spectral projectors for $P\hat{X}P$ satisfy the assumptions of Theorem 4. Therefore, if we take $\{P_j\}_{j \in \mathcal{J}}$ to be the band projectors for $P\hat{X}P$, then Theorem 4 implies that diagonalizing $P_j Y P_j$ for each $j \in \mathcal{J}$ gives an exponentially localized orthogonal basis for $\text{range}(P)$.

4.2 Technical Statement of Results

To formally state our results we will first make two important definitions: *finitely degenerate centers* and *generalized Wannier basis*. Our definition for generalized

Wannier basis differs slightly from those given previously in the literature [MMMP19, MMP20]. We will discuss these differences in more detail in Section 4.2.1.

Definition 4 (Finitely Degenerate Centers). We say that a collection of functions $\{\psi_\alpha\}_{\alpha \in \mathcal{I}} \subseteq L^2(\mathbb{R}^2)$ has *finitely degenerate centers* if:

1. Each ψ_α has a well defined expected position. That is, for all $\alpha \in \mathcal{I}$ the following quantities exist and are finite:

$$\mu_\alpha^X := \langle \psi_\alpha, X \psi_\alpha \rangle \quad \text{and} \quad \mu_\alpha^Y := \langle \psi_\alpha, Y \psi_\alpha \rangle. \quad (4.1)$$

We will refer to the point $(\mu_\alpha^X, \mu_\alpha^Y)$ as the *center point* for ψ_α .

2. The collection of center points for $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ has bounded density. That is, there exists a constant $M < \infty$ such that for all $(x_0, y_0) \in \mathbb{R}^2$ we have

$$\#\{\alpha : (\mu_\alpha^X, \mu_\alpha^Y) \in B_1(x_0, y_0)\} \leq M$$

where $B_1(x_0, y_0)$ is a ball of radius 1 centered at (x_0, y_0) .

Definition 5 (Generalized Wannier Basis). Let $P \in \mathcal{B}(L^2(\mathbb{R}^2))$ be an orthogonal projection. We say that a collection of functions $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ is a *generalized Wannier basis* if there exists a localization function $G(\cdot) : \mathbb{R} \rightarrow \mathbb{R}_+$ and a constant $C > 0$ such that:

1. The collection $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ forms an orthonormal basis for $\text{range}(P)$ with finitely degenerate centers.
2. Each ψ_α is localized about its center point in the sense that

$$\int_{\mathbb{R}^2} G(|\mathbf{x} - (\mu_\alpha^X, \mu_\alpha^Y)|) |\psi_\alpha(\mathbf{x})|^2 \leq C$$

where $(\mu_\alpha^X, \mu_\alpha^Y)$ is as defined in Equation (4.1).

In this chapter, we specifically consider two important special classes of generalized Wannier bases:

1. We say a generalized Wannier bases is *exponentially localized* if we can choose $G(|\mathbf{x}|) = e^{2\gamma|\mathbf{x}|}$ for some $\gamma > 0$.
2. We say a generalized Wannier bases is *s-localized* if we can choose $G(|\mathbf{x}|) = (1 + |\mathbf{x}|^2)^s$ for some $s > 0$.

The formal statement of our result is then the following:

Theorem 5. *Let P be the spectral projector onto σ_0 for a Hamiltonian H satisfying Assumptions 1 and 2. Then the following statements are equivalent:*

1. *P admits a generalized Wannier basis that is exponentially localized.*
2. *P admits a generalized Wannier basis that is s -localized for some $s > 5/2$.*

4.2.1 Connection with Previous Work and Discussions

Generalized Wannier bases in two dimensions have been considered and defined in previous works [NN98, MMMP19, MMP20], however the definition we give in our work slightly differs from these previous definitions. The main difference between our definition of a generalized Wannier basis and the ones given in these previous works lies in the conditions imposed on the center points. In our work, we define the center point of a basis function ψ_α to be its expected position in X and Y . While this requires that each basis element has a well defined expected position, this assumption is satisfied since we assume that P admits an s -localized basis for $s > 5/2$. We then additionally assume that these center points do not cluster arbitrarily strongly to prevent pathological counterexamples.

In the work by Nenciu-Nenciu [NN98], the set of center points were only assumed to be a discrete set. We found this assumption to be problematic as it allows the center points to become arbitrarily strongly clustered. In the work of Marcelli, Monaco, Moscolari, and Panati [MMMP19], the authors assume that the center points are part of a Delone set (a set which is “nowhere dense” and “nowhere sparse”, see

[MMMP19, Definition 5.2]). This Delone set assumption puts a fairly rigid structure on the center points which does not play a role in our argument since we only focus on the localization of the Wannier functions. The definition of a generalized Wannier basis given in the more recent work by Marcelli, Moscolari and Panati [MMP20], on the other hand, is equivalent to the finitely degenerate centers assumption so long as the basis has a well defined expected position.

Before continuing with the remainder of this chapter we will quickly discuss the Localization Dichotomy Conjecture for non-periodic insulators introduced in [MMMP19]. In the periodic case, the Chern number plays an important role in classifying when an exponentially localized basis of Wannier functions exists or not. The natural extension of these ideas to the non-periodic case was introduced in [MMMP19] (see also [CMM18]) and is known as *Chern marker*.

Definition 6 (Chern Marker). Let P be a projection on $L^2(\mathbb{R}^2)$ and χ_L be the indicator function of the set $(-L, L]^2$. The *Chern marker* of P is defined by

$$C(P) := \lim_{L \rightarrow \infty} \frac{2\pi i}{4L^2} \operatorname{tr} \left(\chi_L P \left[[X, P], [Y, P] \right] P \chi_L \right)$$

whenever the limit on the right hand side exists.

With this definition the Localization Dichotomy Conjecture as stated in [MMMP19] is the following:

Conjecture 1 (Localization Dichotomy Conjecture). *Let P be the spectral projector onto σ_0 for a Hamiltonian H satisfying Assumptions 1 and 2. Then the following statements are equivalent:*

- (a) *P admits a generalized Wannier basis that is exponentially localized.*
- (b) *P admits a generalized Wannier basis that is s -localized for $s = 1$.*
- (c) *P is topologically trivial in the sense that its Chern marker $C(P)$ exists and is equal to zero.*

The main result of this work shows that (b) \Rightarrow (a) for $s > 5/2$. In recent work [MMP20], Marcelli, Moscolari, and Panati have shown that (b) \Rightarrow (c) for $s > 5$. Since an exponentially localized basis is also s -localized for any $s \geq 0$, our result combined with the result from [MMP20] implies that (b) \Rightarrow (c) for $s > 5/2$.

While in chapter we only consider systems in two dimensions, we expect that the arguments in the work can be generalized to arbitrarily high dimension by a similar approach to the one taken in Section 3.4.

4.3 Construction of \widehat{X}

Throughout the rest of this chapter, we will assume that P admits an s -localized generalized Wannier basis with $s > 5/2$. That is, there exists an orthonormal basis $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ for $\text{range}(P)$ such that:

1. $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ has finitely degenerate centers;
2. $\{\psi_\alpha\}_{\alpha \in \mathcal{I}}$ is s -localized for some $s > 5/2$ sufficiently large.

Our first step to constructing \widehat{X} will be to observe some important consequences of the finitely degenerate centers assumption.

4.3.1 Consequences of Finitely Degenerate Centers

For each $(m, n) \in \mathbb{Z}^2$ let us define the unit box centered at (m, n) as follows:

$$S_{m,n} := \left[m - \frac{1}{2}, m + \frac{1}{2} \right) \times \left[n - \frac{1}{2}, n + \frac{1}{2} \right).$$

If a basis $\{\psi_\alpha\}$ satisfies the finitely degenerate centers assumption we know that there is some finite number M such that no more than M basis elements have their center in $S_{m,n}$. Using this property, we can relabel our basis as $\{\psi_{m,n}^{(j)}\}_{(m,n) \in \mathbb{Z}^2}$ where $\psi_{m,n}^{(j)}$ has its center in $S_{m,n}$ and j is a degeneracy index which runs from 1 to M . In the

case that the box $S_{m,n}$ has fewer than M basis elements (say it has j^*) then we define $\psi_{m,n}^{(j)} \equiv 0$ for all $j > j^*$.

The importance of this relabelling is that it allows us to essentially discretize the center points of the basis $\{\psi_{m,n}^{(j)}\}$. Recall that if $\psi_{m,n}^{(j)}$ is s -localized then by definition

$$\int (1 + |x_1 - \mu_{m,n,j}^X|^2 + |x_2 - \mu_{m,n,j}^Y|^2)^s |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \leq C. \quad (4.2)$$

where $(\mu_{m,n,j}^X, \mu_{m,n,j}^Y)$ is the center point of $\psi_{m,n}^{(j)}$. Furthermore, by definition we know that:

$$|\mu_{m,n,j}^X - m| \leq \frac{1}{2} \quad \text{and} \quad |\mu_{m,n,j}^Y - n| \leq \frac{1}{2} \quad (4.3)$$

Since $(\mu_{m,n}^X, \mu_{m,n}^Y)$ and (m, n) are close, we have the following lemma:

Lemma 4.3.1. *If $\psi_{m,n}^{(j)}$ satisfies Equation (4.2) for some $s \geq 0$, then it also satisfies*

$$\int (1 + |x_1 - m|^2 + |x_2 - n|^2)^s |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \leq 2^s(C + 1) \quad (4.4)$$

Hence, treating the center point of $\psi_{m,n}^{(j)}$ as (m, n) instead of $(\mu_{m,n}^X, \mu_{m,n}^Y)$ only makes the bounds worse by a constant factor.

Proof. Observe that for any $(x, y) \in \mathbb{R}^2$ and $(m, n) \in \mathbb{R}^2$ we have

$$\begin{aligned} 1 + |x_1 - m|^2 + |x_2 - n|^2 &= |(x_1 - m, x_2 - n, 1)|^2 \\ &= |(x_1 - \mu_{m,n,j}^X, x_2 - \mu_{m,n,j}^Y, 1) - (\mu_{m,n,j}^X - m, \mu_{m,n,j}^Y - n, 0)|^2 \end{aligned} \quad (4.5)$$

Now recall the elementary inequality for any $a, b \in \mathbb{R}^d$ (which is an immediate consequence of triangle inequality):

$$|a + b|^{2s} \leq 2^{2s}(|a|^{2s} + |b|^{2s}).$$

Therefore, using this inequality in (4.5) we have

$$\begin{aligned} (1 + |x_1 - m|^2 + |x_2 - n|^2)^s &\leq 2^{2s} \left(|(x_1 - \mu_{m,n,j}^X, x_2 - \mu_{m,n,j}^Y, 1)|^{2s} + |(\mu_{m,n,j}^X - m, \mu_{m,n,j}^Y - n, 0)|^{2s} \right) \end{aligned}$$

Since $|\mu_{m,n,j}^X - m| \leq \frac{1}{2}$ and $|\mu_{m,n,j}^Y - n| \leq \frac{1}{2}$ it's clear that for any $s \geq 0$, $|(\mu_{m,n,j}^X - m, \mu_{m,n,j}^Y - n, 0)| \leq 1$. Therefore, we conclude that:

$$\begin{aligned} & \int (1 + |x_1 - m|^2 + |x_2 - n|^2)^s |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\ & \leq \int 2^{2s} \left((1 + |x_1 - \mu_{m,n,j}^X|^2 + |x_2 - \mu_{m,n,j}^Y|^2)^s + 1 \right) |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\ & \leq 2^{2s}(C + 1). \end{aligned} \quad \square$$

Another important consequence of knowing an s -localized basis with finitely degenerate centers for range (P) exists is *any* other localized basis must also have finitely degenerate centers.

Lemma 4.3.2. *Suppose that $P \in \mathcal{B}(L^2(\mathbb{R}^2))$ is an orthogonal projector. Suppose further that $\{\psi_\alpha\}$ and $\{\phi_\alpha\}$ are two distinct orthonormal bases for range(P) and both bases are s -localized with $s > 1$. If $\{\psi_\alpha\}$ has finitely degenerate centers then $\{\phi_\alpha\}$ must also have finitely degenerate centers.*

Proof. Given in Appendix A.5. □

Because Lemma 4.3.2 and our assumptions, once we construct an exponentially localized basis for range (P) we know that this basis must necessarily have finitely degenerate centers.

4.3.2 The Construction of \widehat{X}

Since we have discretized the center points of the basis $\{\psi_{m,n}^{(j)}\}$, we can use this discretization to define a new position operator \tilde{X} :

$$\tilde{X} := \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| + QXQ. \quad (4.6)$$

Since $PQ = QP = 0$ it's clear that $\sigma(P\tilde{X}P) \subseteq \mathbb{Z}$. Furthermore, if we assume that the basis $\{\psi_{m,n}^{(j)}\}$ has sufficiently fast algebraic decay then it's possible to show that

$\|\tilde{X} - X\| = O(1)$. Unfortunately, since the basis $\{\psi_{m,n}^{(j)}\}$ only decays algebraically, the band projectors for $P\tilde{X}P$ will generally not be exponentially localized. To address this issue, we use the spectral filter approach used by Hastings in [Has09]. Specifically, we define \hat{X} via the formula:

$$\hat{X} := \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}\tilde{X}e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \quad (4.7)$$

Here Δ is a finite parameter to be chosen as part of our proofs and $f(t)$ is a filter function defined in terms of its Fourier transform as follows:

$$\hat{f}(\xi) = \begin{cases} (1 - |\xi|^2)^3 & |\xi| \leq 1 \\ 0 & |\xi| \geq 1 \end{cases}$$

Note that since $\hat{f}(\xi)$ is $C^2(\mathbb{R}^2)$, $tf(t) \in L^1(\mathbb{R})$. Also, note that $\int f(t) dt = \hat{f}(0) = 1$.

To better understand how this construction gives exponential localization for the band projectors, let's consider the simple case where \tilde{X} and \hat{X} are both finite matrices. In this case, for any $\lambda = (\lambda_x, \lambda_y)$ and $\mu = (\mu_x, \mu_y)$, we can find vectors v_λ and v_μ which are simultaneous eigenvectors of X and Y so that

$$\begin{aligned} Xv_\lambda &= \lambda_x v_\lambda & Yv_\lambda &= \lambda_y v_\lambda \\ Xv_\mu &= \mu_x v_\mu & Yv_\mu &= \mu_y v_\mu \end{aligned}$$

For these vectors we have that

$$\begin{aligned} \langle v_\lambda, \hat{X}v_\mu \rangle &= \int_{\mathbb{R}^2} f(t_1)f(t_2)\langle v_\lambda, e^{i(Xt_1+Yt_2)/\Delta}\tilde{X}e^{-i(Xt_1+Yt_2)/\Delta}v_\mu \rangle dt_1 dt_2 \\ &= \langle v_\lambda, \tilde{X}v_\mu \rangle \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(\lambda_x t_1 + \lambda_y t_2)/\Delta}e^{-i(\mu_x t_1 + \mu_y t_2)/\Delta} dt_1 dt_2 \\ &= \langle v_\lambda, \tilde{X}v_\mu \rangle \left(\int_{\mathbb{R}} f(t_1)e^{i(\lambda_x - \mu_x)t_1/\Delta} dt_1 \right) \left(\int_{\mathbb{R}} f(t_2)e^{i(\lambda_y - \mu_y)t_2/\Delta} dt_2 \right) \\ &= \langle v_\lambda, \tilde{X}v_\mu \rangle \hat{f}\left(\frac{\lambda_x - \mu_x}{\Delta}\right) \hat{f}\left(\frac{\lambda_y - \mu_y}{\Delta}\right) \end{aligned} \quad (4.8)$$

Since \hat{f} is only non-zero on $(-1, 1)$, these steps imply that if $|\lambda_x - \mu_x| \geq \Delta$ or $|\lambda_y - \mu_y| \geq \Delta$ then $\langle v_\lambda, \hat{X}v_\mu \rangle = 0$. This calculation shows that in this simple case

that the formula Equation (4.7) sets the entries of \tilde{X} far from the diagonal to zero (hence \hat{X} is a local operator). Unfortunately, this calculation does not seem to generalize to the continuum case due to the fact we do not have good control on the oscillation of functions from range(Q). Despite this technical difficulty, we can still show that \hat{X} satisfies some technical estimates needed to prove the estimates in Theorem 4.

4.3.3 Proof Organization

The remainder of this chapter is devoted to proving properties of \hat{X} and the operator $P\hat{X}P$ and is organized as follows. Throughout this proof, we will make use of a number of estimates on the projector P which were first stated in Section 2.2.1. In Section 4.4, we show that \hat{X} as constructed above is close to the true position operator X . In Section 4.5, we will prove some technical estimates which imply band projectors of $P\hat{X}P$ are exponentially localized. Finally, in Section 4.6 we will show that $P\hat{X}P$ has uniform spectral gaps so the band projectors for $P\hat{X}P$ exist and are well defined. Having proved these important estimates for \hat{X} , we will finish the proof of Theorem 5 in Section 4.7 by showing that the band projectors of $P\hat{X}P$ satisfy the assumptions of Theorem 4.

4.4 Closeness of \hat{X} and X

The main goal of this section is to prove the following proposition.

Proposition 4.4.1. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 2$, then there exists a finite constant $C > 0$ such that*

$$\|\hat{X} - X\| \leq C.$$

Let's start the proof of this proposition with a straightforward calculation. By definition of \widehat{X} we have that:

$$\begin{aligned}
\widehat{X} - X &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} \tilde{X} e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 - X \\
&= \int_{\mathbb{R}^2} f(t_1)f(t_2) \left(e^{i(Xt_1+Yt_2)/\Delta} \tilde{X} e^{-i(Xt_1+Yt_2)/\Delta} - X \right) dt_1 dt_2 \\
&= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} (\tilde{X} - X) e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \quad (4.9)
\end{aligned}$$

where we have used that $\int f(t) dt = 1$ and the fact that $[X, e^{-i(Xt_1+Yt_2)}] = 0$. Therefore,

$$\begin{aligned}
\|\widehat{X} - X\| &\leq \int_{\mathbb{R}^2} \|f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} (\tilde{X} - X) e^{-i(Xt_1+Yt_2)/\Delta}\| dt_1 dt_2 \\
&\leq \|\tilde{X} - X\| \left(\int_{\mathbb{R}} |f(t_1)| dt_1 \right) \left(\int_{\mathbb{R}} |f(t_2)| dt_2 \right)
\end{aligned}$$

Since $f \in L^1(\mathbb{R})$, the proposition is proved so long as we can show that $\|\tilde{X} - X\|$ is bounded. Let's recall the definition of \tilde{X}

$$\tilde{X} = \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| + QXQ. \quad (4.6, \text{revisited})$$

Now since $P + Q = I$ we have that

$$\begin{aligned}
X - \tilde{X} &= (P + Q)X(P + Q) - \tilde{X} \\
&= PXP + PXQ + QXP + QXQ - \tilde{X} \\
&= \left(PXP - \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| \right) + (PXQ + QXP). \quad (4.10)
\end{aligned}$$

Now at least formally we can write:

$$\begin{aligned}
PXP &= \left(\sum_{m,n,j} |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| \right) X \left(\sum_{m',n',j'} |\psi_{m',n'}^{(j')}\rangle \langle \psi_{m',n'}^{(j')}| \right) \\
&= \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, X \psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}|.
\end{aligned}$$

Since $\{\psi_{m,n}^{(j)}\}$ is an orthonormal basis, we have that when $(m, n, j) \neq (m', n', j')$:

$$\langle \psi_{m,n}^{(j)}, X \psi_{m',n'}^{(j')} \rangle = \langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle.$$

Therefore, we can express the difference from Equation (4.10) as follows:

$$\begin{aligned} PXP - \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| \\ = \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}|. \end{aligned}$$

Hence,

$$\begin{aligned} \|\tilde{X} - X\| &\leq \left\| \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \right\| \\ &\quad + \|PXQ\| + \|QXP\| \end{aligned}$$

Since $\|PXQ\| + \|QXP\|$ is bounded by Corollary 2.2.2(ii) with $\gamma = 0$, to finish the proof we only need to control the operator norm of the first term, which also justifies the expansion above. To do this, we will appeal the following proposition which we prove in Appendix A.7. This proposition is little stronger than we need to prove Proposition 4.4.1, but we will need to use this stronger result as part of the proofs in Section 4.5.

Proposition 4.4.2. *Fix an orthonormal basis $\{\psi_{m,n}^{(j)}\}$. For any $h, g \in L^2(\mathbb{R}^2)$ define $h_{m,n,j}$ and $g_{m',n',j'}$ as follows:*

$$h_{m,n,j} := \int_{\mathbb{R}^2} |\psi_{m,n}^{(j)}(\mathbf{x}) h(\mathbf{x})| d\mathbf{x} \quad g_{m',n',j'} := \int_{\mathbb{R}^2} |\psi_{m',n'}^{(j')}(\mathbf{x}) g(\mathbf{x})| d\mathbf{x}.$$

If $\{\psi_{m,n}^{(j)}\}$ is an s -localized basis with $s > 2$ then there exists an absolute constant $C > 0$ such that

$$\sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| h_{m,n,j} g_{m',n',j'} \leq C \|h\| \|g\|$$

Noting that $h_{m,n,j} = \langle |h|, |\psi_{m,n}^{(j)}| \rangle$ and $g_{m',n',j'} = \langle |\psi_{m',n'}^{(j')}|, |g| \rangle$. This result proves

Proposition 4.4.1 since by definition

$$\begin{aligned}
& \left\| \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \right\| \\
&= \sup_{\|h\|, \|g\|=1} \left| \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle \langle h, \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')}, g \rangle \right| \\
&\leq \sup_{\|h\|, \|g\|=1} \sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| |\langle h, \psi_{m,n}^{(j)} \rangle| |\langle \psi_{m',n'}^{(j')}, g \rangle|.
\end{aligned}$$

4.5 \widehat{X} is exponentially localized

The main goal of this section is to prove the following proposition which gives a precise meaning to the statement “ \widehat{X} is exponentially localized”.

Proposition 4.5.1. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 2$, then there exist finite constants $C_1, C_2 > 0$ such that for any $\mu \in \mathbb{R}$ and any γ sufficiently small:*

$$\|\widehat{X}_\gamma - \widehat{X}\| \leq C_1 \gamma \tag{4.11}$$

$$\|(X - \mu + i)^{-1} [\widehat{X}_\gamma, Y] (X - \mu + i)^{-1}\| \leq C_2 \tag{4.12}$$

In the discrete case, proving Equation (4.11) implies that the matrix entries of \widehat{X} decay exponentially quickly off the diagonal. Therefore, this bound captures at least part of the statement “ \widehat{X} is exponentially localized”. On the other hand, Equation (4.12) controls the non-commutativity of \widehat{X} and Y . The need for this bound arises as a technical condition needed to prove that the band projectors of $P\widehat{X}P$ satisfy the assumptions of Theorem 4 (in particular it is used to prove Equation (4.32b)). Despite this difference in interpretation, the techniques to prove these two bounds are quite similar. We will prove Equation (4.11) in Section 4.5.1 and Equation (4.12) in Section 4.5.2

4.5.1 Proof of Equation (4.11)

As we saw in Equation (4.9) in Section 4.4, using the fact that $\int_{\mathbb{R}} f = 1$ and $[X, e^{-i(Xt_1+Yt_2)/\Delta}] = 0$ we have that:

$$\widehat{X} - X = \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(\tilde{X} - X)e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2.$$

Hence, since $\tilde{X} = P\tilde{X}P + QXQ$ and $X = PXP + QXQ + PXQ + QXP$ we can rewrite $\tilde{X} - X$ in the integrand above and obtain:

$$\begin{aligned} \widehat{X} - X &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(P\tilde{X}P - PXP \\ &\quad - QXP - PXQ)e^{-i(Xt_1+Yt_2)/\Delta} dt \\ &= \int_{\mathbb{R}^2} f(t_1)f(t_2)\left(e^{i(Xt_1+Yt_2)/\Delta}(P\tilde{X}P - PXP)e^{-i(Xt_1+Yt_2)/\Delta} \right. \\ &\quad \left. - e^{i(Xt_1+Yt_2)/\Delta}(QXP + PXQ)e^{-i(Xt_1+Yt_2)/\Delta}\right) dt_1 dt_2. \end{aligned}$$

To reduce clutter in the next few steps, let's define the following shorthands:

$$\begin{aligned} A^{(1)} &:= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(P\tilde{X}P - PXP)e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \\ A^{(2)} &:= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(QXP + PXQ)e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \end{aligned}$$

Using this notation we clearly have that

$$\widehat{X} - X = A^{(1)} - A^{(2)}. \quad (4.13)$$

Multiplying on the left by B_γ and on the right by B_γ^{-1} we have that

$$\widehat{X}_\gamma - X = A_\gamma^{(1)} - A_\gamma^{(2)}, \quad (4.14)$$

where we have made use of our convention for exponentially tilted operators (Section 2.1.1). Using the identities in Equations (4.13) and (4.14) we can rewrite the difference we are interested in bounding as follows:

$$\begin{aligned} \widehat{X}_\gamma - \widehat{X} &= (\widehat{X}_\gamma - X) - (\widehat{X} - X) \\ &= (A_\gamma^{(1)} - A_\gamma^{(2)}) - (A^{(1)} - A^{(2)}) \\ &= (A_\gamma^{(1)} - A^{(1)}) - (A_\gamma^{(2)} - A^{(2)}) \end{aligned}$$

Hence to show that $\|\widehat{X}_\gamma - \widehat{X}\| \leq C_1\gamma$, it is enough to find constants K_1, K_2 so that

$$\|A_\gamma^{(1)} - A^{(1)}\| \leq K_1\gamma$$

$$\|A_\gamma^{(2)} - A^{(2)}\| \leq K_2\gamma$$

We will show the bound for $A^{(1)}$ in Section 4.5.1 and the bound for $A^{(2)}$ in Section 4.5.1.

Bounding $\|A_\gamma^{(1)} - A^{(1)}\|$

To begin, we will first write $PXP - P\tilde{X}P$ as an integral kernel. Repeating the calculations from Section 4.4, we see that we can write the difference $PXP - P\tilde{X}P$ as follows:

$$PXP - P\tilde{X}P = \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}|$$

Therefore, we can define the integral kernel $K : \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}$ as follows:

$$K(\mathbf{x}, \mathbf{y}) = - \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle \psi_{m,n}^{(j)}(\mathbf{x}) \psi_{m',n'}^{(j')}(\mathbf{y}). \quad (4.15)$$

Using this kernel, for any $g \in C_c^\infty(\mathbb{R}^2)$ we have that:

$$((P\tilde{X}P - PXP)g)(\mathbf{x}) = \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y})g(\mathbf{y}) \, d\mathbf{y}.$$

We can then use this kernel to express the action of $A^{(1)}$ on any arbitrary $g \in C_c^\infty(\mathbb{R}^2)$:

$$\begin{aligned} (A^{(1)}g)(\mathbf{x}) &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(x_1t_1+x_2t_2)/\Delta} \left(\int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y})e^{-i(y_1t_1+y_2t_2)/\Delta}g(\mathbf{y}) \right) dt_1 dt_2 \\ &= \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y})g(\mathbf{y}) \left(\int_{\mathbb{R}} f(t_1)e^{i(x_1-y_1)t_1/\Delta} dt_1 \right) \left(\int_{\mathbb{R}} f(t_2)e^{i(x_2-y_2)t_2/\Delta} dt_2 \right) d\mathbf{y} \\ &= \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y})g(\mathbf{y}) \hat{f}\left(\frac{x_1-y_1}{\Delta}\right) \hat{f}\left(\frac{x_2-y_2}{\Delta}\right) d\mathbf{y} \end{aligned}$$

Slightly abusing notation we define

$$\hat{f}\left(\frac{\mathbf{x}-\mathbf{y}}{\Delta}\right) := \hat{f}\left(\frac{x_1-y_1}{\Delta}\right) \hat{f}\left(\frac{x_2-y_2}{\Delta}\right). \quad (4.16)$$

With this notation we have

$$(A^{(1)}g)(\mathbf{x}) = \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y}) \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) g(\mathbf{y}) \, d\mathbf{y}.$$

Now recall our definition for B_γ :

$$B_\gamma = B_{\gamma,(a,b)} = \exp\left(\gamma\sqrt{1 + (X - a)^2 + (Y - b)^2}\right).$$

Since B_γ acts pointwisely, it's easy to see that

$$B_\gamma(P\tilde{X}P - PXP)B_\gamma^{-1}g = e^{\gamma|(x_1-a, x_2-b, 1)|} \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y}) e^{-\gamma|(y_1-a, y_2-b, 1)|} g(\mathbf{y}) \, d\mathbf{y}.$$

Therefore, repeating similar steps gives us that:

$$(A_\gamma^{(1)}g)(\mathbf{x}) = \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y}) e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) g(\mathbf{y}) \, d\mathbf{y} \quad (4.17)$$

and so

$$\begin{aligned} & ((A_\gamma^{(1)} - A^{(1)})g)(\mathbf{x}) \\ &= \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y}) (e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} - 1) \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) g(\mathbf{y}) \, d\mathbf{y}. \end{aligned}$$

Since we are interested in the spectral norm of $A_\gamma^{(1)} - A^{(1)}$, we can use our expression for $(A_\gamma^{(1)} - A^{(1)})g$, take the inner product with any $h \in L^2(\mathbb{R}^2)$, and apply triangle inequality so that the bound to show is the following

$$\int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \left| h(\mathbf{x}) K(\mathbf{x}, \mathbf{y}) E(\mathbf{x}, \mathbf{y}) \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) g(\mathbf{y}) \right| \, d\mathbf{y} \, d\mathbf{x} \leq C\gamma \|g\| \|h\| \quad (4.18)$$

where

$$E(\mathbf{x}, \mathbf{y}) := e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} - 1.$$

Using reverse triangle inequality and elementary calculus we have that:

$$\begin{aligned} |e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} - 1| &\leq |e^{\gamma|(x_1-y_1, x_2-y_2, 1-1)|} - 1| \\ &= |e^{\gamma|\mathbf{x}-\mathbf{y}|} - 1| \\ &\leq \gamma|\mathbf{x} - \mathbf{y}| e^{\gamma|\mathbf{x}-\mathbf{y}|}. \end{aligned}$$

So since \hat{f} is compactly supported on $[-\Delta, \Delta]^2$ we conclude that we can bound Equation (4.18) with the following:

$$\gamma(\sqrt{2}\Delta e^{\gamma\sqrt{2}\Delta}) \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |h(\mathbf{x})K(\mathbf{x}, \mathbf{y})g(\mathbf{y})| \, d\mathbf{y} \, d\mathbf{x}. \quad (4.19)$$

For our final step, we can substitute in the definition of the kernel K from Equation (4.15) to conclude that:

$$\begin{aligned} & \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |h(\mathbf{x})K(\mathbf{x}, \mathbf{y})g(\mathbf{y})| \, d\mathbf{y} \, d\mathbf{x} \\ & \leq \sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X-m)\psi_{m',n'}^{(j')} \rangle| \\ & \quad \times \left(\int_{\mathbb{R}^2} |h(\mathbf{x})\psi_{m,n}^{(j)}(\mathbf{x})| \, d\mathbf{x} \right) \left(\int_{\mathbb{R}^2} |g(\mathbf{y})\psi_{m',n'}^{(j')}(\mathbf{y})| \, d\mathbf{y} \right) \\ & \leq C\|h\|\|g\|, \end{aligned}$$

where the last inequality follows from Proposition 4.4.2. This proves that for all $\gamma \geq 0$

$$\|A_\gamma^{(1)} - A^{(1)}\| \leq \left(C\sqrt{2}\Delta e^{\gamma\sqrt{2}\Delta} \right) \gamma$$

which is what we wanted to show.

Bounding $\|A_\gamma^{(2)} - A^{(2)}\|$

Let's begin by recalling the definitions for $A_\gamma^{(2)}$ and $A^{(2)}$:

$$\begin{aligned} A_\gamma^{(2)} &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(Q_\gamma X P_\gamma + P_\gamma X Q_\gamma)e^{-i(Xt_1+Yt_2)/\Delta} \, dt_1 \, dt_2 \\ A^{(2)} &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(QXP + PXQ)e^{-i(Xt_1+Yt_2)/\Delta} \, dt_1 \, dt_2 \end{aligned}$$

Hence we can write the difference we're interested in as:

$$\int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(Q_\gamma X P_\gamma - QXP + P_\gamma X Q_\gamma - PXQ)e^{-i(Xt_1+Yt_2)/\Delta} \, dt_1 \, dt_2$$

Due to our decay estimates on the projector P , by Corollary 2.2.2(iv), we have that for all γ sufficiently small

$$\|Q_\gamma X P_\gamma - QXP\| = O(\gamma), \quad \text{and} \quad \|P_\gamma X Q_\gamma - PXQ\| = O(\gamma).$$

Hence applying these estimates we have that we can find a constant $C > 0$ such that

$$\|A_\gamma^{(2)} - A^{(2)}\| \leq C\gamma \left(\int |f(t_1)| dt_1 \right) \left(\int |f(t_2)| dt_2 \right)$$

finishing the proof that $\|A_\gamma^{(2)} - A^{(2)}\| = O(\gamma)$.

4.5.2 Proof of Equation (4.12)

To begin this section, let us fix some $\mu \in \mathbb{R}$ and recall the quantity we want to bound:

$$(X - \mu + i)^{-1} [\widehat{X}_\gamma, Y] (X - \mu + i)^{-1}. \quad (4.12, \text{revisited})$$

Similar to the previous section, our first step bounding this quantity will be to rewrite $[\widehat{X}_\gamma, Y]$ into a more friendly form. Using that $[X, Y] = 0$ we have that

$$\begin{aligned} [\widehat{X}_\gamma, Y] &= [\widehat{X}_\gamma - X, Y] \\ &= [B_\gamma(\widehat{X} - X)B_\gamma^{-1}, Y] \\ &= B_\gamma[\widehat{X} - X, Y]B_\gamma^{-1} \\ &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} B_\gamma[\tilde{X} - X, Y]B_\gamma^{-1}e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \end{aligned}$$

We can now decompose the difference $\tilde{X} - X$ into two parts:

$$\tilde{X} - X = \left(P\tilde{X}P - PXP \right) + \left(PXQ + QXP \right).$$

Using this decomposition, let's define $\tilde{A}^{(1)}$ and $\tilde{A}^{(2)}$ as follows:

$$\begin{aligned} \tilde{A}^{(1)} &:= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} B_\gamma[P\tilde{X}P - PXP, Y]B_\gamma^{-1}e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \\ \tilde{A}^{(2)} &:= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} B_\gamma[PXQ + QXP, Y]B_\gamma^{-1}e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \\ &= \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta} [P_\gamma X Q_\gamma + Q_\gamma X P_\gamma, Y] e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \end{aligned}$$

With this notation, clearly

$$\begin{aligned} (X - \mu + i)^{-1} [\widehat{X}_\gamma, Y] (X - \mu + i)^{-1} \\ = (X - \mu + i)^{-1} (\tilde{A}^{(1)} - \tilde{A}^{(2)}) (X - \mu + i)^{-1}. \end{aligned}$$

Similar to Section 4.5.1, we will show that $(X - \mu + i)^{-1} \tilde{A}^{(1)} (X - \mu + i)^{-1}$ is bounded in Section 4.5.2 and $(X - \mu + i)^{-1} \tilde{A}^{(2)} (X - \mu + i)^{-1}$ is bounded in Section 4.5.2.

Bounding $\tilde{A}^{(1)}$

We start by observing

$$\begin{aligned} \|(X - \mu + i)^{-1} A^{(1)} (X - \mu + i)^{-1}\| & \\ & \leq \|(X - \mu + i)^{-1}\| \|A^{(1)}\| \|(X - \mu + i)^{-1}\| \\ & \leq \|A^{(1)}\| \end{aligned}$$

so it suffices to show that $\|A^{(1)}\|$ is bounded. Repeating similar calculations as given in Section 4.5.1 one can easily calculate the action of $\tilde{A}^{(1)}$ for any $g \in C_c^\infty(\mathbb{R}^2)$ as follows (cf. Equation (4.17)):

$$(\tilde{A}^{(1)}g)(\mathbf{x}) := \int_{\mathbb{R}^2} K(\mathbf{x}, \mathbf{y})(x_2 - y_2) e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) g(\mathbf{y}) \, d\mathbf{y}$$

Next, taking the inner product with any $h \in L^2(\mathbb{R}^2)$ we have that:

$$\begin{aligned} \langle h, \tilde{A}^{(1)}g \rangle & \\ & \leq \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |h(\mathbf{x})| |K(\mathbf{x}, \mathbf{y})| |x_2 - y_2| e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} \hat{f}\left(\frac{\mathbf{x} - \mathbf{y}}{\Delta}\right) \, d\mathbf{y} \, d\mathbf{x} \end{aligned}$$

Since by reverse triangle inequality

$$e^{\gamma|(x_1-a, x_2-b, 1)|} e^{-\gamma|(y_1-a, y_2-b, 1)|} \leq e^{\gamma|(x_1-y_1, x_2-y_2, 1-1)|} = e^{\gamma|\mathbf{x}-\mathbf{y}|}$$

using the fact that \hat{f} is supported on $[-\Delta, \Delta]^2$ we conclude that

$$\langle h, \tilde{A}^{(1)}g \rangle \leq \Delta e^{\gamma\sqrt{2}\Delta} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |h(\mathbf{x})| |K(\mathbf{x}, \mathbf{y})| |g(\mathbf{y})| \, d\mathbf{y} \, d\mathbf{x}$$

Hence, applying Proposition 4.4.2 we conclude that

$$\|\tilde{A}^{(1)}\| = \sup_{\|h\|=\|g\|=1} |\langle h, \tilde{A}^{(1)}g \rangle| \leq C \Delta e^{\gamma\sqrt{2}\Delta}$$

completing the proof that $\tilde{A}^{(1)}$ is bounded.

Bounding $\tilde{A}^{(2)}$

Unlike the proof in the previous section, to show that $(X - \mu + i)^{-1}\tilde{A}^{(2)}(X - \mu + i)^{-1}$ is bounded, we will need to use the additional decay provided by $(X - \mu + i)^{-1}$. In this section we will prove the following bounds:

$$\|(X - \mu + i)^{-1}[P_\gamma X Q_\gamma, Y](X - \mu + i)^{-1}\| = O(1) \quad (4.20)$$

$$\|(X - \mu + i)^{-1}[Q_\gamma X P_\gamma, Y](X - \mu + i)^{-1}\| = O(1). \quad (4.21)$$

Proving these estimates show that $\tilde{A}^{(2)}$ is bounded by the following argument

$$\begin{aligned} & \|(X - \mu + i)^{-1}\tilde{A}^{(2)}(X - \mu + i)^{-1}\| \\ &= \left\| \int_{\mathbb{R}^2} f(t_1)f(t_2)e^{i(Xt_1+Yt_2)/\Delta}(X - \mu + i)^{-1}[P_\gamma X Q_\gamma + Q_\gamma X P_\gamma, Y] \right. \\ & \quad \left. \cdot (X - \mu + i)^{-1}e^{-i(Xt_1+Yt_2)/\Delta} dt_1 dt_2 \right\| \\ &\leq \|(X - \mu + i)^{-1}[P_\gamma X Q_\gamma + Q_\gamma X P_\gamma, Y](X - \mu + i)^{-1}\| \left(\int_{\mathbb{R}} |f(t)| dt \right)^2 < \infty \end{aligned}$$

which proves Equation (4.12).

We will only prove Equation (4.20) in this section, Equation (4.21) follows by similar steps. Using that $P_\gamma Q_\gamma = Q_\gamma P_\gamma = 0$ we have that for any $\mu \in \mathbb{R}$:

$$\begin{aligned} [P_\gamma X Q_\gamma, Y] &= [P_\gamma(X - \mu)Q_\gamma, Y] \\ &= P_\gamma(X - \mu)Q_\gamma Y - Y P_\gamma(X - \mu)Q_\gamma \\ &= P_\gamma(X - \mu)[Q_\gamma, Y] + P_\gamma(X - \mu)Y Q_\gamma - [Y, P_\gamma](X - \mu)Q_\gamma - P_\gamma Y(X - \mu)Q_\gamma \end{aligned}$$

where in the last line we have commuted Q_γ and Y in the first term and P_γ and Y in the second term. Since $[Y, X - \mu] = 0$ we see that two of the terms above cancel so we get that:

$$[P_\gamma X Q_\gamma, Y] = P_\gamma(X - \mu)[Q_\gamma, Y] - [Y, P_\gamma](X - \mu)Q_\gamma$$

Hence we have that

$$\begin{aligned}
& \| (X - \mu + i)^{-1} [P_\gamma X Q_\gamma, Y] (X - \mu + i)^{-1} \| \\
&= \| (X - \mu + i)^{-1} (P_\gamma (X - \mu) [Q_\gamma, Y] - [Y, P_\gamma] (X - \mu) Q_\gamma) (X - \mu + i)^{-1} \| \\
&\leq \| (X - \mu + i)^{-1} P_\gamma (X - \mu) \| \| [Q_\gamma, Y] \| + \| [Y, P_\gamma] \| \| (X - \mu) Q_\gamma (X - \mu + i)^{-1} \|.
\end{aligned}$$

Due to Corollary 2.2.2(iii) we know that $\| [P_\gamma, Y] \| = \| [Q_\gamma, Y] \| < \infty$ hence to finish the bound, we only need to show that $\| (X - \mu + i)^{-1} P_\gamma (X - \mu) \|$ and $\| (X - \mu) Q_\gamma (X - \mu + i)^{-1} \|$ are both bounded. This is easy to see however since

$$\begin{aligned}
(X - \mu + i)^{-1} P_\gamma (X - \mu) &= (X - \mu + i)^{-1} [P_\gamma, X] + (X - \mu + i)^{-1} (X - \mu) P_\gamma \\
(X - \mu) Q_\gamma (X - \mu + i)^{-1} &= [X, Q_\gamma] (X - \mu + i)^{-1} + Q_\gamma (X - \mu) (X - \mu + i)^{-1}
\end{aligned}$$

which are both clearly bounded due to Corollary 2.2.2(iii). This proves Equation (4.12) completing the proof of Proposition 4.5.1.

4.6 $P\widehat{X}P$ has uniform spectral gaps

Let us begin this section by first noting that since PXP is essentially self-adjoint and $\|X - \widehat{X}\|$ is bounded (see Section 4.4), then that implies $P\widehat{X}P$ is essentially self-adjoint so the notion of uniform spectral gaps makes sense. In particular, we have the following easy lemma

Lemma 4.6.1. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 2$. Then $P\widehat{X}P$ is essentially self-adjoint.*

Proof. Recall the definitions of \tilde{X} and \widehat{X} :

$$\tilde{X} = \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| + QXQ \quad (4.6, \text{revisited})$$

$$\widehat{X} = \int_{\mathbb{R}^2} f(t_1) f(t_2) e^{i(Xt_1 + Yt_2)/\Delta} \tilde{X} e^{-i(Xt_1 + Yt_2)/\Delta} dt_1 dt_2. \quad (4.7, \text{revisited})$$

Since f is real valued and \tilde{X} is clearly a symmetric operator, it's easy to see that \widehat{X} is also a symmetric operator.

Next, notice that

$$P\widehat{X}P = PXP + P(\widehat{X} - X)P$$

We have shown previously that PXP is essentially self-adjoint under Assumption 3 (see Lemma 3.3.1). Since $\|P(\widehat{X} - X)P\| \leq \|\widehat{X} - X\|$ is bounded due to our proof from Section 4.4, by the Kato-Rellich theorem [RS75a, Theorem X.12], $P\widehat{X}P$ is essentially self-adjoint. \square

Having established essential self-adjointness, the main goal of this section is to prove the following proposition:

Proposition 4.6.2. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 5/2$. Next, define a set of gaps G as follows:*

$$G = \bigcup_{m \in \mathbb{Z}} \left(m + \frac{1}{4}, m + \frac{3}{4} \right). \quad (4.22)$$

If \widehat{X} is as defined in Equation (4.7) then for $\Delta > 0$ sufficiently large, $G \subseteq \rho(P\widehat{X}P)$. Hence for such a choice of Δ , $P\widehat{X}P$ has uniform spectral gaps.

The basic idea behind proving Proposition 4.6.2 is to pick some $\lambda \in G$ and consider $(\lambda - P\widehat{X}P)^{-1}$. Since by construction $\sigma(P\tilde{X}P) \subseteq \mathbb{Z}$ we can formally write:

$$\begin{aligned} (\lambda - P\widehat{X}P)^{-1} &= (\lambda - P\tilde{X}P + P\tilde{X}P - P\widehat{X}P)^{-1} \\ &= (\lambda - P\tilde{X}P)^{-1} \left(I - (P\widehat{X}P - P\tilde{X}P)(\lambda - P\tilde{X}P)^{-1} \right)^{-1}. \end{aligned}$$

If we can show that for some constant C

$$\|(P\widehat{X}P - P\tilde{X}P)(\lambda - P\tilde{X}P)^{-1}\| \leq C\Delta^{-1}, \quad (4.23)$$

then by picking $\Delta \geq (2C)^{-1}$ we have that

$$\begin{aligned} \|(\lambda - P\widehat{X}P)^{-1}\| &\leq \|(\lambda - P\tilde{X}P)^{-1}\| \left\| \left(I - (P\widehat{X}P - P\tilde{X}P)(\lambda - P\tilde{X}P)^{-1} \right)^{-1} \right\| \\ &\leq \left(\frac{1}{4} \right)^{-1} \left(1 - \frac{1}{2} \right)^{-1} = 8, \end{aligned}$$

where we have used that $\lambda \in G$ and $\sigma(P\tilde{X}P) \subseteq \mathbb{Z}$. Hence $\lambda \in \rho(P\hat{X}P)$.

While it is possible to prove the bound in Equation (4.23), we found proving this seems to require $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 3$. We can slightly improve this to $s > 5/2$ by introducing decay from the Green's function $(\lambda - P\tilde{X}P)^{-1}$ "symmetrically".

For this let us define the square root of $(\lambda - P\tilde{X}P)^{-1}$. Explicitly, for any $\lambda \in G$ we define S_λ as follows

$$S_\lambda := |\lambda|^{-1/2}Q + \sum_{m,n,j} |\lambda - m|^{-1/2} |\psi_{m,n}^{(j)}\rangle\langle\psi_{m,n}^{(j)}| \quad (4.24)$$

Note that by construction $[S_\lambda, P] = 0$.

Since $P + Q = I$ and the collection $\{\psi_{m,n}^{(j)}\}$ spans $\text{range}(P)$ we have that:

$$\begin{aligned} \lambda - P\tilde{X}P &= \lambda P + \lambda Q - \sum_{m,n,j} m |\psi_{m,n}^{(j)}\rangle\langle\psi_{m,n}^{(j)}| \\ &= \lambda Q + \sum_{m,n,j} (\lambda - m) |\psi_{m,n}^{(j)}\rangle\langle\psi_{m,n}^{(j)}|. \end{aligned}$$

A simple calculation shows that

$$S_\lambda(\lambda - P\tilde{X}P)S_\lambda = \frac{\lambda}{|\lambda|}Q + \sum_{m,n,j} \frac{\lambda - m}{|\lambda - m|} |\psi_{m,n}^{(j)}\rangle\langle\psi_{m,n}^{(j)}|.$$

Hence, since $\lambda \in \mathbb{R}$, $S_\lambda(\lambda - P\tilde{X}P)S_\lambda$ has eigenvalues ± 1 .

With this definition of S_λ we can now repeat similar steps to before to get

$$\begin{aligned} (\lambda - P\hat{X}P)^{-1} &= (\lambda - P\tilde{X}P + P\tilde{X}P - P\hat{X}P)^{-1} \\ &= S_\lambda \left(S_\lambda(\lambda - P\tilde{X}P)S_\lambda - S_\lambda(P\hat{X}P - P\tilde{X}P)S_\lambda \right)^{-1} S_\lambda. \end{aligned}$$

Therefore if we can show that

$$\|S_\lambda(P\hat{X}P - P\tilde{X}P)S_\lambda\| \leq C\Delta^{-1} \quad (4.25)$$

then by choosing $\Delta \geq (2C)$ the previous argument implies that $\lambda \in \rho(P\hat{X}P)$.

Let's start our proof of Equation (4.25) by considering the difference $P\widehat{X}P - P\widetilde{X}P$. Using the fact that $\int f = 1$ we have that

$$\begin{aligned} P\widehat{X}P - P\widetilde{X}P &= \int_{\mathbb{R}^2} f(t_1)f(t_2)Pe^{i(Xt_1+Yt_2)/\Delta}\widetilde{X}e^{-i(Xt_1+Yt_2)/\Delta}P dt_1 dt_2 - P\widetilde{X}P \\ &= \int_{\mathbb{R}^2} f(t_1)f(t_2)P \left(e^{i(Xt_1+Yt_2)/\Delta}\widetilde{X}e^{-i(Xt_1+Yt_2)/\Delta} - \widetilde{X} \right) P dt_1 dt_2. \end{aligned}$$

For the next few steps, let's define the difference in parenthesis as D :

$$D(t_1, t_2) := e^{i(Xt_1+Yt_2)/\Delta}\widetilde{X}e^{-i(Xt_1+Yt_2)/\Delta} - \widetilde{X}.$$

With this short-hand notation, we have that:

$$\|S_\lambda(P\widehat{X}P - P\widetilde{X}P)S_\lambda\| \leq \int_{\mathbb{R}^2} |f(t_1)||f(t_2)|\|S_\lambda PD(t_1, t_2)PS_\lambda\| dt_1 dt_2 \quad (4.26)$$

We will now use techniques similar to those used by Hastings [Has09] to control Equation (4.26). One important difference between the present work and previous work is that the operators X, Y, \widetilde{X} are not bounded. Despite this fact, due to the multiplication on the left and right by S_λ , we are able to control Equation (4.26) and prove a similar bound to the one proved in Hastings' work [Has09, Lemma 1].

Our first step of controlling Equation (4.26) will be exchange the decay provided by S_λ (which is diagonal in the basis $\{\psi_{m,n}^{(j)}\}$) for $\langle X - \lambda \rangle^{-1/2}$ (which is diagonal in the position basis). Formally, we calculate

$$\begin{aligned} &\|S_\lambda PD(t_1, t_2)PS_\lambda\| \\ &= \|S_\lambda P \langle X - \lambda \rangle^{1/2} \langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2} \langle X - \lambda \rangle^{1/2} PS_\lambda\| \\ &\leq \|S_\lambda P \langle X - \lambda \rangle^{1/2}\| \| \langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2} \| \| \langle X - \lambda \rangle^{1/2} PS_\lambda \| \end{aligned}$$

Intuitively speaking, we should expect that $\|S_\lambda P \langle X - \lambda \rangle^{1/2}\|$ and $\|\langle X - \lambda \rangle^{1/2} PS_\lambda\|$ are both bounded since S_λ is the square root of \widetilde{X} when restricted to $\text{range}(P)$ and X and \widetilde{X} differ by $O(1)$ in the spectral norm. Indeed, we have the following lemma:

Lemma 4.6.3. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finite degenerate centers which is s -localized for some $s > 2$. Then there exists a constant $C > 0$ such that for any $\lambda \in G$:*

$$\begin{aligned}\|S_\lambda P \langle X - \lambda \rangle^{1/2}\| &\leq C \\ \|\langle X - \lambda \rangle^{1/2} P S_\lambda\| &\leq C\end{aligned}$$

Proof. Given in Appendix A.8. □

Combining this lemma with the above calculation and Equation (4.26) we therefore conclude that

$$\begin{aligned}\|S_\lambda(P\hat{X}P - P\tilde{X}P)S_\lambda\| \\ \leq C^2 \int_{\mathbb{R}^2} |f(t_1)| |f(t_2)| \|\langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2}\| dt_1 dt_2\end{aligned}\tag{4.27}$$

For the next few steps, let us define the shorthand

$$\tilde{X}_b := \langle X - \lambda \rangle^{-1/2} \tilde{X} \langle X - \lambda \rangle^{-1/2}.\tag{4.28}$$

Since $\|\tilde{X} - X\| = O(1)$ it's easy to see that for a fixed value of λ , the operator \tilde{X}_b is bounded as an operator acting from $L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^2)$. The subscript b is intended to be suggestive of the fact that \tilde{X}_b is a *bounded* version of \tilde{X} .

We can write the quantity $\langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2}$ in terms of \tilde{X}_b by commuting $\langle X - \lambda \rangle^{-1/2}$ with $e^{i(Xt_1+Yt_2)/\Delta}$ and $e^{-i(Xt_1+Yt_2)/\Delta}$ as follows:

$$\begin{aligned}\langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2} \\ = \langle X - \lambda \rangle^{-1/2} \left(e^{i(Xt_1+Yt_2)/\Delta} \tilde{X} e^{-i(Xt_1+Yt_2)/\Delta} - \tilde{X} \right) \langle X - \lambda \rangle^{-1/2} \\ = e^{i(Xt_1+Yt_2)/\Delta} \tilde{X}_b e^{-i(Xt_1+Yt_2)/\Delta} - \tilde{X}_b.\end{aligned}$$

Therefore, defining $A(t_1, t_2)$ as

$$A(t_1, t_2) = e^{i(Xt_1+Yt_2)/\Delta} \tilde{X}_b e^{-i(Xt_1+Yt_2)/\Delta}$$

we see that by definition

$$\langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2} = A(t_1, t_2) - A(0, 0).$$

We now state an important proposition regarding \tilde{X}_b :

Proposition 4.6.4. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 5/2$. Then for any $\lambda \in G$ there exists a finite constant $C > 0$ such that*

$$\begin{aligned} \|[X, \tilde{X}_b]\| &= \|\langle X - \lambda \rangle^{-1/2} [X, \tilde{X}] \langle X - \lambda \rangle^{-1/2}\| \leq C, \\ \|[Y, \tilde{X}_b]\| &= \|\langle X - \lambda \rangle^{-1/2} [Y, \tilde{X}] \langle X - \lambda \rangle^{-1/2}\| \leq C. \end{aligned} \tag{4.29}$$

Proof. Given in Appendix A.9. □

With this proposition in mind, for any $\phi \in C_c^\infty(\mathbb{R}^2)$ we differentiate $A(t_1, t_2)\phi$ with respect to t_1 to get:

$$\begin{aligned} \partial_{t_1} A(t_1, t_2)\phi &= i\Delta^{-1} e^{i(Xt_1 + Yt_2)/\Delta} (X\tilde{X}_b - \tilde{X}_b X) e^{-i(Xt_1 + Yt_2)/\Delta} \phi \\ &= i\Delta^{-1} e^{i(Xt_1 + Yt_2)/\Delta} [X, \tilde{X}_b] e^{-i(Xt_1 + Yt_2)/\Delta} \phi. \end{aligned}$$

This differentiation step is justified for any $\phi \in C_c^\infty(\mathbb{R}^2)$ since $\tilde{X}_b X$ and $X\tilde{X}_b$ are both bounded operators on $C_c^\infty(\mathbb{R}^2)$. The fact that $\tilde{X}_b X$ is bounded is clear since X is bounded on $C_c^\infty(\mathbb{R}^2)$ and \tilde{X}_b , as defined in (4.28), is a bounded operator. The fact that $X\tilde{X}_b$ is bounded follows from the identity $X\tilde{X}_b = [X, \tilde{X}_b] + \tilde{X}_b X$ which is bounded due to Proposition 4.6.4.

An analogous argument shows that

$$\partial_{t_2} A(t_1, t_2)\phi = i\Delta^{-1} e^{i(Xt_1 + Yt_2)/\Delta} [Y, \tilde{X}_b] e^{-i(Xt_1 + Yt_2)/\Delta} \phi.$$

Due to Proposition 4.6.4, it's easy to check that both $\partial_{t_1} A(t_1, t_2)\phi$ and $\partial_{t_2} A(t_1, t_2)\phi$ are continuous functions of t_1, t_2 so we can apply mean value theorem to conclude

there exists a $(c_1, c_2) \in [0, t_1] \times [0, t_2]$ so that:

$$\begin{aligned} \|(A(t_1, t_2) - A(0))\phi\| &\leq \Delta^{-1}|c_1| \|e^{i(Xc_1+Yc_2)/\Delta}[X, \tilde{X}_b]e^{-i(Xc_1+Yc_2)/\Delta}\phi\| \\ &\quad + \Delta^{-1}|c_2| \|e^{i(Xc_1+Yc_2)/\Delta}[Y, \tilde{X}_b]e^{-i(Xc_1+Yc_2)/\Delta}\phi\| \\ &\leq \Delta^{-1} \left(|t_1| \| [X, \tilde{X}_b] \| + |t_2| \| [Y, \tilde{X}_b] \| \right) \|\phi\| \end{aligned}$$

Since $C_c^\infty(\mathbb{R}^2)$ is dense in $L^2(\mathbb{R}^2)$, this implies that there exists a finite constant C so that

$$\|\langle X - \lambda \rangle^{-1/2} D(t_1, t_2) \langle X - \lambda \rangle^{-1/2}\| \leq C \Delta^{-1} (|t_1| + |t_2|).$$

Hence, substituting this bound into Equation (4.27), we have that

$$\begin{aligned} &\|S_\lambda(P\hat{X}P - P\tilde{X}P)S_\lambda\| \\ &\leq C \Delta^{-1} \int_{\mathbb{R}^2} |f(t_1)| |f(t_2)| (|t_1| + |t_2|) dt_1 dt_2 \\ &\leq C' \Delta^{-1}, \end{aligned}$$

where to get the last line we have used the fact that by construction $f(t), tf(t) \in L^1(\mathbb{R})$. This completes the proof of Proposition 4.6.2 and hence establishes that for Δ sufficiently large $P\hat{X}P$ has uniform spectral gaps.

4.7 The Band Projectors for $P\hat{X}P$ Satisfy the Assumptions of Theorem 4

Over the past few sections, we have proved a number of important properties of the operator \hat{X} . In particular we have shown that:

1. \hat{X} is close to X (Section 4.4)

$$\|\hat{X} - X\| = O(1)$$

2. \hat{X} is exponentially localized (Section 4.5)

$$(a) \quad \|\widehat{X}_\gamma - \widehat{X}\| = O(\gamma)$$

$$(b) \quad \forall \mu \in \mathbb{R}, \|(X - \mu + i)^{-1}[\widehat{X}_\gamma, Y](X - \mu + i)^{-1}\| = O(1)$$

3. $P\widehat{X}P$ has uniform spectral gaps (Section 4.6)

$$\bigcup_{m \in \mathbb{Z}} \left(m + \frac{1}{4}, m + \frac{3}{4} \right) \subseteq \rho(P\widehat{X}P)$$

Our next step will be to use all of these properties to show that if $\{P_j\}_{j \in \mathbb{Z}}$ are the band projectors for $P\widehat{X}P$, then these projectors satisfy the assumptions of Theorem 4.

First, due to the fact that $P\widehat{X}P$ has uniform spectral gaps, we can define the orthogonal projection P_j by the Riesz formula

$$P_j := \frac{1}{2\pi i} P \left(\int_{\mathcal{C}_j} (\lambda - P\widehat{X}P)^{-1} d\lambda \right) P \quad (4.30)$$

where the contour \mathcal{C}_j is chosen so that \mathcal{C}_j encloses the integer j and avoids $\sigma(P\widehat{X}P)$. We will assume without loss of generality that the contour \mathcal{C}_j is chosen so that for all $j \in \mathbb{Z}$ if $\lambda \in \mathcal{C}_j$ then $|\lambda - j| \leq 1$. We can assume this without loss of generality due to the characterization of $\rho(P\widehat{X}P)$ proven in Section 4.6.

As a technical note, the addition of P in the definition of P_j makes it so that $\text{range}(P_j) \subseteq \text{range}(P)$ for all $j \in \mathbb{Z}$ and ensures that $\sum_j P_j = P$. Since P is a projection, we know that $[P\widehat{X}P, P] = 0$ and hence P_j can be equivalently defined as

$$P_j := \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P\widehat{X}P)^{-1} P d\lambda. \quad (4.31)$$

The most technically involved part of showing that P_j satisfies the estimates of Theorem 4 is showing that the resolvent $(\lambda - P\widehat{X}P)^{-1}$ is exponentially localized in following sense:

Proposition 4.7.1. *Suppose that P satisfies decay estimates as in Assumption 3. There exists finite, positive constants (C_1, γ^*) such that for all $0 \leq \gamma \leq \gamma^*$, all $j \in \mathbb{Z}$, and all $\lambda \in \mathcal{C}_j$ we have*

$$\|B_\gamma(\lambda - P\widehat{X}P)^{-1}B_\gamma^{-1}\| = \|(\lambda - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1}\| \leq C_1$$

Once we prove Proposition 4.7.1, we can then prove that P_j satisfies the assumptions of Theorem 4. More specifically, we can show that there exists finite, positive constants (C_1, C_2, C_3, C_4) such that for all j , P_j satisfies the following estimates for all γ sufficiently small:

$$\|P_{j,\gamma} - P_j\| \leq C_2\gamma \tag{4.32a}$$

$$\|[P_{j,\gamma}, Y]\| \leq C_3 \tag{4.32b}$$

$$\|P_{j,\gamma}(X - j)\| \leq C_4 \tag{4.32c}$$

$$\|(X - j)P_{j,\gamma}\| \leq C_4 \tag{4.32d}$$

It is important to note that the constants (C_1, C_2, C_3, C_4) from Proposition 4.7.1 and Equation (4.32) are *independent* of the choice j . While the tools from Chapter 3 allows one to prove these bounds uniformly in j , there are a few subtle technical issues which arise as part of these proofs. For clarity of presentation, in the next few sections we will prove Proposition 4.7.1 and Equation (4.32) for $j = 0$ only. We will then return to discuss the modifications needed to prove the bounds uniformly for $j \neq 0$ in Section 4.7.6.

The remainder of this section is structured as follows. We begin by proving an important technical lemma in Section 4.7.1. We then make use of this lemma in Section 4.7.2 to prove Proposition 4.7.1 for $j = 0$. After proving this proposition, we will prove Equation (4.32a) in Section 4.7.3, Equation (4.32b) in Section 4.7.4, and Equations (4.32c) and (4.32d) in Section 4.7.5 (all for $j = 0$). Finally, in Section 4.7.6, we will show how to generalize the previous proofs to $j \neq 0$. Once we have shown all of these estimates, Theorem 4 then implies Theorem 5 completing the proof of our main theorem.

4.7.1 Projected Position Operators and Their Resolvents

Over the next few sections, we will perform a simple calculation which we will repeat multiple times. Instead of repeating this calculation each time, in this section, we

will show this calculation in detail with an illustrative example. We will then state a technical lemma (Lemma 4.7.2) which extracts the essence of the calculation at the end of this section.

For our illustrative example we will show how to bound the following for $\lambda \in \mathcal{C}_j$ when $j = 0$:

$$XP(\lambda - P\widehat{X}P)^{-1}. \quad (4.33)$$

Intuitively, $XP(\lambda - P\widehat{X}P)^{-1}$ should be bounded since \widehat{X} is close to X and $(\lambda - P\widehat{X}P)^{-1}$ “inverts” \widehat{X} on $\text{range}(P)$.

Formally, we calculate

$$\begin{aligned} & \|XP(\lambda - P\widehat{X}P)^{-1}\| \\ &= \|(X - \widehat{X} + \widehat{X})P(\lambda - P\widehat{X}P)^{-1}\| \\ &\leq \|X - \widehat{X}\| \|(\lambda - P\widehat{X}P)^{-1}\| + \|\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\|. \end{aligned}$$

Since we know that $\|X - \widehat{X}\| = O(1)$, to show that Equation (4.33) is bounded we only need to show that $\widehat{X}P(\lambda - P\widehat{X}P)^{-1}$ is bounded.

Using the fact that $I = Q + P$ we have that

$$\begin{aligned} & \|\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| \\ &= \|(Q + P)\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| \\ &\leq \|Q\widehat{X}P\| \|(\lambda - P\widehat{X}P)^{-1}\| + \|P\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| \end{aligned}$$

The first of these two terms is bounded since $\|(\lambda - P\widehat{X}P)^{-1}\|$ is bounded and

$$\begin{aligned} \|Q\widehat{X}P\| &\leq \|Q(\widehat{X} - X)P\| + \|QXP\| \\ &\leq \|\widehat{X} - X\| + \|QXP\| \end{aligned}$$

where $\|QXP\|$ is bounded by Corollary 2.2.2(ii) with $\gamma = 0$. Finally $P\widehat{X}P(\lambda -$

$P\widehat{X}P)^{-1}$ is bounded since

$$\begin{aligned}
\|P\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| &= \|(P\widehat{X}P - \lambda + \lambda)(\lambda - P\widehat{X}P)^{-1}\| \\
&= \|-I + \lambda(\lambda - P\widehat{X}P)^{-1}\| \\
&\leq 1 + |\lambda| \|(\lambda - P\widehat{X}P)^{-1}\|. \tag{4.34}
\end{aligned}$$

The final bound in Equation (4.34) illustrates the importance of our choice of $\lambda \in \mathcal{C}_j$ where $j = 0$. Since $\lambda \in \mathcal{C}_0$, by construction we know that $|\lambda| = |\lambda - 0| \leq 1$. Therefore,

$$\|P\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| \leq 1 + \|(\lambda - P\widehat{X}P)^{-1}\|$$

which is a constant *independent* of the choice of j . If we were considering $j \neq 0$, then typically we would have that $|\lambda| \gg 1$ which would prevent us from having a uniform bound. As mentioned previously, we will modify the argument in Section 4.7.6 to make it work for $j \neq 0$.

From this calculation, we conclude that $XP(\lambda - P\widehat{X}P)^{-1}$ is bounded by a constant only depending on $\|QXP\|$, $\|X - \widehat{X}\|$, and the gap size of $P\widehat{X}P$. By repeating this calculation multiple times using our decay estimates on P (Assumption 3 and Corollary 2.2.2), we have the following lemma:

Lemma 4.7.2. *Suppose that P is a projector satisfying decay estimates as in Assumption 3. There exists finite, positive constants (C_1, C_2, C_3, C_4) such that for all $\lambda \in \mathcal{C}_j$ where $j = 0$:*

- (i) $\|(\lambda - P\widehat{X}P)^{-1}P\widehat{X}\| \leq C_1$
- (ii) $\|\widehat{X}P(\lambda - P\widehat{X}P)^{-1}\| \leq C_2$
- (iii) $\|(\lambda - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1}P_\gamma\widehat{X}_\gamma\| \leq C_3$
- (iv) $\|(\lambda - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1}P_\gamma X\| \leq C_4$

4.7.2 Proof of Proposition 4.7.1

The main goal of this section is to show that there exists a finite, positive constant C such that for $j = 0$ we have:

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \leq C.$$

This bound is proved by the following chain of implications which hold for all $\lambda \in \mathcal{C}_j$ (where USG is an abbreviation for uniform spectral gaps):

$$\begin{aligned} P\widehat{X}P \text{ has USG} &\implies \|(\lambda - P\widehat{X}P)^{-1}\| < \infty \implies \|(\lambda - P\widehat{X}P_\gamma)^{-1}\| < \infty \\ &\implies \|(\lambda - P_\gamma \widehat{X} P_\gamma)^{-1}\| < \infty \implies \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| < \infty. \end{aligned} \quad (4.35)$$

In words, since $P\widehat{X}P$ has uniform spectral gaps, we know that $\|(\lambda - P\widehat{X}P)^{-1}\| < \infty$ for all $\lambda \in \mathcal{C}_j$. Using this fact, along with our previous estimates on P and \widehat{X} , we can conclude that $\|(\lambda - P\widehat{X}P_\gamma)^{-1}\| < \infty$ for all γ sufficiently small. Once we know that $(\lambda - P\widehat{X}P_\gamma)^{-1}$ is bounded, we can use that estimate to show that $(\lambda - P_\gamma \widehat{X} P_\gamma)^{-1}$ is bounded for all γ sufficiently small. Finally, once we know that $(\lambda - P_\gamma \widehat{X} P_\gamma)^{-1}$ is bounded, we can show that $(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}$ is bounded, finishing the proof of the proposition. These steps will be detailed below.

Bounding $\|(\lambda - P\widehat{X}P_\gamma)^{-1}\|$

We start by performing a formal calculation. Adding and subtracting $P\widehat{X}P$ in the resolvent we want to bound gives that:

$$\begin{aligned} (\lambda - P\widehat{X}P_\gamma)^{-1} &= (\lambda - P\widehat{X}P + P\widehat{X}P - P\widehat{X}P_\gamma)^{-1} \\ &= \left((\lambda - P\widehat{X}P) - P\widehat{X}(P_\gamma - P) \right)^{-1} \\ &= \left(I - (\lambda - P\widehat{X}P)^{-1} P\widehat{X}(P_\gamma - P) \right)^{-1} (\lambda - P\widehat{X}P)^{-1}. \end{aligned}$$

Now observe that

$$\begin{aligned} &\|(\lambda - P\widehat{X}P)^{-1} P\widehat{X}(P_\gamma - P)\| \\ &\leq \|(\lambda - P\widehat{X}P)^{-1} P\widehat{X}\| \|P_\gamma - P\|. \end{aligned}$$

Due to Lemma 4.7.2(i), we know that $(\lambda - P\widehat{X}P)^{-1}P\widehat{X}$ is bounded. We also know that $\|P_\gamma - P\| = O(\gamma)$ by Assumption 3(i) and thus we can pick γ sufficiently small so that

$$\|(\lambda - P\widehat{X}P)^{-1}P\widehat{X}(P_\gamma - P)\| \leq \frac{1}{2}.$$

Therefore, by Neumann series we conclude that for all γ sufficiently small

$$\begin{aligned} \|(\lambda - P\widehat{X}P_\gamma)^{-1}\| &\leq \left\| \left(I - (\lambda - P\widehat{X}P)^{-1}P\widehat{X}(P_\gamma - P) \right)^{-1} (\lambda - P\widehat{X}P)^{-1} \right\| \\ &\leq \left(1 - \frac{1}{2} \right)^{-1} \|(\lambda - P\widehat{X}P)^{-1}\| \end{aligned}$$

which is bounded by a constant due to the fact that $P\widehat{X}P$ has uniform spectral gaps and the choice of λ .

Bounding $\|(\lambda - P_\gamma\widehat{X}P_\gamma)^{-1}\|$

Now that we've shown that $(\lambda - P\widehat{X}P_\gamma)^{-1}$ is bounded, we can bound $(\lambda - P_\gamma\widehat{X}P_\gamma)^{-1}$.

Performing similar formal calculations to before

$$\begin{aligned} (\lambda - P_\gamma\widehat{X}P_\gamma)^{-1} &= (\lambda - P\widehat{X}P_\gamma + P\widehat{X}P_\gamma - P_\gamma\widehat{X}P_\gamma)^{-1} \\ &= \left((\lambda - P\widehat{X}P_\gamma) - (P_\gamma - P)\widehat{X}P_\gamma \right)^{-1} \\ &= (\lambda - P\widehat{X}P_\gamma)^{-1} \left(I - (P_\gamma - P)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} \right)^{-1}. \end{aligned}$$

Similar to before, we will want to show that $\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}$ is bounded by a constant and use that $\|P_\gamma - P\| = O(\gamma)$ to conclude that $(\lambda - P_\gamma\widehat{X}P_\gamma)^{-1}$ is bounded for all γ sufficiently small. Unfortunately, the calculation used to prove Lemma 4.7.2 does *not* apply here. It turns out however that a slight modification of the calculation which proves Lemma 4.7.2 allows us to show that $\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}$ is bounded.

First, let us define the shorthand $E := P_\gamma - P = Q - Q_\gamma$. Observe that

$$Q - Q_\gamma = E \Rightarrow Q = E + Q_\gamma.$$

Using the fact that $I = P + Q$ we have that

$$\begin{aligned}
& \widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} \\
&= (P + Q)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} \\
&= (P + Q_\gamma + E)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} \\
&= (P + Q_\gamma)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} + E\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}
\end{aligned}$$

Moving the term multiplied by E to the left hand side then gives that:

$$\begin{aligned}
(I - E)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} &= (P + Q_\gamma)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} \\
\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1} &= (I - E)^{-1}(P + Q_\gamma)\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}.
\end{aligned}$$

Note that since $\|E\| = \|P_\gamma - P\| = O(\gamma)$, we can pick γ sufficiently small so that $\|(I - E)^{-1}\|$ is bounded. Therefore, taking norms on both sides gives that

$$\begin{aligned}
& \|\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}\| \\
& \leq \|(I - E)^{-1}\| \left(\|P\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}\| + \|Q_\gamma\widehat{X}P_\gamma\| \|(\lambda - P\widehat{X}P_\gamma)^{-1}\| \right)
\end{aligned}$$

This final equation can be easily be seen to be bounded by constant by observing that

$$\begin{aligned}
\|P\widehat{X}P_\gamma(\lambda - P\widehat{X}P_\gamma)^{-1}\| &\leq 1 + |\lambda| \|(\lambda - P\widehat{X}P_\gamma)^{-1}\| \\
\|Q_\gamma\widehat{X}P_\gamma\| &\leq \|Q_\gamma(X - \widehat{X})P_\gamma\| + \|Q_\gammaXP_\gamma\|
\end{aligned}$$

and Corollary 2.2.2(i,ii). Notice again, we require that $\lambda \in \mathcal{C}_j$ for $j = 0$ to conclude that $|\lambda| \leq 1$ which is a constant independent of j .

Bounding $\|(\lambda - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1}\|$

Now that we've shown $(\lambda - P_\gamma\widehat{X}P_\gamma)^{-1}$ is bounded, we can finally finish the proof of Proposition 4.7.1. Similar to before, we have that

$$\begin{aligned}
(\lambda - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1} &= (\lambda - P_\gamma\widehat{X}P_\gamma + P_\gamma\widehat{X}P_\gamma - P_\gamma\widehat{X}_\gamma P_\gamma)^{-1} \\
&= \left((\lambda - P_\gammaXP_\gamma) - P_\gamma(\widehat{X}_\gamma - \widehat{X})P_\gamma \right)^{-1} \\
&= \left(I - (\lambda - P_\gammaXP_\gamma)^{-1}P_\gamma(\widehat{X}_\gamma - \widehat{X})P_\gamma \right)^{-1} (\lambda - P_\gammaXP_\gamma)^{-1}.
\end{aligned}$$

Since

$$\|P_\gamma(\widehat{X}_\gamma - \widehat{X})P_\gamma\| \leq \|P_\gamma\|^2 \|\widehat{X}_\gamma - \widehat{X}\|$$

and in Section 4.5 we showed that $\|\widehat{X}_\gamma - \widehat{X}\| = O(\gamma)$, we can choose γ sufficiently small so that

$$\|(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma (\widehat{X}_\gamma - \widehat{X}) P_\gamma\| \leq \frac{1}{2}$$

and hence for all γ sufficiently small

$$(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \leq \left(1 - \frac{1}{2}\right)^{-1} \|(\lambda - P_\gamma X P_\gamma)^{-1}\|.$$

Combined with the chain of implications in Equation (4.35), we conclude that (for $j = 0$)

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma\| < \infty$$

which finishes the proof of Proposition 4.7.1.

4.7.3 Proof of Equation (4.32a)

Similar to the previous section, let us define the shorthand $E := P_\gamma - P$. We begin by writing down the definition of $P_{j,\gamma}$ and P_j as contour integrals

$$\begin{aligned} P_{j,\gamma} - P_j &= \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma - (\lambda - P \widehat{X} P)^{-1} P \, d\lambda \\ &= \frac{1}{2\pi i} \int_{\mathcal{C}_j} \left((\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} - (\lambda - P \widehat{X} P)^{-1} \right) P_\gamma + (\lambda - P \widehat{X} P)^{-1} E \, d\lambda \end{aligned}$$

Taking norms of both sides then gives that:

$$\begin{aligned} \|P_{j,\gamma} - P_j\| &\leq \frac{\ell(\mathcal{C}_j)}{2\pi} \sup_{\lambda \in \mathcal{C}_j} \left(\|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} - (\lambda - P \widehat{X} P)^{-1}\| \|P_\gamma\| + \|(\lambda - P \widehat{X} P)^{-1}\| \|E\| \right). \end{aligned}$$

Since $\lambda \in \mathcal{C}_j$ and $\|E\| = O(\gamma)$, we know that $\|(\lambda - P \widehat{X} P)^{-1}\| \|E\| = O(\gamma)$. Therefore, to finish the proof of Equation (4.32a) we only need to show the first term is $O(\gamma)$.

Applying the second resolvent identity gives

$$\begin{aligned} & (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} - (\lambda - P \widehat{X} P)^{-1} \\ &= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} (P_\gamma \widehat{X}_\gamma P_\gamma - P \widehat{X} P) (\lambda - P \widehat{X} P)^{-1}. \end{aligned}$$

Next, adding and subtracting various terms gives

$$\begin{aligned} & (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} (P_\gamma \widehat{X}_\gamma P_\gamma - P \widehat{X} P) (\lambda - P \widehat{X} P)^{-1} \\ &= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \left(P_\gamma \widehat{X}_\gamma P_\gamma - (P_\gamma \widehat{X}_\gamma P + P_\gamma \widehat{X}_\gamma P) - P \widehat{X} P \right) (\lambda - P \widehat{X} P)^{-1} \\ &= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \left(P_\gamma \widehat{X}_\gamma E + P_\gamma \widehat{X}_\gamma P + (P_\gamma \widehat{X} P - P_\gamma \widehat{X} P) - P \widehat{X} P \right) (\lambda - P \widehat{X} P)^{-1} \\ &= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} (P_\gamma \widehat{X}_\gamma E + P_\gamma (\widehat{X}_\gamma - \widehat{X}) P + E \widehat{X} P) (\lambda - P \widehat{X} P)^{-1} \end{aligned}$$

The middle term, $P_\gamma (\widehat{X}_\gamma - \widehat{X}) P$ is clearly $O(\gamma)$ since we know that $\|\widehat{X}_\gamma - \widehat{X}\| = O(\gamma)$. Since $\|E\| = O(\gamma)$ to finish the lemma we only need to show that

$$\begin{aligned} & (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma \widehat{X}_\gamma \\ & \widehat{X} P (\lambda - P \widehat{X} P)^{-1} \end{aligned}$$

are both bounded operators. But we already argued that these quantities are bounded in Lemma 4.7.2(ii,iii). Hence Equation (4.32a) is proved.

4.7.4 Proof of Equation (4.32b)

We begin this proof by writing $P_{j,\gamma}$ in terms of its contour integral and taking operator norms:

$$\begin{aligned} \|[P_{j,\gamma}, Y]\| &= \left\| \left[\left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma d\lambda \right), Y \right] \right\| \\ &\leq \frac{\ell(\mathcal{C}_j)}{2\pi} \sup_{\lambda \in \mathcal{C}_j} \|[(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma, Y]\|. \end{aligned}$$

Therefore, to prove Equation (4.32b) it's enough to show that $[(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma, Y]$ is bounded. Expanding this commutator and using the fact that $[(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}, P_\gamma] =$

0, we have that

$$\begin{aligned}
& [(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma, Y] \\
&= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma Y - Y (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma \\
&= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma Y - Y P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \\
&= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma Y (P_\gamma + Q_\gamma) - (P_\gamma + Q_\gamma) Y P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \\
&= [(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}, P_\gamma Y P_\gamma] \\
&\quad + (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma Y Q_\gamma - Q_\gamma Y P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}
\end{aligned}$$

Due to Corollary 2.2.2(ii) we know that $Q_\gamma Y P_\gamma$ and $P_\gamma Y Q_\gamma$ are both bounded. Since $(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}$ is also bounded, we therefore only need to control the first term. A standard commutator identity shows that:

$$\begin{aligned}
& [(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}, P_\gamma Y P_\gamma] \\
&= (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} [P_\gamma \widehat{X}_\gamma P_\gamma, P_\gamma Y P_\gamma] (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}
\end{aligned} \tag{4.36}$$

Now we can rewrite the commutator $[P_\gamma \widehat{X}_\gamma P_\gamma, P_\gamma Y P_\gamma]$ as follows:

$$\begin{aligned}
[P_\gamma \widehat{X}_\gamma P_\gamma, P_\gamma Y P_\gamma] &= P_\gamma \widehat{X}_\gamma P_\gamma Y P_\gamma - P_\gamma Y P_\gamma \widehat{X}_\gamma P_\gamma \\
&= P_\gamma \widehat{X}_\gamma (I - Q_\gamma) Y P_\gamma - P_\gamma Y (I - Q_\gamma) \widehat{X}_\gamma P_\gamma \\
&= P_\gamma [\widehat{X}_\gamma, Y] P_\gamma - P_\gamma \widehat{X}_\gamma Q_\gamma Y P_\gamma + P_\gamma Y Q_\gamma \widehat{X}_\gamma P_\gamma
\end{aligned}$$

Substituting this identity back into Equation (4.36) and taking norms then gives that

$$\begin{aligned}
& \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} [P_\gamma \widehat{X}_\gamma P_\gamma, P_\gamma Y P_\gamma] (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \\
&\leq \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma [\widehat{X}_\gamma, Y] P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \\
&\quad + \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\|^2 \|P_\gamma \widehat{X}_\gamma Q_\gamma\| \|Q_\gamma Y P_\gamma\| \\
&\quad + \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\|^2 \|P_\gamma Y Q_\gamma\| \|Q_\gamma \widehat{X}_\gamma P_\gamma\|.
\end{aligned} \tag{4.37}$$

The last two terms can easily be seen to be bounded using Corollary 2.2.2. In particular,

$$\begin{aligned}
\|P_\gamma \widehat{X}_\gamma Q_\gamma\| &= \|P_\gamma (\widehat{X}_\gamma - \widehat{X} + \widehat{X} - X + X) Q_\gamma\| \\
&\leq \|P_\gamma\| \|\widehat{X}_\gamma - \widehat{X}\| \|Q_\gamma\| + \|P_\gamma\| \|\widehat{X} - X\| \|Q_\gamma\| + \|P_\gamma X Q_\gamma\|.
\end{aligned}$$

Hence, since we've shown that $\|\widehat{X}_\gamma - \widehat{X}\| = O(\gamma)$, $\|\widehat{X} - X\| = O(1)$, and Corollary 2.2.2(i,ii), we conclude that the last two terms in (4.37) are bounded. Therefore, to finish the proof of this lemma we only need to bound the first term in (4.37).

To bound this term, we will appeal to one of the bounds proven in Section 4.5. In particular, in that section we showed that (Equation (4.12)) for any $\mu \in \mathbb{R}$ we have that

$$\|(X - \mu + i)^{-1}[\widehat{X}_\gamma, Y](X - \mu + i)^{-1}\| < \infty \quad (4.12, \text{revisited})$$

Now let's recall the quantity we want to bound

$$(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma [\widehat{X}_\gamma, Y] P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}.$$

Our first step will be to exchange the decay provided by $(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}$ for $(X - \mu + i)^{-1}$ so that we can apply Equation (4.12). To perform this exchange, observe that for any $\mu \in \mathbb{R}$:

$$(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma = (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma (X - \mu + i)(X - \mu + i)^{-1}.$$

Now for any $\mu \in \mathbb{R}$ we have

$$\begin{aligned} & \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma (X - \mu + i)\| \\ & \leq \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma (X - \mu)\| + \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \|P_\gamma\|. \end{aligned}$$

Choosing $\mu = j = 0$ and appealing to Lemma 4.7.2 we conclude there exists a constant C so that

$$\|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma (X + i)\| \leq C.$$

Similarly,

$$\|(X + i) P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \leq C$$

Hence,

$$\begin{aligned}
& \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma [\widehat{X}_\gamma, Y] P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \\
&= \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma (X + i) (X + i)^{-1} [\widehat{X}_\gamma, Y] P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1}\| \\
&\leq C \| (X + i)^{-1} [\widehat{X}_\gamma, Y] P_\gamma (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} \| \\
&\leq C^2 \| (X + i)^{-1} [\widehat{X}_\gamma, Y] (X + i)^{-1} \|
\end{aligned}$$

where to get the last line we have inserted $(X + i)^{-1}(X + i)$ on the right as we did on the left. This final line is bounded due to Equation (4.12), completing the proof of Equation (4.32b).

4.7.5 Proof of Equations (4.32c) and (4.32d)

Since we are considering the special case where $j = 0$, the quantity to show are bounded are $P_{j,\gamma} X$ and $X P_{j,\gamma}$. We only show $\|P_{j,\gamma} X\|$ is bounded, the other bound follows via a similar argument. Writing $P_{j,\gamma}$ in terms of its contour integral gives

$$\begin{aligned}
\|P_{j,\gamma} X\| &= \left\| \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma X \, d\lambda \right\| \\
&\leq \frac{\ell(\mathcal{C}_j)}{2\pi} \sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma X\|
\end{aligned}$$

But $\|(\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma X\|$ is bounded due to Lemma 4.7.2. This completes the proof of Equations (4.32c) and (4.32d).

4.7.6 The Shifting Lemma Revisited

In this section, we review some of the tools which were proven in Appendix A.3 to prove Proposition 4.7.1 and Equation (4.32) with bounds *independent* of the choice j . The key trick is the following simple calculation. Suppose that $\lambda \in \mathcal{C}_j$ for some

$j \neq 0$. We have that

$$\begin{aligned}
(\lambda - P\widehat{X}P)^{-1} &= \left((\lambda - j + j) - P(\widehat{X} - j + j)P \right)^{-1} \\
&= \left((\lambda - j) - P(\widehat{X} - j)P + j(I - P) \right)^{-1} \\
&= \left((\lambda - j) - P(\widehat{X} - j)P + jQ \right)^{-1}
\end{aligned}$$

Now since $PQ = QP = 0$ it can be shown that

$$\begin{aligned}
(\lambda - P\widehat{X}P)^{-1}P &= \left((\lambda - j) - P(\widehat{X} - j)P + jQ \right)^{-1}P \\
&= \left((\lambda - j) - P(\widehat{X} - j)P \right)^{-1}P
\end{aligned} \tag{4.38}$$

Through this trick, we are able to effectively “shift down” the contour \mathcal{C}_j by j . More precisely, using this calculation, in Appendix A.3 we proved the following lemma:

Lemma A.2.5 (Shifting Lemma). *Suppose P satisfies decay estimates as in Assumption 3 and suppose that PXP has uniform spectral gaps with decomposition $\{\sigma_j\}_{j \in \mathbb{Z}}$. For arbitrary $\eta \in \mathbb{C}$, define $\lambda_\eta := \lambda - \eta$ and $X_\eta := X - \eta$. Then the following are equivalent for all γ sufficiently small:*

1. *There exists a $C > 0$, independent of j , such that*

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \leq C$$

2. *There exists a $C' > 0$, independent of j , such that*

$$\sup_{\lambda \in \mathcal{C}_j} \sup_{\eta \in \sigma_j} \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \leq C'$$

Furthermore, if $\|(\lambda - P_\gamma X P_\gamma)^{-1}\|$ is bounded we have for any $j \in \mathbb{Z}$ and $\eta \in \sigma(PXP)$:

$$(\lambda - P_\gamma X P_\gamma)^{-1}P_\gamma = (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}P_\gamma.$$

Since the proof of Lemma A.2.5 only relies on the shifting calculation in Equation (4.38), Lemma A.2.5 also holds if we replace X with \widehat{X} . Choosing $\eta = j$ we have

that by the lemma for all γ sufficiently small

$$\begin{aligned} P_{j,\gamma} &= \int_{\mathcal{C}_j} (\lambda - P_\gamma \widehat{X}_\gamma P_\gamma)^{-1} P_\gamma d\lambda \\ &= \int_{\mathcal{C}_j} \left((\lambda - j) - P_\gamma (\widehat{X}_\gamma - j) P_\gamma \right)^{-1} P_\gamma d\lambda \end{aligned}$$

By replacing λ with $\lambda - j$ and \widehat{X} with $\widehat{X} - j$ in all of the arguments in Sections 4.7.2, 4.7.3, 4.7.4, 4.7.5 it can be checked that instead of a dependence on $|\lambda|$ we have a dependence $|\lambda - j|$ which is bounded by the construction of \mathcal{C}_j . Therefore, we conclude that Proposition 4.7.1 and Equation (4.32) holds with constants uniform in j proving the main theorem.

Chapter 5

Conclusions and Future Work

In Chapter 3, we introduced and proved the correctness of an algorithm for constructing exponentially localized Wannier functions in insulating materials in two dimensions (with clear extensions to higher dimension). Our proof of correctness in this chapter fundamentally relies on the assumption that the projected position operator PXP has uniform spectral gaps.

In Chapter 4, we saw that PXP may not always have uniform spectral gaps in part due to the existence of topological obstructions (e.g. the \mathbb{Z}_2 invariant). Despite this, we were able to show that in two dimension so as long as $\text{range}(P)$ admits a basis which has sufficiently fast algebraic decay then it is possible to construct a new position operator \hat{X} so that $P\hat{X}P$ has uniform spectral gaps. As a consequence of the construction of \hat{X} , we were able to prove a weak form of the localization dichotomy for non-periodic systems in two dimensions: If $\text{range}(P)$ admits a basis which is s -localized for $s > 5/2$, then it also admits a basis which is exponentially localized.

Because of the generality of our results, there are a number of interesting potential future directions for this work.

Applications for Electron Structure Calculations

The results of this dissertation prove the correctness of an algorithm for constructing exponentially localized Wannier functions. Since exponentially localized Wannier functions are commonly used in practice, a natural next step of these results is to apply our algorithm to a real world system.

Applications to the Theory of Topological Insulators

Thus far, a majority of the work on topological insulators has focused on periodic systems only. Through the main proofs in Chapters 3 and 4, we prove that the vanishing of the Chern number is equivalent to the existence of uniform spectral gaps of “ PXP ” in periodic system. One immediate question from this result is whether the uniform spectral gaps condition can be used to establish the full localization dichotomy in non-periodic insulators. As a first step, one could consider using the vanishing of the Chern marker (see Definition (6)), to conclude that an s -localized basis for $\text{range}(P)$ exists for some $s > 0$. Some results in this direction have recently appeared using K -theoretic generalizations of the Chern number [LT20, BM20].

Applications for Data Analysis

Throughout most of our proofs, the fact that the projector P was associated to a Hamiltonian system only played a minor role. So long as the off diagonal entries of the projector P decay reasonably quickly (perhaps not exponentially quickly), most of the details of the proofs in Chapters 3 and 4 will still carry through. Therefore, we expect that performing the sequence of diagonalizations $PXP \rightarrow P_j Y P_j$ will generally always give a well localized basis for $\text{range}(P)$ (so long as PXP has uniform spectral gaps). As such, the algorithm introduced in this dissertation could be applied to construct sparse representations of general data sets, not just those arising from quantum mechanics.

Appendix A

Appendices

A.1 Decay Estimates for Fermi Projectors

In this section we will show that if H is a Hamiltonian satisfying Assumptions 1 and 2 and if P is a spectral projector onto σ_0 then P satisfies the decay estimates from Assumption 3. That is there exist finite, positive constants $(C_1, C_2, C_3, C_4, C_5, \gamma^*)$ such that for all $0 \leq \gamma \leq \gamma^*$ the following bounds hold:

- (i) $\|P_\gamma - P\| \leq C_1\gamma$
- (ii) (a) $\|[P_\gamma, X]\| \leq C_2$
(b) $\|[P_\gamma, Y]\| \leq C_2$
- (iii) (a) $\|[P_\gamma - P, X]\| \leq C_3\gamma$
(b) $\|[P_\gamma - P, Y]\| \leq C_3\gamma$
- (iv) $\|[P, \langle X - \lambda \rangle^{1/2}]\| \leq C_4$
- (v) (a) $\|\langle X - \lambda \rangle^{1/2}[P, X]\langle X - \lambda \rangle^{-1/2}\| \leq C_5$
(b) $\|\langle X - \lambda \rangle^{1/2}[P, Y]\langle X - \lambda \rangle^{-1/2}\| \leq C_5$

The key tool for proving these estimates is to use the Riesz formula for the projector P . Since P is a projector onto σ_0 , we can find a contour \mathcal{C} of finite length enclosing σ_0 such that:

$$P = \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H)^{-1} dz \quad \text{and} \quad \sup_{z \in \mathcal{C}} \|(z - H)^{-1}\| < \infty. \quad (\text{A.1})$$

To streamline our estimates for P , we will now state and prove three useful lemmas:

Lemma A.1.1. *Suppose that H satisfies Assumption 1 and $f, g \in C^2(\mathbb{R}^2)$. Then we have the following identities:*

$$e^f H e^{-f} = H + 2i \nabla f \cdot (i \nabla + A) - \Delta f + \nabla f \cdot \nabla f \quad (\text{A.2})$$

$$e^f [H, g] e^{-f} = -\Delta g + 2i \nabla g \cdot (i \nabla + A) + 2 \nabla g \cdot \nabla f \quad (\text{A.3})$$

Proof. It follows from a direct calculation. \square

Lemma A.1.2. *Suppose that H satisfies Assumptions 1 and 2. Then Δ is H -bounded in the sense that $\mathcal{D}(\Delta) \subset \mathcal{D}(H)$ and there exist constants $a, b > 0$ such that for any $\psi \in \mathcal{D}(H)$,*

$$\|\Delta \psi\| \leq a \|H \psi\| + b \|\psi\|.$$

Proof. Let Assumption 1 on H hold, and let $\psi \in \mathcal{D}(\Delta)$. Then

$$\|\Delta \psi\| = \|(\Delta + H)\psi - H\psi\| \leq \|(\Delta + H)\psi\| + \|H\psi\|. \quad (\text{A.4})$$

Explicitly,

$$\Delta + H = -2iA \cdot \nabla - i \operatorname{div} A + A \cdot A + V.$$

Hence,

$$\|(\Delta + H)\psi\| \leq 4\|A\|_{L^\infty} \sup_{j=1,2} \|\partial_j \psi\| + (\|\operatorname{div} A\|_{L^\infty} + \|A\|_{L^\infty}^2 + \|V\|_{L^\infty}) \|\psi\|. \quad (\text{A.5})$$

Now observe that for any $\epsilon > 0$,

$$\|\partial_j \psi\| \leq \epsilon \|\Delta \psi\| + \frac{1}{\epsilon} \|\psi\| \quad j = 1, 2.$$

Substituting this inequality into (A.5), and then substituting (A.5) into (A.4), we have

$$\begin{aligned} \|\Delta \psi\| &\leq \|H\psi\| + 4\epsilon \|A\|_{L^\infty} \|\Delta \psi\| \\ &+ \left(4\frac{1}{\epsilon} \|A\|_{L^\infty} + \|\operatorname{div} A\|_{L^\infty} + \|A\|_{L^\infty}^2 + \|V\|_{L^\infty} \right) \|\psi\|. \end{aligned} \quad (\text{A.6})$$

Now, by taking ϵ sufficiently small, we can ensure that $1 - 2\epsilon\|A\|_{L^\infty} > 0$. For such ϵ we have that

$$\begin{aligned} \|\Delta\psi\| &\leq (1 - 4\epsilon\|A\|_{L^\infty})^{-1} \|H\psi\| \\ &\quad + (1 - 4\epsilon\|A\|_{L^\infty})^{-1} \left(4\frac{1}{\epsilon}\|A\|_{L^\infty} + \|\operatorname{div}A\|_{L^\infty} + \|A\|_{L^\infty}^2 + \|V\|_{L^\infty} \right) \|\psi\|, \end{aligned} \tag{A.7}$$

which proves the Lemma with

$$\begin{aligned} a &= (1 - 4\epsilon\|A\|_{L^\infty})^{-1} \\ b &= (1 - 4\epsilon\|A\|_{L^\infty})^{-1} \left(4\frac{1}{\epsilon}\|A\|_{L^\infty} + \|\operatorname{div}A\|_{L^\infty} + \|A\|_{L^\infty}^2 + \|V\|_{L^\infty} \right) \end{aligned}$$

and $0 < \epsilon < \frac{1}{4\|A\|_{L^\infty}}$. □

Lemma A.1.3. *Suppose that H satisfies Assumptions 1 and 2. If $z \in \mathcal{C}$, where \mathcal{C} is the contour from Equation (A.1), then there exists an absolute constant C such that for all $v \in \mathbb{R}^2$:*

$$\|v \cdot (i\nabla + A)(z - H)^{-1}\| \leq C\|v\|$$

Proof. The proof is a straightforward consequence of Lemma A.1.2. First, note that using boundedness of \mathbf{v} and A ,

$$\|\mathbf{v} \cdot (-i\nabla + A)\psi\| \leq \|\mathbf{v} \cdot (-i\nabla)\psi\| + 2\|\mathbf{v}\|_\infty\|A\|_\infty\|\psi\|. \tag{A.8}$$

On the other hand,

$$\|\mathbf{v} \cdot (-i\nabla)\psi\| \leq 2\|\mathbf{v}\|_\infty (\|\Delta\psi\| + \|\psi\|). \tag{A.9}$$

Substituting (A.9) into (A.8) gives

$$\|\mathbf{v} \cdot (-i\nabla + A)\psi\| \leq 2\|\mathbf{v}\|_\infty\|\Delta\psi\| + (2\|\mathbf{v}\|_\infty + 2\|\mathbf{v}\|_\infty\|A\|_\infty) \|\psi\|. \tag{A.10}$$

The result now follows upon combining (A.10) with Lemma A.1.2. □

With these three lemmas in hand, we will now prove the first three estimates (i), (ii), (iii) in Appendix A.1.1 and the last two estimates (iv), (v) in Appendix A.1.2

A.1.1 Exponential Localization Bounds

Let us first make use of Lemmas A.1.1 and A.1.3 to prove the following corollary

Corollary A.1.4. *Suppose that H satisfies Assumptions 1 and 2. If $z \in \mathcal{C}$, where \mathcal{C} is the contour from Equation (A.1), then there exists constants $(\gamma^*, K_1, K_2, K_3)$ independent of z such that for all $\gamma \leq \gamma^*$ we have the following bounds:*

1. $\|(H_\gamma - H)(z - H)^{-1}\| \leq K_1\gamma$
2. (a) $\|[H_\gamma, X](z - H)^{-1}\| \leq K_2$
 (b) $\|[H_\gamma, Y](z - H)^{-1}\| \leq K_2$
3. (a) $\|[H_\gamma - H, X](z - H)^{-1}\| \leq K_3\gamma$
 (b) $\|[H_\gamma - H, Y](z - H)^{-1}\| \leq K_3\gamma$

Proof. We will show how to prove $\|[H_\gamma - H, X](z - H)^{-1}\| \leq K_3\gamma$ using Lemmas A.1.1 and A.1.3. The remaining estimates follow by similar steps.

Choosing $f(x, y) = \gamma\sqrt{1 + (x - a)^2 + (y - b)^2}$ and $g(x, y) = x$ with Lemma A.1.1 we have that

$$[H_\gamma, X] = 2ie_1 \cdot (i\nabla + A) + 2\gamma e_1 \cdot \left(\frac{x - a}{\sqrt{1 + (x - a)^2 + (y - a)^2}} \right)$$

Similarly, choosing $f(x, y) \equiv 0$ and $g(x, y) = x$ we have that

$$[H, X] = 2ie_1 \cdot (i\nabla + A).$$

Therefore,

$$[H_\gamma - H, X] = 2\gamma e_1 \cdot \left(\frac{x - a}{\sqrt{1 + (x - a)^2 + (y - a)^2}} \right).$$

Therefore, clearly there exists a constant K_3 such that $\|[H_\gamma - H, X](z - H)^{-1}\| \leq K_3\gamma$. □

Proof of Bound (i)

We calculate

$$\begin{aligned}
P_\gamma - P &= \frac{1}{2\pi i} \int_{\mathcal{C}} B_\gamma (z - H)^{-1} B_\gamma^{-1} - (z - H)^{-1} dz \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H_\gamma)^{-1} - (z - H)^{-1} dz \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H_\gamma)^{-1} (H_\gamma - H) (z - H)^{-1} dz
\end{aligned}$$

where the final line follows by the second resolvent identity. Hence

$$\|P_\gamma - P\| \leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(\|(z - H_\gamma)^{-1}\| \|(H_\gamma - H)(z - H)^{-1}\| \right)$$

The term $(z - H_\gamma)^{-1}$ is bounded since

$$\begin{aligned}
(z - H_\gamma)^{-1} &= (z - H + H - H_\gamma)^{-1} \\
&= (z - H)^{-1} \left(I - (H_\gamma - H)(z - H)^{-1} \right)^{-1}
\end{aligned} \tag{A.11}$$

Due to Corollary A.1.4(1) we know that

$$\|(H_\gamma - H)(z - H)^{-1}\| \leq K_1 \gamma.$$

Therefore if we pick $\gamma \leq (2K_1)^{-1}$ we conclude that

$$\|(z - H_\gamma)^{-1}\| \leq \|(z - H)^{-1}\| \left(1 - \frac{1}{2} \right)^{-1}$$

Using this bound, we therefore conclude that

$$\|P_\gamma - P\| \leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(2 \|(z - H)^{-1}\| \right) (K_1 \gamma)$$

which proves bound (i). □

Proof of Bound (ii)

We will show this bound for X only, the corresponding bound for Y follows by analogous steps. We calculate

$$\begin{aligned}
[P_\gamma, X] &= \frac{1}{2\pi i} \int_{\mathcal{C}} [(z - H_\gamma)^{-1}, X] dz \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H_\gamma)^{-1} [H_\gamma, X] (z - H_\gamma)^{-1} dz
\end{aligned}$$

Hence

$$\|[P_\gamma, X]\| \leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(\|(z - H_\gamma)^{-1}\| \|[H_\gamma, X](z - H_\gamma)^{-1}\| \right).$$

Following the calculation from Equation (A.11) we have that

$$[H_\gamma, X](z - H_\gamma)^{-1} = [H_\gamma, X](z - H)^{-1} \left(I - (H_\gamma - H)(z - H)^{-1} \right)^{-1}.$$

Therefore, following reasoning from Appendix A.1.1, we conclude that for all $\gamma \leq (2K_1)^{-1}$

$$\|[P_\gamma, X]\| \leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left[\left(2\|(z - H)^{-1}\| \right) \left(2\|[H_\gamma, X](z - H)^{-1}\| \right) \right].$$

The above is bounded by a constant due to Corollary A.1.4(2) which proves bound (ii). \square

Proof of Bound (iii)

We will show this bound for X only, the corresponding bound for Y follows by analogous steps. From the calculation in Appendix A.1.1 we have that

$$P_\gamma - P = \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H_\gamma)^{-1} (H_\gamma - H) (z - H)^{-1} dz$$

Hence

$$[P_\gamma - P, X] = \frac{1}{2\pi i} \int_{\mathcal{C}} [(z - H_\gamma)^{-1} (H_\gamma - H) (z - H)^{-1}, X] dz.$$

Now to complete this proof, we need to compute the following commutator

$$[(z - H_\gamma)^{-1} (H_\gamma - H) (z - H)^{-1}, X].$$

This proceeds by an long but straightforward calculation. We start by commuting X with $(z - H)^{-1}$:

$$\begin{aligned} & (z - H_\gamma)^{-1} (H_\gamma - H) (z - H)^{-1} X \\ &= \left((z - H_\gamma)^{-1} (H_\gamma - H) \right) \left(X (z - H)^{-1} + [(z - H)^{-1}, X] \right) \\ &= \left((z - H_\gamma)^{-1} (H_\gamma - H) \right) \left(X + (z - H)^{-1} [H, X] \right) (z - H)^{-1} \end{aligned}$$

Next, commuting $H_\gamma - H$ with X gives us that:

$$\begin{aligned} & (z - H_\gamma)^{-1}(H_\gamma - H)X(z - H)^{-1} \\ &= (z - H_\gamma)^{-1}\left(X(H_\gamma - H) + [H_\gamma - H, X]\right)(z - H)^{-1}. \end{aligned}$$

Finally, commuting $(z - H_\gamma)^{-1}$ with X gives that:

$$\begin{aligned} & (z - H_\gamma)^{-1}X(H_\gamma - H)(z - H)^{-1} \\ &= \left(X(z - H_\gamma)^{-1} + [(z - H_\gamma)^{-1}, X]\right)(H_\gamma - H)(z - H)^{-1} \\ &= \left(X + (z - H_\gamma)^{-1}[H_\gamma, X]\right)(z - H_\gamma)^{-1}(H_\gamma - H)(z - H)^{-1}. \end{aligned}$$

Combining all of these estimates together shows that:

$$\begin{aligned} & [(z - H_\gamma)^{-1}(H_\gamma - H)(z - H)^{-1}, X] \\ &= (z - H_\gamma)^{-1}(H_\gamma - H)(z - H)^{-1}[H, X](z - H)^{-1} \\ &\quad + (z - H_\gamma)^{-1}[H_\gamma - H, X](z - H)^{-1} \\ &\quad + (z - H_\gamma)^{-1}[H_\gamma, X](z - H_\gamma)^{-1}(H_\gamma - H)(z - H)^{-1}. \end{aligned}$$

Hence

$$\begin{aligned} & \|[(z - H_\gamma)^{-1}(H_\gamma - H)(z - H)^{-1}, X]\| \\ &\leq \left(\|(z - H_\gamma)^{-1}\|\right)\left(\|(H_\gamma - H)(z - H)^{-1}\|\right)\left(\|[H, X](z - H)^{-1}\|\right) \\ &\quad + \left(\|(z - H_\gamma)^{-1}\|\right)\left(\|[H_\gamma - H, X](z - H)^{-1}\|\right) \\ &\quad + \left(\|(z - H_\gamma)^{-1}\|\right)\left(\|[H_\gamma, X](z - H_\gamma)^{-1}\|\right)\left(\|(H_\gamma - H)(z - H)^{-1}\|\right). \end{aligned}$$

We showed in Appendix A.1.1 that $\|(z - H_\gamma)^{-1}\|$ is bounded and in Appendix A.1.1 that $\|[H_\gamma, X](z - H_\gamma)^{-1}\|$ is bounded. These bounds combined with Corollary A.1.4 implies bound (iii). \square

A.1.2 Square Root Localization Bounds

Similar to Appendix A.1.1 we will begin this section by stating a corollary which follows from Lemmas A.1.1 and A.1.3.

Corollary A.1.5. *Suppose that H satisfies Assumptions 1 and 2. If $z \in \mathcal{C}$, where \mathcal{C} is the contour from Equation (A.1), then there exists constants (K_4, K_5) independent of z such that for all $\lambda \in \mathbb{R}$:*

1. $\|[H, \langle X - \lambda \rangle^{1/2}](z - H)^{-1}\| \leq K_4$
2. (a) $\|\langle X - \lambda \rangle^{1/2}[H, X]\langle X - \lambda \rangle^{-1/2}(z - H)^{-1}\| \leq K_5$
(b) $\|\langle X - \lambda \rangle^{1/2}[H, Y]\langle X - \lambda \rangle^{-1/2}(z - H)^{-1}\| \leq K_5$

Proof. Applying Lemma A.1.1 with $f(x, y) \equiv 0$ and $g(x, y) = \langle x - \lambda \rangle^{1/2}$ gives

$$[H, \langle X - \lambda \rangle^{1/2}] = \left(\frac{2 - (x - \lambda)^2}{4\langle x - \lambda \rangle^{7/4}} \right) + \left(\frac{2i(x - \lambda)}{2\langle x - \lambda \rangle^{3/2}} \right) e_1 \cdot (i\nabla + A).$$

Hence, $[H, \langle X - \lambda \rangle^{1/2}](z - H)^{-1}$ is clearly bounded by a constant due to Lemma A.1.3.

To get the second and third bounds, simply apply Lemma A.1.1 with $f(x, y) = \ln(\langle x - \lambda \rangle^{1/2})$ and either $g(x, y) = x$ or $g(x, y) = y$ and use a similar argument. \square

Proof of Bound (iv)

We calculate

$$\begin{aligned} [P, \langle X - \lambda \rangle^{1/2}] &= \frac{1}{2\pi i} \int_{\mathcal{C}} [(z - H)^{-1}, \langle X - \lambda \rangle^{1/2}] dz \\ &= \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H)^{-1} [H, \langle X - \lambda \rangle^{1/2}](z - H)^{-1} dz. \end{aligned}$$

Hence

$$\|[P, \langle X - \lambda \rangle^{1/2}]\| \leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(\|(z - H)^{-1}\| \|[H, \langle X - \lambda \rangle^{1/2}](z - H)^{-1}\| \right)$$

which is bounded by a constant due to Corollary A.1.5. \square

Proof of Bound (v)

We will only prove the bound for Y , the bound for X follows by similar steps. We calculate

$$\begin{aligned} [P, Y] &= \frac{1}{2\pi i} \int_{\mathcal{C}} [(z - H)^{-1}, Y] dz \\ &= \frac{1}{2\pi i} \int_{\mathcal{C}} (z - H)^{-1} [H, Y] (z - H)^{-1} dz. \end{aligned}$$

Therefore,

$$\begin{aligned} &\|\langle X - \lambda \rangle^{1/2} [P, Y] \langle X - \lambda \rangle^{-1/2}\| \\ &\leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(\|\langle X - \lambda \rangle^{1/2} (z - H)^{-1} [H, Y] (z - H)^{-1} \langle X - \lambda \rangle^{-1/2}\| \right) \end{aligned}$$

To help with reducing clutter in the next few steps, let us define the shorthand $X_\lambda := X - \lambda$. With this notation, we have that

$$\begin{aligned} &\|\langle X - \lambda \rangle^{1/2} [P, Y] \langle X - \lambda \rangle^{-1/2}\| \\ &\leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \|\langle X_\lambda \rangle^{1/2} (z - H)^{-1} [H, Y] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| \\ &\leq \frac{\ell(\mathcal{C})}{2\pi} \sup_{z \in \mathcal{C}} \left(\|\langle X_\lambda \rangle^{1/2} (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| \|\langle X_\lambda \rangle^{1/2} [H, Y] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| \right) \end{aligned}$$

The first term on the right-hand side in the bracket is clearly bounded since

$$\begin{aligned} &\|\langle X_\lambda \rangle^{1/2} (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| \\ &= \|\langle X_\lambda \rangle^{1/2}, (z - H)^{-1}\| \|\langle X_\lambda \rangle^{-1/2} + (z - H)^{-1}\| \\ &\leq \|(z - H)^{-1} \langle X_\lambda \rangle^{1/2}, H\| \|(z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| + \|(z - H)^{-1}\| \\ &\leq \|(z - H)^{-1}\| \|\langle X_\lambda \rangle^{1/2}, H\| \|(z - H)^{-1}\| + \|(z - H)^{-1}\| \end{aligned}$$

which is bounded due to Corollary A.1.5(1).

To see that

$$\langle X_\lambda \rangle^{1/2} [H, Y] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}$$

is bounded we perform the following calculations

$$\begin{aligned}
& \langle X_\lambda \rangle^{1/2} [H, Y] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2} \\
&= \langle X_\lambda \rangle^{1/2} [H, Y] \langle X_\lambda \rangle^{-1/2} \langle X_\lambda \rangle^{1/2} (z - H)^{-1} \langle X_\lambda \rangle^{-1/2} \\
&= \langle X_\lambda \rangle^{1/2} [H, Y] \langle X_\lambda \rangle^{-1/2} \left([\langle X_\lambda \rangle^{1/2}, (z - H)^{-1}] \langle X_\lambda \rangle^{-1/2} + (z - H)^{-1} \right) \\
&= \langle X_\lambda \rangle^{1/2} [H, Y] \langle X_\lambda \rangle^{-1/2} (z - H)^{-1} \left([\langle X_\lambda \rangle^{1/2}, H] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2} + I \right)
\end{aligned}$$

Hence

$$\begin{aligned}
& \|\langle X_\lambda \rangle^{1/2} [H, Y] (z - H)^{-1} \langle X_\lambda \rangle^{-1/2}\| \\
&\leq \left(\|\langle X_\lambda \rangle^{1/2} [H, Y] \langle X_\lambda \rangle^{-1/2} (z - H)^{-1}\| \right) \left(\|[\langle X_\lambda \rangle^{1/2}, H] (z - H)^{-1}\| \|\langle X_\lambda \rangle^{-1/2}\| + 1 \right)
\end{aligned}$$

Since

$$\begin{aligned}
& \|[\langle X - \lambda \rangle^{1/2}, H] (z - H)^{-1}\|, \text{ and} \\
& \|\langle X - \lambda \rangle^{1/2} [H, Y] \langle X - \lambda \rangle^{-1/2} (z - H)^{-1}\|
\end{aligned}$$

are bounded due to Corollary A.1.5, we conclude bound (v). \square

A.2 Bounds for P_j

Recall that when PXP satisfies the uniform gap assumption (Assumption 4), we can define band projectors

$$P_j := \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - PXP)^{-1} d\lambda \right) P \quad (\text{A.12})$$

for each $j \in \mathcal{J}$, which project onto the spectral subspace corresponding to each separated component σ_j of the spectrum of PXP . Here \mathcal{C}_j denotes a contour enclosing σ_j in the complex plane.

The goal of this section is to prove the following lemma:

Lemma A.2.1. *Let P be an orthogonal projection satisfying Assumption 3 with finite, positive constants (γ', K'_1, K'_2) . Now suppose that PXP has uniform spectral*

gaps in the sense of Assumption 4 with constants (d, D) . If P_j is a band projection onto σ_j then there exists finite, positive constants $(\gamma'', K_1'', K_2'', K_3'')$, independent of j , such that for all $\gamma \leq \gamma''$

1. $\|P_{j,\gamma} - P_j\| \leq K_1'' \gamma$
2. $\|[P_{j,\gamma}, X]\| \leq K_2''$ and $\|[P_{j,\gamma}, Y]\| \leq K_2''$
3. For all $\eta \in \sigma_j$:

$$\|(X - \eta)P_{j,\gamma}\| \leq K_3'' \text{ and } \|P_{j,\gamma}(X - \eta)\| \leq K_3''.$$

The constant γ'' only depends on (γ', K_1', K_2') and (d, D) and is independent of the system size.

Note that Lemma A.2.1 is a re-statement of Lemma 3.3.7, and contains Lemma 3.3.6 as a special case.

The starting point of our proof will be our decay estimates for P (Assumption 3), which established operator norm bounds on the Fermi projector P . In particular, we will use that there exists finite, positive constants (γ', K_1', K_2') so that for all $\gamma \in [0, \gamma']$

1. $\|P_\gamma - P\| \leq K_1' \gamma$
2. $\|[P_\gamma, X]\| \leq K_2'$ and $\|[P_\gamma, Y]\| \leq K_2'$

A.2.1 Proof of key estimate on $(\lambda - P_\gamma X P_\gamma)^{-1}$

The most difficult step in the proof of Lemma A.2.1 is to prove the following proposition, which states that the operator $(\lambda - P_\gamma X P_\gamma)^{-1}$ is bounded uniformly for $\lambda \in \mathcal{C}_j$ for all $j \in \mathcal{J}$ by a constant which is independent of j .

Proposition A.2.2. *There constants $\gamma_0 > 0$ and $C > 0$ such that for all $\gamma \leq \gamma_0$*

$$\sup_{j \in \mathcal{J}} \sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \leq C. \tag{A.13}$$

To see why Proposition A.2.2 is relevant to Lemma A.2.1, recall the contour integral definition (A.12) of P_j and note that

$$\begin{aligned}
P_{j,\gamma} &= B_\gamma \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - PXP)^{-1} d\lambda \right) P B_\gamma^{-1} \\
&= B_\gamma \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - PXP)^{-1} d\lambda \right) (B_\gamma^{-1} B_\gamma) P B_\gamma^{-1} \\
&= \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} B_\gamma (\lambda - PXP)^{-1} B_\gamma^{-1} d\lambda \right) P_\gamma \\
&= \left(\frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma X P_\gamma)^{-1} d\lambda \right) P_\gamma
\end{aligned} \tag{A.14}$$

where in the last step we have used that $[B_\gamma, X] = 0$ and

$$B_\gamma P X P B_\gamma^{-1} = B_\gamma P (B_\gamma^{-1} B_\gamma) X P B_\gamma^{-1} = P_\gamma X P_\gamma.$$

Hence Proposition A.2.2 immediately implies, through (A.14), that for sufficiently small γ , there exists a constant $C > 0$ such that

$$\sup_{j \in \mathcal{J}} \|P_{j,\gamma}\| \leq C.$$

With Proposition A.2.2 established, the other assertions of Lemma A.2.1 follow from relatively straightforward manipulations.

We will prove Proposition A.2.2 across the next few subsections, with the proof of one lemma postponed until Appendix A.3. We start by showing how a naïve approach at bounding (A.13) yields an estimate which is not uniform in j .

Failure of a naïve approach to yield an estimate uniform in j

We start with the formal manipulations

$$\begin{aligned}
(\lambda - P_\gamma X P_\gamma)^{-1} &= (\lambda - PXP_\gamma + PXP_\gamma - P_\gamma X P_\gamma)^{-1} \\
&= (\lambda - PXP_\gamma - (P_\gamma - P)XP_\gamma)^{-1} \\
&= (\lambda - PXP_\gamma)^{-1} (I - (P_\gamma - P)XP_\gamma(\lambda - PXP_\gamma)^{-1})^{-1}.
\end{aligned} \tag{A.15}$$

Recall that $\|P_\gamma - P\| = O(\gamma)$ by Assumption 3. It follows that if

$$(\lambda - PXP_\gamma)^{-1} \text{ and } XP_\gamma(\lambda - PXP_\gamma)^{-1}$$

can be bounded for all $\lambda \in \mathcal{C}_j$ independently of j we are done by taking γ sufficiently small. Unfortunately, a direct attempt to bound $(\lambda - PXP_\gamma)^{-1}$ fails in this respect. More formal manipulations yield:

$$\begin{aligned} (\lambda - PXP_\gamma)^{-1} &= (\lambda - PXP - PX(P_\gamma - P))^{-1} \\ &= (\lambda - PXP - PX(P_\gamma - P))^{-1}(\lambda - PXP)(\lambda - PXP)^{-1} \\ &= (I - (\lambda - PXP)^{-1}PX(P_\gamma - P))^{-1}(\lambda - PXP)^{-1}. \end{aligned}$$

Again, since $\|P_\gamma - P\| = O(\gamma)$ by Assumption 3, we obtain a bound on $(\lambda - PXP_\gamma)^{-1}$ if we can bound

$$(\lambda - PXP)^{-1}PX$$

for all $\lambda \in \mathcal{C}_j$ independently of j . Let

$$Q := I - P$$

denote the orthogonal projector onto the orthogonal complement of range P . Since $P + Q = I$,

$$\begin{aligned} \|(\lambda - PXP)^{-1}PX\| &= \|(\lambda - PXP)^{-1}PX(P + Q)\| \\ &= \|(\lambda - PXP)^{-1}(PXP - \lambda + \lambda + PXQ)\| \tag{A.16} \\ &\leq 1 + |\lambda| \|(\lambda - PXP)^{-1}\| + \|(\lambda - PXP)^{-1}PXQ\|. \end{aligned}$$

It is easy to see that PXQ is bounded, since

$$PXQ = PX(I - P) = PX - PXP = -P[X, P],$$

which is bounded by Assumption 3, and $(\lambda - PXP)^{-1}$ is bounded for all $\lambda \in \mathcal{C}_j$ independently of j by assumption. Substituting these observations into (A.16) yields a bound on $(\lambda - PXP)^{-1}PX$ with the form

$$\|(\lambda - PXP)^{-1}PX\| \leq C + C|\lambda|,$$

which can be bounded uniformly for $\lambda \in \mathcal{C}_j$ for any fixed value of $j \in \mathcal{J}$, but not independently of j .

Remark A.2.3. The inserting of $P_\gamma X P_\gamma - P X P$ in Equation (A.15) is non-obvious. Initially, one might be tempted to insert $P X P - P X P$ instead. To make this step work, one would need to show that

$$\|(P_\gamma X P_\gamma - P X P)(\lambda - P X P)^{-1}\| = O(\gamma).$$

Unfortunately, some numerical tests for finite systems suggest that:

$$\|(P_\gamma X P_\gamma - P X P)(\lambda - P X P)^{-1}\| \sim |\text{system size}| \gamma.$$

Since it does not seem possible to control $\|(P_\gamma X P_\gamma - P X P)(\lambda - P X P)^{-1}\|$ in general, we have to resort to the more complicated argument we give above.

Strategy for proving an estimate which is uniform in j

We now explain how to improve on the j -dependent bound proved in Section A.2.1. First, for each $j \in \mathcal{J}$, let $\eta_j \in \sigma_j$ be arbitrary, and define a j -dependent “shift” of $\lambda - P_\gamma X P_\gamma$ by

$$\begin{aligned} & (\lambda_{\eta_j} - P_\gamma X_{\eta_j} P_\gamma)^{-1}, \\ & \lambda_{\eta_j} := \lambda - \eta_j, \quad X_{\eta_j} := X - \eta_j. \end{aligned} \tag{A.17}$$

We will proceed by the following steps:

1. Using the argument sketched in Section A.2.1, we will bound each shifted operator (A.17) uniformly in λ over the contour $\lambda \in \mathcal{C}_j$, and uniformly over $\eta \in \sigma_j$, by a constant which is independent of $j \in \mathcal{J}$.
2. We will deduce the bound (A.13) from the set of bounds proved in part (1).

Before embarking on the proof of estimate (A.13), we pause to introduce some notation and prove some elementary bounds which follow from Assumption 3.

Notation and Some Easy Estimates

Recall that we defined $Q := I - P$ to be the orthogonal projection onto the orthogonal complement of P . We now make the following further definitions

$$Q_\gamma := B_\gamma Q B_\gamma = I - P_\gamma$$

$$E := P_\gamma - P.$$

We now note some easy estimates which follow from Assumption 3. We will prove the following proposition:

Proposition A.2.4. *For any P satisfying Assumption 3 and for all γ sufficiently small:*

1. $\|P_\gamma - P\| = \|Q - Q_\gamma\| = \|E\| \leq K'\gamma$
2. $\|P_\gamma\| \leq 1 + K'\gamma$, and $\|Q_\gamma\| \leq 1 + K'\gamma$.

For any $\eta \in \mathbb{C}$, let $X_\eta = X - \eta$ and $\lambda_\eta = \lambda - \eta$. Then

3. $\|P_\gamma X_\eta Q_\gamma\| < \infty$ and $\|Q_\gamma X_\eta P_\gamma\| < \infty$.

Proof. (1) An elementary manipulation implies that

$$Q - Q_\gamma = P_\gamma - P = E,$$

from which the claim immediately follows.

(2) The triangle inequality implies that

$$\begin{aligned} \|P_\gamma\| &\leq \|P_\gamma - P\| + \|P\| \\ &\leq 1 + K'_1\gamma. \end{aligned} \tag{A.18}$$

An identical calculation implies $\|Q_\gamma\| \leq 1 + K'_1\gamma$.

(3) Since P is a projection, we have that

$$P_\gamma^2 = B_\gamma P B_\gamma^{-1} B_\gamma P B_\gamma^{-1} = B_\gamma P^2 B_\gamma^{-1} = P_\gamma.$$

Therefore, P_γ is also a projection. An immediate consequence of the fact that P_γ is a projection is $P_\gamma Q_\gamma = P_\gamma - P_\gamma^2 = 0$. Since $P_\gamma Q_\gamma = 0$ we also have that

$$P_\gamma X_\eta Q_\gamma = P_\gamma (X - \eta) Q_\gamma = P_\gamma X Q_\gamma = [P_\gamma, X] Q_\gamma$$

which is bounded due to Corollary 3(i,iii). Similar calculations show that $\|Q_\gamma X_\eta P_\gamma\| < \infty$. \square

Estimating the j -dependent shifted operators (A.17)

We now move on to bounding each of the j -dependent shifted operators (A.17) uniformly in λ over the contour $\lambda \in \mathcal{C}_j$, and uniformly in $\eta \in \sigma_j$, by a constant independent of $j \in \mathcal{J}$.

For simplicity of notation, we will drop the subscript j from η_j in this section. Assuming for now that $(\lambda_\eta - P X_\eta P_\gamma)^{-1}$ is well defined, then an identical calculation to (A.15) gives

$$(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} = (\lambda_\eta - P X_\eta P_\gamma)^{-1} \left(I - E X_\eta P_\gamma (\lambda_\eta - P X_\eta P_\gamma)^{-1} \right)^{-1},$$

where $E := P_\gamma - P$. If we could show that

$$(\lambda_\eta - P X_\eta P_\gamma)^{-1} \text{ and } X_\eta P_\gamma (\lambda_\eta - P X_\eta P_\gamma)^{-1} \tag{A.19}$$

are both bounded, then since $\|E\| = O(\gamma)$ we can choose γ sufficiently small so that $(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}$ can be written as a product of bounded operators and we are done.

We will first prove that $\|(\lambda_\eta - P X_\eta P_\gamma)^{-1}\|$ is bounded and then we will then use that result to prove that $\|X_\eta P_\gamma (\lambda_\eta - P X_\eta P_\gamma)^{-1}\|$ is bounded.

Bounding $(\lambda_\eta - P X_\eta P_\gamma)^{-1}$

Essentially the same calculations as in (A.2.1) give the following

$$(\lambda_\eta - P X_\eta P_\gamma)^{-1} = \left(I - (\lambda_\eta - P X_\eta P)^{-1} P X_\eta E \right)^{-1} (\lambda_\eta - P X_\eta P)^{-1}.$$

Hence

$$\|(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| \leq \left\| \left(I - (\lambda_\eta - PX_\eta P)^{-1} PX_\eta E \right)^{-1} \right\| \|(\lambda_\eta - PX_\eta P)^{-1}\|. \quad (\text{A.20})$$

To show that the first term is bounded it is enough to show that for γ sufficiently small

$$\|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta E\| \leq \frac{1}{2}.$$

Inserting $P + Q = I$, we have that

$$\begin{aligned} \|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta\| &= \|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta (P + Q)\| \\ &\leq \|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta P\| + \|(\lambda_\eta - PX_\eta P)^{-1}\| \|PX_\eta Q\| \\ &\leq 1 + |\lambda_\eta| \|(\lambda_\eta - PX_\eta P)^{-1}\| + \|(\lambda_\eta - PX_\eta P)^{-1}\| \|PX_\eta Q\|. \end{aligned}$$

By the definition of the contour \mathcal{C}_j (recall Assumption 4 and Definition 2), we know that both $|\lambda_\eta|$ and $\|(\lambda_\eta - PX_\eta P)^{-1}\|$ are both bounded by constants which are independent of $\eta \in \sigma_j$ and j . Since by Proposition A.2.4, we also know that $\|PX_\eta Q\|$ is bounded, we can conclude that $\|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta\|$ is bounded by a constant independent of λ and j .

Since $\|E\| \leq K'_1 \gamma$ if we pick γ so that

$$\gamma \leq (2K'_1)^{-1} \left(1 + \left(|\lambda_\eta| + \|PX_\eta Q\| \right) \|(\lambda_\eta - PX_\eta P)^{-1}\| \right)^{-1}$$

we see that

$$\|(\lambda_\eta - PX_\eta P)^{-1} PX_\eta E\| \leq \frac{1}{2}$$

and therefore by Equation A.20, $\|(\lambda_\eta - PX_\eta P_\gamma)^{-1}\|$ is bounded uniformly for $\lambda \in \mathcal{C}_j$ by a constant independent of j .

Bounding $X_\eta P_\gamma (\lambda_\eta - PX_\eta P_\gamma)^{-1}$

The key trick proving this bound is noticing that $E = Q - Q_\gamma$ and therefore $Q = Q_\gamma + E$. Inserting a copy of $(P + Q)$ into the quantity we want to bound gives

$$\begin{aligned} X_\eta P_\gamma (\lambda_\eta - PX_\eta P_\gamma)^{-1} &= (P + Q) X_\eta P_\gamma (\lambda_\eta - PX_\eta P_\gamma)^{-1} \\ &= (P + Q_\gamma + E) X_\eta P_\gamma (\lambda_\eta - PX_\eta P_\gamma)^{-1} \end{aligned} \quad (\text{A.21})$$

Now we can move the term containing E on the right hand side of Equation A.21 to get:

$$(I - E)X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1} = (P + Q_\gamma)X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}$$

Since $\|E\| \leq K'_1 \gamma$ so long as we pick $\gamma \leq (2K'_1)^{-1}$ we can invert $(I - E)$ to get:

$$X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1} = (I - E)^{-1}(P + Q_\gamma)X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}$$

Therefore,

$$\begin{aligned} & \|X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| \\ & \leq \|(I - E)^{-1}\| \left(\|PX_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| + \|Q_\gamma X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| \right). \end{aligned}$$

Now to finish the proof we only need to show that both

$$PX_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1} \text{ and } Q_\gamma X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}$$

are bounded independent of λ and j . However, with the estimates we have now both of these bounds are fairly easy:

$$\|PX_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| \leq 1 + |\lambda_\eta| \|(\lambda_\eta - PX_\eta P_\gamma)^{-1}\|$$

$$\|Q_\gamma X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}\| \leq \|Q_\gamma X_\eta P_\gamma\| \|(\lambda_\eta - PX_\eta P_\gamma)^{-1}\|.$$

By the proof in Section A.2.1, we know that $\|(\lambda_\eta - PX_\eta P_\gamma)^{-1}\|$ is bounded. Since $|\lambda_\eta|$ is bounded by the construction of \mathcal{C}_j and from Proposition A.2.4 we know that $\|Q_\gamma X_\eta P_\gamma\|$ is also bounded, by the above logic we conclude that $X_\eta P_\gamma(\lambda_\eta - PX_\eta P_\gamma)^{-1}$ is bounded. Therefore, by the above logic, for all γ sufficiently small the operator $\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\|$ is bounded uniformly for $\lambda \in \mathcal{C}_j$ by a constant which is independent of $j \in \mathcal{J}$. Since our arguments make no reference to any particular $\eta \in \sigma_j$, this estimate is also uniform in $\eta \in \sigma_j$.

Deducing the key estimate (A.13) from the uniform bound proved on the shifted operators (A.17)

The key estimate (A.13) can be deduced from the uniform bound proved on the shifted operators (A.17) in the previous section via the following Lemma, whose

proof we postpone until Appendix A.3.

Lemma A.2.5. *Suppose P satisfies Assumption 3 with constants (γ', K'_1, K'_2) and suppose that PXP has uniform spectral gaps with decomposition $\{\sigma_j\}_{j \in \mathcal{J}}$ and corresponding contours $\{\mathcal{C}_j\}_{j \in \mathcal{J}}$. Then the following are equivalent for all $0 \leq \gamma < \gamma'$:*

1. *There exists a $C > 0$, independent of j , such that*

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \leq C.$$

There exists a $C' > 0$, independent of j , such that for each $j \in \mathcal{J}$:

$$\sup_{\lambda \in \mathcal{C}_j} \sup_{\eta_j \in \sigma_j} \|(\lambda_{\eta_j} - P_\gamma X_{\eta_j} P_\gamma)^{-1}\| \leq C'$$

Furthermore, for any $0 \leq \gamma < \gamma'$ if $\|(\lambda - P_\gamma X P_\gamma)^{-1}\|$ is bounded we have for any $j \in \mathcal{J}$, $\lambda \in \mathcal{C}_j$, and $\eta_j \in \sigma_j$:

$$(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma = (\lambda_{\eta_j} - P_\gamma X_{\eta_j} P_\gamma)^{-1} P_\gamma.$$

Proof. Given in Appendix A.3. □

With Proposition A.2.2 proved, we can now proceed to prove the assertions of Lemma A.2.1.

A.2.2 Proof of Lemma A.2.1(1)

Let $\eta \in \sigma_j$ be arbitrary. Writing $P_{j,\gamma}$ and P_j in terms of their contour integrals gives:

$$P_{j,\gamma} - P_j = \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma - (\lambda - PXP)^{-1} P d\lambda.$$

Similar to the proof in Section A.2.1, we will want to work with the shifted versions of $(\lambda - P_\gamma X P_\gamma)^{-1}$ and $(\lambda - PXP)^{-1}$. Due to Lemma A.2.5 we know that:

$$(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma = (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma$$

$$(\lambda - PXP)^{-1} P = (\lambda_\eta - PX_\eta P)^{-1} P.$$

Therefore, we have that

$$\begin{aligned}
& P_{j,\gamma} - P_j \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma - (\lambda - P X P)^{-1} P d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma - (\lambda_\eta - P X_\eta P)^{-1} P d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} \left((\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} - (\lambda_\eta - P X_\eta P)^{-1} \right) P + (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} (P_\gamma - P) d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} \left((\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} - (\lambda_\eta - P X_\eta P)^{-1} \right) P + (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} E d\lambda.
\end{aligned}$$

Therefore

$$\begin{aligned}
& \|P_{j,\gamma} - P_j\| \\
&\leq \frac{\ell(\mathcal{C}_j)}{2\pi} \left(\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} - (\lambda_\eta - P X_\eta P)^{-1}\| \|P\| + \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \|E\| \right).
\end{aligned}$$

The second term is $O(\gamma)$ since $\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\|$ is bounded and $\|E\| = O(\gamma)$.

Therefore to finish the proof we need only need to show the first term is $O(\gamma)$.

Using the second resolvent identity we get

$$\begin{aligned}
& (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} - (\lambda_\eta - P X_\eta P)^{-1} \\
&= (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} (P_\gamma X_\eta P_\gamma - P X_\eta P) (\lambda_\eta - P X_\eta P)^{-1} \\
&= (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} (P_\gamma X_\eta P_\gamma - P_\gamma X_\eta P + P_\gamma X_\eta P - P X_\eta P) (\lambda_\eta - P X_\eta P)^{-1} \\
&= (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} (P_\gamma X_\eta E + E X_\eta P) (\lambda_\eta - P X_\eta P)^{-1} \\
&= (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta E (\lambda_\eta - P X_\eta P)^{-1} + (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} E X_\eta P (\lambda_\eta - P X_\eta P)^{-1}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
& \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} - (\lambda_\eta - P X_\eta P)^{-1}\| \\
&\leq \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta\| \|E\| \|(\lambda_\eta - P X_\eta P)^{-1}\| \\
&\quad + \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \|E\| \|X_\eta P (\lambda_\eta - P X_\eta P)^{-1}\|
\end{aligned}$$

Since we already know that $\|(\lambda_\eta - PX_\eta P)^{-1}\|$ and $\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\|$ are bounded and $\|E\| = O(\gamma)$ we only need to show that $\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta\|$ and $\|X_\eta P(\lambda_\eta - PX_\eta P)^{-1}\|$ are bounded.

This is straightforward since

$$\begin{aligned}
& \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta\| \\
&= \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta (P_\gamma + Q_\gamma)\| \\
&\leq \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma X_\eta P_\gamma\| + \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \|P_\gamma X_\eta Q_\gamma\| \\
&\leq 1 + |\lambda_\eta| \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| + \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \|P_\gamma X_\eta Q_\gamma\|,
\end{aligned}$$

which is bounded by our previous estimates.

Repeating similar steps for $X_\eta P(\lambda_\eta - PX_\eta P)^{-1}$ (where one inserts $P + Q$ instead of $P_\gamma + Q_\gamma$) shows that $X_\eta P(\lambda_\eta - PX_\eta P)^{-1}$ is bounded. Therefore, by the previous logic, we conclude that $\|P_{j,\gamma} - P_j\| = O(\gamma)$ as we wanted to show.

A.2.3 Proof of Lemma A.2.1(2)

We will show that $\|[P_{j,\gamma}, Y]\|$ is bounded, that $\|[P_{j,\gamma}, X]\|$ is also bounded follows by similar calculations. By definition we have:

$$[P_{j,\gamma}, Y] = \frac{1}{2\pi i} \int_{\mathcal{C}_j} [(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma, Y] d\lambda.$$

Hence

$$\|[P_{j,\gamma}, Y]\| \leq \frac{\ell(\mathcal{C}_j)}{2\pi} \sup_{\lambda \in \mathcal{C}_j} \|[(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma, Y]\|.$$

Noticing that

$$\begin{aligned}
& (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma - P_\gamma (\lambda - P_\gamma X P_\gamma)^{-1} \\
&= (\lambda - P_\gamma X P_\gamma)^{-1} [P_\gamma (\lambda - P_\gamma X P_\gamma) - (\lambda - P_\gamma X P_\gamma) P_\gamma] (\lambda - P_\gamma X P_\gamma)^{-1},
\end{aligned}$$

and hence $[(\lambda - P_\gamma X P_\gamma)^{-1}, P_\gamma] = 0$, we have:

$$\begin{aligned}
[(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma, Y] &= [(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma, Y] \\
&= (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma Y - Y P_\gamma (\lambda - P_\gamma X P_\gamma)^{-1} \\
&= (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma Y (P_\gamma + Q_\gamma) - (P_\gamma + Q_\gamma) Y P_\gamma (\lambda - P_\gamma X P_\gamma)^{-1} \\
&= [(\lambda - P_\gamma X P_\gamma)^{-1}, P_\gamma Y P_\gamma] \\
&\quad + (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma Y Q_\gamma - Q_\gamma Y P_\gamma (\lambda - P_\gamma X P_\gamma)^{-1}.
\end{aligned} \tag{A.22}$$

The last two terms in Equation (A.22) are bounded since $\|Q_\gamma Y P_\gamma\|$ and $\|P_\gamma Y Q_\gamma\|$ are bounded (see Proposition A.2.4) and we showed that $\|(\lambda - P_\gamma X P_\gamma)^{-1}\|$ is bounded in Section A.2.1. Therefore, to show that $\|[P_{j,\gamma}, Y]\|$ is bounded it suffices to show that $\|[(\lambda - P_\gamma X P_\gamma)^{-1}, P_\gamma Y P_\gamma]\|$ is bounded.

An elementary commutator identity gives that

$$[(\lambda - P_\gamma X P_\gamma)^{-1}, P_\gamma Y P_\gamma] = (\lambda - P_\gamma X P_\gamma)^{-1} [P_\gamma Y P_\gamma, P_\gamma X P_\gamma] (\lambda - P_\gamma X P_\gamma)^{-1}.$$

Since P_γ is idempotent, an easy calculation shows that (proven below in Lemma A.2.6):

$$[P_\gamma Y P_\gamma, P_\gamma X P_\gamma] = -P_\gamma [[X, P_\gamma], [Y, P_\gamma]].$$

Hence

$$\begin{aligned}
\|[(\lambda - P_\gamma X P_\gamma)^{-1}, P_\gamma Y P_\gamma]\| &\leq \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \| [P_\gamma Y P_\gamma, P_\gamma X P_\gamma] \| \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \\
&= \|P_\gamma [[X, P_\gamma], [Y, P_\gamma]]\| \|(\lambda - P_\gamma X P_\gamma)^{-1}\|^2 \\
&\leq \|P_\gamma\| \| [[X, P_\gamma], [Y, P_\gamma]] \| \|(\lambda - P_\gamma X P_\gamma)^{-1}\|^2 \\
&\leq 2 \|P_\gamma\| \| [X, P_\gamma] \| \| [Y, P_\gamma] \| \|(\lambda - P_\gamma X P_\gamma)^{-1}\|^2
\end{aligned}$$

and so from the bounds in Proposition A.2.4 and above logic, $\|[P_{j,\gamma}, Y]\|$ is bounded.

Lemma A.2.6. *Suppose that P is idempotent (i.e. $P^2 = P$) and $[X, Y] = 0$ then*

$$[PXP, PYP] = P[[X, P], [Y, P]]$$

Proof. Defining $Q := I - P$, this is just a straightforward calculation:

$$\begin{aligned}
[PXP, PYP] &= PXPYP - PYPXP \\
&= PX(I - Q)YP + PY(I - Q)YP \\
&= PYQXP - PXQYP + PXYYP - PYYXP \\
&= PYQXP - PXQYP \\
&= PYQ[X, P] - PXQ[Y, P] \\
&= P[Y, Q][X, P] - P[X, Q][Y, P] \\
&= -P[Y, P][X, P] + P[X, P][Y, P] \\
&= P[[X, P], [Y, P]].
\end{aligned}$$

In the above calculation, we have made use of the fact that $PQ = QP = 0$ and so $QXP = QPX + Q[X, P] = Q[X, P]$. \square

A.2.4 Proof of Lemma A.2.1(3)

For this section, let us fix some $\eta \in \sigma_j$, we will prove that $\|(X - \eta)P_{j,\gamma}\|$ is bounded. The fact that $\|P_{j,\gamma}(X - \eta)\|$ is bounded follows by essentially the same steps. Recalling we define $\lambda_\eta := \lambda - \eta$ and $X_\eta := X - \eta$ and using Lemma A.2.5 we have

$$\begin{aligned}
(X - \eta)P_{j,\gamma} &= \frac{1}{2\pi i} \int_{\mathcal{C}_j} (X - \eta)(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} X_\eta (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} P_\gamma d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} X_\eta P_\gamma (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} d\lambda \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}_j} (P_\gamma + Q_\gamma) X_\eta P_\gamma (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} d\lambda.
\end{aligned}$$

where we have used that P_γ commutes with $(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}$. Therefore,

$$\|(X - \eta)P_{j,\gamma}\| \leq \frac{\ell(\mathcal{C}_j)}{2\pi} \left(\|P_\gamma X_\eta P_\gamma (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| + \|Q_\gamma X_\eta P_\gamma\| \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \right).$$

Note that

$$\|P_\gamma X_\eta P_\gamma (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \leq 1 + |\lambda_\eta| \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\|.$$

Therefore, since $\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\|$ and $\|Q_\gamma X_\eta P_\gamma\|$ are both bounded, we can conclude that $\|(X - \eta)P_{j,\gamma}\|$ is bounded as we wanted to show.

A.3 Shifting Lemma

Let's recall the result we would like to prove:

Lemma A.3.1. *Suppose P satisfies Assumption 3 with constants (γ', K'_1, K'_2) and suppose that PXP has uniform spectral gaps with decomposition $\{\sigma_j\}_{j \in \mathcal{J}}$ and corresponding contours $\{\mathcal{C}_j\}_{j \in \mathcal{J}}$. For arbitrary $\eta \in \mathbb{C}$, define $\lambda_\eta := \lambda - \eta$ and $X_\eta := X - \eta$. Then the following are equivalent for all $0 \leq \gamma < \gamma'$:*

1. *There exists a $C > 0$, independent of j , such that*

$$\sup_{\lambda \in \mathcal{C}_j} \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \leq C$$

2. *There exists a $C' > 0$, independent of j , such that*

$$\sup_{\lambda \in \mathcal{C}_j} \sup_{\eta \in \sigma_j} \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \leq C'$$

Furthermore, for any $\gamma < \gamma'$ if $\|(\lambda - P_\gamma X P_\gamma)^{-1}\|$ is bounded we have for any $j \in \mathcal{J}$ and $\eta_j \in \mathcal{C}_j$:

$$(\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma = (\lambda_{\eta_j} - P_\gamma X_{\eta_j} P_\gamma)^{-1} P_\gamma.$$

The basic steps to prove this lemma are the following:

$$\begin{aligned} (\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1} &= (\lambda - \eta - P_\gamma (X - \eta) P_\gamma)^{-1} \\ &= (\lambda - \eta - P_\gamma X P_\gamma + \eta P_\gamma)^{-1} \\ &= (\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1}. \end{aligned} \tag{A.23}$$

Since $P_\gamma + Q_\gamma = I$, because of this calculation we know that

$$\begin{aligned} \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| &= \|(\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1}\| \\ &\leq \|(\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1} P_\gamma\| + \|(\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1} Q_\gamma\|. \end{aligned}$$

Since $P_\gamma Q_\gamma = Q_\gamma P_\gamma = 0$, we should expect that shifting by ηQ_γ should not change what happens on range(P_γ). Similarly, the action of $P_\gamma X P_\gamma$ should not change what happens on range(Q_γ). This observation leads us to expect that:

$$(\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1} P_\gamma = (\lambda - P_\gamma X P_\gamma)^{-1} P_\gamma \quad (\text{A.24})$$

$$(\lambda - P_\gamma X P_\gamma - \eta Q_\gamma)^{-1} Q_\gamma = (\lambda - \eta Q_\gamma)^{-1} Q_\gamma. \quad (\text{A.25})$$

By similar reasoning:

$$(\lambda - \eta Q_\gamma)^{-1} Q_\gamma = (\lambda - \eta + \eta P_\gamma)^{-1} Q_\gamma = (\lambda - \eta)^{-1} Q_\gamma. \quad (\text{A.26})$$

Assuming Equations (A.24), (A.25), (A.26) are true, we conclude that:

$$\|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| \leq \|(\lambda - P_\gamma X P_\gamma)^{-1}\| \|P_\gamma\| + |\lambda - \eta|^{-1} \|Q_\gamma\|. \quad (\text{A.27})$$

Since P satisfies Assumption 3 we know that $\|P_\gamma\|$ and $\|Q_\gamma\|$ are bounded. Because of the uniform spectral gaps assumption on PXP , since we have chosen $\eta \in \sigma_j$ and $\lambda \in \mathcal{C}_j$ we also know that $|\lambda - \eta|^{-1}$ is bounded by a constant independent of j and η . Therefore, Equation (A.27) shows that

$$\|(\lambda - P_\gamma X P_\gamma)^{-1}\| < \infty \implies \|(\lambda_\eta - P_\gamma X_\eta P_\gamma)^{-1}\| < \infty.$$

We can prove the reverse implication by instead starting with the calculation

$$\begin{aligned} (\lambda - P_\gamma X P_\gamma)^{-1} &= (\lambda - \eta + \eta - P_\gamma(X - \eta + \eta)P_\gamma)^{-1} \\ &= (\lambda_\eta - P_\gamma X_\eta P_\gamma + \eta Q_\gamma)^{-1}, \end{aligned}$$

and proceeding along similar steps.

What remains to finish the proof of Lemma A.2.5 is to prove that Equations (A.24), (A.25), (A.26) are all true. For this, we have the following technical lemma:

Lemma A.3.2. *Let \tilde{P}, \tilde{Q} be any pair of bounded operators such that $\tilde{P}\tilde{Q} = \tilde{Q}\tilde{P} = 0$. Next, let A, B be possibly unbounded operators densely defined on a common domain \mathcal{D} . Suppose further that $\|[\tilde{P}, A]\|$ both $\|[\tilde{Q}, B]\|$ are bounded.*

If $\tilde{\lambda} \in \mathbb{C}$ is any scalar such that $\|(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}\|$ is bounded then $\|(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})^{-1}\tilde{P}\|$ is also bounded and

$$(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}\tilde{P} = (\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})^{-1}\tilde{P}.$$

Note that applying Lemma A.3.2 three times proves that Equations (A.24), (A.25), (A.26) are all true.

The assumption that $\|[\tilde{P}, A]\|$ and $\|[\tilde{Q}, B]\|$ are bounded is purely a technical assumption which ensures that $\tilde{P}A\tilde{P}$ and $\tilde{Q}B\tilde{Q}$ are a well defined operators on \mathcal{D} . To see, why observe that

$$\tilde{P}A\tilde{P} = \tilde{P}[A, \tilde{P}] + \tilde{P}\tilde{P}A \text{ and } \tilde{Q}B\tilde{Q} = \tilde{Q}[B, \tilde{Q}] + \tilde{Q}\tilde{Q}B.$$

For our purposes, the only unbounded operator we will need to be careful with is the operator X . Since P satisfies Assumption 3 we know that $\|[P_\gamma, X]\| = \|[Q_\gamma, X]\| < \infty$, therefore we may apply Lemma A.3.2 without worry.

Proof of Lemma A.3.2. First, note that $\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{P}B\tilde{P}$ is injective on $\text{range}(P)$ since for arbitrary non-zero $v \in \text{range}(P) \cap \mathcal{D}$,

$$\begin{aligned} \left\| \left(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q} \right) v \right\| &= \left\| \left(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q} \right) \tilde{P}v \right\| \\ &= \left\| \left(\tilde{\lambda} + \tilde{P}A\tilde{P} \right) v \right\| \geq \|(\lambda + PAP)^{-1}\|^{-1}\|v\|. \end{aligned}$$

Now observe that since $\tilde{P}\tilde{Q} = \tilde{Q}\tilde{P} = 0$

$$[(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q}), (\tilde{\lambda} + \tilde{P}A\tilde{P})] = 0.$$

Since $(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}$ is well defined, this implies that

$$[(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q}), (\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}] = 0$$

Since $\tilde{Q}\tilde{P} = 0$ we also have that

$$\begin{aligned} (\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})\tilde{P} &= (\tilde{\lambda} + \tilde{P}A\tilde{P})\tilde{P} \\ \iff (\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})\tilde{P} &= \tilde{P} \\ \iff (\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}\tilde{P} &= \tilde{P}. \end{aligned}$$

The final equality implies that $\text{range}(\tilde{P}) \subseteq \text{range}(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})$. Since $(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}$ is bounded we can conclude that $(\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})$ is invertible on $\text{range}(\tilde{P})$ and so

$$(\tilde{\lambda} + \tilde{P}A\tilde{P})^{-1}\tilde{P} = (\tilde{\lambda} + \tilde{P}A\tilde{P} + \tilde{Q}B\tilde{Q})^{-1}\tilde{P}.$$

□

A.4 Uniform Spectral Gaps and the Chern Number

In this section we connect the uniform spectral gap assumption (Assumption 4) to the existing well-developed theory of exponentially-localized Wannier functions in crystalline insulators. Specifically, we prove that if the uniform spectral gap assumption (Assumption 4) holds for a two-dimensional *crystalline* insulator, then it is possible to construct an analytic and periodic Bloch frame for the Fermi projection. It is well established that existence of such a frame is equivalent to triviality of the Chern number, a topological invariant associated to the Fermi projection, and to the existence of exponentially-localized composite Wannier functions defined via integration with respect to quasi-momentum over the Brillouin zone [Clo64, DC64, Nen83, HS88, Nen91, BPC⁺07, Pan07, MPPT18]. To our knowledge, the observation that the uniform spectral gap assumption (Assumption 4) is sufficient for the construction of an analytic and periodic Bloch frame is original to the mathematical literature, although it is implicit in the works of Soluyanov and

Vanderbilt [SV11b, SV11a, TGV14, GAY⁺17, WZS⁺18], and the techniques required for the proof are basically known [CHN16, CLPS17].

We will make the connection between the operator PXP and existence of a periodic and analytic Bloch frame through the hybrid Wannier functions (HWFs) first described in [SPR01] (see also [Niu91]). The key observation is that, with an appropriate Bloch frame, HWFs are exact eigenfunctions of PXP [Niu91, SV11b, SV11a, TGV14, GAY⁺17, WZS⁺18]. We will see that the uniform spectral gap assumption (Assumption 4) gives a sufficient condition for the frame to be analytic and periodic over the whole Brillouin zone.

The structure of this section is as follows. We will first recall the aspects of Bloch theory which are necessary to state our results in Section A.4.1. We will then make our assumptions precise and state the theorem which we will prove (Theorem 6) in Section A.4.2. We will then construct an analytic frame over the whole Brillouin zone which is periodic with respect to *one* of the components of the quasi-momentum, and derive a condition under which this gauge is also periodic with respect to the other component (Section A.4.3). We will then introduce the hybrid Wannier functions which diagonalize PXP and show that the uniform spectral gap assumption implies the condition necessary for the frame just constructed to be periodic with respect to both components of the quasi-momentum (Section A.4.4).

A.4.1 Notation and Bloch theory in two spatial dimensions

We consider Hamiltonians with the form (recall Assumption 1)

$$H = (i\nabla + A)^2 + V, \tag{A.28}$$

where $A \in L^\infty(\mathbb{R}^2; \mathbb{R}^2)$, $\operatorname{div} A \in L^\infty(\mathbb{R}^2; \mathbb{R})$, and $V \in L^\infty(\mathbb{R}^2; \mathbb{R})$ are real functions. Let Λ denote a two-dimensional lattice generated by non-parallel lattice vectors $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^2$, i.e.

$$\Lambda = \{m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2 : (m_1, m_2) \in \mathbb{Z}^2\}. \tag{A.29}$$

We assume that the functions A and V are periodic with respect to Λ in the sense that for all $\mathbf{x} \in \mathbb{R}^2$

$$A(\mathbf{x} + \mathbf{v}) = A(\mathbf{x}), \quad V(\mathbf{x} + \mathbf{v}) = V(\mathbf{x}) \text{ for all } \mathbf{v} \in \Lambda. \quad (\text{A.30})$$

Define $L_j := |\mathbf{v}_j|, j = 1, 2$. We work with coordinates defined with respect to the lattice vectors \mathbf{v}_1 and \mathbf{v}_2 so that for $\mathbf{x} \in \mathbb{R}^2$,

$$\mathbf{x} = x\mathbf{v}_1 + y\mathbf{v}_2 \quad (\text{A.31})$$

for $(x, y) \in \mathbb{R}^2$. We let Ω denote a fundamental cell of the lattice Λ , i.e.

$$\Omega := \{x\mathbf{v}_1 + y\mathbf{v}_2 : (x, y) \in [0, 1]^2\}. \quad (\text{A.32})$$

For any $\mathbf{k} \in \mathbb{R}^2$, let $L_{\mathbf{k}}^2$ denote the space of L^2 functions on Ω with “ \mathbf{k} -quasi-periodic” boundary conditions

$$L_{\mathbf{k}}^2 := \{f(\mathbf{x}) \in L^2(\Omega) : f(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{k} \cdot \mathbf{v}} f(\mathbf{x}) \quad \forall \mathbf{v} \in \Lambda\}, \quad (\text{A.33})$$

and let L_{per}^2 denote the same space but with periodic boundary conditions

$$L_{per}^2 := \{f(\mathbf{x}) \in L^2(\Omega) : f(\mathbf{x} + \mathbf{v}) = f(\mathbf{x}) \quad \forall \mathbf{v} \in \Lambda\}. \quad (\text{A.34})$$

The operator H restricted to any of the spaces $L_{\mathbf{k}}^2$ is self-adjoint and has compact resolvent. Its spectrum therefore consists only of real eigenvalues which can be ordered with multiplicity as

$$E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq \dots \leq E_n(\mathbf{k}) \leq \dots \quad (\text{A.35})$$

The functions $\mathbf{k} \mapsto E_n(\mathbf{k})$ are known as Bloch band functions, and the associated $L_{\mathbf{k}}^2$ -eigenfunctions of these eigenvalues $\Phi_n(\mathbf{x}, \mathbf{k})$ are known as Bloch functions. The parameter \mathbf{k} is known as the quasi-momentum (or crystal momentum).

The dual lattice is defined by

$$\Lambda^* := \{m_1\mathbf{w}_1 + m_2\mathbf{w}_2 : (m_1, m_2) \in \mathbb{Z}^2\}, \quad (\text{A.36})$$

where \mathbf{w}_1 and \mathbf{w}_2 are defined by the relations

$$\mathbf{v}_i \cdot \mathbf{w}_j = 2\pi\delta_{ij} \quad i, j = 1, 2. \quad (\text{A.37})$$

We work with coordinates defined with respect to the lattice vectors \mathbf{w}_1 and \mathbf{w}_2 so that

$$\mathbf{k} = \frac{k_1}{2\pi}\mathbf{w}_1 + \frac{k_2}{2\pi}\mathbf{w}_2. \quad (\text{A.38})$$

Since $L^2_{\mathbf{k}+\mathbf{w}} = L^2_{\mathbf{k}}$ for any $\mathbf{w} \in \Lambda^*$, the Bloch band functions (A.35) and associated eigenprojections $P_n(\mathbf{k})$ are periodic with respect to Λ^* . There is thus no loss in restricting attention to \mathbf{k} only in a fundamental cell of the dual lattice which we denote by \mathcal{B} and refer to as the Brillouin zone (see Remark A.4.1)

$$\mathcal{B} := \left\{ \frac{k_1}{2\pi}\mathbf{w}_1 + \frac{k_2}{2\pi}\mathbf{w}_2 : (k_1, k_2) \in [-\pi, \pi]^2 \right\}. \quad (\text{A.39})$$

The Bloch functions $\Phi_n(\mathbf{x}, \mathbf{k})$ extend naturally to functions on \mathbb{R}^2 using the boundary condition (A.33). These functions form a complete set in $L^2(\mathbb{R}^2)$ in the following sense (see [Gel50, OK64, PBL78] for proofs). For any $f \in L^2(\mathbb{R}^2)$, define the Bloch-Floquet coefficients

$$\tilde{f}_n(\mathbf{k}) := \langle \Phi_n(\cdot, \mathbf{k}) | f(\cdot) \rangle_{L^2(\mathbb{R}^2)} \quad n \geq 1, \mathbf{k} \in \mathcal{B}. \quad (\text{A.40})$$

Then, for a suitable normalization of the $\Phi_n(\mathbf{x}, \mathbf{k})$,

$$f(\mathbf{x}) = \sum_{n \geq 1} \int_{\mathcal{B}} \tilde{f}_n(\mathbf{k}) \Phi_n(\mathbf{x}, \mathbf{k}) \, d\mathbf{k}. \quad (\text{A.41})$$

It follows that the $L^2(\mathbb{R}^2)$ -spectrum of H is simply the union of the set of closed intervals swept out by the maps $\mathbf{k} \mapsto E_n(\mathbf{k})$ as \mathbf{k} varies over the Brillouin zone, i.e.

$$\sigma(H) = \bigcup_{n \in \mathbb{N}} \bigcup_{\mathbf{k} \in \mathcal{B}} E_n(\mathbf{k}). \quad (\text{A.42})$$

The eigenvalues (A.35) and associated Bloch functions can equivalently be obtained by noting that $\Phi_n(\mathbf{x}, \mathbf{k}) \in L^2_{\mathbf{k}}$ is an eigenfunction of H with eigenvalue $E_n(\mathbf{k})$ if and only if $\chi_n(\mathbf{x}, \mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{x}} \Phi_n(\mathbf{x}, \mathbf{k})$ is an eigenfunction of the operator

$$H(\mathbf{k}) := (\mathbf{k} + A - i\nabla)^2 + V \quad (\text{A.43})$$

acting on L_{per}^2 with eigenvalue $E_n(\mathbf{k})$. Each $\chi_n(\mathbf{x}, \mathbf{k})$ is known as a “periodic Bloch function”. The eigenprojections $P_{per,n}(\mathbf{k})$ onto periodic Bloch functions satisfy the symmetry

$$P_{per,n}(\mathbf{k} + \mathbf{w}) = e^{-i\mathbf{w}\cdot\mathbf{k}} P_{per,n}(\mathbf{k}) e^{i\mathbf{w}\cdot\mathbf{k}} \quad \forall \mathbf{w} \in \Lambda^*. \quad (\text{A.44})$$

Remark A.4.1. Note that generally speaking the Brillouin zone refers to the fundamental cell of the dual lattice defined as the set of points closer to the origin of the reciprocal lattice than to any other reciprocal lattice points (Wigner-Seitz cell), which does not agree with the definition (A.39) for every Bravais lattice. Here we abuse notation because for our purposes it is simpler to work with the rectangular geometry (A.39).

A.4.2 Problem statement

We at this point make our assumptions precise. Let H be a periodic Schrödinger operator as in (A.28).

Assumption 5. *We assume that there exists a positive integer N such that the N th and $(N + 1)$ th Bloch band functions of H are separated by a uniform gap, i.e.*

$$E_{gap} := \min_{\mathbf{k} \in \mathcal{B}} |E_{N+1}(\mathbf{k}) - E_N(\mathbf{k})| > 0. \quad (\text{A.45})$$

Assumption 5 is essentially Assumption 2 specialized to the crystalline case. Note that we do not assume gaps between the other Bloch band functions $E_n(\mathbf{k})$ where $1 \leq n \leq N$. We define the Fermi projection $P : L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^2)$ as the orthogonal projection onto the set of Bloch functions associated with the first N bands, i.e.

$$Pf(\mathbf{x}) = \sum_{n=1}^N \int_{\mathcal{B}} \langle \Phi_n(\cdot, \mathbf{k}) | f(\cdot) \rangle_{L^2(\mathbb{R}^2)} \Phi_n(\mathbf{x}, \mathbf{k}) d\mathbf{k}. \quad (\text{A.46})$$

Because of the gap assumption (Assumption 5), we could equivalently define P via a Riesz projection as in (3.3). It is useful to introduce orthogonal projections $P(\mathbf{k}) :$

$L_{\mathbf{k}}^2 \rightarrow L_{\mathbf{k}}^2$ onto the sets of Bloch functions associated with the first N bands for each $\mathbf{k} \in \mathcal{B}$, i.e.

$$P(\mathbf{k})f(\mathbf{x}) = \sum_{n=1}^N \langle \Phi_n(\cdot, \mathbf{k}) | f(\cdot) \rangle_{L_{\mathbf{k}}^2} \Phi_n(\mathbf{x}, \mathbf{k}). \quad (\text{A.47})$$

We finally introduce orthogonal projections $P_{per}(\mathbf{k}) : L_{per}^2 \rightarrow L_{per}^2$ onto the sets of periodic Bloch functions associated with the first N bands for each $\mathbf{k} \in \mathcal{B}$, i.e.

$$P_{per}(\mathbf{k})f(\mathbf{x}) = \sum_{n=1}^N \langle \chi_n(\cdot, \mathbf{k}) | f(\cdot) \rangle_{L_{per}^2} \chi_n(\mathbf{x}, \mathbf{k}). \quad (\text{A.48})$$

We now introduce the precise concept of a Bloch frame.

Definition 7. A Bloch frame is a choice of basis for $\text{range } P_{per}(\mathbf{k})$ at every $\mathbf{k} \in \mathcal{B}$, i.e. a collection of maps

$$\begin{aligned} \mathcal{B} &\rightarrow (L_{per}^2)^N \\ \mathbf{k} &\mapsto (\Xi_1(\mathbf{x}, \mathbf{k}), \dots, \Xi_N(\mathbf{x}, \mathbf{k})), \end{aligned} \quad (\text{A.49})$$

where the set $(\Xi_1(\mathbf{x}, \mathbf{k}), \dots, \Xi_N(\mathbf{x}, \mathbf{k}))$ is a basis for $\text{range } P_{per}(\mathbf{k})$ at every $\mathbf{k} \in \mathcal{B}$. We say the Bloch frame is analytic if every map $\mathbf{k} \mapsto \Xi_n(\mathbf{x}, \mathbf{k}), 1 \leq n \leq N$ is (real) analytic for all $\mathbf{k} \in \mathcal{B}$. We say the Bloch frame is periodic if every map $\mathbf{k} \mapsto \Xi_n(\mathbf{x}, \mathbf{k}), 1 \leq n \leq N$ satisfies

$$\Xi_n(\mathbf{x}, \mathbf{k} + \mathbf{w}) = e^{-i\mathbf{w} \cdot \mathbf{x}} \Xi_n(\mathbf{x}, \mathbf{k}) \quad 1 \leq n \leq N, \forall \mathbf{w} \in \Lambda^*. \quad (\text{A.50})$$

We will prove that

Theorem 6. *Let P be the Fermi projection of a periodic Hamiltonian as in (A.46), and assume the spectral gap Assumption 5. Recall the coordinates introduced in (A.31), and define the operator X by*

$$Xf(x, y) = L_1 x f(x, y). \quad (\text{A.51})$$

Then, if the operator PXP satisfies the uniform spectral gap assumption (Assumption 4), an analytic and periodic Bloch function gauge in the sense of Definition 7 exists.

We will prove Theorem 6 across the following sections. Recall that we have introduced natural \mathbf{k} -space coordinates (k_1, k_2) (A.38). We will first construct a Bloch function gauge which is analytic over the Brillouin zone and periodic with respect to k_1 . We will then prove that, whenever the uniform spectral gap assumption on PXP holds, this gauge must also be periodic with respect to k_2 .

A.4.3 Proof of Theorem 6: Parallel transport unitaries and construction of an analytic gauge periodic with respect to k_1

We first recall the notion of parallel transport of periodic Bloch functions (see [CHN16] for more detail).

Recall we define $P_{per}(k_1, k_2)$ to be the L^2_{per} -projection onto the set of periodic Bloch functions at k_1, k_2 , i.e. onto the span of $\{\chi_n(\mathbf{x}, k_1, k_2)\}_{1 \leq n \leq N}$. The operators $P_{per}(k_1, k_2)$ satisfy the following symmetries, which follow from symmetry of the operator $H(\mathbf{k})$ (A.43)

$$\begin{aligned} e^{-i\mathbf{w}_2 \cdot \mathbf{x}} P_{per}(k_1, k_2) e^{i\mathbf{w}_2 \cdot \mathbf{x}} &= P_{per}(k_1, k_2 + 2\pi) \\ e^{-i\mathbf{w}_1 \cdot \mathbf{x}} P_{per}(k_1, k_2) e^{i\mathbf{w}_1 \cdot \mathbf{x}} &= P_{per}(k_1 + 2\pi, k_2). \end{aligned} \tag{A.52}$$

Following Kato [Kat95], we define unitaries $T_{k_2}(k_1)$ for each fixed $k_2 \in [-\pi, \pi]$ and for $k_1 \in [-\pi, \pi]$ by the ODE

$$\begin{aligned} i\partial_{k_1} T_{k_2}(k_1) &= i[\partial_{k_1} P_{per}(k_1, k_2), P_{per}(k_1, k_2)] T_{k_2}(k_1) \\ T_{k_2}(0) &= I. \end{aligned} \tag{A.53}$$

We note three properties of these unitaries. First, the identity (see [Kat95, Chapter 2 §4])

$$P_{per}(k_1, k_2) T_{k_2}(k_1) = T_{k_2}(k_1) P_{per}(0, k_2) \tag{A.54}$$

shows that $T_{k_2}(k_1)$ restricted to $\text{range}(P_{per}(0, k_2))$ maps to $\text{range}(P_{per}(k_1, k_2))$ bijectively.

tively. Second, using the symmetries (A.52), we have that, for example,

$$\begin{aligned} i\partial_{k_1} \left(e^{-i\mathbf{w}_2 \cdot \mathbf{x}} T_{k_2}(k_1) e^{i\mathbf{w}_2 \cdot \mathbf{x}} \right) &= i[\partial_{k_1} P_{per}(k_1, k_2 + 2\pi), P_{per}(k_1, k_2 + 2\pi)] \left(e^{-i\mathbf{w}_2 \cdot \mathbf{x}} T_{k_2}(k_1) e^{i\mathbf{w}_2 \cdot \mathbf{x}} \right) \\ e^{-i\mathbf{w}_2 \cdot \mathbf{x}} T_{k_2}(0) e^{i\mathbf{w}_2 \cdot \mathbf{x}} &= I, \end{aligned} \quad (\text{A.55})$$

and hence (since they satisfy the same initial value problems)

$$T_{k_2+2\pi}(k_1) = e^{-i\mathbf{w}_2 \cdot \mathbf{x}} T_{k_2}(k_1) e^{i\mathbf{w}_2 \cdot \mathbf{x}}, \quad T_{k_2}(k_1 + 2\pi) = e^{-i\mathbf{w}_1 \cdot \mathbf{x}} T_{k_2}(k_1) e^{i\mathbf{w}_1 \cdot \mathbf{x}}. \quad (\text{A.56})$$

Third, by the method of successive approximations (see [CL55]), the maps $k_1 \mapsto T_{k_2}(k_1)$ and $k_2 \mapsto T_{k_2}(k_1)$ are both (real) analytic since $P_{per}(k_1, k_2)$ is analytic in both variables. It is clear that by the same calculations we can also define unitaries $T_{k_1}(k_2)$ where $k_1 \in [-\pi, \pi]$ is fixed and $k_2 \in [-\pi, \pi]$ with analogous properties.

We first construct a Bloch frame which is periodic with respect to k_2 as follows. Let $\{\Xi_n(\mathbf{x}, 0, 0)\}_{1 \leq n \leq N}$ be an arbitrary basis of the span of $\{\chi_n(\mathbf{x}, 0, 0)\}_{1 \leq n \leq N}$. Define

$$\Xi_n(\mathbf{x}, 0, k_2) := T_0(k_2) \Xi_n(\mathbf{x}, 0, 0) \quad 1 \leq n \leq N, k_2 \in [-\pi, \pi]. \quad (\text{A.57})$$

By analyticity of $T_0(k_2)$, the $\Xi_n(\mathbf{x}, 0, k_2)$ are analytic with respect to k_2 . Using symmetry of $P_{per}(k_1, k_2)$ (A.52) we have that

$$\Xi_m(\mathbf{x}, 0, -\pi) = e^{i\mathbf{w}_2 \cdot \mathbf{x}} \sum_{n=1}^N U_{mn} \Xi_n(\mathbf{x}, 0, \pi) \quad (\text{A.58})$$

where $U = \{U_{mn}\}_{1 \leq m \leq N, 1 \leq n \leq N}$ is a unitary $N \times N$ matrix with eigenvalues $(\lambda_1, \dots, \lambda_N)$. By unitarity we can write U as

$$U = QDQ^*, \quad D := \text{diag}(\lambda_1, \dots, \lambda_N), \quad (\text{A.59})$$

where Q is the matrix whose columns are the normalized eigenvectors of U , $\lambda_1, \dots, \lambda_N$ denotes the eigenvalues of U , and $\text{diag}(v)$ denotes the diagonal matrix with the components of the vector v along its diagonal. Again by unitarity, we have that each eigenvalue of U can be written $\lambda_m = e^{i\Gamma_m}$ where Γ_m is real and $-\pi \leq \Gamma_m \leq \pi$. We define the matrix log of U in the usual way via spectral calculus as

$$\log U := Q (\log D) Q^*, \quad \log D := \text{diag}(\Gamma_1, \dots, \Gamma_N). \quad (\text{A.60})$$

To obtain a periodic frame along the line $k_1 = 0$ we define

$$\exp\left(-i\frac{k_2 \log U}{2\pi}\right) := Q \exp\left(-i\frac{k_2 \log D}{2\pi}\right) Q^* \quad (\text{A.61})$$

where

$$\exp\left(-i\frac{k_2 \log D}{2\pi}\right) := \text{diag}\left(e^{-i\frac{\Gamma_1 k_2}{2\pi}}, \dots, e^{-i\frac{\Gamma_N k_2}{2\pi}}\right). \quad (\text{A.62})$$

We then define a new frame along the line $k_1 = 0$ by

$$\tilde{\Xi}_n(\mathbf{x}, 0, k_2) := \exp\left(-i\frac{k_2 \log U}{2\pi}\right) \Xi_n(\mathbf{x}, 0, k_2). \quad (\text{A.63})$$

The $\tilde{\Xi}_n(\mathbf{x}, 0, k_2)$ are clearly analytic with respect to k_2 , and are now periodic in the sense that

$$\tilde{\Xi}_n(\mathbf{x}, 0, -\pi) = e^{i\mathbf{w}_2 \cdot \mathbf{x}} \tilde{\Xi}_n(\mathbf{x}, 0, \pi). \quad (\text{A.64})$$

We now extend this frame to the whole Brillouin zone by defining

$$\tilde{\Xi}_n(\mathbf{x}, k_1, k_2) := T_{k_2}(k_1) \tilde{\Xi}_n(\mathbf{x}, 0, k_2) \quad 1 \leq n \leq N, (k_1, k_2) \in [-\pi, \pi]^2. \quad (\text{A.65})$$

Using the properties of $T_{k_2}(k_1)$ the $\tilde{\Xi}_n(\mathbf{x}, k_1, k_2)$ are analytic with respect to both k_1 and k_2 , and periodic with respect to k_2 since for any $k_1 \in [-\pi, \pi]$,

$$\begin{aligned} \tilde{\Xi}_n(\mathbf{x}, k_1, -\pi) &= T_{-\pi}(k_1) \tilde{\Xi}_n(\mathbf{x}, 0, -\pi) = e^{i\mathbf{w}_2 \cdot \mathbf{x}} T_\pi(k_1) e^{-i\mathbf{w}_2 \cdot \mathbf{x}} e^{i\mathbf{w}_2 \cdot \mathbf{x}} \tilde{\Xi}_n(\mathbf{x}, 0, \pi) \\ &= e^{i\mathbf{w}_2 \cdot \mathbf{x}} T_\pi(k_1) \tilde{\Xi}_n(\mathbf{x}, 0, \pi) \\ &= e^{i\mathbf{w}_2 \cdot \mathbf{x}} \tilde{\Xi}_n(\mathbf{x}, k_1, \pi), \end{aligned} \quad (\text{A.66})$$

where the second equality is by (A.56) and (A.64). Note that using (A.53) the frame satisfies the following ‘‘parallel transport’’ property with respect to k_1

$$\left\langle \tilde{\Xi}_m(\mathbf{x}, k_1, k_2) \left| \partial_{k_1} \tilde{\Xi}_n(\mathbf{x}, k_1, k_2) \right\rangle_{L_{per}^2} \quad 1 \leq m, n \leq N, (k_1, k_2) \in [-\pi, \pi]^2. \quad (\text{A.67})$$

Having constructed a frame which is analytic and periodic with respect to k_2 , we now aim to ‘‘mend’’ the gauge so that it is also periodic with respect to k_1 . We will see that this is not always possible while preserving periodicity with respect to k_2 .

For each k_2 , the gauge so far constructed will not in general be periodic with respect to k_1 , but must satisfy

$$\tilde{\Xi}_m(\mathbf{x}, -\pi, k_2) = e^{i\mathbf{w}_1 \cdot \mathbf{x}} \sum_{n=1}^N U_{mn}(k_2) \tilde{\Xi}_n(\mathbf{x}, \pi, k_2) \quad k_2 \in [-\pi, \pi] \quad (\text{A.68})$$

for a family of $N \times N$ unitary matrices $U(k_2) = \{U_{mn}(k_2)\}_{1 \leq m \leq N, 1 \leq n \leq N}$ depending analytically and periodically on $k_2 \in [-\pi, \pi]$.

We now require a Lemma, whose proof is similar to Section 2.7.4 of [CHN16], see also Kato [Kat95].

Lemma A.4.2. *Let $\phi(\tau)$ be a family of unitary $N \times N$ matrices depending analytically and periodically on $\tau \in [-\pi, \pi]$. Then there exist analytic and periodic functions*

$$\begin{aligned} [-\pi, \pi] &\rightarrow \mathbb{R}^N \\ \tau &\mapsto \mathbf{v}_n(\tau) \end{aligned} \quad (\text{A.69})$$

for $1 \leq n \leq N$ such that $\mathbf{v}_n(\tau)$ is an eigenvector of $\phi(\tau)$ for every $\tau \in [-\pi, \pi]$.

Proof. We start by noting that the roots of the characteristic polynomial of $\phi(\tau)$ are branches of analytic functions of τ with only algebraic singularities [Kat95]. It follows that the number of eigenvalues of $\phi(\tau)$ is a constant with the exception of finitely many points in the interval $[-\pi, \pi]$, which implies that every eigenvalue of $\phi(\tau)$ is either degenerate for all τ or non-degenerate except at finitely many τ . It follows that we can find τ^* such that every eigenvalue which is not degenerate for every $\tau \in [-\pi, \pi]$ is non-degenerate. We can define projections onto each eigenvector, or degenerate family of eigenvectors, in a neighborhood of τ^* via the Riesz projection formula

$$Q_n(\tau) := \frac{1}{2\pi i} \int_{\gamma_n} (z - \phi(\tau))^{-1} dz, \quad (\text{A.70})$$

where γ_n is a contour enclosing exactly one eigenvalue of $\phi(\tau^*)$. It is clear that the projection is analytic in a neighborhood of τ^* . We next note that each projection can be analytically continued over the whole interval $[-\pi, \pi]$, even through eigenvalue

crossings (see Rellich [RB69]). By periodicity of $\phi(\tau)$ and using the formula (A.70), the projections $Q_n(\tau)$ are also 2π -periodic. We can now define eigenvectors which are analytic in τ by defining parallel transport unitaries associated to the projections $Q_n(\tau)$ as in (A.53). To make these eigenvectors periodic as well we use the same trick as in (A.63), i.e. we use the matrix log of the unitary mapping the eigenvectors at $\tau^* + 2\pi$ to those at τ^* to rotate the eigenvectors so that they are periodic. \square

Using Lemma A.4.2 we can write $U(k_2)$ as

$$U(k_2) = Q(k_2)D(k_2)Q^*(k_2), \quad D(k_2) := \text{diag}(\lambda_1(k_2), \dots, \lambda_N(k_2)) \quad (\text{A.71})$$

where $Q(k_2)$ is the matrix whose columns are normalized eigenvectors of $U(k_2)$, *chosen to be periodic with respect to k_2* , and $\lambda_1(k_2), \dots, \lambda_N(k_2)$ are the eigenvalues of $U(k_2)$.

We now define

$$\check{\Xi}_m(x, k_1, k_2) = \sum_{n=1}^N Q_{mn}(k_2) \tilde{\Xi}_n(x, k_1, k_2) \quad 1 \leq m \leq N, (k_1, k_2) \in [-\pi, \pi]^2. \quad (\text{A.72})$$

The new frame $\{\check{\Xi}_n(\mathbf{x}, k_1, k_2)\}_{1 \leq n \leq N}$ retains analyticity and periodicity with respect to k_2 , and now satisfies, instead of (A.68),

$$\check{\Xi}_n(\mathbf{x}, -\pi, k_2) = e^{i\omega_1 \cdot \mathbf{x}} \lambda_n(k_2) \check{\Xi}_n(\mathbf{x}, \pi, k_2) \quad 1 \leq n \leq N. \quad (\text{A.73})$$

We finally shift the frame once more as

$$\check{\Xi}_n(\mathbf{x}, k_1, k_2) = e^{-i\frac{\Gamma_n(k_2)k_1}{2\pi}} \check{\Xi}_n(\mathbf{x}, k_1, k_2) \quad 1 \leq n \leq N, (k_1, k_2) \in [-\pi, \pi]^2, \quad (\text{A.74})$$

where $\Gamma_n(k_2)$ is, for each $1 \leq n \leq N$ and each $k_2 \in [-\pi, \pi]$, the logarithm of $\lambda_n(k_2)$ chosen such that $k_2 \mapsto \Gamma_n(k_2)$ is analytic and $-\pi < \Gamma_n(0) < \pi$. By construction, the frame $\{\check{\Xi}_n(\mathbf{x}, k_1, k_2)\}_{1 \leq n \leq N}$ is analytic and periodic with respect to k_1 , but it is possible that the shift (A.74) breaks periodicity with respect to k_2 because periodicity of the $\lambda_n(k_2)$ does not imply periodicity of the $\Gamma_n(k_2)$, only periodicity mod 2π , i.e. it is only guaranteed that

$$\Gamma_n(\pi) = \Gamma_n(-\pi) \pmod{2\pi} \quad 1 \leq n \leq N. \quad (\text{A.75})$$

If $\Gamma_n(\pi) \neq \Gamma_n(-\pi)$, the frame will not retain periodicity with respect to k_2 . We will see in the next section that when PXP satisfies the uniform spectral gap assumption (Assumption 4), it must be that

$$\Gamma_n(\pi) = \Gamma_n(-\pi) \quad 1 \leq n \leq N \quad (\text{A.76})$$

and hence the construction described above must yield an analytic and periodic gauge with respect to k_1 and k_2 .

Remark A.4.3. Using periodicity of the Brillouin zone and of the complex exponential function it is natural to consider the maps $k_2 \mapsto \Gamma_n(k_2)$ for $1 \leq n \leq N$ as maps from $S^1 \rightarrow S^1$. The condition (A.76) then has the geometric interpretation that the winding numbers of all of the maps $k_2 \mapsto \Gamma_n(k_2)$ are zero.

A.4.4 Proof of Theorem 6: the PXP gap assumption implies

$$(A.76)$$

In the previous section we constructed a Bloch frame $\{\check{\Xi}_n(\mathbf{x}, k_1, k_2)\}_{1 \leq n \leq N}$ which was analytic and periodic with respect to k_1 and periodic with respect to k_2 if and only if (A.76) holds. In this section we show that the PXP gaps assumption (Assumption 4) implies (A.76).

We now introduce a basis of $PL^2(\mathbb{R}^2)$ which diagonalizes the operator PXP . Note that via Bloch theory (the operator PXP is invariant under translations with respect to \mathbf{v}_2 , see Remark A.4.4) it suffices to consider the operator PXP restricted to the family of spaces

$$\begin{aligned} L_{k_2}^2 &:= \{f(\mathbf{x}) \in L^2(\Upsilon) : f(\mathbf{x} + \mathbf{v}_2) = e^{i\mathbf{k} \cdot \mathbf{v}_2} f(\mathbf{x})\} \\ &= \{f(x, y) \in L^2(\Upsilon) : f(x, y + 1) = e^{ik_2} f(x, y)\}, \end{aligned} \quad (\text{A.77})$$

where $k_2 \in [0, 2\pi]$ and Υ denotes the strip

$$\Upsilon := \{x\mathbf{v}_1 + y\mathbf{v}_2 : x \in \mathbb{R}, y \in [0, 1]\}. \quad (\text{A.78})$$

Define $P(k_2) : L_{k_2}^2 \rightarrow L_{k_2}^2$ by

$$P(k_2)f(\mathbf{x}) = \sum_{n=1}^N \int_{-\pi}^{\pi} \langle \Phi_n(\cdot, k_1, k_2) | f(\cdot) \rangle_{L_{k_2}^2} \Phi_n(\mathbf{x}, k_1, k_2) dk_1, \quad (\text{A.79})$$

then the restrictions of the operator PXP to the spaces $L_{k_2}^2$ are the operators $P(k_2)XP(k_2) : L_{k_2}^2 \rightarrow L_{k_2}^2$ where $k_2 \in [-\pi, \pi]$. In particular, we have

$$\sigma(PXP) = \bigcup_{k_2 \in [-\pi, \pi]} \sigma(P(k_2)XP(k_2)). \quad (\text{A.80})$$

We define quasi-Bloch functions (functions which span range $P(k_1, k_2)$ but are not necessarily individually eigenfunctions of H) by multiplying each of the components of the Bloch frame by $e^{i\mathbf{k} \cdot \mathbf{x}} = e^{i[k_1x + k_2y]}$ so that

$$\check{\Psi}_n(\mathbf{x}, k_1, k_2) = e^{i[k_1x + k_2y]} \check{\Xi}_n(\mathbf{x}, k_1, k_2). \quad (\text{A.81})$$

In particular, we can equivalently define $P(k_2)$ in terms of the quasi-Bloch functions as

$$P(k_2)f(\mathbf{x}) = \sum_{n=1}^N \int_{-\pi}^{\pi} \langle \check{\Psi}_n(\cdot, k_1, k_2) | f(\cdot) \rangle_{L_{k_2}^2} \check{\Psi}_n(\mathbf{x}, k_1, k_2) dk_1. \quad (\text{A.82})$$

We define hybrid Wannier functions (HWFs) for each $M \in \mathbb{Z}$ by integrating the quasi-Bloch functions with respect to k_1 along lines of constant k_2

$$H_n(\mathbf{x}, M, k_2) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \check{\Psi}_n(\mathbf{x}, k_1, k_2) e^{-ik_1M} dk_1 \quad 1 \leq n \leq N. \quad (\text{A.83})$$

Remark A.4.4. Here we invoke Bloch theory in two dimensions when translation symmetry holds only in one direction. The manipulations needed to make the theory rigorous can be found in, for example [FLTW16].

We claim that, if the Bloch functions are formed using the frame just constructed (i.e. after the shift (A.74)) and the operator X is defined as in (A.51), that $H_n(\mathbf{x}, M, k_2)$ is an exact eigenfunction of $P(k_2)XP(k_2)$ for every $k_2 \in [-\pi, \pi]$ and $1 \leq n \leq N$. To see this, first note that

$$P(k_2)XP(k_2)H_n(\mathbf{x}, M, k_2) = \frac{1}{2\pi} P(k_2) \int_{-\pi}^{\pi} L_1 x e^{i[k_1x + k_2y]} \check{\Xi}_n(\mathbf{x}, k_1, k_2) e^{-ik_1M} dk_1. \quad (\text{A.84})$$

Since $xe^{i[k_1x+k_2y]} = -i\partial_{k_1}e^{i[k_1x+k_2y]}$ and integrating by parts we have

$$\begin{aligned} &= \frac{-iL_1}{2\pi}P(k_2) [\check{\Psi}(\mathbf{x}, k_1, k_2)e^{-ik_1M}]_{-\pi}^{\pi} \\ &\quad + \frac{iL_1}{2\pi}P(k_2) \int_{-\pi}^{\pi} \sum_{m=1}^N \langle \check{\Xi}_m(\cdot, k_1, k_2) | \partial_{k_1} \check{\Xi}_n(\cdot, k_1, k_2) \rangle \check{\Psi}_m(\mathbf{x}, k_1, k_2) e^{-ik_1M} \quad (\text{A.85}) \\ &\quad + \check{\Psi}_n(\mathbf{x}, k_1, k_2)(-iM)e^{-ik_1M} dk_1, \end{aligned}$$

where we have expanded $\partial_{k_1} \check{\chi}_n(\mathbf{x}, k_1, k_2)$ in terms of the other elements of the Bloch frame, with $\langle | \rangle$ denoting the L_{per}^2 inner product. Since $\check{\Psi}_n(\mathbf{x}, k_1, k_2)$ is 2π -periodic with respect to k_1 , the first term of (A.85) vanishes. Now recall that using (A.74),

$$\partial_{k_1} \check{\Xi}_n(\mathbf{x}, k_1, k_2) = -i \frac{\Gamma_n(k_2)}{2\pi} \check{\Xi}_n(\mathbf{x}, k_1, k_2) + e^{-i \frac{\Gamma_n(k_2)k_1}{2\pi}} \partial_{k_1} \check{\Xi}_n(\mathbf{x}, k_1, k_2), \quad (\text{A.86})$$

where $\langle \check{\Xi}_m(\cdot, k_1, k_2) | \partial_{k_1} \check{\Xi}_n(\mathbf{x}, k_1, k_2) \rangle = 0$ for all $1 \leq m, n \leq N$ by (A.67). Hence (A.85) simplifies to

$$\begin{aligned} &P(k_2)XP(k_2)H_n(\mathbf{x}, M, k_2) \\ &= (L_1M + \bar{x}(k_2))H_n(\mathbf{x}, M, k_2), \end{aligned} \quad (\text{A.87})$$

where

$$\bar{x}_n(k_2) := \frac{L_1\Gamma_n(k_2)}{2\pi} \quad (\text{A.88})$$

is known as the n th Wannier charge center ‘‘at k_2 ’’. Since M is arbitrary, we see that the spectrum of $P(k_2)XP(k_2)$ is the union of shifted copies of $L_1\mathbb{Z}$

$$\sigma(P(k_2)XP(k_2)) = \bigcup_{1 \leq n \leq N} \{L_1\mathbb{Z} + \bar{x}_n(k_2)\}. \quad (\text{A.89})$$

Recall that in the previous section we constructed an analytic Bloch frame which is always periodic with respect to k_1 , and periodic with respect to k_2 under condition (A.76). We will now show that if (A.76) does not hold, the spectrum of PXP must equal the whole real line \mathbb{R} , which is clearly inconsistent with the uniform spectral gap assumption. It then immediately follows that if the uniform spectral gap assumption does hold, (A.76) must hold and hence the frame constructed in the previous section must be analytic and periodic with respect to both k_1 and k_2 .

Let us suppose that (A.76) does not hold, i.e. that for some $1 \leq n_0 \leq N$ we have

$$\Gamma_{n_0}(\pi) \neq \Gamma_{n_0}(-\pi). \quad (\text{A.90})$$

From (A.75), we have that $|\Gamma_{n_0}(\pi) - \Gamma_{n_0}(-\pi)| \geq 2\pi$, so by analyticity of the map $k_2 \mapsto \Gamma_{n_0}(k_2)$ we see that the map $k_2 \mapsto \bar{x}_{n_0}(k_2)$ must sweep out the whole interval $[0, L_1]$. It now follows immediately from (A.80) that

$$\sigma(PXP) = \mathbb{R}, \quad (\text{A.91})$$

which is a contradiction of the uniform spectral gaps assumption (Assumption 4). We conclude that the uniform spectral gap assumption on PXP implies that $\Gamma_n(\pi) = \Gamma_n(-\pi)$ for every $1 \leq n \leq N$ and Theorem 6 follows.

Remark A.4.5. The proof of Theorem 6 generalizes without difficulty to tight-binding models under analogous assumptions, the only difference being that L_{per}^2 is finite-dimensional.

Numerical computations of the spectra of $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{M}\right) P(k_2)$ where $k_2 \in [-\pi, \pi]$ for the Haldane model (where $N = 1$) are shown in Figure A.1. Here M denotes the number of cells in the X direction. Since formally

$$\frac{M}{2\pi} \text{Im} \log \exp\left(\frac{2\pi i X}{M}\right) = X \bmod M, \quad (\text{A.92})$$

we expect the spectra of $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{M}\right) P(k_2)$ approximate those of $P(k_2)XP(k_2)$ while respecting periodic boundary conditions (see Resta [Res98]). The computations illustrate clearly that the uniform spectral gap assumption fails when the model is in its topological phase because each eigenvalue of $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{M}\right) P(k_2)$ sweeps out an interval of width $\frac{2\pi}{M}$ as k_2 is varied over the interval $[-\pi, \pi]$, so that the union of the spectra is the whole interval $[-\pi, \pi]$. Similar figures appear in the works of Soluyanov, Vanderbilt and coauthors [SV11b, SV11a, TGV14, GAY⁺17, WZS⁺18].

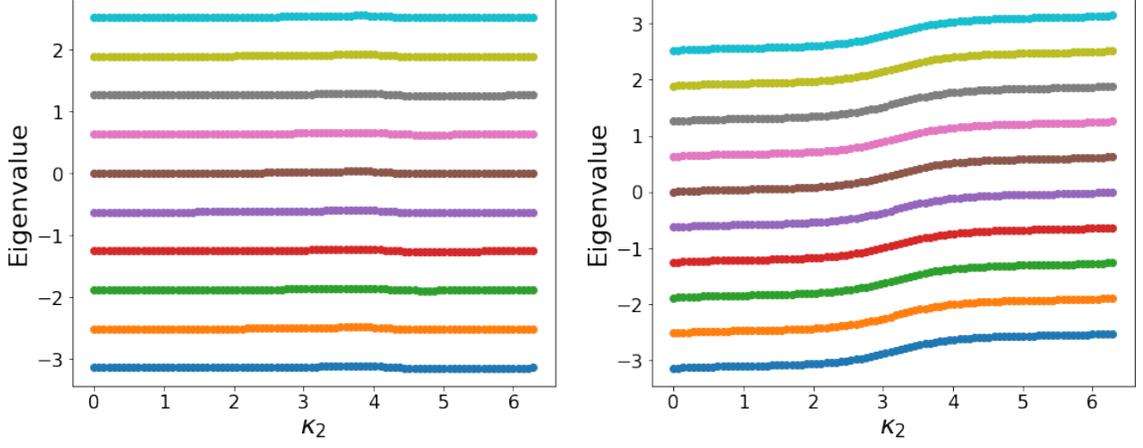


Figure A.1: Eigenvalues of $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{10}\right) P(k_2)$ as a function of k_2 , computed from the Haldane model on a 10×90 lattice with periodic boundary conditions in its non-topological (left) phase and topological (right) phase. Note that for large M , $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{M}\right) P(k_2) \approx \frac{1}{M} P(k_2) X P(k_2)$. Eigenvalues of $\text{Im} \log P(k_2) \exp\left(\frac{2\pi i X}{10}\right) P(k_2)$ sweep out closed intervals of width $\frac{2\pi}{10}$ as k_2 is varied from 0 to 2π so that the spectrum of $\text{Im} \log P \exp\left(\frac{2\pi i X}{10}\right) P$ does not have gaps. In the non-topological phase, eigenvalues of $\text{Im} \log P \exp\left(\frac{2\pi i X}{10}\right) P$ return to their original values after k_2 is varied from 0 to 2π .

A.5 Proof of Lemma 4.3.2

Let's recall the statement we want to prove:

Lemma 4.3.2. *Suppose that $P \in \mathcal{B}(L^2(\mathbb{R}^2))$ is an orthogonal projector. Suppose further that $\{\psi_\alpha\}$ and $\{\phi_\alpha\}$ are two distinct orthonormal bases for $\text{range}(P)$ and both bases are s -localized with $s > 1$. If $\{\psi_\alpha\}$ has finitely degenerate centers then $\{\phi_\alpha\}$ must also have finitely degenerate centers.*

Proof. For this proof let $\chi_{L,(x_0,y_0)}$ denote the characteristic function

$$\chi_{L,(x_0,y_0)} = \begin{cases} 1 & \mathbf{x} \in \left[x_0 - \frac{L}{2}, x_0 + \frac{L}{2} \right] \times \left[y_0 - \frac{L}{2}, y_0 + \frac{L}{2} \right] \\ 0 & \text{otherwise.} \end{cases}$$

and let $\|\cdot\|_F$ denote the Fröbenius norm (Schatten 2-norm). Since ψ_α has finitely degenerate centers we can relabel it as $\{\psi_{m,n}^{(j)}\}$ as we did in Section 4.3.1 where $(m,n) \in \mathbb{Z}^2$ and $j \in \{1, \dots, M\}$. Since $\{\psi_{m,n}^{(j)}\}$ forms an orthonormal basis, for any $(x_0, y_0) \in \mathbb{R}^2$ by the definition of the Fröbenius norm we have that:

$$\|\chi_{L,(x_0,y_0)}P\|_F^2 = \sum_{m,n,j} \|\chi_{L,(x_0,y_0)}P\psi_{m,n}^{(j)}\|^2 = \sum_{j=1}^M \sum_{m,n} \|\chi_{L,(x_0,y_0)}\psi_{m,n}^{(j)}\|^2$$

Our basic strategy of this proof will be to first show that if $\{\psi_{m,n}^{(j)}\}$ is an s -localized basis with $s > 1$ with finitely degenerate centers then $\|\chi_{L,(x_0,y_0)}P\|_F^2 = O(L^2)$. This estimate essentially puts a limit on how strongly the center points for a localized bases from $\text{range}(P)$ can cluster. If a basis for $\text{range}(P)$ does not satisfy the finitely degenerate centers condition, then its center points cluster arbitrarily strongly, which allows us to violate the $O(L^2)$ bound leading to a contradiction.

We'll start by proving the estimate for $\|\chi_{L,(x_0,y_0)}P\|_F^2$. Towards these ends, let's split the sum over m, n into two parts

$$A := \mathbb{Z}^2 \cap \text{supp}(\chi_{2L,(x_0,y_0)})$$

$$A^c := \mathbb{Z}^2 \setminus A.$$

Note that the side length in the definition of A is $2L$ not L . Since $2L > L$, we have the following estimate for all $(m, n) \in A^c$

$$\begin{aligned}
& \|\chi_{L,(x_0,y_0)}\psi_{m,n}^{(j)}\|^2 \\
&= \int_{\mathbb{R}^2} \chi_{L,(x_0,y_0)}(\mathbf{x}) |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\
&= \int_{\mathbb{R}^2} \chi_{L,(x_0,y_0)}(\mathbf{x}) \frac{\langle \mathbf{x} - (m, n) \rangle^{2(1+\epsilon)}}{\langle \mathbf{x} - (m, n) \rangle^{2(1+\epsilon)}} |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\
&\leq \frac{1}{\langle (m-L, n-L) \rangle^{2(1+\epsilon)}} \int_{\mathbb{R}^2} \chi_{L,(x_0,y_0)}(\mathbf{x}) \langle \mathbf{x} - (m, n) \rangle^{2(1+\epsilon)} |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\
&\leq \frac{C}{(1 + (m-L)^2 + (n-L)^2)^{1+\epsilon}}.
\end{aligned}$$

where in the second to last line we have used the following pointwise inequality which holds for all $(m, n) \in A^c$

$$\frac{\chi_{L,(x_0,y_0)}(\mathbf{x})}{\langle \mathbf{x} - (m, n) \rangle^{2(1+\epsilon)}} \leq \frac{1}{\langle (m-L, n-L) \rangle^{2(1+\epsilon)}}$$

and in the final line we have used our assumption that $\psi_{m,n}$ is s -localized for some $s > 1$ to choose ϵ sufficiently small so that

$$\int_{\mathbb{R}^2} \langle \mathbf{x} - (m, n) \rangle^{2(1+\epsilon)} |\psi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \leq C.$$

Using this estimate we have that

$$\begin{aligned}
\|\chi_{L,(x_0,y_0)}P\|_F^2 &= \sum_{j=1}^M \sum_{m,n} \|\chi_{L,(x_0,y_0)}\psi_{m,n}^{(j)}\|^2 \\
&= \sum_{j=1}^M \sum_{(m,n) \in A} \|\chi_{L,(x_0,y_0)}\psi_{m,n}^{(j)}\|^2 + \sum_{j=1}^M \sum_{(m,n) \in A^c} \|\chi_{L,(x_0,y_0)}\psi_{m,n}^{(j)}\|^2 \\
&\leq \sum_{j=1}^M \sum_{(m,n) \in A} 1 + \sum_{j=1}^M \sum_{(m,n) \in A^c} \frac{C}{(1 + (m-L)^2 + (n-L)^2)^{2(1+\epsilon)}} \\
&\leq 4ML^2 + \sum_{(m,n) \in \mathbb{Z}^2} \frac{CM}{(1 + (m-L)^2 + (n-L)^2)^{2(1+\epsilon)}} \\
&\leq 4ML^2 + C'
\end{aligned}$$

where C' is an absolute constant independent of L .

Next, towards a contradiction, let's suppose that the basis $\{\phi_\alpha\}$ does not have finitely degenerate centers. By definition, this means that for every $N \in \mathbb{Z}_+$ we can find a ball $B_1(x_N, y_N)$ so that this ball has more than N center points in it. Recall our notation for the unit box centered at (m, n) :

$$S_{m,n} := \left[m - \frac{1}{2}, m + \frac{1}{2} \right) \times \left[n - \frac{1}{2}, n + \frac{1}{2} \right)$$

Using basic planar geometry, it's easy to see that each ball of radius 1 overlaps with at most 4 of these unit boxes. Therefore, for each (x_N, y_N) (a center point for a box) we can also find a pair of integers $(m_N, n_N) \in \mathbb{Z}^2$ so that the box S_{m_N, n_N} contains at least $\frac{N}{4}$ center points.

While we are assuming that $\{\phi_\alpha\}$ does not have finitely degenerate centers, since this basis is s -localized with $s > 1$, we can still relabel this basis as $\{\phi_{m,n}^{(j)}\}$ where the degeneracy index j may run through an infinite number values.

Since $\phi_{m,n}^{(j)}$ is s -localized for some $s > 1$, we also have that for all (m, n, j)

$$\begin{aligned} \|(1 - \chi_{L,(m,n)})\phi_{m,n}^{(j)}\|^2 &= \int_{\mathbb{R}^2} (1 - \chi_{L,(m,n)}(\mathbf{x})) |\phi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\ &= \int_{\mathbb{R}^2} (1 - \chi_{L,(m,n)}(\mathbf{x})) \frac{\langle \mathbf{x} - (m, n) \rangle^2}{\langle \mathbf{x} - (m, n) \rangle^2} |\phi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\ &\leq \frac{1}{\sqrt{1 + 2L^2}} \int_{\mathbb{R}^2} \langle \mathbf{x} - (m, n) \rangle^2 |\phi_{m,n}^{(j)}(\mathbf{x})|^2 d\mathbf{x} \\ &\leq \frac{C''}{\sqrt{1 + 2L^2}}. \end{aligned}$$

where in the last line we have used the fact that $\phi_{m,n}^{(j)}$ is s -localized with $s > 1$. Since the constant C'' is uniform in (m, n, j) , we may find a real number L^* so that for all (m, n, j)

$$\begin{aligned} \|(1 - \chi_{L^*,(m,n)})\phi_{m,n}^{(j)}\|^2 &\leq \frac{1}{2} \\ \implies \|\chi_{L^*,(m,n)}\phi_{m,n}^{(j)}\|^2 &\geq \frac{1}{2}. \end{aligned}$$

Since by assumption $\{\phi_{m,n}^{(j)}\}$ does not have finitely degenerate centers, there must be an index $(m^*, n^*) \in \mathbb{Z}^2$ so that there are more than $4(4M(L^*)^2 + C')$ center points in the box S_{m^*, n^*} . This is a contradiction as

$$\begin{aligned} \|\chi_{L^*, (m^*, n^*)} P\|_F^2 &= \sum_{m, n, j} \|\chi_{L^*, (m^*, n^*)} \phi_{m, n}^{(j)}\|^2 \\ &\geq \sum_{j=1}^{\lceil 4(4M(L^*)^2 + C') \rceil} \|\chi_{L^*, (m^*, n^*)} \phi_{m^*, n^*}^{(j)}\|^2 \\ &\geq 2(4M(L^*)^2 + C') \end{aligned}$$

which violates our previous bound. Hence $\{\phi_\alpha\}$ must also have finitely degenerate centers. \square

A.6 Technical Lemmas

We collect two technical lemmas here which will be used in other parts of the proof.

A.6.1 Decay Lemma

Recall, for each $(k, \ell) \in \mathbb{Z}^2$ we define the unit box centered at (k, ℓ)

$$S_{k, \ell} := \left[k - \frac{1}{2}, k + \frac{1}{2} \right) \times \left[\ell - \frac{1}{2}, \ell + \frac{1}{2} \right)$$

Also recall our special notation for the characteristic function for $S_{k, \ell}$

$$\chi_{k, \ell}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in S_{k, \ell} \\ 0 & \mathbf{x} \notin S_{k, \ell} \end{cases}$$

Using this notation, we now state the following result:

Lemma A.6.1. *For any $s_1, s_2 \geq 0$, any $(m, n) \in \mathbb{Z}^2$, any $(k, \ell) \in \mathbb{Z}^2$, and any $v \in L^2(\mathbb{R}^2)$ then*

$$\|\chi_{k, \ell} v\| \leq \frac{2^{s_1 + s_2} \|\chi_{k, \ell} (|X - m| + 1)^{s_1} (|Y - n| + 1)^{s_2} v\|}{\langle m - k \rangle^{s_1} \langle n - \ell \rangle^{s_2}} \quad (\text{A.93})$$

where $\langle x \rangle$ is the Japanese bracket $\langle x \rangle := \sqrt{1 + x^2}$.

Proof. Instead of proving Equation (A.93) directly we will instead prove that:

$$\|\chi_{k,\ell}v\| \leq \frac{\|\chi_{k,\ell}(|X - m| + 1)^{s_1}(|Y - n| + 1)^{s_2}v\|}{\||m - k| + 1/2|^{s_1}\| |n - \ell| + 1/2|^{s_2}} \quad (\text{A.94})$$

Proving Equation (A.94) is sufficient since for all $a \in \mathbb{Z}$ one can check that

$$\sqrt{1 + a^2} \leq 2||a| + 1/2|.$$

Therefore, for any $(m, n) \in \mathbb{Z}^2$ and any $(k, \ell) \in \mathbb{Z}^2$ we have that

$$\begin{aligned} ||m - k| + 1/2|^{-s_1} &\leq 2^{s_1} \langle m - k \rangle^{-s_1} \\ ||n - \ell| + 1/2|^{-s_2} &\leq 2^{s_2} \langle n - \ell \rangle^{-s_2}. \end{aligned}$$

Hence, the proving Equation (A.94) implies Equation (A.93).

We will now prove Equation (A.94) in the case where $m \neq k$ and $n \neq \ell$; the other cases follow easily using similar arguments. Our main tool for proving Equation (A.94) will be to use “strip” characteristic functions in X and Y :

$$\begin{aligned} \chi\{|x_1 - m| \leq d\}(\mathbf{x}) &= \begin{cases} 1 & |x_1 - m| \leq d \\ 0 & \text{otherwise.} \end{cases} \\ \chi\{|x_2 - n| \leq d\}(\mathbf{x}) &= \begin{cases} 1 & |x_2 - n| \leq d \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

The key observation is that characteristic functions

$$\chi_{k,\ell} \quad \text{and} \quad \chi\{|x_1 - m| \leq |m - k| - 1/2\}$$

have disjoint supports (up to a set of measure zero). Therefore,

$$\chi_{k,\ell} = \chi_{k,\ell}(1 - \chi\{|x_1 - m| \leq |m - k| - 1/2\}). \quad (\text{A.95})$$

Using Equation (A.95) for any function v we have that:

$$\begin{aligned}
\|\chi_{k,\ell}v\|^2 &= \int_{\mathbb{R}^2} \chi_{k,\ell}|v(\mathbf{x})|^2 d\mathbf{x} \\
&= \int_{\mathbb{R}^2} \chi_{k,\ell}(1 - \chi\{|x_1 - m| \leq |m - k| - 1/2\})|v(\mathbf{x})|^2 d\mathbf{x} \\
&= \int_{\mathbb{R}^2} \chi_{k,\ell}(1 - \chi\{|x_1 - m| \leq |m - k| - 1/2\}) \frac{(1 + |x_1 - m|)^{2s_1}}{(1 + |x_1 - m|)^{2s_1}} |v(\mathbf{x})|^2 d\mathbf{x}
\end{aligned}$$

Since

$$1 - \chi\{|x_1 - m| \leq |m - k| - 1/2\} = \chi\{|x_1 - m| > |m - k| - 1/2\}$$

we have

$$\begin{aligned}
(1 - \chi\{|x_1 - m| \leq |m - k| - 1/2\}) \frac{1}{(1 + |x_1 - m|)^{2s_1}} \\
= \chi\{|x_1 - m| > |m - k| - 1/2\} \frac{1}{(1 + |x_1 - m|)^{2s_1}} \leq \frac{1}{(|m - k| + 1/2)^{2s_1}}
\end{aligned}$$

Hence

$$\begin{aligned}
\|\chi_{k,\ell}v\|^2 &\leq \frac{1}{(|m - k| + 1/2)^{2s_1}} \int_{\mathbb{R}^2} \chi_{k,\ell}(1 + |x_1 - m|)^{2s_1}|v(\mathbf{x})|^2 d\mathbf{x} \\
&= \frac{\|\chi_{k,\ell}(1 + |X - m|)^{s_1}v\|^2}{(|m - k| + 1/2)^{2s_1}}
\end{aligned}$$

We will now apply a similar argument $\|\chi_{k,\ell}(1 + |X - m|)^{s_1}v\|^2$. By similar reasoning to Equation (A.95), we have that

$$\chi_{k,\ell} = \chi_{k,\ell}(1 - \chi\{|x_2 - n| \leq |n - \ell| - 1/2\}). \quad (\text{A.96})$$

Therefore,

$$\begin{aligned}
\|\chi_{k,\ell}(1 + |X - m|)^{s_1}v\|^2 &= \int_{\mathbb{R}^2} \chi_{k,\ell}(1 + |x_1 - m|)^{2s_1}|v(\mathbf{x})|^2 d\mathbf{x} \\
&= \int_{\mathbb{R}^2} \chi_{k,\ell}(1 - \chi\{|x_2 - n| \leq |n - \ell| - 1/2\})(1 + |x_1 - m|)^{2s_1}|v(\mathbf{x})|^2 d\mathbf{x} \\
&= \int_{\mathbb{R}^2} \chi_{k,\ell}(1 - \chi\{|x_2 - n| \leq |n - \ell| - 1/2\}) \frac{(1 + |x_1 - m|)^{2s_1}(1 + |x_2 - n|)^{2s_2}}{(1 + |x_2 - n|)^{2s_2}} |v(\mathbf{x})|^2 d\mathbf{x}.
\end{aligned}$$

Hence, repeating a similar argument to before we conclude that:

$$\|\chi_{k,\ell}v\|^2 \leq \frac{\|\chi_{k,\ell}(1+|X-m|)^{s_1}(1+|Y-n|)^{s_2}v\|^2}{(|m-k|+1/2)^{2s_1}(|n-\ell|+1/2)^{2s_2}}.$$

This proves Equation (A.94) proving the lemma. \square

A.6.2 Product to Sum Bound

Lemma A.6.2. *For any $s_1, s_2 \geq 0$, any $(m, n) \in \mathbb{R}^2$, and any $v \in L^2(\mathbb{R}^2)$ we have the following inequality:*

$$\begin{aligned} & \|(1+|X-m|)^{s_1}(1+|Y-n|)^{s_2}v\| \\ & \leq \|(1+|X-m|)^{s_1+s_2}v\| + \|(1+|Y-n|)^{s_1+s_2}v\|. \end{aligned}$$

Proof. Observe that the result is trivial if $s_1 = 0$ or $s_2 = 0$ so we can assume without loss of generality that $s_1 > 0$ and $s_2 > 0$.

By definition we have that:

$$\begin{aligned} & \|(1+|X-m|)^{s_1}(1+|Y-n|)^{s_2}v\|^2 \\ & = \int_{\mathbb{R}^2} (1+|x_1-m|)^{2s_1}(1+|x_2-n|)^{2s_2}|v(\mathbf{x})|^2 d\mathbf{x}. \end{aligned}$$

Since $s_1, s_2 > 0$ we can apply Young's product inequality with $p = \frac{s_1+s_2}{s_1}$ and $q = \frac{s_1+s_2}{s_2}$ so that

$$\begin{aligned} & (1+|x_1-m|)^{2s_1}(1+|x_2-n|)^{2s_2} \\ & \leq \frac{1}{p}(1+|x_1-m|)^{2s_1p} + \frac{1}{q}(1+|x_2-n|)^{2s_2q} \\ & \leq \frac{1}{p}(1+|x_1-m|)^{2(s_1+s_2)} + \frac{1}{q}(1+|x_2-n|)^{2(s_1+s_2)} \end{aligned}$$

Hence, using this pointwise bound:

$$\begin{aligned} & \|(1+|X-m|)^{s_1}(1+|Y-n|)^{s_2}v\|^2 \\ & \leq \frac{1}{p}\|(1+|X-m|)^{s_1+s_2}v\|^2 + \frac{1}{q}\|(1+|Y-n|)^{s_1+s_2}v\|^2 \end{aligned}$$

The result follows by taking square roots, using that $\sqrt{a^2+b^2} \leq |a|+|b|$, and observing that $\max\{p^{-1/2}, q^{-1/2}\} \leq 1$ \square

A.7 Proof of Proposition 4.4.2

We'll start this section by recalling the proposition we want to prove:

Proposition 4.4.2. *Fix an orthonormal basis $\{\psi_{m,n}^{(j)}\}$. For any $h, g \in L^2(\mathbb{R}^2)$ define $h_{m,n,j}$ and $g_{m',n',j'}$ as follows:*

$$h_{m,n,j} := \int_{\mathbb{R}^2} |\psi_{m,n}^{(j)}(\mathbf{x})h(\mathbf{x})| d\mathbf{x} \quad g_{m',n',j'} := \int_{\mathbb{R}^2} |\psi_{m',n'}^{(j')}(\mathbf{x})g(\mathbf{x})| d\mathbf{x}.$$

If $\{\psi_{m,n}^{(j)}\}$ is an s -localized basis with $s > 2$ then there exists an absolute constant C such that

$$\sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| h_{m,n,j} g_{m',n',j'} \leq C \|h\| \|g\|$$

The core idea of this estimate is to make use of a modified version of Young's convolution inequality. Let's start by recalling the standard Young's convolution inequality for three functions [LL97, Theorem 4.2]:

Theorem 7 (Young's Convolution Inequality, Discrete Case). *Suppose that g, h, k are functions so that $g \in \ell^p(\mathbb{Z}^2)$, $h \in \ell^q(\mathbb{Z}^2)$, $k \in \ell^r(\mathbb{Z}^2)$ where $p, q, r \geq 1$ and*

$$\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 2.$$

Then we have the following bound:

$$\sum_{m,n} \sum_{m',n'} |g[m',n']k[m - m', n - n']h[m,n]| \leq \|g\|_{\ell^p} \|k\|_{\ell^r} \|h\|_{\ell^q}$$

Roughly speaking, one can think of the proof of the proposition as applying this inequality with $p = q = 2$ and $r = 1$ where

$$\begin{aligned} h &= h_{m,n,j} \\ g &= g_{m',n',j'} \\ k &= |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle|. \end{aligned}$$

It is important to note that $|\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle|$ is not a convolution kernel so Young's convolution inequality does not directly apply. Despite this, some minor modifications to the proof of Young's convolution inequality let us derive a similar result for our specific case.

With this argument in mind, in the following sections we prove the following two lemmas:

Lemma A.7.1. *If $h \in L^2(\mathbb{R}^2)$ and the collection $\{\psi_{m,n}^{(j)}\}$ is an s -localized orthonormal basis for $s > 2$ with finitely degenerate centers then there exists a finite constant $C > 0$ such that*

$$\sum_{m,n,j} h_{m,n,j}^2 = \sum_{m,n,j} \left(\int_{\mathbb{R}^2} |\psi_{m,n}^{(j)}(\mathbf{x})h(\mathbf{x})| d\mathbf{x} \right)^2 \leq C\|h\|^2.$$

Lemma A.7.2. *If the collection $\{\psi_{m,n}^{(j)}\}$ is an s -localized orthonormal basis for $s > 2$ with finitely degenerate centers then there exists a finite constant $C' > 0$ such that:*

$$\sup_{m,n,j} \left(\sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| \right) \leq C'$$

$$\sup_{m',n',j'} \left(\sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| \right) \leq C'$$

Assuming these lemmas are true, we can now complete the proof of Proposition 4.4.2. First, by applying Cauchy-Schwarz to the sum over (m, n, j) and (m', n', j') we get:

$$\begin{aligned} & \sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| h_{m,n,j} g_{m',n',j'} \\ &= \sum_{m,n,j} \sum_{m',n',j'} \left(|\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle|^{1/2} h_{m,n,j} \right) \left(|\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle|^{1/2} g_{m',n',j'} \right) \\ &\leq \left(\sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| h_{m,n,j}^2 \right)^{1/2} \\ &\quad \times \left(\sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m)\psi_{m',n'}^{(j')} \rangle| g_{m',n',j'}^2 \right)^{1/2} \end{aligned}$$

Next, since all of the terms in the summand are positive, we can take the supremum over (m, n, j) in the first sum and the supremum over (m', n', j') in the second sum to get:

$$\begin{aligned} & \sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| h_{m,n,j}^2 \\ & \leq \left(\sup_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \right) \left(\sum_{m,n,j} h_{m,n,j}^2 \right) \\ & \sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| g_{m',n',j'}^2 \\ & \leq \left(\sup_{m',n',j'} \sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \right) \left(\sum_{m',n',j'} g_{m',n',j'}^2 \right) \end{aligned}$$

Hence applying Lemma A.7.1 and Lemma A.7.2 we conclude that there exists a constant C

$$\sum_{m,n,j} \sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| h_{m,n,j} g_{m',n',j'} \leq C \|h\| \|g\|$$

proving the proposition.

We now turn to prove Lemmas A.7.1 and A.7.2. Our main technique for proving these results is to insert a partition of unity of the form:

$$\sum_{k,\ell} \chi_{k,\ell}(\mathbf{x}) = 1$$

where

$$\chi_{k,\ell}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in [k - \frac{1}{2}, k + \frac{1}{2}) \times [\ell - \frac{1}{2}, \ell + \frac{1}{2}) \\ 0 & \text{otherwise.} \end{cases}$$

We prove two technical lemmas (Lemmas A.6.1 and A.6.2) which relate the characteristic functions $\chi_{k,\ell}$ to the basis $\{\psi_{m,n}^{(j)}\}$ in Appendix A.6.

A.7.1 Proof of Lemma A.7.1

Before starting this proof, we will recall an alternate statement of Young's convolution inequality which follows from a duality argument applied to Theorem 7:

Theorem 8 (Young's Convolution Inequality, Discrete Case, Alternative Statement).

Suppose that g, k are functions so that $g \in \ell^p(\mathbb{Z}^2)$, $k \in \ell^q(\mathbb{Z}^2)$ where $p, q, r \geq 1$ and

$$\frac{1}{p} + \frac{1}{q} = 1 + \frac{1}{r}.$$

Then we have the following bound:

$$\sum_{m,n} \left(\sum_{m',n'} |g[m', n'] k[m - m', n - n']| \right)^r \leq \|g\|_{\ell^p}^r \|k\|_{\ell^q}^r$$

Inserting the partition of unity $\sum_{k,\ell} \chi_{k,\ell} = 1$ to the quantity we want to bound gives:

$$\begin{aligned} & \sum_{m,n,j} \left(\int_{\mathbb{R}^2} |\psi_{m,n}^{(j)}(\mathbf{x}) h(\mathbf{x})| d\mathbf{x} \right)^2 \\ &= \sum_{m,n,j} \left(\sum_{k,\ell} \int_{\mathbb{R}^2} |\chi_{k,\ell}(\mathbf{x}) \psi_{m,n}^{(j)}(\mathbf{x}) h(\mathbf{x})| d\mathbf{x} \right)^2 \\ &\leq \sum_{m,n,j} \left(\sum_{k,\ell} \|\chi_{k,\ell} \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} h\| \right)^2 \\ &\leq M \sup_j \sum_{m,n} \left(\sum_{k,\ell} \|\chi_{k,\ell} \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} h\| \right)^2 \end{aligned} \tag{A.97}$$

where in the second to last line we have used the Cauchy-Schwarz inequality. The key observation here is to note that the sequence $\{\|\chi_{k,\ell} h\|\}_{(k,\ell) \in \mathbb{Z}^2}$ is square summable.

In particular, we have that

$$\sum_{k,\ell} \|\chi_{k,\ell} h\|^2 = \sum_{k,\ell} \int \chi_{k,\ell} |h(\mathbf{x})|^2 d\mathbf{x} = \int |h(\mathbf{x})|^2 d\mathbf{x} = \|h\|^2.$$

By applying Lemma A.6.1 with $s_1 = s_2 = 1 + \epsilon$ and Lemma A.6.2 we have for any $\epsilon > 0$:

$$\begin{aligned} \|\chi_{k,\ell} \psi_{m,n}^{(j)}\| &\leq \frac{C_1 \|(|X - m| + 1)^{1+\epsilon} (|Y - n| + 1)^{1+\epsilon} \psi_{m,n}^{(j)}\|}{\langle m - k \rangle^{1+\epsilon} \langle n - \ell \rangle^{1+\epsilon}} \\ &\leq \frac{C_1 (\|(|X - m| + 1)^{2+2\epsilon} \psi_{m,n}^{(j)}\| + \|(|Y - n| + 1)^{2+2\epsilon} \psi_{m,n}^{(j)}\|)}{\langle m - k \rangle^{1+\epsilon} \langle n - \ell \rangle^{1+\epsilon}} \end{aligned}$$

Hence, assuming $\psi_{m,n}^{(j)}$ is s -localized with $s > 2$, we can pick ϵ sufficiently small so that

$$\|\chi_{k,\ell}\psi_{m,n}^{(j)}\| \leq \frac{C_2}{\langle m-k \rangle^{1+\epsilon}\langle n-\ell \rangle^{1+\epsilon}}.$$

Substituting this inequality into Equation (A.97) the sum to bound is therefore:

$$\sum_{m,n} \left(\sum_{k,\ell} \frac{\|\chi_{k,\ell}h\|}{\langle m-k \rangle^{1+\epsilon}\langle n-\ell \rangle^{1+\epsilon}} \right)^2 \quad (\text{A.98})$$

where we have dropped the supremum over j since the summand no longer depends on j . Now notice that Equation (A.98) is the ℓ^2 norm squared of a convolution. Since

$$\|\chi_{k,\ell}h\| \in \ell^2(\mathbb{Z}^2) \quad \text{and} \quad \frac{1}{\langle m \rangle^{1+\epsilon}\langle n \rangle^{1+\epsilon}} \in \ell^1(\mathbb{Z}^2)$$

applying Young's convolution inequality with $p = r = 2$, and $q = 1$, we conclude that

$$\sum_{m,n} \left(\sum_{k,\ell} \frac{\|\chi_{k,\ell}h\|}{\langle m-k \rangle^{1+\epsilon}\langle n-\ell \rangle^{1+\epsilon}} \right)^2 \leq C\|h\|^2$$

and the lemma is proved.

A.7.2 Proof of Lemma A.7.2

Let us begin this proof by recalling the bounds we want to show

$$\begin{aligned} \sup_{m,n,j} \left(\sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X-m)\psi_{m',n'}^{(j')} \rangle| \right) &\leq C' \\ \sup_{m',n',j'} \left(\sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X-m)\psi_{m',n'}^{(j')} \rangle| \right) &\leq C'. \end{aligned}$$

Our first observation is that these two bounds are in fact equivalent. Since $\{\psi_{m,n}^{(j)}\}$ forms an orthonormal basis, we have that whenever $(m, n, j) \neq (m', n', j')$

$$\langle \psi_{m,n}^{(j)}, (X-m)\psi_{m',n'}^{(j')} \rangle = \langle \psi_{m,n}^{(j)}, (X-m')\psi_{m',n'}^{(j')} \rangle \quad (\text{A.99})$$

Since Equation (A.99) is also true when $(m, n, j) = (m', n', j')$, it follows that for any fixed choice of (m', n', j') we have

$$\sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X-m)\psi_{m',n'}^{(j')} \rangle| = \sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X-m')\psi_{m',n'}^{(j')} \rangle|$$

Therefore, the bounds we want to show are

$$\begin{aligned} \sup_{m,n,j} \left(\sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \right) &\leq C' \\ \sup_{m',n',j'} \left(\sum_{m,n,j} |\langle \psi_{m,n}^{(j)}, (X - m') \psi_{m',n'}^{(j')} \rangle| \right) &\leq C'. \end{aligned}$$

Using the fact that X is self-adjoint we easily see that the second bound is equivalent to the first bound by making the relabeling $(m, n, j) \Leftrightarrow (m', n', j')$.

For the rest of this argument, let us take (m, n, j) to be fixed and prove a bound which is independent of the choice of (m, n, j) . Inserting a partition of unity of characteristic functions $\sum_{k,\ell} \chi_{k,\ell} = 1$ we have that:

$$\begin{aligned} &\sum_{m',n',j'} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \\ &\leq \sum_{m',n',j'} \sum_{k,\ell} |\langle \chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}, \psi_{m',n'}^{(j')} \rangle| \\ &\leq \sum_{m',n',j'} \sum_{k,\ell} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \\ &\leq M \left(\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \right) \\ &\leq M \left(\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \|\chi_{k,\ell} (|X - m| + 1) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \right) \end{aligned} \quad (\text{A.100})$$

where in the last line we have used the pointwise bound $(x - m)^2 \leq (|x - m| + 1)^2$.

Applying Lemma A.6.1 with $s_1 = s_2 = 1 + \epsilon$ gives us that:

$$\|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \leq \frac{C_1 \|\chi_{k,\ell} (|X - m'| + 1)^{1+\epsilon} (|Y - n'| + 1)^{1+\epsilon} \psi_{m',n'}^{(j')}\|}{\langle m' - k \rangle^{1+\epsilon} \langle n' - \ell \rangle^{1+\epsilon}} \quad (\text{A.101})$$

Next, applying Lemma A.6.1 with $s_1 = s_2 = 1/2 + \epsilon$ gives that:

$$\begin{aligned} &\|\chi_{k,\ell} (|X - m| + 1) \psi_{m,n}^{(j)}\| \\ &\leq \frac{C_2 \|\chi_{k,\ell} (|X - m| + 1)^{3/2+\epsilon} (|Y - n| + 1)^{1/2+\epsilon} \psi_{m,n}^{(j)}\|}{\langle m - k \rangle^{1/2+\epsilon} \langle n - \ell \rangle^{1/2+\epsilon}}. \end{aligned} \quad (\text{A.102})$$

Applying Lemma A.6.2 to upper bound Equation (A.101) gives:

$$\begin{aligned}
\|\chi_{k\ell}\psi_{m',n'}^{(j')}\| &\leq \frac{C_1\|\chi_{k,\ell}(|X-m'|+1)^{1+\epsilon}(|Y-n'|+1)^{1+\epsilon}\psi_{m',n'}^{(j')}\|}{\langle m'-k \rangle^{1+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \\
&\leq \frac{C_1(\|(|X-m'|+1)^{2+2\epsilon}\psi_{m',n'}^{(j')}\| + \|(|Y-n'|+1)^{2+2\epsilon}\psi_{m',n'}^{(j')}\|)}{\langle m'-k \rangle^{1+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \\
&\leq \frac{C_3}{\langle m'-k \rangle^{1+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}}. \tag{A.103}
\end{aligned}$$

In the last line, we have used the fact that by assumption $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 2$, so we can pick ϵ sufficiently small so that

$$\|(|X-m'|+1)^{2+2\epsilon}\psi_{m',n'}^{(j')}\| + \|(|Y-n'|+1)^{2+2\epsilon}\psi_{m',n'}^{(j')}\|$$

is bounded by a constant.

Plugging Equation (A.102) and Equation (A.103) into Equation (A.100) we have that we can find a constant C_4 such that:

$$\begin{aligned}
&\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \|\chi_{k,\ell}(|X-m|+1)\psi_{m,n}^{(j)}\| \|\chi_{k\ell}\psi_{m',n'}^{(j')}\| \\
&\leq \sum_{m',n'} \sum_{k,\ell} \frac{C_4\|\chi_{k,\ell}(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|}{\langle m-k \rangle^{1/2+\epsilon}\langle n-\ell \rangle^{1/2+\epsilon}\langle m'-k \rangle^{1+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}}.
\end{aligned}$$

Treating (m, n, j) as a constant we can group the summand into two parts

$$\begin{aligned}
A_{k,\ell} &:= \frac{\|\chi_{k,\ell}(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|}{\langle m-k \rangle^{1/2+\epsilon}\langle n-\ell \rangle^{1/2+\epsilon}} \\
B_{m'-k,n'-\ell} &:= \frac{1}{\langle m'-k \rangle^{1+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}}.
\end{aligned}$$

With this notation the sum we wish to bound can be written as:

$$\sum_{m',n'} \sum_{k,\ell} A_{k,\ell} B_{m'-k,n'-\ell}. \tag{A.104}$$

However the above sum is the ℓ^1 -norm of a convolution. Therefore, if we can show that $A_{k,\ell} \in \ell^1(\mathbb{Z}^2)$ and $B_{m',n'} \in \ell^1(\mathbb{Z}^2)$ then by applying Young's convolution inequality (Theorem 8) with $p = q = r = 1$ we can conclude that Equation (A.104) is bounded, completing the proof of Lemma A.7.2.

It's easy to see that $B_{m',n'} \in \ell^1(\mathbb{Z}^2)$ for any $\epsilon > 0$ by integral test so we only need to show that $A_{k,\ell} \in \ell^1(\mathbb{Z}^2)$. Applying Cauchy-Schwarz inequality

$$\begin{aligned} \sum_{k,\ell} A_{k,\ell} &= \sum_{k,\ell} \frac{\|\chi_{k,\ell}(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|}{\langle m-k \rangle^{1/2+\epsilon}\langle n-\ell \rangle^{1/2+\epsilon}} \\ &\leq \left(\sum_{k,\ell} \|\chi_{k,\ell}(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|^2 \right)^{1/2} \\ &\quad \times \left(\sum_{k,\ell} \frac{1}{\langle m-k \rangle^{1+2\epsilon}\langle n-\ell \rangle^{1+2\epsilon}} \right)^{1/2} \\ &\leq C_4 \|(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\| \end{aligned}$$

where in the last line we have made use of the fact that $\sum_{k,\ell} \chi_{k,\ell} = 1$. Since by assumption $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 2$, by applying Lemma A.6.2 we conclude that

$$\|(|X-m|+1)^{3/2+\epsilon}(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|$$

is bounded for all ϵ sufficiently small. This completes the proof of Lemma A.7.2.

A.8 Square Root Bounds

In this section, we will prove the following lemma which includes Lemma 4.6.3 as a special case.

Lemma A.8.1. *Suppose that P is a projector satisfying decay estimates as Assumption 3. Suppose further that P admits a basis with finite degenerate centers which is s -localized for some $s > 2$. Then there exists a constant $C > 0$ such that for any $\lambda \in G$ (recall that G is the set of gaps defined in Equation (4.22)):*

$$\begin{aligned} \|S_\lambda P \langle X - \lambda \rangle^{1/2}\| &\leq C \\ \|\langle X - \lambda \rangle^{1/2} P S_\lambda\| &\leq C \\ \|S_\lambda^{-1} P \langle X - \lambda \rangle^{-1/2}\| &\leq C \\ \|\langle X - \lambda \rangle^{-1/2} P S_\lambda^{-1}\| &\leq C \end{aligned}$$

Lemma A.8.1 follows as an easy corollary of the following result and our decay estimates on P (Assumption 3 and Corollary 2.2.2):

Lemma A.8.2. *Suppose that P is a projector satisfying decay estimates as Assumption 3. Suppose further that P admits a basis with finite degenerate centers which is s -localized for some $s > 2$. Then there exists a constant $C' > 0$ such that for any $\lambda \in G$:*

$$\|PS_\lambda^{-1}P - P\langle X - \lambda \rangle^{1/2}P\| \leq C'$$

Let's assume Lemma A.8.2 is true and prove Lemma A.8.1. We will return to prove Lemma A.8.2 in the next section (Appendix A.8.1).

Proof of Lemma A.8.1. We will show that

$$\begin{aligned} \|S_\lambda P\langle X - \lambda \rangle^{1/2}\| &\leq C \\ \|S_\lambda^{-1}P\langle X - \lambda \rangle^{-1/2}\| &\leq C \end{aligned}$$

the other two bounds follow by using the fact for any bounded operator $\|A\| = \|A^\dagger\|$.

For the first bound, we calculate

$$\begin{aligned} S_\lambda P\langle X - \lambda \rangle^{1/2} &= S_\lambda P\left(\langle X - \lambda \rangle^{1/2} - S_\lambda^{-1} + S_\lambda^{-1}\right) \\ &= S_\lambda P\left(\langle X - \lambda \rangle^{1/2} - S_\lambda^{-1}\right) + P \\ &= S_\lambda P\left(\langle X - \lambda \rangle^{1/2} - S_\lambda^{-1}\right)(P + Q) + P \\ &= S_\lambda P\left(\langle X - \lambda \rangle^{1/2} - S_\lambda^{-1}\right)P + S_\lambda P\langle X - \lambda \rangle^{1/2}Q + P, \end{aligned}$$

where we have used that $[P, S_\lambda] = 0$, $P + Q = I$, and $PQ = QP = 0$. Therefore, we have that

$$\begin{aligned} &\|S_\lambda P\langle X - \lambda \rangle^{1/2}\| \\ &\leq \|S_\lambda\| \left(\|P\langle X - \lambda \rangle^{1/2}P - PS_\lambda^{-1}P\| + \|P\langle X - \lambda \rangle^{1/2}Q\| \right) + 1 \\ &\leq \|S_\lambda\| \left(\|P\langle X - \lambda \rangle^{1/2}P - PS_\lambda^{-1}P\| + \|[P, \langle X - \lambda \rangle^{1/2}]\| \right) + 1. \end{aligned}$$

Now observe that $\|P\langle X - \lambda \rangle^{1/2}P - PS_\lambda^{-1}P\|$ is bounded due to Lemma A.8.2 and $\|[P, \langle X - \lambda \rangle^{1/2}]\|$ is bounded due to decay estimates on P (Assumption 3(iv)). Hence the first bound is proved.

For the second bound, we calculate

$$\begin{aligned} S_\lambda^{-1}P\langle X - \lambda \rangle^{-1/2} &= \left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2} + \langle X - \lambda \rangle^{1/2}\right)P\langle X - \lambda \rangle^{-1/2} \\ &= \left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2}\right)P\langle X - \lambda \rangle^{-1/2} + \langle X - \lambda \rangle^{1/2}P\langle X - \lambda \rangle^{-1/2} \\ &= \left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2}\right)P\langle X - \lambda \rangle^{-1/2} + [\langle X - \lambda \rangle^{1/2}, P]\langle X - \lambda \rangle^{-1/2} + P \end{aligned}$$

Hence, using the fact that $\|\langle X - \lambda \rangle^{-1/2}\| \leq 1$, we get the upper bound

$$\begin{aligned} &\|S_\lambda^{-1}P\langle X - \lambda \rangle^{-1/2}\| \\ &\leq \left\| \left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2}\right)P \right\| + \|[\langle X - \lambda \rangle^{1/2}, P]\| + 1 \\ &\leq \|P\left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2}\right)P\| + \|Q\langle X - \lambda \rangle^{1/2}P\| + \|[\langle X - \lambda \rangle^{1/2}, P]\| + 1 \\ &\leq \|P\left(S_\lambda^{-1} - \langle X - \lambda \rangle^{1/2}\right)P\| + 2\|[\langle X - \lambda \rangle^{1/2}, P]\| + 1 \end{aligned}$$

which is bounded due to Lemma A.8.2 and Assumption 3(iv) as before. \square

A.8.1 Proof of Lemma A.8.2

The proof of this lemma follows very closely with the proof of Lemma A.7.2 from Appendix A.7. Writing out these two expressions in terms of the basis $\{\psi_{m,n}^{(j)}\}$ we have that:

$$\begin{aligned} PS_\lambda^{-1}P &= \sum_{m,n,j} |m - \lambda|^{1/2} |\psi_{m,n}^{(j)}\rangle \langle \psi_{m,n}^{(j)}| \\ P\langle X - \lambda \rangle^{1/2}P &= \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, \langle X - \lambda \rangle^{1/2} \psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \end{aligned}$$

Since $\{\psi_{m,n}^{(j)}\}$ is orthonormal, we have that when $(m, n, j) \neq (m', n', j')$:

$$\begin{aligned} \langle \psi_{m,n}^{(j)}, \langle X - \lambda \rangle^{1/2} \psi_{m',n'}^{(j')} \rangle &= \langle \psi_{m,n}^{(j)}, \left(\langle X - \lambda \rangle^{1/2} - |m - \lambda|^{1/2}\right) \psi_{m',n'}^{(j')} \rangle \\ &= \langle \psi_{m,n}^{(j)}, \left(\langle X - \lambda \rangle^{1/2} - |m' - \lambda|^{1/2}\right) \psi_{m',n'}^{(j')} \rangle \end{aligned} \quad (\text{A.105})$$

Therefore, we can express the difference $PS_\lambda^{-1}P - P\langle X - \lambda \rangle^{1/2}P$ as follows:

$$\begin{aligned} & PS_\lambda^{-1}P - P\langle X - \lambda \rangle^{1/2}P \\ &= - \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)} | \left(\langle X - \lambda \rangle^{1/2} - |m' - \lambda|^{1/2} \right) \psi_{m',n'}^{(j')} \rangle | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} | \end{aligned}$$

Now by Schur's test, to show that $PS_\lambda^{-1}P - P\langle X - \lambda \rangle^{1/2}P$ is a bounded operator, it's enough to show that:

$$\begin{aligned} & \sup_{m,n,j} \sum_{m',n',j'} | \langle \psi_{m,n}^{(j)} | \left(\langle X - \lambda \rangle^{1/2} - |m - \lambda|^{1/2} \right) \psi_{m',n'}^{(j')} \rangle | < \infty \\ & \sup_{m',n',j'} \sum_{m,n,j} | \langle \psi_{m,n}^{(j)} | \left(\langle X - \lambda \rangle^{1/2} - |m' - \lambda|^{1/2} \right) \psi_{m',n'}^{(j')} \rangle | < \infty \end{aligned}$$

Due to Equation (A.105) and the fact that X is self-adjoint, we can see that the above two bounds are equivalent so it is enough to prove the first of these bounds.

Inserting the partition of unity $\sum_{k,\ell} \chi_{k,\ell} = 1$ we have that

$$\begin{aligned} & \sum_{m',n',j'} \sum_{k,\ell} | \langle \chi_{k,\ell} \psi_{m,n}^{(j)} | \left(\langle X - \lambda \rangle^{1/2} - |m - \lambda|^{1/2} \right) \psi_{m',n'}^{(j')} \rangle | \\ & \leq \sum_{m',n',j'} \sum_{k,\ell} \| \chi_{k,\ell} \left(\langle X - \lambda \rangle^{1/2} - |m - \lambda|^{1/2} \right) \psi_{m,n}^{(j)} \| \| \chi_{k,\ell} \psi_{m',n'}^{(j')} \| \\ & \leq \sum_{m',n',j'} \sum_{k,\ell} \| \chi_{k,\ell} (|X - m| + 1)^{1/2} \psi_{m,n}^{(j)} \| \| \chi_{k,\ell} \psi_{m',n'}^{(j')} \|. \end{aligned}$$

To get the last line we have used the following sequence of pointwise inequalities:

$$\begin{aligned} & | \langle x - \lambda \rangle^{1/2} - |m - \lambda|^{1/2} |^2 \\ & \leq | \langle x - \lambda \rangle - |m - \lambda| | \quad \text{(elementary)} \\ & = | \sqrt{(x - \lambda)^2 + 1^2} - \sqrt{(m - \lambda)^2 + 0^2} | \\ & \leq \sqrt{(x - m)^2 + 1} \quad \text{(reverse triangle inequality)} \\ & \leq |x - m| + 1. \quad \text{(elementary)} \end{aligned}$$

Therefore, the quantity we want to bound is

$$\begin{aligned} & \sum_{m',n',j'} \sum_{k,\ell} \|\chi_{k,\ell}(|X-m|+1)^{1/2}\psi_{m,n}^{(j)}\| \|\chi_{k,\ell}\psi_{m',n'}^{(j')}\| \\ & \leq M \left(\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \|\chi_{k,\ell}(|X-m|+1)^{1/2}\psi_{m,n}^{(j)}\| \|\chi_{k,\ell}\psi_{m',n'}^{(j')}\| \right) \end{aligned} \quad (\text{A.106})$$

In the proof of Lemma A.7.2, we showed that the following expression is bounded when P admits a basis which is s -localized for $s > 2$ (see Equation (A.100)):

$$\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \|\chi_{k,\ell}(|X-m|+1)\psi_{m,n}^{(j)}\| \|\chi_{k,\ell}\psi_{m',n'}^{(j')}\|.$$

Since $(|X-m|+1)^{1/2} \leq (|X-m|+1)$ this calculation implies that Equation (A.106) is bounded, completing the proof of Lemma 4.6.3.

A.9 Proof of Proposition 4.6.4

Let us start this section by recalling the proposition we want to prove:

Proposition 4.6.4. *Suppose that P is a projector satisfying decay estimates as Assumption 3. Suppose further that P admits a basis with finitely degenerate centers which is s -localized for some $s > 5/2$. Then for any $\lambda \in G$ there exists a finite constant $C > 0$ such that*

$$\begin{aligned} \|\langle X - \lambda \rangle^{-1/2} [X, \tilde{X}] \langle X - \lambda \rangle^{-1/2}\| & \leq C, \\ \|\langle X - \lambda \rangle^{-1/2} [Y, \tilde{X}] \langle X - \lambda \rangle^{-1/2}\| & \leq C. \end{aligned} \quad (\text{A.107})$$

The core idea of this proof is to rewrite the commutators we are interested in bounding into different parts we can control.

Let's begin by considering the commutator $[Y, \tilde{X}]$. Using that $Y = PYP + PYQ + QYP + QYQ$ and $\tilde{X} = P\tilde{X}P + QXQ$ we have:

$$\begin{aligned} [Y, \tilde{X}] &= [PYP + PYQ + QYP + QYQ, P\tilde{X}P + QXQ] \\ &= [PYP + PYQ + QYP, P\tilde{X}P] + [PYQ + QYP + QYQ, QXQ] \end{aligned}$$

where we have used that $PQ = QP = 0$. Grouping the terms with $PYQ + QYP$ together then gives us:

$$[Y, \tilde{X}] = [PYP, P\tilde{X}P] + [QYQ, QXQ] + [PYQ + QYP, \tilde{X}]$$

Performing similar calculations for $[X, \tilde{X}]$ gives us

$$\begin{aligned} [X, \tilde{X}] &= [PXP, P\tilde{X}P] + [QXQ, QXQ] + [PXQ + QXP, \tilde{X}] \\ &= [PXP, P\tilde{X}P] + [PXQ + QXP, \tilde{X}] \end{aligned}$$

Therefore, we have three types of terms to bound:

1. $[QYQ, QXQ]$ (see Appendix A.9.1)
2. $[PXQ + QXP, \tilde{X}]$ and $[PYQ + QYP, \tilde{X}]$ (see Appendix A.9.2)
3. $[PXP, P\tilde{X}P]$ and $[PYP, P\tilde{X}P]$ (see Appendix A.9.3)

While $[QYQ, QXQ]$ can be bounded without using the decay terms, $\langle X - \lambda \rangle^{-1/2}$ (see Appendix A.9.1), bounding the other terms requires making use of this additional decay (see Appendix A.9.2 and Appendix A.9.3).

A.9.1 Bounding $[QXQ, QYQ]$ term

Using the fact that $Q = I - P$ and $[X, Y] = 0$ we easily calculate that

$$\begin{aligned} [QXQ, QYQ] &= QXQYQ - QYQXQ \\ &= QX(I - P)YQ - QY(I - P)XQ \\ &= QXYQ - QXPYQ - QYXQ + QYPXQ \\ &= QYPXQ - QXPYQ \end{aligned}$$

Therefore,

$$\begin{aligned} \|[QXQ, QYQ]\| &= \|QYPXQ - QXPYQ\| \\ &\leq \|QYP\| \|PXQ\| + \|QXP\| \|PYQ\| \end{aligned}$$

but this is bounded due to Corollary 2.2.2(i) with $\gamma = 0$.

A.9.2 Bounding $[PXQ + QXP, \tilde{X}]$ and $[PYQ + QYP, \tilde{X}]$ terms

In this section, we will show how to bound

$$\langle X - \lambda \rangle^{-1/2} [PYQ, \tilde{X}] \langle X - \lambda \rangle^{-1/2}.$$

Bounding $\langle X - \lambda \rangle^{-1/2} [QYP, \tilde{X}] \langle X - \lambda \rangle^{-1/2}$ and the other two terms follows using similar steps.

Expanding this commutator gives us

$$\begin{aligned} [PYQ, \tilde{X}] &= [PYQ, \tilde{X} - \lambda] \\ &= PYQ(\tilde{X} - \lambda) - (\tilde{X} - \lambda)PYQ. \end{aligned}$$

Let's start by considering the term

$$\langle X - \lambda \rangle^{-1/2} PYQ(\tilde{X} - \lambda) \langle X - \lambda \rangle^{-1/2}.$$

Inserting a copy of $\langle X - \lambda \rangle^{1/2} \langle X - \lambda \rangle^{-1/2}$ gives us that

$$\begin{aligned} &\langle X - \lambda \rangle^{-1/2} PYQ(\tilde{X} - \lambda) \langle X - \lambda \rangle^{-1/2} \\ &= \left(\langle X - \lambda \rangle^{-1/2} PYQ \langle X - \lambda \rangle^{1/2} \right) \left(\langle X - \lambda \rangle^{-1/2} (\tilde{X} - \lambda) \langle X - \lambda \rangle^{-1/2} \right) \end{aligned}$$

due to Corollary 2.2.2(v), we know that $\langle X - \lambda \rangle^{-1/2} PYQ \langle X - \lambda \rangle^{1/2}$ is bounded. The second term can be seen to be bounded by adding and subtracting X :

$$\begin{aligned} &\| \langle X - \lambda \rangle^{-1/2} (\tilde{X} - \lambda) \langle X - \lambda \rangle^{-1/2} \| \\ &= \| \langle X - \lambda \rangle^{-1/2} (\tilde{X} - X + X - \lambda) \langle X - \lambda \rangle^{-1/2} \| \\ &\leq \| \tilde{X} - X \| + \| \langle X - \lambda \rangle \langle X - \lambda \rangle^{-1} \| \\ &\leq \| \tilde{X} - X \| + 1. \end{aligned}$$

Hence, these terms are bounded.

A.9.3 Bounding $[PXP, P\tilde{X}P]$ and $[PYP, P\tilde{X}P]$ terms

In this section we will show how to bound the following quantities

$$\begin{aligned} & \langle X - \lambda \rangle^{-1/2} [PXP, P\tilde{X}P] \langle X - \lambda \rangle^{-1/2} \\ & \langle X - \lambda \rangle^{-1/2} [PYP, P\tilde{X}P] \langle X - \lambda \rangle^{-1/2}. \end{aligned}$$

We'll start by writing the commutators $[PXP, P\tilde{X}P]$ and $[PYP, P\tilde{X}P]$ in terms of the basis $\{\psi_{m,n}^{(j)}\}$.

$$\begin{aligned} [PXP, P\tilde{X}P] &= \left[\sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, X\psi_{m',n'}^{(j')} | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} |, P\tilde{X}P \right] \\ &= \sum_{m,n,j} \sum_{m',n',j'} \langle \psi_{m,n}^{(j)}, X\psi_{m',n'}^{(j')} \rangle \left(P\tilde{X}P | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} | - | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} | P\tilde{X}P \right) \\ &= \sum_{m,n,j} \sum_{m',n',j'} (m - m') \langle \psi_{m,n}^{(j)}, X\psi_{m',n'}^{(j')} \rangle | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} | \end{aligned} \quad (\text{A.108})$$

A similar calculation shows that

$$[PYP, P\tilde{X}P] = \sum_{m,n,j} \sum_{m',n',j'} (m - m') \langle \psi_{m,n}^{(j)}, Y\psi_{m',n'}^{(j')} \rangle | \psi_{m,n}^{(j)} \rangle \langle \psi_{m',n'}^{(j')} |. \quad (\text{A.109})$$

Since S_λ is diagonal in the basis $\{\psi_{m,n}^{(j)}\}$ it will significantly simplify our arguments if we replace the decay provided by $\langle X - \lambda \rangle^{-1/2}$ with S_λ . Using Lemma A.8.1 we have that

$$\begin{aligned} & \| \langle X - \lambda \rangle^{-1/2} [PXP, P\tilde{X}P] \langle X - \lambda \rangle^{-1/2} \| \\ & \leq \| \langle X - \lambda \rangle^{-1/2} P [PXP, P\tilde{X}P] P \langle X - \lambda \rangle^{-1/2} \| \\ & \leq \| \langle X - \lambda \rangle^{-1/2} P S_\lambda^{-1} \| \| S_\lambda [PXP, P\tilde{X}P] S_\lambda \| \| S_\lambda^{-1} P \langle X - \lambda \rangle^{-1/2} \| \\ & \leq C^2 \| S_\lambda [PXP, P\tilde{X}P] S_\lambda \| \end{aligned}$$

Similar calculations for Y show that

$$\| \langle X - \lambda \rangle^{-1/2} [PYP, P\tilde{X}P] \langle X - \lambda \rangle^{-1/2} \| \leq C^2 \| S_\lambda [PYP, P\tilde{X}P] S_\lambda \|$$

Hence it suffices to show that $S_\lambda[PXP, P\tilde{X}P]S_\lambda$ and $S_\lambda[PYP, P\tilde{X}P]S_\lambda$ are both bounded. Using the expressions for $[PXP, P\tilde{X}P]$ and $[PYP, P\tilde{X}P]$ from Equations (A.108) and (A.109), we get

$$\begin{aligned} & S_\lambda[PXP, P\tilde{X}P]S_\lambda \\ &= \sum_{m,n,j} \sum_{m',n',j'} \frac{(m-m')}{|\lambda-m|^{1/2}|\lambda-m'|^{1/2}} \langle \psi_{m,n}^{(j)}, X\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \end{aligned}$$

$$\begin{aligned} & S_\lambda[PYP, P\tilde{X}P]S_\lambda \\ &= \sum_{m,n,j} \sum_{m',n',j'} \frac{(m-m')}{|\lambda-m|^{1/2}|\lambda-m'|^{1/2}} \langle \psi_{m,n}^{(j)}, Y\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \end{aligned}$$

Therefore, to finish the proof of Proposition 4.6.4, we will prove the following proposition:

Proposition A.9.1. *If $\{\psi_{m,n}^{(j)}\}$ is an s -localized basis with $s > 5/2$, then there exists an absolute constant C such that for all $\lambda \in G$ (recall that G is the set of gaps defined in Equation (4.22)) we have*

$$\left\| \sum_{m,n,j} \sum_{m',n',j'} \frac{(m-m')}{|\lambda-m|^{1/2}|\lambda-m'|^{1/2}} \langle \psi_{m,n}^{(j)}, X\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \right\| \leq C \quad (\text{A.110})$$

$$\left\| \sum_{m,n,j} \sum_{m',n',j'} \frac{(m-m')}{|\lambda-m|^{1/2}|\lambda-m'|^{1/2}} \langle \psi_{m,n}^{(j)}, Y\psi_{m',n'}^{(j')} \rangle |\psi_{m,n}^{(j)}\rangle \langle \psi_{m',n'}^{(j')}| \right\| \leq C. \quad (\text{A.111})$$

A.9.4 Proof of Proposition A.9.1

In this section, we will only prove Equation (A.110), Equation (A.111) follows by analogous steps.

To bound Equation (A.110), we will use Schur's test. Recall that Schur's test tells us that if T is a linear operator defined by the discrete kernel $K(m, n, j, m', n', j')$:

$$Tf(m, n, j) = \sum_{m',n',j'} K(m, n, j, m', n', j')f(m', n', j')$$

and if for some real, positive functions p, q we have

$$\sum_{m', n', j'} |K(m, n, j, m', n', j')| q(m', n', j') \leq \alpha p(m, n, j) \quad \text{and}$$

$$\sum_{m, n} p(m, n, j) |K(m, n, j, m', n', j')| \leq \beta q(m', n', j').$$

then $\|T\| \leq \sqrt{\alpha\beta}$. Equation (A.110) can be viewed as the operator norm of an operator defined by the following discrete kernel:

$$K(m, n, j, m', n', j') := \frac{(m - m')}{|\lambda - m|^{1/2} |\lambda - m'|^{1/2}} \langle \psi_{m, n}^{(j)}, X \psi_{m', n'}^{(j')} \rangle.$$

Choosing $p(m, n, j) = |\lambda - m|^{-1/2}$ and $q(m', n', j') = |\lambda - m'|^{-1/2}$ and applying Schur's test we see that it is enough to find α, β such that

$$\sum_{m', n', j'} \frac{|m' - m|}{|\lambda - m'| |\lambda - m|^{1/2}} |\langle \psi_{m, n}^{(j)}, X \psi_{m', n'}^{(j')} \rangle| \leq \frac{\alpha}{|\lambda - m|^{1/2}}$$

$$\sum_{m, n, j} \frac{|m' - m|}{|\lambda - m'|^{1/2} |\lambda - m|} |\langle \psi_{m, n}^{(j)}, X \psi_{m', n'}^{(j')} \rangle| \leq \frac{\beta}{|\lambda - m'|^{1/2}}$$

Multiplying both sides of the first inequality by $|\lambda - m|^{1/2}$ gives that we need to show that:

$$\sum_{m', n', j'} \frac{|m' - m|}{|\lambda - m'|} |\langle \psi_{m, n}^{(j)}, X \psi_{m', n'}^{(j')} \rangle| \leq \alpha \quad (\text{A.112})$$

Similarly, multiplying both sides of the second inequality by $|\lambda - m'|^{1/2}$ gives that we need to show that:

$$\sum_{m, n, j} \frac{|m' - m|}{|\lambda - m|} |\langle \psi_{m, n}^{(j)}, X \psi_{m', n'}^{(j')} \rangle| \leq \beta \quad (\text{A.113})$$

Since X is self-adjoint, proving the bound in Equation (A.112) immediately implies Equation (A.113) with $\alpha = \beta$ by performing the change of index $(m, n, j) \leftrightarrow (m', n', j')$. Hence, we will focus on Equation (A.112) for the remainder of this section.

Similar to the proof of Proposition 4.4.2 in Appendix A.7, our main technique for proving Equation (A.112) will be inserting a partition unity of the form:

$$\sum_{k, \ell} \chi_{k, \ell}(\mathbf{x}) = 1$$

where

$$\chi_{k,\ell}(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in [k - \frac{1}{2}, k + \frac{1}{2}) \times [\ell - \frac{1}{2}, \ell + \frac{1}{2}) \\ 0 & \text{otherwise.} \end{cases}$$

Since $\{\psi_{m,n}^{(j)}\}$ is an orthonormal basis $\langle \psi_{m,n}^{(j)}, \psi_{m',n'}^{(j')} \rangle = 0$ whenever $(m, n, j) \neq (m', n', j')$. Therefore, we easily see that

$$\begin{aligned} & \sum_{m',n',j'} \frac{|m' - m|}{|\lambda - m'|} |\langle \psi_{m,n}^{(j)}, X \psi_{m',n'}^{(j')} \rangle| \\ &= \sum_{m',n',j'} \frac{|m' - m|}{|\lambda - m'|} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle|. \end{aligned}$$

Now we can insert our partition of unity to get

$$\begin{aligned} & \sum_{m',n',j'} \frac{|m' - m|}{|\lambda - m'|} |\langle \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \\ & \leq \sum_{m',n',j'} \sum_{k,\ell} \frac{|m' - m|}{|\lambda - m'|} |\langle \chi_{k,\ell} \psi_{m,n}^{(j)}, (X - m) \psi_{m',n'}^{(j')} \rangle| \\ & \leq \sum_{m',n',j'} \sum_{k,\ell} \frac{|m' - m|}{|\lambda - m'|} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \\ & \leq M \left(\sup_{j'} \sum_{m',n'} \sum_{k,\ell} \frac{|m' - m|}{|\lambda - m'|} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \right) \quad (\text{A.114}) \end{aligned}$$

Using the fact that $|m - m'| \leq |m - k| + |m' - k|$, we can now upper bound Equation (A.114) by the sum of the following two terms:

$$\sum_{m',n'} \sum_{k,\ell} \frac{|m - k|}{|\lambda - m'|} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\| \quad (\text{A.115})$$

$$\sum_{m',n'} \sum_{k,\ell} \frac{|m' - k|}{|\lambda - m'|} \|\chi_{k,\ell} (X - m) \psi_{m,n}^{(j)}\| \|\chi_{k,\ell} \psi_{m',n'}^{(j')}\|. \quad (\text{A.116})$$

We will bound Equation (A.115) in Appendix A.9.4 and Equation (A.116) in Appendix A.9.4.

Bounding Equation (A.115)

For this proof, we will fix a choice of (m, n, j) and prove a bound which is uniform in (m, n, j) . Using Lemma A.6.1 with $s_1 = 1/2 + \epsilon$ and $s_2 = 1 + \epsilon$ we have that for

any $\epsilon > 0$

$$\|\chi_{k,\ell}\psi_{m',n'}^{(j')}\| \leq \frac{C_1\|\chi_{k,\ell}(|X-m'|+1)^{1/2+\epsilon}(|Y-n'|+1)^{1+\epsilon}\psi_{m',n'}^{(j')}\|}{\langle m'-k \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \quad (\text{A.117})$$

Next, using Lemma A.6.2

$$\begin{aligned} & \|\chi_{k,\ell}(|X-m'|+1)^{1/2+\epsilon}(|Y-n'|+1)^{1+\epsilon}\psi_{m',n'}^{(j')}\| \\ & \leq \|(|X-m'|+1)^{3/2+2\epsilon}\psi_{m',n'}^{(j')}\| + \|(|Y-n'|+1)^{3/2+2\epsilon}\psi_{m',n'}^{(j')}\| \end{aligned}$$

but this quantity is bounded by a constant, C_2 , since we assume that the basis $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 5/2$. Therefore, we can upper bound Equation (A.115) with

$$\begin{aligned} & \sum_{m',n'} \sum_{k,\ell} \frac{|m-k|}{|\lambda-m'|} \|\chi_{k,\ell}(X-m)\psi_{m,n}^{(j)}\| \|\chi_{k,\ell}\psi_{m',n'}^{(j')}\| \\ & \leq C_2 \sum_{m',n'} \sum_{k,\ell} \frac{|m-k|}{|\lambda-m'|} \frac{\|\chi_{k,\ell}(X-m)\psi_{m,n}^{(j)}\|}{\langle m'-k \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \end{aligned}$$

Applying Lemma A.6.1 with $s_1 = 1$ and $s_2 = 1/2 + \epsilon$ we also have that

$$\begin{aligned} & \|\chi_{k,\ell}(X-m)\psi_{m,n}^{(j)}\| \\ & \leq \frac{C_3\|\chi_{k,\ell}(|X-m|+1)^2(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|}{\langle m-k \rangle\langle n-\ell \rangle^{1/2+\epsilon}} \quad (\text{A.118}) \end{aligned}$$

To reduce clutter, in the next few steps let us define:

$$A_{k,\ell} := \|\chi_{k,\ell}(|X-m|+1)^2(|Y-n|+1)^{1/2+\epsilon}\psi_{m,n}^{(j)}\|. \quad (\text{A.119})$$

Note that we have excluded the dependence on (m, n, j) in our notation since we have fixed a choice (m, n, j) for this proof. With this definition and the bound from Equation (A.118) we have that

$$\begin{aligned} & \sum_{m',n'} \sum_{k,\ell} \frac{|m-k|}{|\lambda-m'|} \frac{\|\chi_{k,\ell}(X-m)\psi_{m,n}^{(j)}\|}{\langle m'-k \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \\ & \leq C_2C_3 \sum_{m',n'} \sum_{k,\ell} \frac{|m-k|}{|\lambda-m'|} \frac{A_{k,\ell}}{\langle m-k \rangle\langle n-\ell \rangle^{1/2+\epsilon}} \frac{1}{\langle m'-k \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \\ & \leq C_2C_3 \sum_{m',n'} \sum_{k,\ell} \frac{1}{|\lambda-m'|} \frac{A_{k,\ell}}{\langle n-\ell \rangle^{1/2+\epsilon}\langle m'-k \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \\ & \leq C_2C_3 \sum_{n',\ell} \frac{1}{\langle n-\ell \rangle^{1/2+\epsilon}\langle n'-\ell \rangle^{1+\epsilon}} \left(\sum_{m',k} \frac{A_{k,\ell}}{|\lambda-m'| \langle m'-k \rangle^{1/2+\epsilon}} \right) \quad (\text{A.120}) \end{aligned}$$

Let's focus our attention on the sum over (m', k)

$$\sum_{m', k} \frac{A_{k, \ell}}{|\lambda - m'| \langle m' - k \rangle^{1/2 + \epsilon}}$$

Since λ , ℓ , and (m, n, j) are fixed this is a sum of the form

$$\sum_{m'} \sum_k a[k] b[m'] c[m' - k]$$

which is clearly the ℓ^1 -norm of a convolution. Therefore, by Young's convolution inequality (Theorem 7) with $p = 2$, $q = 1 + \frac{\epsilon}{2}$ and $r = (2 - \frac{1}{p} - \frac{1}{q})^{-1} = \frac{2(2+\epsilon)}{2+3\epsilon}$ we have that

$$\begin{aligned} & \sum_{m', k} \frac{A_{k, \ell}}{|\lambda - m'| \langle m' - k \rangle^{1/2 + \epsilon}} \\ & \leq \left(\sum_k A_{k, \ell}^2 \right)^{1/2} \left(\sum_{m'} \frac{1}{|\lambda - m'|^{1 + \epsilon/2}} \right)^{1/q} \left(\sum_{m'} \frac{1}{\langle m' \rangle^{(1/2 + \epsilon)r}} \right)^{1/r} \end{aligned} \quad (\text{A.121})$$

It's easy to check that

$$\left(\frac{1}{2} + \epsilon \right) r = \frac{2 + 5\epsilon + 2\epsilon^2}{2 + 3\epsilon} = 1 + \epsilon + O(\epsilon^2)$$

so for $\epsilon > 0$ sufficiently small the last two terms in Equation (A.121) are bounded by a constant, C_4 . Therefore, we conclude that

$$\sum_{m', k} \frac{A_{k, \ell}}{|\lambda - m'| \langle m' - k \rangle^{1/2 + \epsilon}} \leq C_4 \left(\sum_k A_{k, \ell}^2 \right)^{1/2}. \quad (\text{A.122})$$

Using this bound in Equation (A.120) then gives:

$$\begin{aligned} & \sum_{m', n'} \sum_{k, \ell} \frac{|m - k|}{|\lambda - m'|} \frac{\|\chi_{k, \ell}(X - m)\psi_{m, n}^{(j)}\|}{\langle m' - k \rangle^{1/2 + \epsilon} \langle n' - \ell \rangle^{1 + \epsilon}} \\ & \leq C_3 C_4 C_5 \sum_{n', \ell} \frac{1}{\langle n - \ell \rangle^{1/2 + \epsilon} \langle n' - \ell \rangle^{1 + \epsilon}} \left(\sum_k A_{k, \ell}^2 \right)^{1/2}. \end{aligned}$$

Similar to before, this sum is the ℓ^1 -norm of a convolution in n', ℓ . Therefore, by Young's convolution inequality (Theorem 7) with $p = q = 2$, $r = 1$ we have that

$$\begin{aligned} & \sum_{n', \ell} \frac{1}{\langle n - \ell \rangle^{1/2+\epsilon} \langle n' - \ell \rangle^{1+\epsilon}} \left(\sum_k A_{k, \ell}^2 \right)^{1/2} \\ & \leq \left(\sum_{k, \ell} A_{k, \ell}^2 \right)^{1/2} \left(\sum_{\ell} \frac{1}{\langle n - \ell \rangle^{1+2\epsilon}} \right)^{1/2} \left(\sum_{n'} \frac{1}{\langle n' \rangle^{1+\epsilon}} \right) \end{aligned}$$

The last two sums are clearly bounded for any $\epsilon > 0$ so to finish the bounding Equation (A.115), we only need to show the first sum is bounded. Recalling the definition of $A_{k, \ell}$ as Equation (A.119):

$$\begin{aligned} \sum_{k, \ell} A_{k, \ell}^2 &= \sum_{k, \ell} \|\chi_{k, \ell} (|X - m| + 1)^2 (|Y - n| + 1)^{1/2+\epsilon} \psi_{m, n}^{(j)}\|^2 \\ &= \|(|X - m| + 1)^2 (|Y - n| + 1)^{1/2+\epsilon} \psi_{m, n}^{(j)}\|^2. \end{aligned}$$

Applying Lemma A.6.2, we see that this quantity is bounded by a constant so long as we assume that $\{\psi_{m, n}^{(j)}\}$ is bounded with $s > 5/2$. This finishes the proof that Equation (A.115) is bounded.

Bounding Equation (A.116)

This bound follows by essentially the same argument as used to bound Equation (A.115); we only include it for completeness. Similar to before, we will fix a choice of (m, n, j) and prove a bound which is uniform in (m, n, j) .

Using Lemma A.6.1 with $s_1 = 3/2 + \epsilon$ and $s_2 = 1/2 + \epsilon$ we have that for any $\epsilon > 0$

$$\|\chi_{k, \ell} \psi_{m', n'}^{(j')}\| \leq \frac{C_1 \|\chi_{k, \ell} (|X - m'| + 1)^{3/2+\epsilon} (|Y - n'| + 1)^{1/2+\epsilon} \psi_{m', n'}^{(j')}\|}{\langle m' - k \rangle^{3/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \quad (\text{A.123})$$

Next, using Lemma A.6.2

$$\begin{aligned} & \|\chi_{k, \ell} (|X - m'| + 1)^{3/2+\epsilon} (|Y - n'| + 1)^{1/2+\epsilon} \psi_{m', n'}^{(j')}\| \\ & \leq \|(|X - m'| + 1)^{2+2\epsilon} \psi_{m', n'}^{(j')}\| + \|(|Y - n'| + 1)^{2+2\epsilon} \psi_{m', n'}^{(j')}\| \end{aligned}$$

but this quantity is bounded by a constant, C_2 , since we assume that the basis $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 5/2$. Therefore, we can upper bound Equation (A.116) with

$$\begin{aligned} & \sum_{m',n'} \sum_{k,\ell} \frac{|m' - k|}{|\lambda - m'|} \|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\| \|\chi_{k,\ell}\psi_{m',n'}^{(j')}\| \\ & \leq C_2 \sum_{m',n'} \sum_{k,\ell} \frac{|m' - k|}{|\lambda - m'|} \frac{\|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\|}{\langle m' - k \rangle^{3/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \\ & \leq C_2 \sum_{m',n'} \sum_{k,\ell} \frac{1}{|\lambda - m'|} \frac{\|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\|}{\langle m' - k \rangle^{1/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \end{aligned}$$

Applying Lemma A.6.1 with $s_1 = 0$ and $s_2 = 1 + \epsilon$ we also have that

$$\begin{aligned} & \|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\| \\ & \leq \frac{C_3 \|\chi_{k,\ell}(|X - m| + 1)(|Y - n| + 1)^{1+\epsilon}\psi_{m,n}^{(j)}\|}{\langle n - \ell \rangle^{1+\epsilon}} \end{aligned} \quad (\text{A.124})$$

To reduce clutter, in the next few steps let us define (recall that we have fixed (m, n, j)):

$$\tilde{A}_{k,\ell} := \|\chi_{k,\ell}(|X - m| + 1)(|Y - n| + 1)^{1+\epsilon}\psi_{m,n}^{(j)}\|. \quad (\text{A.125})$$

With this definition and the bound from Equation (A.124), we have that

$$\begin{aligned} & \sum_{m',n'} \sum_{k,\ell} \frac{1}{|\lambda - m'|} \frac{\|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\|}{\langle m' - k \rangle^{1/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \\ & \leq C_2 C_3 \sum_{m',n'} \sum_{k,\ell} \frac{1}{|\lambda - m'|} \frac{\tilde{A}_{k,\ell}}{\langle n - \ell \rangle^{1+\epsilon} \langle m' - k \rangle^{1/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \\ & \leq C_2 C_3 \sum_{n',\ell} \frac{1}{\langle n - \ell \rangle^{1+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \left(\sum_{m',k} \frac{\tilde{A}_{k,\ell}}{|\lambda - m'| \langle m' - k \rangle^{1/2+\epsilon}} \right) \end{aligned} \quad (\text{A.126})$$

Using our calculation from Appendix A.9.4 (Equation (A.122)), we know that

$$\begin{aligned} & \sum_{m',n'} \sum_{k,\ell} \frac{1}{|\lambda - m'|} \frac{\|\chi_{k,\ell}(X - m)\psi_{m,n}^{(j)}\|}{\langle m' - k \rangle^{1/2+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \\ & \leq C_4 \sum_{n',\ell} \frac{1}{\langle n - \ell \rangle^{1+\epsilon} \langle n' - \ell \rangle^{1/2+\epsilon}} \left(\sum_k \tilde{A}_{k,\ell}^2 \right)^{1/2} \\ & \leq \left(\sum_{k,\ell} \tilde{A}_{k,\ell}^2 \right)^{1/2} \left(\sum_\ell \frac{1}{\langle n - \ell \rangle^{1+\epsilon}} \right) \left(\sum_{n'} \frac{1}{\langle n' \rangle^{1+2\epsilon}} \right)^{1/2}, \end{aligned}$$

where in the last line we have used Young's convolution inequality (Theorem 7) with $p = q = 2$ and $r = 1$. Recalling the definition of $\tilde{A}_{k,\ell}$ we have that

$$\begin{aligned} \sum_{k,\ell} \tilde{A}_{k,\ell}^2 &= \sum_{k,\ell} \|\chi_{k,\ell}(|X - m| + 1)(|Y - n| + 1)^{1+\epsilon} \psi_{m,n}^{(j)}\|^2 \\ &= \|(|X - m| + 1)(|Y - n| + 1)^{1+\epsilon} \psi_{m,n}^{(j)}\|^2 \end{aligned}$$

which is bounded by a constant due to Lemma A.6.2 and the assumption that $\{\psi_{m,n}^{(j)}\}$ is s -localized with $s > 5/2$. This finishes the proof that Equation (A.116) is bounded, completing the proof of Proposition A.9.1.

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Biography

Kevin Stubbs earned a B.S. in Mathematics and a B.S. in Computer Engineering from the University of Maryland – College Park in May 2015. In August 2015, he then moved to Durham, North Carolina to pursue a PhD in Mathematics at Duke University. While at Duke, Kevin received the James B. Duke fellowship as well as the National Science Foundation’s Graduate Research fellowship. Upon completion of his degree in May 2021, Kevin will take up a position at the Institute for Pure and Applied Mathematics at UCLA as part of a Simons Postdoctoral Fellowship.