Computation of bound states of semi-infinite matrix Hamiltonians with applications to edge states of two-dimensional materials

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Abstract

We present a novel numerical method for the computation of bound states of semi-infinite matrix Hamiltonians which model electronic states localized at edges of one and two-dimensional materials (edge states) in the tight-binding limit. The na"ive approach fails: arbitrarily large finite truncations of the Hamiltonian have spectrum which does not correspond to spectrum of the semi-infinite problem (spectral pollution). Our method, which overcomes this difficulty, is to accurately compute the Green’s function of the semi-infinite Hamiltonian by imposing an appropriate boundary condition at the semi-infinite end; then, the spectral data is recovered via Riesz projection. We demonstrate our method’s effectiveness by a study of edge states at a graphene zig-zag edge in the presence of defects, including atomic vacancies. Our method may also be used to study states localized at domain wall-type edges in one and two-dimensional materials where the edge Hamiltonian is infinite in both directions; we demonstrate this for the case of dimerized honeycomb structures joined along a zig-zag edge.
1 Introduction

When computing the electronic states of crystalline materials it is typical to first treat the material as infinite in all directions of periodicity, leading to an infinite periodic bulk Hamiltonian which is naturally analyzed using the Bloch transform (see [3], for example). The eigenstates of this Hamiltonian, known as bulk states, are quasi-periodic with respect to the crystal lattice and hence extensive throughout the material.

It is well-known that materials may host additional electronic edge states which decay rapidly away from the physical edge of the material. Such states are bound states of a semi-infinite edge Hamiltonian obtained by truncating the infinite bulk Hamiltonian in one direction and imposing a Dirichlet boundary condition at the truncation. Such states play an important role in the theory of the quantum Hall effect and of topological insulators, and are of independent interest for wave-guiding applications because of their robustness to certain classes of local perturbations [10, 12, 14, 4, 17].

In this work we study the numerical computation of bound states of semi-infinite edge Hamiltonians which model electronic states localized at the boundary of one and two-dimensional materials, such as graphene, in the tight-binding limit. The computation is complicated by the fact that arbitrarily large finite truncations of the Hamiltonian have spectrum which does not correspond to spectrum of the semi-infinite problem. We propose a method which overcomes this difficulty. The key idea of our method is that the Green’s function of the edge Hamiltonian may be computed accurately by truncating the Hamiltonian while imposing an appropriate boundary condition at the semi-infinite end. The spectrum and eigenstates of the original Hamiltonian may then be recovered via Riesz projection. Our method has a wide range of applicability: it may be adapted to a large class of edge Hamiltonians derived from tight-binding models of one or two-dimensional materials, and also to discretizations of continuous PDE models of such materials (see [7], for example).

The rest of the paper is organized as follows. In Section 2 we explain the appearance of spectral pollution in naïve computations and the main idea of our method using the SSH model, a one-dimensional model which has most of the essential features of the general case. In Section 3 we introduce our method in detail, again focusing on the SSH model. In Sections 4 and 6 we demonstrate the effectiveness of our method through studies of bound states at the zig-zag edge of graphene in the presence of atomic vacancies and of bound states at the interface of two dimerized graphene structures joined along a zig-zag edge. We provide a proof of the validity of our method which covers the examples considered in this work in Section 5.

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Figure 2.1: Illustration of the fully infinite bulk (top) and semi-infinite edge (bottom) SSH Hamiltonians without disorder. A sites are red; B sites are blue. $t_1$ and $t_2$ are the hopping amplitudes between neighboring sites.

2 Spectral pollution in a one-dimensional model: the SSH model

In this section, in order to motivate and clearly lay out the ideas behind our method, we restrict attention to a one-dimensional model which has most of the features of the general case: the (non-interacting) SSH model. This model, named for Su, Schrieffer, and Heeger \cite{SSH1980}, is a well-known tight-binding model of a one-dimensional chain of atomic sites which supports edge states. The structure of this section is as follows.

In Section \ref{sec:bulk}, we review the definition and spectrum (known as the bulk spectrum) of the SSH bulk Hamiltonian (illustrated in Figure \ref{fig:bulk}). In Sections \ref{sec:left-edge} and \ref{sec:left-edge-spectrum} we review the definition of the SSH left edge Hamiltonian (illustrated in Figure \ref{fig:edge}). In the absence of disorder, the spectrum of this Hamiltonian, which we refer to as the edge spectrum, can be explicitly computed by introducing a transfer matrix. Since this idea will play a key role in our main method, we review this calculation in detail.

In Section \ref{sec:disorder}, we introduce a disordered edge Hamiltonian whose spectral data can no longer be computed by hand. In Section \ref{sec:pollution} we demonstrate and explain the appearance of spectral pollution in na"ive numerical computations of the spectrum of the disordered edge Hamiltonian. Finally, in Section \ref{sec:nonlinear} we present a computational method which eliminates spectral pollution at the cost of making the problem nonlinear.

The stage will then be set for us to present, in Section \ref{sec:greens}, the main focus of the paper: a linear method which we refer to as the Green's function method which accurately computes spectral data of disordered edge Hamiltonians.

2.1 SSH bulk Hamiltonian and bulk spectrum

In this section, we review the definition and spectrum of the SSH bulk Hamiltonian (Figure \ref{fig:bulk}). We consider an electron (we ignore spin) "hopping" along a one-dimensional infinite periodic lattice (chain) of atomic sites with hopping amplitudes that alternate between sites along the chain. A fundamental cell of the chain consists of any two neighboring...
sites, which we label $A$ and $B$. We introduce the notation

$$\psi_m = \begin{bmatrix} \psi_m^A \\ \psi_m^B \end{bmatrix} \in \mathbb{C}^2, \quad m \in \mathbb{Z},$$

(2.1)

to represent the restriction of the electron wavefunction $\psi \in l^2(\mathbb{Z}; \mathbb{C}^2)$ to the $m$th fundamental cell of the chain. Denoting the intra- and inter-cell hopping amplitudes by $t_1$ and $t_2$ (for simplicity, we ignore all hopping other than between nearest-neighbors and assume that $t_1$ and $t_2$ are real and non-zero throughout), the bulk Hamiltonian $H_{\text{bulk}}$ is defined by its action on the $m$th fundamental cell by

$$[H_{\text{bulk}} \psi]_m = \begin{bmatrix} t_1 \psi_{m+1}^B + t_2 \psi_{m-1}^B \\ t_1 \psi_{m+1}^A + t_2 \psi_{m-1}^A \end{bmatrix}, \quad m \in \mathbb{Z}.\ \ \ (2.2)$$

Periodicity of the bulk Hamiltonian (2.2) implies, via Bloch’s theorem, that all (generalized) eigenfunctions $\Phi$ of $H_{\text{bulk}}$ are $k$-quasi-periodic: $\Phi_{m+1}(k) = e^{ik} \Phi_m(k) \ m \in \mathbb{Z}$ for $k \in [-\pi, \pi]$. They may therefore be expressed in the form

$$\Phi_m(k) = e^{ikm} \chi(k) \quad m \in \mathbb{Z}, \quad k \in [-\pi, \pi]$$

(2.3)

where $\chi(k) \in \mathbb{C}^2$ is independent of $m$. Substituting (2.3) into the eigenequation $H_{\text{bulk}} \Phi = E \Phi$, we obtain a $k$-dependent eigenvalue problem for $\chi$,

$$\begin{bmatrix} 0 & t^*(k) \\ t(k) & 0 \end{bmatrix} \chi(k) = E \chi(k) \quad k \in [-\pi, \pi]$$

(2.4)

whose eigenvalues are:

$$E^\pm(k) = \pm |t(k)| \quad k \in [-\pi, \pi].$$

(2.5)

The spectrum of (2.2), $\sigma(H_{\text{bulk}})$, is therefore the union of the real intervals (known as spectral bands) swept out by the functions $\pm |t(k)|$ as $k$ is varied over the interval $[-\pi, \pi]$. If $|\frac{t_2}{t_1}| = 1$, then $\sigma(H_{\text{bulk}})$ consists of a single interval. If $|\frac{t_2}{t_1}| \neq 1$, then $\sigma(H_{\text{bulk}})$ consists of two intervals, separated by a gap which contains 0.

The (generalized) eigenvectors (2.3) corresponding to the eigenvalues $E^\pm(k)$ are known as bulk states. These states do not decay as $m \to \pm \infty$.

### 2.2 SSH edge Hamiltonian and computation of edge spectrum via a transfer matrix

We now review the definition and spectrum of the SSH left edge Hamiltonian (Figure 2.1b). We define this Hamiltonian by restricting the bulk Hamiltonian $H_{\text{bulk}}$ to $l^2(\mathbb{N}; \mathbb{C}^2)$ and im-
posing a Dirichlet boundary condition at \( m = 0 \).

\[
[H^L_{\text{edge}} \psi]_m = \begin{bmatrix} t_1 \psi^B_m + t_2 \psi^B_{m-1} \\ t_1 \psi^A_m + t_2 \psi^A_{m+1} \end{bmatrix}, \quad m \in \mathbb{N}
\]  
\[\psi_0 = 0.\]  
\[(2.6)\]

As \( m \to \infty \), the Hamiltonians \( H^L_{\text{edge}} \) and \( H^L_{\text{bulk}} \) are identical, and hence by the Weyl criterion the essential spectrum of \( H^L_{\text{edge}} \) is equal to the spectrum of \( H^L_{\text{bulk}} \):

\[
\sigma_{\text{ess}}(H^L_{\text{edge}}) = \sigma(H^L_{\text{bulk}}).\]  
\[(2.7)\]

Since \( H^L_{\text{edge}} \) is not periodic it may have discrete spectrum, which would correspond to bound states. Since the technique involved will inform the numerical method we introduce below, we now show in detail that, depending on \( t_1 \) and \( t_2 \), \( H^L_{\text{edge}} \) either has no bound states or has precisely one bound state, whose eigenvalue is 0.

Let \( \psi \) be a bound state of \( H^L_{\text{edge}} \) with eigenvalue \( E \), i.e.,

\[
H^L_{\text{edge}} \psi = E \psi, \quad \psi \in l^2(\mathbb{N}; \mathbb{C}^2).
\]  
\[(2.8)\]

Using the definition of \( H^L_{\text{edge}} \), we have that (2.8) is equivalent to requiring that the components of \( \psi \) must satisfy the following second-order linear difference equation with periodic coefficients,

\[
t_1 \psi^A_{m-1} + t_2 \psi^A_m = E \psi^B_{m-1}, \quad t_1 \psi^B_m + t_2 \psi^B_{m-1} = E \psi^A_m, \quad m \in \mathbb{N}, \quad m \geq 2
\]  
\[(2.9)\]

with the initial condition

\[
\begin{bmatrix} \psi^A_1 \\ \psi^B_1 \end{bmatrix} = c \begin{bmatrix} 1 \\ \frac{E}{t_2} \end{bmatrix},
\]  
\[(2.10)\]

where \( c \) is an arbitrary constant which can be chosen such that the bound state is \( l^2(\mathbb{N}; \mathbb{C}^2) \)-normalized. The difference equation (2.9) may be re-stated as

\[
\psi_m = T \psi_{m-1}, \quad m \in \mathbb{N}, \quad m \geq 2,
\]  
\[(2.11)\]

\[
T := \begin{bmatrix} t_2 & 0 \\ E & -t_1 \end{bmatrix}^{-1} \begin{bmatrix} -t_1 & E \\ 0 & t_2 \end{bmatrix} = \begin{bmatrix} -\frac{t_1}{t_2} E \frac{t_2}{t_1} - t_2/2 \\ \frac{t_1}{t_2} E \frac{t_2}{t_1} - t_2 \end{bmatrix}.
\]  
\[(2.12)\]

The matrix \( T \) is known as the transfer matrix; it is analogous to the monodromy matrix which appears in the study of second-order linear ODEs with periodic coefficients (Hill’s equation) [15, 3, 5]. The transfer matrix, more precisely its spectrum, will play a crucial role in the method we present in Section 3.

Since the determinant of the transfer matrix is 1, its spectrum is constrained as follows:

**Lemma 2.1.** Let \( A \) be any \( 2 \times 2 \) matrix with entries in \( \mathbb{C} \). If the determinant of \( A \) is 1, the eigenvalues of \( A \) satisfy precisely one of the following possibilities:

(A1) \( A \) has non-degenerate eigenvalues \( \lambda \) and \( \lambda^{-1} \) such that \( |\lambda| < 1 \) and \( |\lambda^{-1}| > 1 \)

(A2) \( A \) has non-degenerate eigenvalues \( \lambda \) and \( \lambda^{-1} \) such that \( |\lambda| = |\lambda^{-1}| = 1 \)
A has one degenerate eigenvalue equal to 1 or −1.

In the context of Hill’s equation this trichotomy underlies Floquet’s theorem [15, 6, 5]. In order for $E$ to be an eigenvalue of $H_{\text{edge}}^L$, we require that its eigenvector $\psi$ must be in $l^2(\mathbb{N}; \mathbb{C}^2)$; hence, by (2.11), $E$ must be such that the transfer matrix $T$ realizes possibility (A1) of Lemma 2.1. The following is now immediate upon imposing the initial condition (2.10).

**Lemma 2.2.** $E$ is an eigenvalue of $H_{\text{edge}}^L$ if and only if $T$ has an eigenvalue $\lambda$ such that $|\lambda| < 1$ whose associated eigenvector is $\begin{bmatrix} 1; & \frac{E}{\lambda} \end{bmatrix}^T$.

Starting from Lemma 2.2, the proof of the following is then straightforward.

**Proposition 2.3.** When $|\frac{t_2}{t_1}| \leq 1$, $H_{\text{edge}}^L$ has no bound states. When $|\frac{t_2}{t_1}| > 1$, $H_{\text{edge}}^L$ has precisely one bound state with eigenvalue $E = 0$ given explicitly by

$$\psi_m = c \begin{bmatrix} (\frac{t_1}{t_2})^{m-1} & 0 \end{bmatrix}, \quad m \in \mathbb{N}, \quad (2.13)$$

where $c$ is an arbitrary complex constant.

The spectrum of $H_{\text{edge}}^L$ is now completely characterized: The essential spectrum is equal to that of the bulk Hamiltonian, $H_{\text{bulk}}$, by the Weyl criterion (2.7); and Proposition 2.3 characterizes the discrete spectrum of $H_{\text{edge}}^L$. The bound state (2.13) is known as an **edge state** because it decays away from the edge of the material.

**Remark 2.1.** The existence of bound states of edge Hamiltonians has, in certain cases, been related to topological invariants associated with the associated bulk Hamiltonian. This link is known as the bulk-boundary correspondence (see [12, 8, 3], and references within, for example).

### 2.3 The SSH right edge Hamiltonian

The right edge Hamiltonian $H_{\text{edge}}^R$ is defined analogously to $H_{\text{edge}}^L$ by restricting $H_{\text{bulk}}$ to $l^2(-\mathbb{N}; \mathbb{C}^2)$ and imposing $\psi_0 = 0$. By analogous arguments to those given above,

$$\sigma_{\text{ess}}(H_{\text{edge}}^R) = \sigma(H_{\text{bulk}}). \quad (2.14)$$

The discrete spectrum of $H_{\text{edge}}^R$ is then characterized by the following:

**Proposition 2.4.** When $|\frac{t_2}{t_1}| \leq 1$, $H_{\text{edge}}^R$ has no bound states. When $|\frac{t_2}{t_1}| > 1$, $H_{\text{edge}}^R$ has precisely one bound state with eigenvalue $E = 0$ given explicitly by

$$\psi_m = c \begin{bmatrix} 0 & (\frac{t_1}{t_2})^{1+m} \end{bmatrix}, \quad m \in -\mathbb{N}, \quad (2.15)$$

where $c$ is an arbitrary complex constant.
2.4 Disordered SSH edge Hamiltonian

We now consider a generalization of the SSH left edge Hamiltonian where the hopping amplitudes $t_1$ and $t_2$ are (non-zero) functions of the cell index $m$: $t_1(m)$ describes the intra-cell hopping within the $m$th cell; and $t_2(m)$ describes the inter-cell hopping between the $m$th and $(m+1)$th cells. We also now allow for onsite potentials $V^\sigma(m)$, $\sigma \in \{A,B\}$, which we will assume to be real. Under such a general perturbation, the spectrum of the edge Hamiltonian is no longer computable by hand and hence a computational method is called for.

We will assume that the edge Hamiltonian is \textit{eventually periodic} in the following sense.

\textbf{Assumption 2.1 (Periodicity of bulk medium).} There exists a non-negative integer $M \geq 0$ such that for all $m > M$:

- $t_1(m) = t_1^\infty$ and $t_2(m) = t_2^\infty$, where $t_1^\infty$ and $t_2^\infty$ are non-zero real numbers
- $V^\sigma(m) = 0$ for $\sigma \in \{A,B\}$.

For a schematic illustrating Assumption 2.1, see Figure 2.2. In summary, the Hamiltonian we consider is

$$\tilde{H}_{\text{edge}}^L \psi_m = \left[ t_1(m) \psi^B_m + t_2(m-1) \psi^B_{m-1} \right] \psi^A_m + \left[ V^A(m) \psi^A_m \right] \psi^B_m \quad m \in \mathbb{N}$$

$t_j(m) = t_j^\infty$ and $V^\sigma(m) = 0$ for $m > M$ \quad $j \in \{1,2\}, \sigma \in \{A,B\}$

$$\psi_0 = 0.$$  \hspace{1cm} (2.16)

\textbf{Remark 2.2.} Our method relies on eventual periodicity of the edge Hamiltonian. Assumption 2.1 is one example of such periodicity; however, more general perturbations of the left edge Hamiltonian, $H_{\text{edge}}^L$, and other choices of bulk structures can be treated with our method. In Section 5 we prove that our method is applicable to arbitrary eventually periodic edge Hamiltonians with two sites per unit cell. Our methods can be extended to arbitrary banded (finite-range hopping) and self-adjoint Hamiltonians which are eventually periodic at the cost of making the proofs more involved; we leave the details to a future work.

We will refer to $\tilde{H}_{\text{edge}}^L$, as defined by (2.16), as the \textit{disordered left edge Hamiltonian}. We consider the eigenvalue problem,

$$\tilde{H}_{\text{edge}}^L \psi = E \psi \quad \psi \in l^2(\mathbb{N}; \mathbb{C}^2).$$  \hspace{1cm} (2.17)
Under Assumption 2.1, the Hamiltonians $\tilde{H}^L_{\text{edge}}$ and $H_{\text{bulk}}$ (with $t_1$ and $t_2$ replaced by $t_1^\infty$ and $t_2^\infty$) are identical as $m \to \infty$; hence, by the Weyl criterion,

$$\sigma_{\text{ess}}(\tilde{H}^L_{\text{edge}}) = \sigma(H_{\text{bulk}}).$$

(2.18)

It remains only to compute the discrete spectrum of $\tilde{H}^L_{\text{edge}}$. The eigenvalue problem (2.17) is equivalent to the second-order difference equation,

$$t_1(m-1)\psi^A_{m-1} + t_2(m-1)\psi^A_m + V^B(m-1)\psi^B_{m-1} = E\psi^B_{m-1} \quad m \in \mathbb{N}, m \geq 2$$

subject to the initial condition,

$$[\psi^A_1 \psi^B_1] = c \begin{bmatrix} 1 & E - V^A(1) \\ t_1(1) & t_2(1) \end{bmatrix},$$

(2.20)

where $c$ denotes an arbitrary constant. Under Assumption 2.1 we can solve the second-order difference equation (2.19) for $m \geq M + 2$ via a transfer matrix,

$$\psi_m = T^\infty \psi_{m-1} \quad T^\infty := \begin{bmatrix} -t_1^\infty & E \\ t_1^\infty & E^2 - t_2^\infty \end{bmatrix} \quad m \in \mathbb{N}, m \geq M + 2.$$

(2.21)

The following generalization of Lemma 2.2 to the disordered setting is now clear; this lemma is the foundation of our main computational method.

**Lemma 2.5.** Let $\psi_m$ denote the solution of the system (2.19) – (2.20) for $m \in \{1, \ldots, M+1\}$. Then $E$ is an eigenvalue of $\tilde{H}^L_{\text{edge}}$ if and only if $T^\infty$ has an eigenvalue with norm less than 1 whose associated eigenvector is $\psi_{M+1}$.

In contrast to the left edge Hamiltonian without disorder $H^L_{\text{edge}}$, depending on the values of $V^A(m), V^B(m), t_1(m)$, and $t_2(m)$, $\tilde{H}^L_{\text{edge}}$ may have eigenvalues other than 0 and hence Proposition 2.3 does not generalize to this setting (see Remark 2.3 for a partial generalization). In Section 2.5 we study the problem of accurately computing the discrete spectrum of $\tilde{H}^L_{\text{edge}}$ and explain the failure of a naive approach to this problem.

**Remark 2.3.** Proposition 2.3 does not generalize to the disordered setting, since $\tilde{H}^L_{\text{edge}}$ may have eigenvalues other than zero -- see Figure 3.2. However, when $V^\sigma(m) = 0$ for $\sigma \in \{A, B\}$ and all $m \in \mathbb{N}$, the following partial generalization holds. When $|t_2^\infty| \leq 1$, $E = 0$ is not an eigenvalue of $\tilde{H}^L_{\text{edge}}$. When $|t_2^\infty| > 1$, $E = 0$ is an eigenvalue of $\tilde{H}^L_{\text{edge}}$, with associated bound state:

$$\psi_m = c \begin{bmatrix} -t_1(m-1) \\ t_2(m-1) \end{bmatrix}^{m-1} \quad m \in \mathbb{N},$$

(2.22)

where $c$ is an arbitrary complex constant.

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2.5 Spectral pollution associated with finite truncation of the semi-infinite Hamiltonian

In this section, we consider a na"ıve approach to computing the edge states of the disordered left-edge Hamiltonian $\tilde{H}^L_{\text{edge}}$ and show that this approach yields inaccurate results.

A simple approach to solving the eigenvalue problem (2.17) consists of imposing a Dirichlet boundary condition at some large value of the cell index $m$, i.e., solving the eigenvalue problem,

$$\tilde{H}^L_{\text{trunc}}\psi = E\psi \quad \psi \in l^2(\{1,\ldots,\mathcal{M}\};\mathbb{C}^2) \quad (2.23)$$

for some choice of $\mathcal{M} \gg M$, where $M$ is the integer appearing in Assumption 2.1 and where $\tilde{H}^L_{\text{trunc}}$ is defined by

$$[\tilde{H}^L_{\text{trunc}}\psi]_m = \left[ \begin{array}{c} t_1(m)\psi^B_m + t_2(m-1)\psi^B_{m-1} \\ t_1(m)\psi^A_m + t_2(m)\psi^A_{m+1} \\ V^A(m)\psi^A_m \\ V^B(m)\psi^B_m \end{array} \right] \quad m \in \{1,\ldots,\mathcal{M}\}$$

$$t_j(m) = t_j^\infty \quad V^\sigma(m) = 0 \quad m \in \{M,\ldots,\mathcal{M}\}, \quad j \in \{1,2\}, \quad \sigma \in \{A,B\}$$

We call this method the hard truncation method (see Figure 2.3 for an illustration). Such an approach is motivated by the observation that bound state solutions of the eigenvalue problem (2.17) must decay as $m \to \infty$; one might na"ıvely expect that treating near-zero entries of $\psi$ as precisely zero would have little effect on the solution. On the other hand, setting $\psi_{M+1} = 0$ is clearly inconsistent with Lemma 2.5. We now show that this approach produces inaccurate results, even for large $\mathcal{M}$, and explain why.

For $m \geq M$, the action of the Hamiltonian (2.24) is identical to the action of the right edge Hamiltonian $H^R_{\text{edge}}$ (see Section 2.3) with $t_1 = t_1^\infty$ and $t_2 = t_2^\infty$ and its edge shifted from $m = 0$ to $\mathcal{M} + 1$. $H^R_{\text{edge}}$ has an exact zero eigenvalue with associated eigenfunction decaying away from the right edge when $|t_2^\infty| > |t_1^\infty|$ (see Proposition 2.4). For $\mathcal{M} \gg M$, the truncation of this eigenfunction to the set $\{1,\ldots,\mathcal{M}\}$ will be an approximate eigenvector of (2.24) with eigenvalue zero when $|t_2^\infty| > |t_1^\infty|$. The presence of this approximate eigenvector has the effect of polluting the computation.

To see the effect that the approximate eigenvector decaying away from the right edge has on the computation, consider the truncation of the edge Hamiltonian without disorder...
where \( t_1(m) = t_1, \ t_2(m) = t_2, \) and \( V^A(m) = V^B(m) = 0 \) for all \( m, \)

\[
[H_{\text{trunc}}^L \psi]_m = \begin{bmatrix} t_1 \psi^B_m + t_2 \psi^B_{m-1} \\ t_1 \psi^A_m + t_2 \psi^A_{m+1} \end{bmatrix} \quad m \in \{1, ..., M\}
\]

(2.25)

When \( \frac{|t_2|}{|t_1|} > 1 \) and \( M \) is sufficiently large, the truncations of the bound states (2.13) and (2.15) to the set \( \{1, ..., M\} \) are approximate eigenfunctions of (2.25) with eigenvalue 0. By taking appropriate linear combinations of these approximate eigenvectors, two exact eigenvectors of (2.25) can be produced (see Figure 2.4) whose associated eigenvalues are of \( O(e^{-M}) \). The situation is analogous to the case of two well-separated potential wells related by a symmetry in the semi-classical regime (see [11, 18] for example).

**Remark 2.4.** The problem described above can be avoided when \( \frac{|t_2|}{|t_1|} > 1 \) by truncating the chain in the middle of a cell (i.e. after an A site) rather than at the end of a cell (i.e. after a B site). The right edge is then well described by \( H^R_{\text{edge}} \), the right-edge Hamiltonian, but with \( t_1 \) replaced by \( t_2^\infty \) and \( t_2 \) replaced by \( t_1^\infty \) which has no edge state when \( \frac{|t_2|}{|t_1|} \leq 1 \). The method which we describe below has the advantage that it may be applied without modification to all possible choices of \( t_1^\infty \) and \( t_2^\infty \) equally well and generalizes naturally to the two-dimensional cases we consider below.

### 2.6 Direct attempt at imposing appropriate boundary conditions at right end leads to a nonlinear eigenvalue problem

In the previous section we saw that hard truncation of the eigenvalue problem (2.17) leads to inaccurate results because of the presence of an approximate eigenvector decaying away from the right edge. In this section we show how the difficulty described above may be overcome by imposing a more appropriate boundary condition on the Hamiltonian \( \tilde{H}_{\text{edge}}^L \) at

![Figure 2.4: Plot of bound states of the truncated left edge Hamiltonian \( H_{\text{trunc}}^L \) without disorder (2.25) (eigenvalues \( \pm 9.16 \times 10^{-5} \)) (plotted with cyan \( \times \)s and red circles) compared with the unique bound state (eigenvalue \( E = 0 \)) of the semi-infinite left edge Hamiltonian \( H_{\text{edge}}^L \) (black filled circles). The results of the computations differ significantly.](image.png)
its semi-infinite end, but that doing so directly leads to a nonlinear eigenvalue problem. Our main numerical method (presented in Section 3) builds on this basic idea, but does so in a way which avoids nonlinearity.

Lemma 2.5 suggests the route forward: we solve the system (2.19), but instead of imposing a Dirichlet boundary condition after some large number of cells \( M \gg M \), we diagonalize \( T_\infty \) and then impose the condition that \( \psi_{M+1} \) is proportional to an eigenvector of the transfer matrix \( T_\infty \) whose eigenvalue has norm less than 1.

The existence of a unique such eigenvector is guaranteed whenever \( E \) does not lie in the essential spectrum of \( \tilde{H}_\text{edge} \) by Lemma 2.1. If no such eigenvector exists, it must be that one of possibilities (A2) or (A3) of Lemma 2.1 holds for the matrix \( T_\infty \). But either possibility implies the existence of a bounded (generalized) eigenvector of \( \tilde{H}_\text{edge} \) with eigenvalue \( E \) and hence we have a contradiction of \( E \notin \sigma_{\text{ess}}(\tilde{H}_\text{edge}) \).

By Lemma 2.5, we impose this condition without any loss of solutions since all bound states of \( \tilde{H}_\text{edge} \) satisfies this condition. The remainder of the semi-infinite bound state can then be recovered by repeated application of \( T_\infty \) to \( \psi_{M+1} \).

Unfortunately, since \( T_\infty \) depends on the eigenvalue \( E \), this method yields a nonlinear matrix eigenvalue problem of the form,

\[
EI - \begin{pmatrix}
  V^A(1) & t_1(1) & t_2(2) & \cdots & t_1(M) & V^B(M) & t_2(M) & 0 \\
  t_1(1) & V^B(1) & \cdots & \ddots & t_1(M) & 0 & \cdots & 0 \\
  \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
  \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
  t_2(M) & 0 & \cdots & \cdots & t_2(M) & 0 & \cdots & 0 \\
  \xi^B(E) & E - \xi^A(E) & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix} \begin{pmatrix}
  \psi_1^A \\
  \psi_1^B \\
  \vdots \\
  \psi_M^A \\
  \psi_M^B \\
  \psi_{M+1}^A \\
  \psi_{M+1}^B \\
\end{pmatrix} = 0,
\]

(2.26)

where \([\xi^A(E), \xi^B(E)]^T\) denotes the eigenvector of \( T_\infty \) whose associated eigenvalue has norm less than 1. Such problems can be solved via an iterative method. In the next section we will present a superior method which does not require solving a nonlinear eigenvalue problem.

3 Green’s function method

In this section we introduce our main method, which we refer to as the Green’s function method. Rather than trying to compute eigenvectors of \( \tilde{H}_\text{edge} \) directly, as in (2.26), we compute the associated spectral projection operator. This is done by computing the resolvent (or Green’s function) of the Hamiltonian and then recovering the projection via the Riesz projection formula (given below). In Section 3.2 we show how all relevant spectral information can be recovered using this method.

**Theorem 3.1** (Riesz projection). Let \( H \) be a self-adjoint operator on a Hilbert space \( \mathcal{H} \). Let \( \mathcal{C} \) denote a positively oriented contour in the complex plane which (1) does not intersect \( \sigma(H) \), (2) encloses finitely many eigenvalues of \( H \), and (3) does not enclose any other part of \( \sigma(H) \). Then,

\[
\Gamma := \frac{1}{2\pi i} \int_{\mathcal{C}} G(z) \, dz, \quad G(z) := (z - H)^{-1}
\]

(3.1)
is an orthogonal projection operator; in particular, it is the spectral projection onto the associated eigenspace of the eigenvalues enclosed in the contour \( \mathcal{C} \).

**Remark 3.1.** Physically speaking, \( \Gamma \) can be interpreted as the density matrix of a system for which the states corresponding to the eigenvalues enclosed by \( \mathcal{C} \) are all filled and all other states are empty.

Note that our method does not yield information about all of the discrete spectrum of \( \tilde{H}_\text{edge} \), only information about eigenvalues within the contour \( \mathcal{C} \). In practice this is not a problem: typically one is only interested in eigenvalues within the gap between essential spectrum (recall that \( \sigma_{\text{ess}}(\tilde{H}_\text{edge}) \) has a gap containing 0 whenever \( |\frac{t_2}{t_1}| \neq 1 \)). One therefore simply chooses the contour \( \mathcal{C} \) in such a way as to encircle a large subinterval of the gap without intersecting with the essential spectrum.

### 3.1 Computation of truncated Green’s function of disordered edge Hamiltonian \( \tilde{H}_\text{edge} \)

Since the remainder of any eigenstate of \( \tilde{H}_\text{edge} \) can be recovered by repeated application of the transfer matrix, it suffices to compute only the upper left \( 2M \times 2M \) block of the spectral projection \( \Gamma \). Consequently, by (3.1), we only need to determine how to compute the upper-left \( 2M \times 2M \) block of the Green’s function, \( G(z) \). We now show how to compute this block of \( G(z) \), after first introducing some notation.

For values of \( z \in \mathbb{C} \) where the definition makes sense, the Green’s function \( G(z) \) of \( \tilde{H}_\text{edge} \) is defined as the bounded inverse of the operator \( (zI - \tilde{H}_\text{edge}) \) on \( l^2(\mathbb{N}; \mathbb{C}^2) \),

\[
(zI - \tilde{H}_\text{edge})G(z) = I.
\]  

(3.2)

Equation (3.2) may now be expressed column by column as follows. For notational clarity, we suppress column indices and \( z \)-dependence of entries of \( G(z) \) so that we replace \( G_{\sigma,\sigma'}^{m,m'}(z) \) by \( G_{m,m'}^\sigma \).

\[
zG_1^A - V^A(1)G_1^A - t_1(1)G_1^B = \delta_{1,m'}^A,\sigma'
\]  

(3.4)

\[
zG_{m-1}^B - V^B(m-1)G_{m-1}^B - t_1(m-1)G_m^A - t_2(m-1)G_m^B = \delta_{m-1,m'}^B,\sigma'
\]  

\[
zG_m^A - V^A(m)G_m^A - t_1(m)G_m^B - t_2(m-1)G_{m-1}^B = \delta_{m,m'}^A,\sigma'
\]  

(3.5)

Here \( \delta_{m,m'}^{\sigma,\sigma'} \) denotes the \( (m, \sigma) \)-th entry of the vector with 1 in its \( (m', \sigma') \)-th entry and 0 in all its other entries. We solve the system (3.5) for the upper left \( 2M \times 2M \) block of \( G(z) \) as
follows. For \( m' \leq M \) and \( m \geq M + 2 \), the system (3.5) reduces to

\[
z G_{m-1}^B - t_1^\infty G_{m-1}^A - t_2^\infty G_m^A = 0, \quad z G_m^A - t_1^\infty G_m^B - t_2^\infty G_{m-1}^B = 0, \quad m \in \mathbb{N}, m \geq M + 2. \tag{3.6}
\]

The system (3.6) may be solved via a transfer matrix which depends on \( z \)

\[
\begin{bmatrix}
G_m^A \\
G_m^B
\end{bmatrix} = T^\infty(z) \begin{bmatrix}
G_{m-1}^A \\
G_{m-1}^B
\end{bmatrix}, \quad T^\infty(z) := \begin{bmatrix}
t_1^\infty & \frac{z}{t_2^\infty} - \frac{t_1^\infty}{t_2^\infty} \\
\frac{-z}{t_2^\infty} & \frac{z}{t_1^\infty} - \frac{t_2^\infty}{t_1^\infty}
\end{bmatrix} \quad m \geq M + 2. \tag{3.7}
\]

In order to ensure that \( G(z) \) is a bounded operator on \( l^2(\mathbb{Z}; \mathbb{C}^2) \), we solve the system (3.5) for each \( m' \in \{1, \ldots, M\} \) and \( \sigma' \in \{A, B\} \) and \( m \in \{1, \ldots, M+1\} \), \( \sigma \in \{A, B\} \) subject to the constraint that

\[
\begin{bmatrix}
G_{M+1}^A \\
G_{M+1}^B
\end{bmatrix} = c \begin{bmatrix}
\xi_A(z) \\
\xi_B(z)
\end{bmatrix} \quad c \in \mathbb{C}, \tag{3.8}
\]

where \([\xi_A(z), \xi_B(z)]^T\) denotes the eigenvector of \( T^\infty(z) \) whose associated eigenvalue has norm less than one and \( c \) denotes an arbitrary constant. By an identical argument to that given in Section 2.6 (see also Section 5), a unique such eigenvector exists as long as \( z \) does not lie in the essential spectrum of \( \hat{H}_{\text{edge}}^L \). This leads to the following matrix equation for the \((\sigma', m')\)th column of \( G(z) \),

\[
\begin{bmatrix}
V_A(1) & t_1(1) & \cdots & 0 & t_2(M) \\ t_1(1) & V_B(1) & t_2(2) & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ t_1(M) & 0 & t_2(M) \\ \xi_B(z) & \xi_B(z) & \cdots & \cdots & \cdots
\end{bmatrix} \begin{bmatrix}
G_1^A \\
G_1^B \\
\vdots \\
G_M^A \\
G_M^B
\end{bmatrix} = \begin{bmatrix}
\delta_{1,m'}^A,\sigma' \\
\delta_{1,m'}^B,\sigma' \\
\vdots \\
\delta_{M,m'}^A,\sigma' \\
\delta_{M,m'}^B,\sigma'
\end{bmatrix} \tag{3.9}
\]

Since \( z \) is fixed a priori, the matrix problem (3.9) can be solved directly, in contrast to the problem (2.26). We discuss how to recover the eigenvalues and eigenfunctions of \( \hat{H}_{\text{edge}}^L \) from the upper left \( 2M \times 2M \) block of \( G(z) \) in Section 3.2.

The choice to impose the boundary condition (3.8) in the \( M+1 \)th cell is to some extent arbitrary; the results of our method do not change if this boundary condition is imposed in any cell whose index is greater than \( M \). However, choosing \( M+1 \) clearly minimizes the size of the matrix problem (3.9) to solve and is hence optimal. For a numerical verification that our results do not depend on this choice see Figure 3.1.

### 3.2 Recovery of spectral data from the truncated Green’s function

We now discuss how to recover the eigenvalues and eigenstates of \( \hat{H}_{\text{edge}}^L \) from the truncated Green’s function computed in the previous section. The upper left \( 2M \times 2M \) block of the spectral projection \( \Gamma \) may be found by numerically evaluating the contour integral (3.1) using the upper-left \( 2M \times 2M \) block of \( G(z) \) computed in the previous section (see [9] for methods which dramatically speed up the evaluation of this integral). For notational simplicity, let
Figure 3.1: Plot of a bound state (eigenvalue $E = -0.3837$) of the disordered edge Hamiltonian $\tilde{H}^L_{\text{edge}}$ (2.16) (edge state) computed with the Green’s function method for 3 different choices of truncation cell when $M = 4$. We plot the result of truncating in cells $M + 1 = 5$ (cyan $\times$s), 7 (red circles), and 9 (black filled circles). For $m = 1$ to 4, the three computations agree exactly. In this example $t_1^\infty = 1$ and $t_2^\infty = 2$ and we model disorder by drawing values of the hopping amplitudes $t_j(m), j \in \{1, 2\}$, and onsite potentials $V^\sigma(m), \sigma \in \{A, B\}$ from normal distributions with mean equal to their values for $m > M$ and standard deviation $0.5$.

us define

$$\Gamma_{\text{trunc}} := \text{upper-left } 2M \times 2M \text{ block of } \Gamma.$$ (3.10)

The truncated spectral projection, $\Gamma_{\text{trunc}}$, is not sufficient for recovering all eigenvalues and eigenfunctions of $\tilde{H}^L_{\text{edge}}$. The missing information can be recovered by also using the upper-left $2M \times 2M$ block of the operator $\tilde{H}^L_{\text{edge}} \Gamma$, which may be computed via a contour integral, similarly to $\Gamma$.

$$\tilde{H}^L_{\text{edge}} \Gamma = \frac{1}{2\pi i} \int_C \tilde{H}^L_{\text{edge}} G(z) \, dz = \frac{1}{2\pi i} \int_C z G(z) \, dz, \quad G(z) = (z - \tilde{H}^L_{\text{edge}})^{-1},$$ (3.11)

where the second equality is clear by analyticity of the operator $(z - \tilde{H}^L_{\text{edge}})G(z) = I$. The upper left $2M \times 2M$ block of $\tilde{H}^L_{\text{edge}} \Gamma$ may now be computed similarly to that of $\Gamma$. We define

$$(\tilde{H}^L_{\text{edge}} \Gamma)_{\text{trunc}} := \text{upper left } 2M \times 2M \text{ block of } \tilde{H}^L_{\text{edge}} \Gamma.$$ (3.12)

The eigenvalues of $\tilde{H}^L_{\text{edge}}$ within the contour $C$ and their associated eigenvectors may now be computed from the matrices $\Gamma_{\text{trunc}}$ and $(\tilde{H}^L_{\text{edge}} \Gamma)_{\text{trunc}}$ by steps $A$ and $B$ as follows.

Step $A$: Non-zero eigenvalues of $\tilde{H}^L_{\text{edge}}$ within the contour $C$ and their associated eigenvectors are clearly in one-to-one correspondence with the non-zero eigenvalues of $(\tilde{H}^L_{\text{edge}} \Gamma)_{\text{trunc}}$ and their associated eigenvectors. However, the eigenvalues of $(\tilde{H}^L_{\text{edge}} \Gamma)_{\text{trunc}}$ and those of $\tilde{H}^L_{\text{edge}}$ are not equal. Specifically, let $\psi$ be an eigenvector of $\tilde{H}^L_{\text{edge}}$ with associated eigenvalue $E$. 


Figure 3.2: Example bound states (above, absolute value plotted) and spectra (below) of two realizations of the disordered SSH edge Hamiltonian (2.16). In spectral plots, essential spectrum (computed using Bloch theory) is shown as a blue line, while eigenvalues are labeled by $\times$s. The associated eigenvalue of each bound state which is plotted in the above figures is plotted with the same color in the figures below. To generate (a) and (b), we drew the values of the hopping amplitudes $t_1(m)$ and $t_2(m)$ from normal distributions with distinct mean values. To generate (a), we set all onsite potentials $V^\sigma(m) = 0$. To generate (b), we drew the values of the onsite potentials $V^A(m)$ and $V^B(m)$ from normal distributions with means of equal magnitude and opposite sign. For further details, see Section 3.3.

Then $\Gamma_{\text{trunc}}$ acts on the first $2M$ entries of $\psi$ (denoted here by $\psi_{\text{trunc}}$) by

$$\Gamma_{\text{trunc}} \psi_{\text{trunc}} = \langle \psi_{\text{trunc}} | \psi_{\text{trunc}} \rangle \psi_{\text{trunc}}$$

and hence $(\tilde{H}_\text{edge}^L \Gamma)_{\text{trunc}}$ acts by

$$(\tilde{H}_\text{edge}^L \Gamma)_{\text{trunc}} \psi_{\text{trunc}} = E \langle \psi_{\text{trunc}} | \psi_{\text{trunc}} \rangle \psi_{\text{trunc}}.$$

Here, $\langle | \rangle$ denotes the standard complex inner product on $\mathbb{C}^{2M}$. It follows that eigenvectors $\psi_{\text{trunc}}$ of $\tilde{H}_\text{edge}^L \Gamma$ with non-zero associated eigenvalues $E_{\text{trunc}}$ are truncations of eigenvectors $\psi$ of $\tilde{H}_\text{edge}^L$ with eigenvalue,

$$E = \frac{E_{\text{trunc}}}{N_{\text{trunc}}}$$

where $N_{\text{trunc}} := \langle \psi_{\text{trunc}} | \psi_{\text{trunc}} \rangle$.

**Step B:** As for the zero eigenvalues of $\tilde{H}_\text{edge}^L$, note that it is impossible to identify eigenvectors of $\tilde{H}_\text{edge}^L$ with eigenvalue precisely zero by only diagonalizing $(\tilde{H}_\text{edge}^L \Gamma)_{\text{trunc}}$, since these eigenvectors will be indistinguishable from vectors in the null space of $\Gamma$. These eigenvectors must be computed by diagonalizing the spectral projection $\Gamma_{\text{trunc}}$ on the orthogonal complement of the space of eigenvectors of $(\tilde{H}_\text{edge}^L \Gamma)_{\text{trunc}}$ with non-zero eigenvalues and identifying the non-zero eigenspace.
3.3 Results: disordered SSH edge Hamiltonian

Using the Green’s function method described in Sections 3.1 and 3.2, we computed two examples of discrete spectrum of the edge Hamiltonian (2.16) lying in the gap between bands of essential spectrum when \( t_2^\infty = 1.6 \) and \( t_1^\infty = 1 \) with disorder up to the \( M = 40 \)th cell. Our results are shown in Figure 3.2 and were produced as follows.

To generate Figure 3.2a, we drew the values of the functions \( t_1(m) \) and \( t_2(m) \) for \( m \leq M \) from normal distributions with standard deviation 0.5 and means equal to \( t_1^\infty \) and \( t_2^\infty \), respectively. We then set the functions \( V^A(m) = V^B(m) = 0 \) for \( m \leq M \). In this case, we find that (2.16) has an eigenvalue which is precisely 0 corresponding to an eigenfunction which decays rapidly away from the edge of the chain (confirming Remark 2.3). In addition, we see bound states with non-zero eigenvalues whose associated eigenfunctions are localized away from the edge.

To generate Figure 3.2b, we again drew the values of the functions \( t_1(m) \) and \( t_2(m) \) for \( m \leq M \) from normal distributions with standard deviation 0.5 and means equal to \( t_1^\infty \) and \( t_2^\infty \). We then drew the functions \( V^A(m) \) and \( V^B(m) \) for \( m \leq M \) from a normal distribution with standard deviations 0.5 and means 0. In this case, we find again one bound state which decays rapidly away from the edge and multiple bound states whose associated eigenvectors are localized away from the edge. Note that the eigenvalue of the eigenvector which decays rapidly away from the edge is no longer 0 in this case.

4 Application to edge states of honeycomb structures

In Section 3, we introduced the Green’s function method for computing the bound states of the disordered SSH edge Hamiltonian. In this section, we show that our method may be applied to computing bound states at edges of a two-dimensional graphene-like structure with disorder when the disorder satisfies a periodicity condition. In Section 6, we consider the application of our method to more general honeycomb structures.

4.1 Graphene bulk Hamiltonian

We first review the bulk Hamiltonian of a graphene-like structure (see [16] for details). Making analogous assumptions to those made in our treatment of the SSH model introduced in Section 1, we consider a single electron without spin hopping on a two-dimensional honeycomb lattice. Each fundamental cell, labeled by integers \( m \) and \( n \), of such a lattice hosts two atoms, which we label \( A \) and \( B \). We introduce the notation

\[
\psi_{m,n} = \begin{bmatrix} \psi^A_{m,n} \\ \psi^B_{m,n} \end{bmatrix},
\]  

(4.1)

to denote the restriction of the electron wavefunction \( \psi \in l^2(\mathbb{Z}^2; \mathbb{C}^2) \) to the \((m, n)\)th fundamental cell of the lattice. The bulk Hamiltonian of a graphene-like structure then reads

\[
[H_{\text{bulk}} \psi]_{m,n} = -t \begin{bmatrix} \psi^B_{m,n} + \psi^B_{m-1,n} + \psi^B_{m,n-1} \\ \psi^A_{m,n} + \psi^A_{m+1,n} + \psi^A_{m,n+1} \end{bmatrix} \quad m, n \in \mathbb{Z}^2.
\]  

(4.2)

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where \( t \) is a real non-zero constant. Bloch’s theorem in this context implies that bounded eigenfunctions of \( H_{\text{bulk}} \) have the form
\[
\Phi_{m,n}(k_1, k_2) = e^{i[k_1 m + k_2 n]} \chi(k_1, k_2),
\]
where \( \chi(k_1, k_2) \) satisfies the eigenvalue problem,
\[
- t \begin{bmatrix} 0 & f^*(k_1, k_2) \\ f(k_1, k_2) & 0 \end{bmatrix} \chi(k_1, k_2) = E(k_1, k_2) \chi(k_1, k_2) \quad (k_1, k_2) \in [-\pi, \pi]^2
\]
\[
f(k_1, k_2) := 1 + e^{i k_1} + e^{i k_2},
\]
whose eigenvalues may be readily computed:
\[
E^\pm(k_1, k_2) = \pm t |f(k_1, k_2)| \quad (k_1, k_2) \in [-\pi, \pi]^2.
\]
The functions \( E^\pm(k_1, k_2) \) sweep out surfaces which touch at roots of the function \( f(k_1, k_2) \) which occur at the points \( \left( \frac{2\pi}{3}, -\frac{2\pi}{3} \right) \) and \( \left( -\frac{2\pi}{3}, \frac{2\pi}{3} \right) \), which are known as Dirac points. It follows that the spectrum of \( H_{\text{bulk}} \) is a single closed interval.

### 4.2 Graphene zig-zag edge Hamiltonian

The zig-zag edge Hamiltonian \( H_{\text{edge}}^{\text{ZZ}} \) is defined by restricting \( H_{\text{bulk}} \) to \( l^2(\mathbb{N} \times \mathbb{Z}; \mathbb{C}^2) \) and imposing a Dirichlet boundary condition at \( m = 0 \),
\[
[H_{\text{edge}}^{\text{ZZ}} \psi]_{m,n} = -t \begin{bmatrix} \psi_{m,n}^B + \psi_{m-1,n}^B + \psi_{m,n-1}^B \\ \psi_{m,n}^A + \psi_{m+1,n}^A + \psi_{m,n+1}^A \end{bmatrix} \quad m, n \in \mathbb{N} \times \mathbb{Z}
\]
\[
\psi_{0,n} = 0.
\]
In contrast to \( H_{\text{bulk}} \), the Hamiltonian \( H_{\text{edge}}^{\text{ZZ}} \) is periodic only with respect to \( n \). Without loss of generality we may impose the Bloch periodicity condition on the wavefunction in the \( n \) direction only,
\[
\psi_{m,n+1} = e^{i k_{\parallel}} \psi_{m,n} \quad m, n \in \mathbb{N} \times \mathbb{Z}.
\]
Imposing (4.7) leads to a one-dimensional problem which depends on \( k_{\parallel} \in [-\pi, \pi] \) as a parameter,
\[
[H_{\text{edge}}^{\text{ZZ}}(k_{\parallel}) \psi]_m = -t \begin{bmatrix} (1 + e^{-ik_{\parallel}}) \psi_m^B + \psi_{m-1}^B \\ (1 + e^{ik_{\parallel}}) \psi_m^A + \psi_{m+1}^A \end{bmatrix} \quad m \in \mathbb{N}
\]
\[
\psi_0 = 0.
\]
Since \( H_{\text{edge}}^{\text{ZZ}} \) is identical to the bulk Hamiltonian \( H_{\text{bulk}} \) as \( m \to \infty \), the essential spectrum of \( H_{\text{edge}}^{\text{ZZ}}(k_{\parallel}) \) is precisely the intervals swept out by the functions \( k_1 \mapsto E^\pm(k_1, k_{\parallel}) \), \( k_1 \in [-\pi, \pi] \) and hence has a gap whenever \( k_{\parallel} \notin \left\{ -\frac{2\pi}{3}, \frac{2\pi}{3} \right\} \).

A standard calculation \[16\] which closely parallels the earlier discussion of the SSH edge Hamiltonian without disorder (2.6) shows that 0 is an eigenvalue of \( H_{\text{edge}}^{\text{ZZ}}(k_{\parallel}) \) if and only if \( k_{\parallel} \in [-\pi, -\frac{2\pi}{3}) \cup (\frac{2\pi}{3}, \pi] \), and that \( H_{\text{edge}}^{\text{ZZ}} \) has no other eigenvalues. The spectrum of \( H_{\text{edge}}^{\text{ZZ}} \)
is thus completely characterized.

4.3 Graphene edge Hamiltonian with disorder satisfying a periodicity condition

We now consider the effect of local perturbations of the Hamiltonian $H_{\text{edge}}^{ZZ}$. Specifically, we allow for inter-atom hopping amplitudes $t_j(m,n), j \in \{0,1,2\}$ and for onsite potentials $V^\sigma(m,n), \sigma \in \{A,B\}$ which depend on the cell indices $m,n$, making the following assumptions.

**Assumption 4.1** (Periodicity of bulk medium). There exists a non-negative integer $M$ such that for all $m > M$, $V^\sigma(m,n) = 0$ and $t_j(m,n) = t$ for all $n \in \mathbb{Z}$, $\sigma \in \{A,B\}$, and $j \in \{0,1,2\}$.

**Assumption 4.2** (Periodicity of disorder along edge). There exists a positive integer $N$ such that $V^\sigma(m,n + N) = V^\sigma(m,n)$ and $t_j(m,n + N) = t_j(m,n)$ for all $m \in \mathbb{N}$, $n \in \mathbb{Z}$, $j \in \{0,1,2\}$, and $\sigma = \{A,B\}$.

**Remark 4.1.** Our method may be used to study the effect of more general disorder which doesn’t satisfy Assumption 4.2 for any $N$. This leads to an approximate numerical method known as the supercell method (see e.g., [1]). Under Assumption 4.2 our method is exact.

In summary, we consider the disordered edge Hamiltonian,

$$
\left[ H_{\text{edge}}^{ZZ} \right]_{m,n} = -\left[ t_0(m,n)\psi_m^n + t_1(m,n)\psi_{m-1,n} + t_2(m,n)\psi_{m,n-1} \right] + \left[ V^A(m,n)\psi^A_{m,n} \right] + \left[ V^B(m,n)\psi^B_{m,n} \right],
$$

where $V^\sigma(m,n) = 0$ and $t_j(m,n) = t$ for $m \in \mathbb{N}$ and $m > M, n \in \mathbb{Z}, j \in \{0,1,2\}, \sigma \in \{A,B\}$

$$
V^\sigma(m,n + N) = V^\sigma(m,n) \text{ and } t_j(m,n + N) = t_j(m,n) \text{ for } m \in \mathbb{N}, n \in \mathbb{Z}, \sigma \in \{A,B\}
$$

$$
\psi_{0,n} = 0 \text{ for } n \in \mathbb{Z}.
$$

Under Assumption 4.2, there is no loss of generality in imposing the quasi-periodic boundary condition with respect to $n$,

$$
\psi_{m,n+N} = e^{ik_\parallel N}\psi_{m,n}, \quad m, n \in \mathbb{N} \times \mathbb{Z}.
$$

It is clear that this boundary condition is $\frac{2\pi}{N}$-periodic and hence we may restrict $k_\parallel \in \left[-\frac{\pi}{N}, \frac{\pi}{N}\right]$. Imposing (4.10) leads to the $k_\parallel$-dependent eigenvalue problem defined on a single
supercell:

\[
\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_{\parallel}) \psi_{m,n} = - t_0(m,n)\psi_{m+1,n}^B + t_1(m,n)\psi_{m-1,n}^B + t_2(m,n)\psi_{m,n-1}^B + V^A(m,n)\psi_{m,n}^A + V^B(m,n)\psi_{m,n}^B
\]

where

\[V^\sigma(m,n) = 0\] and \(t_j(m,n) = t\) for \(m \in \mathbb{N}\) and \(m > M, n \in \{1, \ldots, N\}\), \(j \in \{0,1,2\}, \sigma \in \{A,B\}\)

\[t_2(m,0) = t_2(m,N)\] for \(m \in \mathbb{N}\)

\[\psi_{0,n} = 0\] for \(n \in \{1, \ldots, N\}\)

\[\psi_{m,0} = e^{-ik_{\parallel}N}\psi_{m,N} \quad \psi_{m,N+1} = e^{ik_{\parallel}N}\psi_{m,1}\] for \(m \in \mathbb{N}\).

(4.11)

The following Lemma, which we prove in Section 5, characterizes the essential spectrum of \(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_{\parallel})\).

**Lemma 4.1.** Fix \(k_{\parallel} \in [-\frac{\pi}{N}, \frac{\pi}{N}]\). Let \(\omega_1, \ldots, \omega_N\) denote the \(N\) roots of the algebraic equation

\[\omega^N = e^{iNk_{\parallel}}, \quad (4.12)\]

and define \(k_j := \arg \omega_j\) for each \(j \in \{1, \ldots, N\}\). Then:

\[\sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_{\parallel})) = \bigcup_{j=1}^N \sigma_{\text{ess}}(H_{\text{edge}}^{\text{ZZ}}(k_j)) \quad (4.13)\]

where \(H_{\text{edge}}^{\text{ZZ}}\) is the zig-zag edge Hamiltonian without disorder (4.8).

We now focus on computing the discrete spectrum.

It is useful at this point to introduce notation:

\[\tilde{\psi} := [\tilde{\psi}_1^A, \tilde{\psi}_1^B, \tilde{\psi}_2^A, \tilde{\psi}_2^B, \ldots]^T,\]

where \(\tilde{\psi}_m^\sigma := [\psi_{m,1}^\sigma, \ldots, \psi_{m,N}^\sigma]^T, \quad m \in \mathbb{N}, \sigma \in \{A,B\}\) (4.14)

in terms of which the Hamiltonian \(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_{\parallel})\) may be put into the form

\[
\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_{\parallel}) \tilde{\psi}_m = \begin{pmatrix}
0 & t_2(m,2) & t_2(m,3) & \cdots & t_2(m,N) \\
t_2(m,2) & 0 & \cdots & \cdots & \cdots \\
t_2(m,3) & \cdots & 0 & \cdots & \cdots \\
\vdots & \cdots & \cdots & \cdots & \cdots \\
t_2(m,N) & \cdots & \cdots & \cdots & 0 \\
0 & \cdots & \cdots & \cdots & 0 \\
e^{ik_{\parallel}N}t_2(m,1)
\end{pmatrix} \quad m \in \mathbb{N}
\]

(4.15)

where \(t_{0,m}, t_{1,m}, \text{ and } V_m^\sigma\) are \(N \times N\) matrices with diagonal elements \(t_0(m,1), \ldots, t_0(m,N), t_1(m,1), \ldots, t_1(m,N), \text{ and } V^\sigma(m,1), \ldots, V^\sigma(m,N)\) (where \(m \in \mathbb{N}\) and \(\sigma \in \{A,B\}\) respectively, and \(t_{2,m}(k_{\parallel})\) is defined for \(N \neq 1\) as the \(N \times N\) matrix

\[
t_{2,m}(k_{\parallel}) := \begin{pmatrix}
0 & t_2(m,2) & t_2(m,3) & \cdots & t_2(m,N) \\
0 & 0 & \cdots & \cdots & \cdots \\
t_2(m,2) & 0 & \cdots & \cdots & \cdots \\
\vdots & \cdots & \cdots & \cdots & \cdots \\
t_2(m,N) & \cdots & \cdots & \cdots & 0 \\
0 & \cdots & \cdots & \cdots & 0 \\
e^{ik_{\parallel}N}t_2(m,1)
\end{pmatrix}, \quad m \in \mathbb{N}, \sigma \in \{A,B\}.
\]

(4.16)
When \( N = 1 \), we define \( t_{2,m}(k) = t_2(m)e^{ik} \). In a similar way as for the SSH edge Hamiltonian (see Section 2), computations of the spectrum of (4.15) based on truncation of the Hamiltonian at some large value of \( m \) yield inaccurate results, and hence we are motivated to adapt the Green’s function method of Section 3 to this context.

### 4.4 Green’s function method for zig-zag edge Hamiltonian with disorder

For values of \( z \in \mathbb{C} \) where the definition makes sense, the Green’s function \( G(z) \) of \( \tilde{H}_{\text{edge}}(k) \) (4.11) is defined as the bounded inverse of the operator \( \tilde{H}_{\text{edge}}(k) \) on \( l^2(\mathbb{N} \times \{1,...,N\}; \mathbb{C}^2) \),

\[
\left(zI - \tilde{H}_{\text{edge}}(k)\right)G(z) = I. \tag{4.17}
\]

It is natural to label entries of \( G(z) \) similarly to those of the wavefunction \( \psi \), so that the \( m \), \( n \)th component of the part of \( G(z) \) which acts on the \( m' \), \( n' \)th fundamental cell is written

\[
\begin{bmatrix}
G_{m,n,m',n'}^A(z) & G_{m,n,m',n'}^B(z) \\
G_{m,n,m',n'}^B(z) & G_{m,n,m',n'}^B(z)
\end{bmatrix}.
\tag{4.18}
\]

It is useful at this point to suppress column indices and \( z \)-dependence of entries of \( G(z) \) so that we replace \( G_{m,n,m',n'}^\sigma(z) \) by \( G_{m,n}^\sigma \) and then introduce vector notation analogous to that introduced for the wavefunction \( \psi \) (4.14),

\[
\tilde{G}_{m}^\sigma := [G_{m,1}^\sigma,...,G_{m,N}^\sigma]^T.
\tag{4.19}
\]

Equation (4.17) may now be written as

\[
\begin{align*}
(z - V_{m}^A)\tilde{G}_{m}^A + t(t_0 + t_2)(k)\tilde{G}_{m}^I &= \delta_{1,n,m',n'}^A, \\
(z - V_{m-1}^B)\tilde{G}_{m-1}^B - (t_0 + t_2)(k)\tilde{G}_{m-1}^A &= \delta_{m-1,n,m',n'}^B, \\
(z - V_{m}^A)\tilde{G}_{m}^A - t_2 \tilde{G}_{m-1}^B - (t_0 + t_2)(k)\tilde{G}_{m}^I &= \delta_{m,n,m',n'}^A, \quad m \in \mathbb{N}
\end{align*}
\tag{4.20}
\]

where \( \sigma' \in \{A, B\} \) and \( m', n' \) vary over \( \mathbb{N} \) and \( \{1,...,N\} \) respectively, and where \( \delta_{m,n,m',n'}^{\sigma,\sigma'} \) denotes the \( (m,n,\sigma) \)th entry of the vector whose \( (m',n',\sigma') \)th entry is 1 and whose other entries are zero.

By Assumption 4.1, for each fixed \( \sigma' \in \{A, B\} \) and \( m', n' \in \{1,...,M\} \times \{1,...,N\} \) and \( m \geq M + 2 \), the system (4.20) reduces to the system

\[
\begin{align*}
z\tilde{G}_{m-1}^B - t(I + J(k))\tilde{G}_{m-1}^A - t\tilde{G}_{m}^I &= 0, \\
z\tilde{G}_{m}^A - tI\tilde{G}_{m-1}^B - t(I + J(k))^*\tilde{G}_{m}^B &= 0 \quad m \geq M + 2,
\end{align*}
\tag{4.22}
\]
where for $N \neq 1$, $J(k\parallel)$ is the $N \times N$ matrix

$$J(k\parallel) := \begin{bmatrix} 0 & 1 \\ 0 & 1 \\ \vdots & \vdots \\ e^{ik\parallel}N & 0 \end{bmatrix}, \quad (4.23)$$

and for $N = 1$ $J(k\parallel) = e^{ik\parallel}$. Assuming that the matrix

$$D := \begin{bmatrix} zI & -t(I + J(k\parallel)) \\ -tI & 0 \end{bmatrix} \quad (4.24)$$

is invertible (see Remark 4.2), the system (4.22) may be solved by a $z$-dependent transfer matrix which depends also on $k\parallel$,

$$T^\infty(z; k\parallel) := \begin{bmatrix} zI & -t(I + J(k\parallel)) \\ -tI & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 & tI \\ t(I + J(k\parallel)) & -zI \end{bmatrix}. \quad (4.25)$$

To ensure that $G(z)$ is a bounded operator on $l^2(\mathbb{N} \times \{1, \ldots, N\}; \mathbb{C}^2)$, we now solve the system (4.20)-(4.21) subject to the constraint that $[G_{m,m'}^A, G_{m,m'}^B]^T$ lies in the space of eigenvectors of $T^\infty(z; k\parallel)$ whose associated eigenvalues have norm less than one.

In contrast to the case of the SSH model where the transfer matrix has size $2 \times 2$ (2.21), here the transfer matrix has size $2N \times 2N$. Since Lemma 2.1 does not generalize to this case, it is unclear how many linearly independent eigenvectors of $T^\infty(z; k\parallel)$ whose eigenvalues have norm less than one exist, and hence how many boundary conditions must be enforced when we compute the solution of the system (4.20)-(4.21). In Section 5 we prove that whenever $z \notin \sigma_{ess}(\tilde{H}_{\text{edge}}^Z(k\parallel))$ precisely $N$ such eigenvectors exist and hence our method can be generalized naturally to this setting.

**Remark 4.2.** The matrix $D$ (4.24) is not always invertible. For example, when $N = 1$ and $k = \pi$, then $I + J(k\parallel) = 1 + e^{i\pi} = 0$ and hence $D$ has determinant zero. Our method can be extended to this setting at the cost of introducing more machinery; we leave the details to a future work.

### 4.5 Results: disordered zig-zag edge of a graphene-like structure

In Figure 4.1, we present results of computations using the method developed in Section 4. We studied the effect of multiple atomic vacancies on a bound state of the Hamiltonian $\tilde{H}_{\text{edge}}^Z(k\parallel)$ (4.11) (edge state) with eigenvalue 0. We observed that the edge state persisted despite this perturbation.
Figure 4.1: Persistence of an edge state of a graphene-like structure under perturbation. In Figure 4.1a, a bound state of the zig-zag edge Hamiltonian (4.11) (edge state) when $N = 5$, $k_{\parallel} = \frac{1}{5} \left(-\frac{2\pi}{30}\right)$, $V^\sigma(m, n) = 0$, $\sigma \in \{A, B\}$, and $t_j(m, n) = t_j \in \{0, 1, 2\}$ for all $m, n \in \mathbb{N} \times \mathbb{Z}$ is plotted. We find that this bound state has eigenvalue precisely 0. The absolute value $|\psi|$ and the argument $\arg \psi$ of the wave function at each lattice point is represented by the radius and color, respectively, of the circle at that point. In Figure 4.1b, an edge state of the zig-zag edge Hamiltonian (4.11) with multiple atomic vacancies is plotted. One way of modeling atomic vacancies is to add large onsite potentials at these sites. We observe that the edge state survives the perturbation: the Hamiltonian retains a bound state with eigenvalue 0.
5 Green’s function method in general

In this section we prove that whenever \( z \notin \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{ZZ}) \) the transfer matrix \( T^\infty(z; k_\parallel) \) (4.25) has precisely \( N \) eigenvectors whose associated eigenvalues have norm \(< 1\). This is the essential step in generalizing the Green’s function method detailed in Section 3 to the more general case described in Section 4. This is also the key step in generalizing our method to the case of more general honeycomb structures which we consider in Section 6. In the process we will prove Lemma 4.1 which gives a simple characterization of \( \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{ZZ}) \).

The result is given in the following lemma.

**Lemma 5.1.** Fix \( k_\parallel \in [-\pi/N, \pi/N] \). Let \( k_j \) be defined for each \( j \in \{1, \ldots, N\} \) as in Lemma 4.1. Let \( \tilde{H}_{\text{edge}}^{ZZ}(k_\parallel) \) be as in (4.11) and \( H_{\text{edge}}^{ZZ}(k_j) \) be the zig-zag edge Hamiltonian without disorder defined by (4.8). Then the following assertions hold:

(L1) The essential spectrum of \( \tilde{H}_{\text{edge}}^{ZZ}(k_\parallel) \) may be characterized as follows

\[
\sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{ZZ}(k_\parallel)) = \bigcup_{j=1}^{N} \sigma_{\text{ess}}(H_{\text{edge}}^{ZZ}(k_j)) \quad (5.1)
\]

(L2) Assume that

\[
z \notin \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{ZZ}(k_\parallel)), \text{ i.e. } z \notin \sigma_{\text{ess}}(H_{\text{edge}}^{ZZ}(k_j)) \text{ for all } j \in \{1, \ldots, N\}. \quad (5.2)
\]

Then the matrix \( T^\infty(z; k_\parallel) \) displayed in (4.25) has \( N \) linearly independent eigenvectors whose associated eigenvalues have norm \(< 1\) and \( N \) linearly independent eigenvectors whose associated eigenvalues have norm \(> 1\).

**Proof.** The proof is by explicit construction as follows.

First note that when \( N = 1 \), the statement follows immediately from Lemma 2.1 as follows. If either of possibilities (A2) or (A3) of Lemma 2.1 holds for the matrix \( T^\infty(z; k_\parallel) \), then \( T^\infty(z; k_\parallel) \) has an eigenvalue of norm 1, which implies the existence of a bounded (generalized) eigenvector of \( \tilde{H}_{\text{edge}}^{ZZ}(k_\parallel) \) with eigenvalue \( z \) and hence \( z \in \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{ZZ}(k_\parallel)) \). If this is not the case, then possibility (A1) of Lemma 2.1 must be realized and the statement holds.

When \( N > 1 \), observe that the system (4.22) is 1-periodic with respect to \( n \). It follows that we may assume without loss of solutions that \( G^\sigma_{m,n} \) is \( k \)-quasiperiodic with respect to \( n \),

\[
G^\sigma_{m,n+1} = e^{ik} G^\sigma_{m,n} \quad m \in \mathbb{N}, n \in \{1, \ldots, N\}, \sigma \in \{A, B\}. \quad (5.3)
\]

The values of \( k \) consistent with the condition

\[
G^\sigma_{m,N+1} = e^{iNk_\parallel} G^\sigma_{m,1} \quad m \in \mathbb{N}, \sigma \in \{A, B\}, \quad (5.4)
\]

which was assumed (4.10) when we wrote down the form of the Hamiltonian (4.11), are precisely the \( k_j \) defined by equation (4.12).

Upon substituting, for each \( k_j \):

\[
\tilde{G}^\sigma_m = [G^\sigma_{m,1}, e^{ik_1} G^\sigma_{m,1}, \ldots, e^{i(N-1)k_j} G^\sigma_{m,1}]^T, \quad \sigma = \{A, B\} \quad (5.5)
\]
into (4.22), we obtain a second-order difference equation for \(G_{m,1}^A\) and \(G_{m,1}^B\) which is precisely what we would have obtained had we sought the Green’s function of the zig-zag edge Hamiltonian without disorder \(H_{\text{edge}}^{\text{ZZ}}(k_j)\) defined by (4.8).

If \(z \in \sigma_{\text{ess}}(H_{\text{edge}}^L(k_j))\), then the transfer matrix of this system has at least one eigenvector whose associated eigenvalue has norm 1. We can extend this eigenvector (via (5.5)) to an eigenvector of \(T^\infty(z; k_j)\) with the same eigenvalue. Such an eigenvector corresponds to a bounded (extended) eigenvector of \(\tilde{H}_{\text{edge}}^{\text{ZZ}}\) with eigenvalue \(z\), which implies \(z \in \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_j))\) and hence

\[
\sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_j)) \subset \bigcup_{j=1}^N \sigma_{\text{ess}}(H_{\text{edge}}^{\text{ZZ}}(k_j)).
\]

(5.6)

On the other hand, by repeating this procedure for each \(j \in \{1, ..., N\}\) we obtain a basis of eigenvectors of \(T^\infty(z; k_j)\) and hence the opposite inclusion also holds. Hence (L1) is proved.

If on the other hand \(z \notin \sigma_{\text{ess}}(H_{\text{edge}}^{\text{ZZ}}(k_j))\), then the transfer matrix of this system has one eigenvector whose associated eigenvalue has norm \(<1\) and one eigenvector whose associated eigenvalue has norm \(>1\). By construction, we can extend these eigenvectors (via (5.5)) to eigenvectors of \(T^\infty(z; k_j)\) with equal associated eigenvalues. If such eigenvectors exist for every \(j \in \{1, ..., N\}\), then we have constructed precisely \(N\) eigenvectors of \(T^\infty(z; k_j)\) whose associated eigenvalues have norm \(<1\) and \(N\) whose associated eigenvalues have norm \(>1\). If \(z \in \sigma_{\text{ess}}(H_{\text{edge}}^{\text{ZZ}}(k_j))\) for any \(j \in \{1, ..., N\}\) then \(z \in \sigma_{\text{ess}}(\tilde{H}_{\text{edge}}^{\text{ZZ}}(k_j))\) by (5.1). Thus (L2) is proved.

Although we have proved Lemma 5.1 for the particular model introduced in Section 4, the argument clearly generalizes to arbitrary edge Hamiltonians with two sites per unit cell which are eventually periodic both along and perpendicular to the edge. Our methods can be extended to arbitrary banded (finite range hopping) and self-adjoint Hamiltonians which are periodic with respect to \(m\) and \(n\) for sufficiently large \(m\) at the cost of making the proofs more involved; we leave the details to a future work (see also Remark 4.2).

6 General honeycomb structures and domain wall edges

A natural generalization of the bulk Hamiltonian (4.2) is

\[
[H_{\text{bulk}}\psi]_{m,n} = - \begin{bmatrix} t_0 \psi_{m,n}^B + t_1 \psi_{m-1,n}^B + t_2 \psi_{m,n-1}^B \\ t_0 \psi_{m,n}^A + t_1 \psi_{m+1,n}^A + t_2 \psi_{m,n+1}^A \\ V_A \psi_{m,n}^A \\ V_B \psi_{m,n}^B \end{bmatrix}, \quad m, n \in \mathbb{Z} \times \mathbb{Z}.
\]

(6.1)

where the onsite potentials \(V_A, V_B\) are assumed real, and the hopping amplitudes \(t_0, t_1, t_2\) are assumed real and non-zero.

Unlike the graphene-like structure we considered in Section 4, such a structure may have a bulk spectral gap. Such structures may host edge states, i.e., eigenstates of the analogous edge Hamiltonians in this setting of (4.6) and (4.11). As long as assumptions analogous to Assumptions 4.1-4.2 hold, then our methods generalize naturally to this case. Since no new ideas are necessary for this computation, we ignore this problem in this work. Instead, we will study states localized at interfaces between two different structures of the form (6.1) known as domain wall edges. Note that this situation leads to Hamiltonians which are no
longer semi-infinite, but infinite in both directions; and hence two boundary conditions must be imposed.

**Remark 6.1.** One-dimensional domain walls may be created by considering the interface of two differently configured chains described by the SSH model. The present discussion of general honeycomb structures and domain wall interfaces may be repeated for this model, but since the mathematical structure of this model is similar to (6.1) we do not discuss this here.

We consider the following edge Hamiltonian describing the interface of two differently configured honeycomb structures,

\[
[H_{\text{edge}}^{\text{ZZ}}]_{m,n} = \begin{bmatrix}
  t_{0}^{-\infty}\psi_{m,n}^{-1,0} + t_{1}^{-\infty}\psi_{m-1,n}^{-1,1} + t_{2}^{-\infty}\psi_{m,n-1}^{-1,2} \\
  t_{0}^{-\infty}\psi_{m,n}^{-0,0} + t_{1}^{-\infty}\psi_{m+1,n}^{-0,1} + t_{2}^{-\infty}\psi_{m,n+1}^{-0,2}
\end{bmatrix} + \begin{bmatrix}
  V_{m,n}^{-\infty,0} \\
  V_{m,n}^{-\infty,2}
\end{bmatrix}
\]

\[m, n \in \mathbb{N} \times \mathbb{Z} \]

\[H_{\text{edge}}^{\text{ZZ}}]_{0,n} = \begin{bmatrix}
  t_{0}^{-\infty}\psi_{0,n}^{-1,0} + t_{1}^{-\infty}\psi_{-1,n}^{-1,1} + t_{2}^{-\infty}\psi_{0,n-1}^{-1,2} \\
  t_{0}^{-\infty}\psi_{0,n}^{-0,0} + t_{1}^{-\infty}\psi_{1,n}^{-0,1} + t_{2}^{-\infty}\psi_{0,n+1}^{-0,2}
\end{bmatrix} + \begin{bmatrix}
  V_{0,n}^{-\infty,0} \\
  V_{0,n}^{-\infty,2}
\end{bmatrix}
\]

\[n \in \mathbb{Z} \]

\[H_{\text{edge}}^{\text{ZZ}}]_{m,n} = \begin{bmatrix}
  t_{0}^{-\infty}\psi_{m,n}^{-1,0} + t_{1}^{-\infty}\psi_{m-1,n}^{-1,1} + t_{2}^{-\infty}\psi_{m,n-1}^{-1,2} \\
  t_{0}^{-\infty}\psi_{m,n}^{-0,0} + t_{1}^{-\infty}\psi_{m+1,n}^{-0,1} + t_{2}^{-\infty}\psi_{m,n+1}^{-0,2}
\end{bmatrix} + \begin{bmatrix}
  V_{m,n}^{-\infty,0} \\
  V_{m,n}^{-\infty,2}
\end{bmatrix}
\]

\[m, n \in -\mathbb{N} \times \mathbb{Z}. \quad (6.2)\]

**Remark 6.2.** Note that in contrast to the semi-infinite edge Hamiltonians we have considered up to this point whose essential spectrum is equal to that of a single bulk Hamiltonian, the essential spectrum of the edge Hamiltonian (6.2) is clearly the union of those of the the bulk Hamiltonians at positive and negative infinity.

As usual, since the Hamiltonian is periodic with respect to $n$, Bloch’s theorem states that the eigenstates can be chosen to satisfy the boundary condition $\psi_{m,n+1} = e^{ik_{||}}\psi_{m,n}$. For a given $k_{||}$, this yields the following system of equations,

\[
[H_{\text{edge}}^{\text{ZZ}}]_{m} = \begin{bmatrix}
  (t_{0}^{-\infty} + t_{1}^{-\infty}e^{-ik_{||}})\psi_{m}^{B} + t_{1}^{+\infty}\psi_{m-1}^{B} \\
  (t_{0}^{+\infty} + t_{1}^{+\infty}e^{ik_{||}})\psi_{m}^{B} + t_{1}^{-\infty}\psi_{m+1}^{B}
\end{bmatrix} + \begin{bmatrix}
  V_{m}^{+,0} \\
  V_{m}^{+,2}
\end{bmatrix}
\]

\[m \in \mathbb{N} \]

\[
[H_{\text{edge}}^{\text{ZZ}}]_{0} = \begin{bmatrix}
  (t_{0}^{-\infty} + t_{1}^{-\infty}e^{-ik_{||}})\psi_{0}^{B} + t_{1}^{-\infty}\psi_{-1}^{B} \\
  (t_{0}^{+\infty} + t_{1}^{+\infty}e^{ik_{||}})\psi_{0}^{B} + t_{1}^{+\infty}\psi_{1}^{B}
\end{bmatrix} + \begin{bmatrix}
  V_{0}^{+,0} \\
  V_{0}^{+,2}
\end{bmatrix}
\]

\[\quad (6.3)\]

\[
[H_{\text{edge}}^{\text{ZZ}}]_{m} = \begin{bmatrix}
  (t_{0}^{-\infty} + t_{2}^{-\infty}e^{-ik_{||}})\psi_{m}^{B} + t_{1}^{+\infty}\psi_{m-1}^{B} \\
  (t_{0}^{+\infty} + t_{2}^{+\infty}e^{ik_{||}})\psi_{m}^{B} + t_{1}^{-\infty}\psi_{m+1}^{B}
\end{bmatrix} + \begin{bmatrix}
  V_{m}^{-\infty,0} \\
  V_{m}^{-\infty,2}
\end{bmatrix}
\]

\[m \in -\mathbb{N}. \]

Depending on the values of the parameters $t_{j}^{\pm\infty}, V_{\sigma,\pm\infty}, j \in \{0, 1, 2\}, \sigma \in \{A, B\}$ the Hamiltonian $H_{\text{edge}}^{\text{ZZ}}$ may have $l^{2}(\mathbb{Z} ; \mathbb{C}^{2})$-eigenvectors. This is the case, for example, if $V_{\sigma,\pm\infty} = 0, \sigma \in \{A, B\}$ and either

\[
\frac{|t_{j}^{\infty}|}{|t_{j}^{-\infty}|} < 1 \quad \text{and} \quad \frac{|t_{j}^{-\infty}|}{|t_{j}^{\infty}|} < 1, \quad \text{or} \quad \frac{|t_{j}^{\infty}|}{|t_{j}^{-\infty}|} > 1 \quad \text{and} \quad \frac{|t_{j}^{-\infty}|}{|t_{j}^{\infty}|} < 1. \quad (6.4)
\]

See, for example, [13]. We can also study disordered edges under analogous assumptions to Assumptions 4.1.4.2. Specifically, we allow for inter-atom hopping amplitudes $t_{j}(m, n), j \in \{0, 1, 2\}$ and onsite potentials $V_{\sigma}(m, n)$ which depend on the cell indices $m, n$ and, for the onsite potentials, $\sigma \in \{A, B\}$. The restrictions we make are summed up in the following assumptions.
Assumption 6.1 (Periodicity of bulk medium). There exist a non-negative integer $M_+$ such that for all $m > M_+$, $V^\sigma(m, n) = V^\sigma,\infty$ and $t_j(m, n) = t_j^\infty$ for all $n \in \mathbb{Z}$, $\sigma = A, B$, and $j \in \{0, 1, 2\}$ and a negative integer $M_-$ such that for all $m < M_-$, $V^\sigma(m, n) = V^\sigma,-\infty$ and $t_j(m, n) = t_j^-\infty$ for all $n \in \mathbb{Z}$, $\sigma = A, B$, and $j \in \{0, 1, 2\}$.

Assumption 6.2 (Periodicity of disorder along edge). There exists a positive integer $N$ such that $V^\sigma(m, n + N) = V^\sigma(m, n)$ and $t_j(m, n + N) = t_j(m, n)$ for all $m \in \mathbb{Z}$, $n \in \mathbb{Z}$, $j \in \{0, 1, 2\}$, and $\sigma = A, B$.

Under Assumptions 6.1 and 6.2, the problem is reduced to the study of the following Hamiltonian on a single supercell,

$$[\tilde{H}_{\text{edge}}(k\|)\psi]_{m,n} = -\left[t_0(m,n)\psi^B_{m,n} + t_1(m-1,n)\psi^B_{m-1,n} + t_2(m,n)\psi^B_{m,n-1}\right] + \left[V^A(m,n)\psi^A_{m,n} + V^B(m,n)\psi^B_{m,n}\right]$$

$m, n \in \mathbb{Z} \times \{1, ..., N\}$

$$t_2(m, N + 1) = t_2(m, 1) \text{ for } m \in \mathbb{Z} \text{ and } n \in \{1, ..., N\}$$

$$V^\sigma(m, n) = V^\sigma,\infty \text{ and } t_j(m, n) = t_j^\infty \text{ for } m \in \mathbb{Z}, m > M_+, n \in \{1, ..., N\}, j \in \{0, 1, 2\}, \sigma \in \{A, B\}$$

$$V^\sigma(m, n) = V^\sigma,-\infty \text{ and } t_j(m, n) = t_j^-\infty \text{ for } m \in \mathbb{Z}, m < M_-, n \in \{1, ..., N\}, j \in \{0, 1, 2\}, \sigma \in \{A, B\}$$

$$\psi_{0,n} = 0 \text{ for } n \in \{1, ..., N\} \quad \psi_{m,0} = e^{-ik\|N}\psi_{m,N} \quad \psi_{m,N+1} = e^{ik\|N}\psi_{m,1} \text{ for } m \in \mathbb{Z}.$$  

(6.5)

The discussions of the previous sections have clear parallels in this setting, with the complication that the edge Hamiltonian is now fully infinite in $m$, and hence two boundary conditions to be imposed.

In Section 6.1 we present results of numerical computations for the case

$$V^\sigma,\pm\infty = 0, \sigma \in \{A, B\}, \text{ and } t_0^-\infty = t_1^-\infty, \frac{|t_2^-\infty|}{|t_1^-\infty|} > 1, \text{ and } t_0^\infty = t_1^\infty, \frac{|t_2^\infty|}{|t_1^\infty|} < 1.$$  

(6.6)

This case is of particular interest because the hard truncation method applied in this case yields clearly inaccurate results.

6.1 Results: zig-zag domain wall edge in a dimerized honeycomb structure

In this section we present results of numerical computations of edge states of the Hamiltonian (6.5) when the bulk structures far from the domain wall edge are defined by (6.6).

In Figure 6.1, we show that the Green’s function method produces correct edge dispersion curves in a case where the hard truncation method yields clearly inaccurate results. The appearance of spurious eigenvalues in this case was noted by Lee-Thorp and Weinstein (see Chapter 26, in particular Figure 26.7, of [13]).

In Figure 6.2a we plot one of the four-fold degenerate eigenvalue zero bound states of (6.5) with $k\| = \frac{\pi}{3}$ when all onsite potentials and hopping amplitudes are set equal to their values far from the domain wall edge. In Figure 6.2b we plot a bound state of (6.5) with
Figure 6.1: (a) Dispersion curves $E(k_\parallel)$ of the edge Hamiltonian (6.2) computed with the hard truncation method, and (b) dispersion curves of the edge Hamiltonian (6.2) computed using the Green’s function method. Zero eigenvalues are plotted with red $\times$’s, while all other eigenvalues are plotted in blue. For $k_\parallel$ in a neighborhood of $\pi$, hard truncation of the Hamiltonian yields spurious zero modes which are eliminated when the proper boundary conditions are applied.

$k_\parallel = \frac{\pi}{4}$ and eigenvalue 0 which persists even in the presence of strong onsite potentials modeling atomic vacancies at the edge.

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Figure 6.2: (a) Plot of one of the four-fold degenerate zero eigenvalue bound states of the Hamiltonian (6.5) when $k_{\parallel} = \frac{\pi}{4}$ when the bulk structures far from the domain wall edge are defined by (6.6) without disorder. The absolute value $|\psi|$ and argument $\arg \psi$ of the wavefunction at each point on the lattice is represented by the radius and color, respectively, of the circle at each point. (b) An edge state of the Hamiltonian (6.5) when $k_{\parallel} = \frac{\pi}{4}$ under Assumption (6.6) with atomic vacancies at the edge modeled by large onsite potentials. We observe that in this case the Hamiltonian has a single non-degenerate bound state with eigenvalue 0.
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