# Wave dynamics in locally periodic structures by multiscale analysis


**Alexander B. Watson**


Submitted in partial fulfillment of the
requirements for the degree
of Doctor of Philosophy
in the Graduate School of Arts and Sciences


**COLUMBIA UNIVERSITY**

2017

# ABSTRACT

## Wave dynamics in locally periodic structures by multiscale analysis

## Alexander B. Watson

We study the propagation of waves in spatially non-homogeneous media, focusing on Schrödinger's equation of quantum mechanics and Maxwell's equations of electromagnetism. We assume that medium variation occurs over two distinct length scales: a short 'fast' scale with respect to which the variation is *periodic*, and a long 'slow' scale over which the variation is smooth. Let $\epsilon$ denote the ratio of these scales. We focus primarily on the time evolution of asymptotic solutions (as $\epsilon \downarrow 0$) known as *semiclassical wavepackets*. Such solutions generalize exact time-dependent Gaussian solutions and ideas of Heller [40] and Hagedorn [36] to periodic media. Our results are as follows:

1. To leading order in $\epsilon$ and up to the 'Ehrenfest' time-scale $t \sim \ln 1/\epsilon$, the center of mass and average (quasi-)momentum of the semiclassical wavepacket satisfy the equations of motion of the classical Hamiltonian given by the wavepacket's *Bloch band energy*. Our first result is to derive all corrections to these dynamics proportional to $\epsilon$. These corrections consist of terms proportional to the Bloch band's *Berry curvature* and terms which describe coupling to the evolution of the wavepacket envelope. These results rely on the assumption that the wavepacket's Bloch band energy is *non-degenerate*.

2. We then consider the case where, in one spatial dimension, a semiclassical wavepacket is incident on a *Bloch band crossing*, a point in phase space where the wavepacket's Bloch band energy is *degenerate*. By a rigorous matched asymptotic analysis, we show that at the time the wavepacket meets the crossing point a second wavepacket, associated with the other Bloch band involved in the crossing, is excited. Our result can be seen as a rigorous justification of the Landau-Zener formula in this setting.

3. Our final result generalizes the recent work of Fefferman, Lee-Thorp, and Weinstein [25] on

one-dimensional 'edge' states. We characterize the bound states of a Schrödinger operator with a periodic potential perturbed by multiple well-separated domain wall 'edge' modulations, by proving a theorem on the near zero eigenstates of an emergent Dirac operator.

# Table of Contents

# List of Figures

# Acknowledgments

I would like to express my deep gratitude for the guidance of my academic advisor Professor Michael Weinstein throughout the completion of this work. It has been a privilege to learn from someone with such passion for science and patience for sharing knowledge with others.

I am also hugely grateful to Professor Jianfeng Lu of Duke University for his encouragement and many contributions to the research described in this thesis. Chapters 2 and 4 of this thesis in particular are the direct result of our collaboration.

I am also very grateful to the other members of my thesis committee: Professors Nanfang Yu, Guillaume Bal, and Qiang Du, and to Professors George Hagedorn, Christof Sparber, and Tomoki Ohsawa, who each contributed stimulating discussions and criticisms which significantly influenced this research.

I would also like to acknowledge the important contributions of Professor Steven Golowich of MIT Lincoln Labs during the early months of this work, in particular for making us aware of the work of Bliokh et al. [7] on the spin Hall effect of light. Attempting to clearly understand this phenomenon has motivated much of the research described in this thesis, most directly Chapter 2.

This thesis would not have been possible without generous funding from NSF Grant No. DMS-1412560 and Simons Foundation Math + X Investigator Award No. 376319 (Michael I. Weinstein).

Finally, I would like to thank my family for their constant encouragement and support.

For Mary, James and Roger.

# Chapter 1

# Introduction

In this work we study the propagation of waves in media with a local periodic structure which varies adiabatically (i.e. over a length scale much longer than the scale of periodicity) through the material. More precisely, we derive approximate solutions of time-dependent partial differential equation (PDE) models of waves in such media and prove convergence of these approximate solutions to exact solutions in the limit where the ratio of the 'fast' periodic scale to the 'slow' scale of variation of the local periodic structure approaches zero. We will henceforth refer to this ratio as $\epsilon$ and will describe these solutions as being *asymptotic* in the limit $\epsilon \downarrow 0$. We focus our attention on Schrödinger's equation and Maxwell's equations, which in this context respectively model the dynamics of electrons propagating in crystalline solids with defects, and the propagation of light through photonic analogs of such structures known as 'photonic crystals'.

For the majority of this work, we will be concerned with localized, propagating pulses, or *wavepackets*. It is well understood that the dynamics of such pulses depends crucially on the spectral properties (more precisely, the 'Floquet-Bloch band structure') of the periodic differential operator obtained by holding the 'slow' dependence of the equation fixed at each position in space. Depending on this 'local' band structure, the effective dynamics of the wavepacket may be 'ballistic propagation' described by a transport equation, or 'dispersion' governed by a Schrödinger equation, for example. The simplest derivation of these effective dynamics is by a multi-scale WKB-type expansion in the small parameter $\epsilon$ (see [11], for example).

These derivations break down, however, in two significant ways. First, at *caustics* in the characteristic flow, where one must make a modified ansatz in order to correctly capture the dynamics (see [69], for example). Second, when the wavepacket is spectrally localized near to *degenerate points* in the local Bloch band structure. Bloch band degeneracies often arise due to symmetries of a periodic structure, and their existence can have considerable physical consequences. For example, the 'Dirac points' of graphene which give rise to its novel transport properties are Bloch band degeneracies caused by the particular 'honeycomb lattice' symmetries of its atomic structure [28]. In order to address this deficiency of standard methods we have studied a family of asymptotic solutions known as *semiclassical wavepackets.* Such solutions obey a particular scaling with respect to the small parameter $\epsilon$ which makes them particularly appropriate for studying the dynamics nearby to Bloch band degeneracies, and do not suffer from the emergence of caustics.

In the final chapter of this work we prove a theorem on the near zero eigenstates of a Dirac operator which emerges in the study of bound states of a periodic Schrödinger operator perturbed by multiple domain wall 'edge' modulations. Our result implies that the Schrödinger operator supports multiple nearly degenerate 'edge states', which bifurcate from the continuous spectrum of the unperturbed periodic operator. Our result represents a generalization of the recent works of Fefferman, Lee-Thorp, and Weinstein [25; 27]. Such states are of great interest for applications because of their *robustness* to local perturbations in the medium.

The structure of this work is as follows:

**Corrections to effective dynamics for semiclassical wavepackets away from Bloch band degeneracies (Chapter 2)** We construct asymptotic solutions of Schrödinger's equation and Maxwell's equations in 'locally periodic' media of semiclassical wavepacket type under the assumption that the wavepacket avoids any Bloch band degeneracies. By computing all corrections to the asymptotic solution up to and including terms of order $\epsilon^{1/2}$ we are able to derive a new Hamiltonian system describing the coupled evolution of the wavepacket's center of mass, (quasi-)momentum, and wave envelope up to and including all corrections proportional to $\epsilon$. These corrections include terms proportional to the Bloch band's *Berry curvature* (Theorems 2.1.1 and 2.1.2, Sections 2.1-2.4). The research described in this Chapter is joint with J. Lu and M. I. Weinstein. Sections 2.1-2.4 and Appendices A.1-A.6 were published in [73].

**The dynamics of a semiclassical wavepacket incident on a band crossing in one spatial dimension (Chapter 3)** Working in one spatial dimension we derive the dynamics of a wavepacket which is accelerated through a *Bloch band crossing*. We show that at the time the wavepacket's Bloch band energy becomes degenerate, a second wavepacket is excited which is associated with the other band involved in the crossing (Theorems 3.3.2 and 3.3.3, Sections 3.1-3.5). To our knowledge this is the first result on the propagation of an explicit wavepacket asymptotic solution through a Bloch band degeneracy. The research described in this chapter is joint with M. I. Weinstein.

**Bound states of a Schrödinger operator with a periodic potential perturbed by multiple domain wall modulations (Chapter 4)** Again working in one spatial dimension, we prove a theorem (Theorem 4.2.1) describing the near zero eigenstates of a Dirac operator which emerges in the study of bound states of a periodic Schrödinger operator perturbed by multiple domain wall 'edge' modulations. We proceed by a Lyapunov-Schmidt reduction which allows us, in the limit where the distance between domain walls is large, to reduce the full Dirac eigenvalue problem to an effective two-by-two matrix eigenvalue problem (Sections 4.1-4.4). The research described in this Chapter is joint with J. Lu and M. I. Weinstein.

We give a more detailed summary of these results in Sections 1.1-1.4 before presenting our work in full detail in the remainder of this thesis.

## 1.1 PDEs of interest and semiclassical wavepacket asymptotic solutions

We now state the PDEs we study in the remainder of this work and give a general introduction to semiclassical wavepacket asymptotic solutions. We study the Schrödinger equation for $\psi^\epsilon(x,t) : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$ depending on a real parameter which we take to be small $\epsilon \ll 1$:

$$\begin{aligned} i\epsilon\partial_t \psi^\epsilon &= -\frac{1}{2}\epsilon^2 \Delta_x \psi^\epsilon + U\left(\frac{x}{\epsilon}, x\right)\psi^\epsilon \\ \psi^\epsilon(x,0) &= \psi_0^\epsilon(x). \end{aligned} \tag{1.1.1}$$

Here, we assume that $U$ is a real, smooth function of both arguments which is *periodic* with respect to some lattice $\Lambda$ in its first argument:

$$\forall v \in \Lambda, \quad U(z+v,x) = U(z,x) \tag{1.1.2}$$

at every value of $z, x \in \mathbb{R}^d$. It is useful to define the class of *separable* potentials which may be written as a sum:

$$U(z,x) = V(z) + W(x) \tag{1.1.3}$$

where $V$ is smooth and periodic with respect to the lattice $\Lambda$ and $W$ is smooth. Studying (1.1.1) when the potential is separable turns out to be considerably easier than the general case.

We are also interested in the time-dependent Maxwell system for the electromagnetic fields $E^\delta(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^3, H^\delta(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^3$ in matter depending on a small parameter $\delta \ll 1$ given by:

$$\partial_t \begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = \begin{pmatrix} 0 & \nabla \times \\ -\nabla \times & 0 \end{pmatrix} \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix}, \qquad \nabla \cdot \begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = 0 \tag{1.1.4}$$

together with the *constitutive relations*:

$$\begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = \begin{pmatrix} \varepsilon\left(\frac{x}{\delta}, x\right) & \chi^\dagger\left(\frac{x}{\delta}, x\right) \\ \chi\left(\frac{x}{\delta}, x\right) & \mu\left(\frac{x}{\delta}, x\right) \end{pmatrix} \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix}. \tag{1.1.5}$$

Here, we assume that each entry in the matrix of constitutive relations is smooth in both arguments and periodic with respect to a lattice $\Lambda$ in its first argument, and such that the matrix as a whole is positive-definite and Hermitian at each value of $x \in \mathbb{R}^3$. Note that when studying Maxwell's equations it is convenient to label the small parameter $\delta$ rather than $\epsilon$ to avoid confusion with the dielectric tensor $\varepsilon$.

We now describe the family of *semiclassical wavepacket* asymptotic solutions of the Schrödinger equation (1.1.1) in the simplest case, when the potential $U(z,x)$ is separable (1.1.3). The first proof of these results is due to Carles and Sparber [61], building on ideas of Hagedorn [36] and Heller [40]. Let $E_n(p)$ denote a Bloch band dispersion function of the Schrödinger operator with periodic co-efficients $-\frac{1}{2}\Delta_z + V(z)$. Let $p_0$ denote a point in the first Brillouin zone $\mathcal{B}$ such that the Bloch band is non-degenerate i.e. $E_{n-1}(p_0) < E_n(p_0) < E_{n+1}(p_0)$. Let $q_0 \in \mathbb{R}^d$ be such that the Hamiltonian dynamical system:

$$\begin{aligned} &\dot{q}(t) = \nabla_p E_n(p(t)), \quad \dot{p}(t) = -\nabla_q W(q(t)) \\ &q(0) = q_0, \quad p(0) = p_0 \end{aligned} \tag{1.1.6}$$

has a smooth solution for all $t \in [0, \infty)$ such that the Bloch band remains non-degenerate along the curve $p(t)$:

$$\forall t \in [0,\infty),\ E_{n-1}(p(t)) < E_n(p(t)) < E_{n+1}(p(t)), \tag{1.1.7}$$

and let $a_0(y) \in \mathcal{S}(\mathbb{R}^d)$ denote an arbitrary Schwartz class function. Then, the solution $\psi^\epsilon$ of the initial value problem (1.1.1) with $U$ as in (1.1.3) and *semiclassical wavepacket* initial data given by:

$$\psi_0^\epsilon(x) = \epsilon^{-d/4} e^{ip_0\cdot[x-q_0]/\epsilon} a_0\left(\frac{x-q_0}{\epsilon^{1/2}}\right)\chi_n(z;p_0) \tag{1.1.8}$$

evolves as a *modulated semiclassical wavepacket* plus a corrector function $\eta^\epsilon(x,t)$ for all $t \in [0,\infty)$:

$$\psi^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot[x-q(t)]/\epsilon} a\left(\frac{x-q(t)}{\epsilon^{1/2}},t\right)\chi_n(z;p(t)) + \eta^\epsilon(x,t) \tag{1.1.9}$$

Here, $S(t)$ denotes the action associated with the path $q(t), p(t)$, $a(y,t)$ satisfies a Schrödinger equation with time-dependent coefficients:

$$\begin{aligned} &i\partial_t a = \frac{1}{2}(-i\nabla_y)\cdot D_p^2 E_n(p(t))(-i\nabla_y)a + \frac{1}{2}y\cdot D_q^2 W(q(t))ya + \nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))a \\ &a(y,0) = a_0(y), \end{aligned} \tag{1.1.10}$$

where $D_p^2 E_n, D_q^2 W$ denote the Hessian matrices of $E_n, W$, $d \geq 1$ denotes the spatial dimension, and $\mathcal{A}_n$ denotes the Berry connection:

$$\mathcal{A}_n(p) := i\left\langle \chi_n(\cdot;p) \middle| \nabla_p \chi_n(\cdot;p)\right\rangle_{L^2(\Omega)}. \tag{1.1.11}$$

Here, $\Omega$ is a unit cell of the lattice $\Lambda$. The corrector function $\eta^\epsilon$ satisfies the bound:

$$\|\eta^\epsilon(\cdot,t)\|_{L^2} \leq C\epsilon^{1/2}e^{ct} \tag{1.1.12}$$

for constants $C > 0, c > 0$ which are independent of $\epsilon, t$. The bound (1.1.12) implies that the semiclassical wavepacket ansatz provides an asymptotic (in the limit $\epsilon \downarrow 0$) description of the dynamics of the PDE up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$.

## 1.2 Higher order effective dynamics for semiclassical wavepackets away from Bloch band degeneracies

By a natural extension of the argument given in Section 1.1, it is possible to derive higher order analogs of (1.1.9) such that the corrector function $\eta^\epsilon(x,t)$ satisfy bounds of the form $C\epsilon^{j/2}e^{ct}$ for any $j \in \{1,2,...\}$. We demonstrate this for the case $j = 2$ in Chapter 2; see Theorem 2.1.1 and

Sections 2.1.2 and 2.3 for details. We can then study the evolution of observables such as the center of mass:

$$\mathcal{Q}^\epsilon(t) := \int_{\mathbb{R}^d} x|\psi^\epsilon(x,t)|^2 \, \mathrm{d}x \tag{1.2.1}$$

of the solution using these asymptotic expressions. Our result (Theorem 2.1.2; see Sections 2.1.2 and 2.4 for details) is that (1.2.1) satisfies a system which, when $d = 3$, takes the form:

$$\begin{aligned}
\dot{\mathcal{Q}}^\epsilon(t) &= \nabla_{\mathcal{P}^\epsilon}\mathcal{H}_n(\mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t)) + \epsilon\left\{ -\dot{\mathcal{P}}^\epsilon(t)\times\nabla_{\mathcal{P}^\epsilon}\times\mathcal{A}_n(\mathcal{P}^\epsilon(t)) + C_1[a^\epsilon](t) \right\}, \\
\dot{\mathcal{P}}^\epsilon(t) &= \underbrace{-\nabla_{\mathcal{Q}^\epsilon}\mathcal{H}_n(\mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t))}_{\substack{\text{Dynamics generated by} \\ \text{`Bloch band' Hamiltonian} \\ \mathcal{H}_n := E_n(\mathcal{P}^\epsilon)+W(\mathcal{Q}^\epsilon)}} + \epsilon\Big\{ \underbrace{\qquad\qquad\qquad\qquad}_{\substack{\text{Anomalous velocity due to} \\ \text{Berry curvature}}} \underbrace{+C_2[a^\epsilon](t)}_{\substack{\text{`Particle-field'} \\ \text{coupling to} \\ \text{envelope } a^\epsilon}} \Big\} \\
i\partial_t a^\epsilon &= \mathscr{H}_n^\epsilon(t)a^\epsilon; \quad \mathscr{H}_n^\epsilon(t) := \underbrace{-\frac{1}{2}\nabla_y\cdot D^2_{\mathcal{P}^\epsilon}E_n(\mathcal{P}^\epsilon(t))\nabla_y + \frac{1}{2}y\cdot D^2_{\mathcal{Q}^\epsilon}W(\mathcal{Q}^\epsilon(t))y}_{\substack{\text{Quantum harmonic oscillator Hamiltonian} \\ \text{with parametric forcing through } \mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t)}}.
\end{aligned} \tag{1.2.2}$$

Here, $\mathcal{P}^\epsilon(t)$ denotes another observable associated with the solution which can be thought of as the average 'quasi-momentum' of the wavepacket, and $a^\epsilon(y,t)$ is the wavepacket envelope function. The 'particle-field' coupling terms $C_1(t), C_2(t)$ are original to our work and can have a significant impact on the effective dynamics.

In the remainder of Chapter 2 we sketch how the above theory generalizes to the case where $U(z,x)$ is 'non-separable', i.e. cannot be written in the form (1.1.3), (Section 2.5) and to the full Maxwell system (1.1.4)-(1.1.5) (Section 2.6), and then present examples of systems where expressions for the Berry curvature can be worked out explicitly (Section 2.7).

## 1.3 Dynamics at a one dimensional band crossing

We then consider the simplest possible relaxation of the 'isolated band' assumption (1.1.7). We specialize to one spatial dimension ($d = 1$), assume that the potential $U$ is separable (1.1.3), and then consider the problem:

**Problem.** *What are the dynamics generated by equation* (1.1.1) *with initial conditions given by a wavepacket associated with a band* $E_n$ *which is then driven by the external potential* $W$ *through a point in phase space where the Bloch band* $E_n$ *is degenerate?*

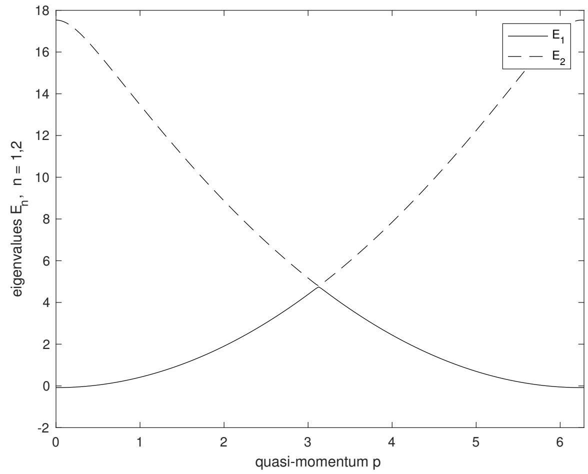



Figure 1.1: Plot of the two lowest Bloch band dispersion functions $E_1(p), E_2(p)$ when $V(z) = 4\cos(4\pi z)$. Note that the band functions are equal (degenerate) when $p = \pi$. This crossing turns out to be "trivial" (see Example 2).

More precisely, suppose that two bands $E_n(p), E_{n+1}(p)$ touch at a quasi-momentum $p^*$ in the Brillouin zone, but are otherwise non-degenerate in a neighborhood of $p^*$ (see Figure 1.1). Then, we study a wavepacket associated with the band $E_n$ initially localized in phase space on a classical trajectory $(q(t), p(t))$ generated by $\mathcal{H}_n := E_n(p) + W(q)$ which encounters the crossing after some finite time $t^*$: for some $t^* > 0$, $\lim_{t \uparrow t^*} p(t) = p^*$.

Our results can be roughly stated as follows; we give a more precise statement in Section 3.2. Assume that the wavepacket is *driven* through the crossing so that $\lim_{t \uparrow t^*} \dot{p}(t) \neq 0$ (Assumption 3). Then:

1. (Theorem 3.3.2) For $t \ll t^*$ and for any fixed positive integer $N$, the solution of (1.1.1) is a wavepacket associated with the band $E_n$ up to errors of $o(\epsilon^N)$ in $L^2$. As $t \uparrow t^*$, this 'single-band' description fails to capture the dynamics of the PDE to any order in $\epsilon$ higher than 1, because of an excited wave associated with the band $E_{n+1}$ whose norm grows to be of order $\epsilon^{1/2}$ for $t \sim t^*$. The precise limit of validity of the 'single-band' description as $t \uparrow t^*$ may be explicitly characterized.

2. (Theorem 3.3.3) For $t \sim t^*$ and $t \gg t^*$ the solution of (1.1.1) up to errors of $o(\epsilon^{1/2})$ is the sum of two semiclassical wavepackets: a wavepacket associated with the band $E_{n+1}$ with $L^2$-norm

proportional to 1 and a wavepacket associated with the band $E_n$ with $L^2$-norm proportional to $\epsilon^{1/2}$. The precise form of both wavepackets can be explicitly characterized.

Our proof relies on the existence of *smooth continuations* of the Bloch band dispersion functions $E_n, E_{n+1}$ through the crossing point $p^*$ (see Property 2 and Figures 3.2 and 3.4). Such continuations always exist in one spatial dimension (see Theorem 3.3.1). Our proof does not readily generalize to cases where no such continuation exists; for example at 'conical', or 'Dirac' points which occur in dimensions $d \geq 2$ [28]. We believe that the propagation of wavepackets through such crossings may be treated by adapting the methods of Hagedorn [37] who studied such cases in the context of the Born-Oppenheimer approximation of molecular dynamics.

## 1.4 Bound states of a periodic Schrödinger operator perturbed by domain wall modulations

The final problem we consider is that of determining the bound states of a Schrödinger operator in one spatial dimension with a periodic potential perturbed adiabatically by one or more *domain walls*. The model we consider is:

$$- \partial_x^2 + V_e(x) + \delta \kappa(\delta x) W_o(x), \tag{1.4.1}$$

where $\delta \ll 1$ is a small parameter. Here $V_e$ denotes a smooth, 1-periodic potential which may be written as an even-index cosine series and $W_o$ denotes a smooth, 1-periodic potential which is the sum of a cosine series with only odd-index terms. The function $\kappa(\zeta)$, which is constant as $|\zeta| \rightarrow \infty$, defines the *domain wall modulations* in the structure. 'Topologically protected' bound states of the operator (1.4.1) were constructed in the limit as $\delta \downarrow 0$ by Fefferman, Lee-Thorp and Weinstein in [26; 25] (see also [27] for the two-dimensional case) in the case where $\kappa(\zeta)$ is smooth and satisfies the asymptotics:

$$\lim_{\zeta \uparrow \infty} \kappa(\zeta) = \kappa_\infty > 0, \quad \lim_{\zeta \downarrow -\infty} \kappa(\zeta) = \kappa_{-\infty} < 0. \tag{1.4.2}$$

It was furthermore demonstrated that the existence of such states is tied to the existence of a robust (up to perturbations of $\kappa$ which do not change (1.4.2)) *zero mode* of the Dirac operator:

$$\mathcal{D}_\kappa := \begin{pmatrix} i\partial_\zeta & \kappa(\zeta) \\ \kappa(\zeta) & -i\partial_\zeta \end{pmatrix} \tag{1.4.3}$$

when $\kappa$ satisfies the asymptotics (1.4.2). More generally if the function $\kappa$ converges to non-zero constants $\kappa_\infty, \kappa_{-\infty}$ as $|\zeta| \to \infty$, but not necessarily with different signs as in (1.4.2), then the same argument given in [26; 25] implies that any eigenvalue of $\mathcal{D}_\kappa$ in the 'mass gap' in the essential spectrum:

$$(-\min|\kappa_{\pm\infty}|, \min|\kappa_{\pm\infty}|), \tag{1.4.4}$$

will lead to a bound state of the Schrödinger operator (1.4.1) in the limit $\delta \downarrow 0$. We are therefore motivated to study bound states of the operator $\mathcal{D}_\kappa$ for more general functions $\kappa$ converging to non-zero constants at infinity.

Let $\kappa_L$ denote the 'two domain wall' function (see Figure 1.2):

$$\kappa_L(x) = \begin{cases} -\kappa(x+L) & \text{for } -\infty \leq x \leq 0 \\ \kappa(x-L) & \text{for } 0 \leq x \leq \infty \end{cases} \tag{1.4.5}$$

where $\kappa$ denotes a 'domain wall' potential function which we assume to be *smooth*, *monotone increasing*, *odd*, and to satisfy:

$$\kappa(x) = \begin{cases} -\kappa_\infty & \text{if } x \leq -1 \\ \kappa_\infty & \text{if } x \geq 1 \end{cases}. \tag{1.4.6}$$

Then, our result (Theorem 4.2.1, see Sections 4.2, 4.4, C.1 for details) is that for sufficiently large $L \gg 1$, the Dirac operator (1.4.3) with $\kappa$ replaced by $\kappa_L$ (1.4.5) has two bound states with near-zero eigenvalues and eigenfunctions which may be characterized up to errors of any polynomial order in the small parameter $e^{-2L}$. Our analysis extends to 3 or more domain wall modulations, see Section 4.3.

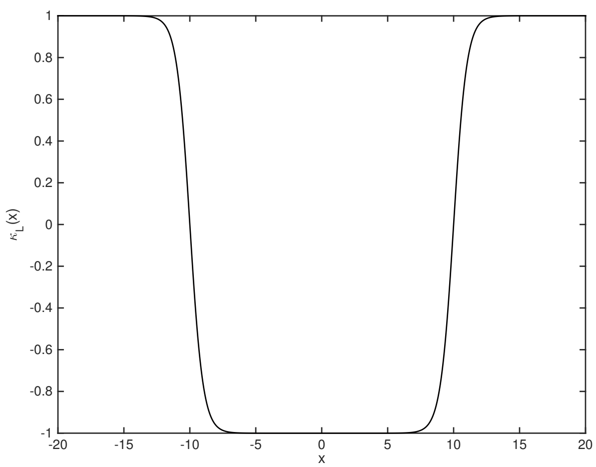



Figure 1.2: The “two domain wall” function $\kappa_L(x)$ (1.4.5) with $\kappa(x) = \tanh(x)$ (which approximately satisfies (1.4.6)), $L = 10$.

# Chapter 2

# Semiclassical wavepacket solutions and effective 'particle-field' dynamics

*The research detailed in this chapter is joint with J. Lu and M. I. Weinstein. Sections 2.1-2.4 and Appendices A.1-A.6 were published in [73] with minor alterations. We present extensions of this work in Sections 2.5-2.7 and Appendix A.7.*

## 2.1 Introduction

In this work we study the non-dimensionalized time-dependent Schrödinger equation for $\psi^\epsilon(x,t) : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}$:

$$\begin{aligned} & i\epsilon\partial_t\psi^\epsilon = -\frac{1}{2}\epsilon^2\Delta_x\psi^\epsilon + V\left(\frac{x}{\epsilon}\right)\psi^\epsilon + W(x)\psi^\epsilon \\ & \psi^\epsilon(x,0) = \psi_0^\epsilon(x). \end{aligned} \tag{2.1.1}$$

Here, $\epsilon$ is a positive real parameter which we assume to be small: $\epsilon \ll 1$. We assume throughout that the function $V$ is smooth and periodic with respect to a $d$-dimensional lattice $\Lambda$ so that:

$$V(z+v) = V(z) \text{ for all } v \in \Lambda, z \in \mathbb{R}^d, \tag{2.1.2}$$

and that $W$ is sufficiently smooth with uniformly bounded derivatives. Equation (2.1.1) is a well-studied model in condensed matter physics of the dynamics of an electron in a crystal under the independent-particle approximation [3], whose periodic effective potential due to the atomic nuclei is specified by $V$, under the influence of a 'slowly varying' external electric field generated by $W$.

In this work we rigorously derive a family of explicit asymptotic solutions of (2.1.1) known as *semiclassical wavepackets*. We then derive the equations of motion of the center of mass and average quasi-momentum of these solutions, including corrections proportional to $\epsilon$.

At order $\epsilon^0$, the mean position and momentum of the semi-classical wavepacket evolve along the classical trajectories associated with the 'Bloch band' Hamiltonian $\mathcal{H}_n := E_n(p) + W(q)$, where $p \mapsto E_n(p)$ is the dispersion relation associated with the $n^{th}$ spectral (Bloch) band of the periodic Schrödinger operator $-\frac{1}{2}\Delta_z + V(z)$. The order $\epsilon$ corrections to the leading order equations of motion depend on the gauge-invariant Berry curvature of the Bloch band and the wavepacket envelope. Through order $\epsilon$, the system governing appropriately defined mean position $\mathcal{Q}^\epsilon(t)$, mean momentum $\mathcal{P}^\epsilon(t)$ and wave-amplitude profile $a^\epsilon(y,t)$ is a closed system of Hamiltonian type (Theorem 2.1.2). When $d = 3$, this system takes the form:

$$
\begin{aligned}
\dot{\mathcal{Q}}^\epsilon(t) &= \nabla_{\mathcal{P}^\epsilon}\mathcal{H}_n(\mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t)) + \epsilon\left\{ -\dot{\mathcal{P}}^\epsilon(t) \times \nabla_{\mathcal{P}^\epsilon} \times \mathcal{A}_n(\mathcal{P}^\epsilon(t)) + C_1[a^\epsilon](t) \right\} \\
\dot{\mathcal{P}}^\epsilon(t) &= \underbrace{-\nabla_{\mathcal{Q}^\epsilon}\mathcal{H}_n(\mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t))}_{\substack{\text{Dynamics generated by}\\ \text{`Bloch band' Hamiltonian}\\ \mathcal{H}_n := E_n(\mathcal{P}^\epsilon)+W(\mathcal{Q}^\epsilon)}} + \epsilon\Big\{ \underbrace{\qquad\qquad\qquad\qquad}_{\substack{\text{Anomalous velocity due to}\\ \text{Berry curvature}}} \underbrace{+C_2[a^\epsilon](t)}_{\substack{\text{`Particle-field'}\\ \text{coupling to}\\ \text{envelope } a^\epsilon}} \Big\},
\end{aligned}
\tag{2.1.3}
$$

$$
i\partial_t a^\epsilon = \mathscr{H}_n^\epsilon(t) a^\epsilon; \quad \mathscr{H}_n^\epsilon(t) := \underbrace{-\frac{1}{2}\nabla_y \cdot D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t))\nabla_y + \frac{1}{2} y \cdot D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) y}_{\substack{\text{Quantum harmonic oscillator Hamiltonian}\\ \text{with parametric forcing through } \mathcal{Q}^\epsilon(t),\mathcal{P}^\epsilon(t)}}.
$$

Here, $D^2_{\mathcal{P}^\epsilon}E_n, D^2_{\mathcal{Q}^\epsilon}W$ denote Hessian matrices and $\mathcal{A}_n$ is the Berry connection (2.1.26). For the explicit forms of $C_1[a], C_2[a]$ and the generalization of (2.1.3) to arbitrary dimensions $d \geq 1$, see (2.1.46). The derivation of the form of the anomalous velocity displayed in (2.1.3) is given in Remark 2.1.12.

The 'particle-field' dynamical system (2.1.3) appears to be new, and contains terms which are not accounted for in the works of Niu et al. [76]. The system reduces, in the case of Gaussian initial data and zero periodic background $V = 0$, to that presented in Proposition 4.4 of Ref. [55] (see also Ref. [56]).

The asymptotic solutions and effective Hamiltonian system (2.1.3) provide an approximate description of the dynamics of the full PDE (2.1.1) up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$, known to be the general limit of applicability of wavepacket, or coherent state, approximations [66]. The validity of the approximation relies on an extension of the result of Carles and Sparber [61] (Theorem 2.1.1)

Our methods are applicable when the wavepacket is spectrally localized in a Bloch band which has crossings (degeneracies), as long as the distance in phase space between the average quasi-momentum of the wavepacket and any crossing is uniformly bounded below independent of $\epsilon$ (see Assumption 2.1.1). We do not attempt a description of wavepacket dynamics when this distance $\downarrow 0$ (propagation through a band crossing), or at an avoided crossing where the separation between bands is proportional to $\epsilon$. We believe that both of these cases may be studied by adapting the work of Hagedorn and Joye [37; 39] on wavepacket dynamics in the Born-Oppenheimer approximation of molecular dynamics to the model (2.1.1).

Our methods are also applicable, with some modifications (see Section 2.1.5), to potentials with the general two-scale form $U\left(\frac{x}{\epsilon}, x\right)$ where $U$ is periodic in its first argument:

$$U(z+v,x) = U(z,x) \text{ for all } z, x \in \mathbb{R}^d, v \in \Lambda \tag{2.1.4}$$

and $U(z,x)$ is 'nonseparable', i.e., cannot be written as the sum of a periodic potential $V(z)$ and an 'external' potential $W(x)$. For details, see Section 2.5. For ease of presentation we consider in this work only the 'separable' case (2.1.1).

The semiclassical wavepacket ansatz was introduced by Heller [40] and Hagedorn [36] to study the uniform background case ($V = 0$) of (2.1.1). See also related work on Gaussian beams [62]. Hagedorn then extended this theory to the case where the potential $W(x)$ is replaced by an $x$-dependent operator in his study of the Born-Oppenheimer approximation of molecular dynamics [37]. Semiclassical wavepacket solutions of (2.1.1) in the periodic background case ($V \neq 0$) were then constructed by Carles and Sparber [61].

The anomalous velocity term in (2.1.3) was first derived by Karplus and Luttinger [44]. For a derivation in terms of Berry curvature of the Bloch band, see Chang and Niu [15] (see also Ref. [76]). It was then derived rigorously by Panati, Spohn, and Teufel [57] (see also [23]). This term is responsible for the 'intrinsic contribution' to the anomalous Hall effect which occurs in solids with broken time-reversal symmetry (see Nagaosa et al.[52] and references therein). The anomalous velocity due to Berry curvature is better known in optics as the spin Hall effect of light and was experimentally observed by Bliokh et al.[7].

### 2.1.1 Dimensional analysis, derivation of equation (2.1.1)

In this section we derive the non-dimensionalized equation (2.1.1) starting with the Schrödinger equation in physical units:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta_x\psi + V(x)\psi + W(x)\psi \tag{2.1.5}$$

where $\hbar$ is the reduced Planck constant, and $m$ is the mass of an electron. This analysis is based on those given in Refs. [23; 4]. Define $l$ as the lattice constant, and let $\tau$ denote the quantum time scale:

$$\tau = \frac{ml^2}{\hbar}. \tag{2.1.6}$$

Let $L, T$ denote macroscopic length and time-scales. We assume that the periodic potential $V$ acts on the 'fast quantum scale' and the $W$ acts on the 'slow macroscopic scale':

$$V(x) = \frac{ml^2}{\tau^2}\tilde{V}\left(\frac{x}{l}\right), W(x) = \frac{mL^2}{T^2}\tilde{W}\left(\frac{x}{L}\right). \tag{2.1.7}$$

After re-scaling $x, t$ by the macroscopic length and time-scales:

$$\tilde{x} := \frac{x}{L}, \tilde{t} := \frac{t}{T}, \tilde{\psi}(\tilde{x}, \tilde{t}) := \psi(x, t), \tag{2.1.8}$$

(2.1.5) becomes:

$$\frac{i\hbar}{T}\partial_{\tilde{t}}\tilde{\psi} = -\frac{\hbar^2}{2mL^2}\Delta_{\tilde{x}}\tilde{\psi} + \frac{ml^2}{\tau^2}\tilde{V}\left(\frac{L\tilde{x}}{l}\right)\psi + \frac{mL^2}{T^2}\tilde{W}\left(\tilde{x}\right)\psi. \tag{2.1.9}$$

We now identify two dimensionless parameters. Let $h$ denote a scaled Planck's constant, and $\epsilon$ the ratio of the lattice constant to the macroscopic scale:

$$h := \frac{\hbar T}{mL^2}, \epsilon := \frac{l}{L}. \tag{2.1.10}$$

Writing (2.1.9) in terms of $h, \epsilon$ and dropping the tildes we arrive at:

$$ih\partial_t\psi^{h,\epsilon} = -\frac{h^2}{2}\Delta_x\psi^{h,\epsilon} + \frac{h^2}{\epsilon^2}V\left(\frac{x}{\epsilon}\right)\psi^{h,\epsilon} + W(x)\psi^{h,\epsilon} \tag{2.1.11}$$

where we have written $\psi^{h,\epsilon}(x,t)$ to emphasize the dependence of the solution on both parameters. We obtain the problem depending only on $\epsilon$ (2.1.1) by setting $h = \epsilon$. Therefore, the limit $\epsilon \downarrow 0$ in (2.1.1) corresponds to sending to zero the ratio of the lattice spacing $l$ to the scale of inhomogeneity $L$ and Planck's constant (appropriately re-scaled) to zero at the same rate.

**Remark 2.1.1.** *Other scalings of the Schrödinger* (2.1.11) *have been considered. For example, the scaling corresponding to $h$ fixed and $\epsilon \downarrow 0$ is considered in Refs. [2; 60; 42], and for the nonlinear Schrödinger / Gross-Pitaevskii (NLS/GP) equation in Refs. [68; 8]. Here, the dynamics are governed by a homogenized effective mass Schrödinger equation (linear, respectively, nonlinear). The articles Refs. [42; 8] concern the bifurcations of bound states of* (2.1.11) *or NLS/GP from spectral band edges into spectral gaps of the periodic potential, $V$. Another scaling where such band-edge bifurcations arise due to an oscillatory, localized and mean-zero potential, $W$, is considered in Refs. [20; 21; 18; 19]. In this case, a subtle higher order effective potential correction to the classical homogenized Schrödinger operator is required to capture the bifurcation.*

### 2.1.2 Statement of results

In order to state our results we require some background on the spectral theory of the Schrödinger operator:

$$H := -\frac{1}{2}\Delta_z + V(z) \tag{2.1.12}$$

where $V$ is periodic with respect to a $d$-dimensional lattice $\Lambda$[46; 63]. Let $\Lambda^*$ denote the dual lattice to $\Lambda$, and define the first Brillouin zone $\mathcal{B}$ to be a fundamental period cell. Consider the family of self-adjoint eigenvalue problems parameterized by $p \in \mathcal{B}$:

$$\begin{aligned} &H(p)\chi(z;p) = E(p)\chi(z;p) \\ &\chi(z+v;p) = \chi(z;p) \text{ for all } z \in \mathbb{R}^d, v \in \Lambda \\ &H(p) := \frac{1}{2}(p - i\nabla_z)^2 + V(z). \end{aligned} \tag{2.1.13}$$

For fixed $p$, known as the quasi-momentum, the spectrum of the operator (2.1.13) is real and discrete and the eigenvalues can be ordered with multiplicity:

$$E_1(p) \le E_2(p) \le ... \le E_n(p) \le ... \tag{2.1.14}$$

For fixed $p$, the associated normalized eigenfunctions $\chi_n(z;p)$ are a basis of the space:

$$L^2_{per} := \left\{ f \in L^2_{loc} : f(z+v) = f(z) \text{ for all } v \in \Lambda, z \in \mathbb{R}^d \right\} \tag{2.1.15}$$

Varying $p$ over the Brillouin zone, the maps $p \mapsto E_n(p)$ are known as the spectral band functions. Their graphs are called the dispersion surfaces of $H$. The set of all dispersion surfaces as $p$ varies over $\mathcal{B}$ is called the band structure of $H$ (2.1.12). Any function in $L^2(\mathbb{R}^d)$ can be written as a superposition of Bloch waves:

$$\left\{\Phi_n(z;p) = e^{ipz}\chi_n(z;p) : n \in \mathbb{N}, p \in \mathcal{B}\right\}; \tag{2.1.16}$$

see (2.2.8). Moreover, the $L^2$-spectrum of the operator (2.1.12) is the union of the real intervals swept out by the spectral band functions $E_n(p)$:

$$\sigma(H)_{L^2(\mathbb{R}^d)} = \cup_{n\in\mathbb{R}} \left\{E_n(p) : p \in \mathcal{B}\right\}. \tag{2.1.17}$$

The map $p \mapsto E_n(p)$ extends to a map on $\mathbb{R}^d$ which is periodic with respect to the reciprocal lattice $\Lambda^*$:

$$\text{for any } b \in \Lambda^*,\ E_n(p+b) = E_n(p). \tag{2.1.18}$$

If the eigenvalue $E_n(p)$ is simple, then: (up to a constant phase shift) $\chi_n(z;p+b) = e^{-ib\cdot z}\chi_n(z;p)$. A more detailed account of the Floquet-Bloch theory which we require, in particular results on the regularity of the maps $p \to E_n(p), \chi_n(z;p)$, can be found in Section 2.2.

We will make the following assumptions throughout:

**Assumption 2.1.1** (Uniformly isolated band assumption)**.** *Let $E_n(p)$ be an eigenvalue band function of the periodic Schrödinger operator (2.1.12). Assume that $(q_0,p_0) \in \mathbb{R}^d \times \mathbb{R}^d$ are such that the flow generated by the classical Hamiltonian $\mathcal{H}_n(q,p) := E_n(p) + W(q)$:*

$$\begin{aligned} \dot{q}(t) &= \nabla_p E_n(p(t)) \\ \dot{p}(t) &= -\nabla_q W(q(t)) \\ q(0), p(0) &= q_0, p_0 \end{aligned} \tag{2.1.19}$$

*has a unique smooth solution $(q(t),p(t)) \in \mathbb{R}^d \times \mathbb{R}^d, \forall t \geq 0$, and that there exists a constant $M > 0$ such that:*

$$\inf_{m\neq n} |E_m(p(t)) - E_n(p(t))| \geq M \text{ for all } t \geq 0. \tag{2.1.20}$$

*That is, the nth spectral band is uniformly isolated along the classical trajectory $(q(t),p(t))$.*

**Assumption 2.1.2.** $\sum_{|\alpha|=1,2,3,4} |\partial_x^\alpha W(x)| \in L^\infty(\mathbb{R}^d)$.

**Remark 2.1.2.** *An example of $W$ satisfying Assumption 2.1.2 is the 'Stark' potential $W(x) = E\cdot x$ for any constant vector $E \in \mathbb{R}^d$. Assumption 2.1.2 may be significantly weakened. For example, a* *refinement of our methods would allow us to deal with any function $W$ with finite order polynomial growth at infinity. This larger class of admissable potentials would include the quantum harmonic oscillator potential $W(x) = \frac{1}{2} x \cdot M x$ where $M$ is any real positive definite $d \times d$ matrix.*

**Remark 2.1.3.** *Our methods may be adapted to work with time-dependent external potentials $W(x,t)$ which are smooth in $x$ and continuous in $t$ as long as there exists a constant $C > 0$ such that for all $t \geq 0 : \sum_{|\alpha|=1,2,3,4} |\partial_x^\alpha W(x,t)| \leq C$.*

### 2.1.3 Dynamics of semiclassical wavepackets in a periodic background

Our first result is an extension of Theorem 1.7 of Carles and Sparber [61]:

**Theorem 2.1.1.** *Let Assumptions 2.1.1 and 2.1.2 hold. Let $a_0(y), b_0(y) \in \mathcal{S}(\mathbb{R}^d)$. Let $S(t)$ denote the classical action along the path $(q(t), p(t))$:*

$$S(t) = \int_0^t p(t') \cdot \nabla_p E_n(p(t')) - E_n(p(t')) - W(q(t'))\, dt'. \tag{2.1.21}$$

*Let $a(y,t)$ satisfy:*

$$\begin{aligned} i\partial_t a(y,t) &= \mathscr{H}(t) a(y,t) \\ a(y,0) &= a_0(y), \end{aligned} \tag{2.1.22}$$

*where:*

$$\mathscr{H}(t) := -\frac{1}{2} \nabla_y \cdot D_p^2 E_n(p(t)) \nabla_y + \frac{1}{2} y \cdot D_q^2 W(q(t)) y. \tag{2.1.23}$$

*And let $b(y,t)$ satisfy:*

$$\begin{aligned} i\partial_t b(y,t) &= \mathscr{H}(t) b(y,t) + \mathscr{I}(t) a(y,t) \\ b(y,0) &= b_0(y), \end{aligned} \tag{2.1.24}$$

*where $\mathscr{H}(t)$ is as in (2.1.23) and:*

$$\begin{aligned} \mathscr{I}(t) := &-\frac{1}{6} \nabla_p \left[ \nabla_y \cdot D_p^2 E_n(p(t)) \nabla_y \right] \cdot (-i\nabla_y) + \frac{1}{6} \nabla_q \left[ y \cdot D_q^2 W(q(t)) y \right] \cdot y \\ &+ \nabla_p \left[ \nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t)) \right] \cdot (-i\nabla_y) + \nabla_q \left[ \nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t)) \right] \cdot y. \end{aligned} \tag{2.1.25}$$

*Here $\mathcal{A}_n(p)$ denotes the $n$th band Berry connection:*

$$\mathcal{A}_n(p) := i \left\langle \chi_n(\cdot; p)) \right| \nabla_p \chi_n(\cdot; p) \rangle_{L^2(\Omega)} \tag{2.1.26}$$

*where $\Omega$ denotes a fundamental period cell of the lattice $\Lambda$. Let $\phi_B(t)$ be the Berry phase associated with transport of $\chi_n$ along the path $p(t) \in \mathcal{B}$ given by:*

$$\phi_B(t) = \int_0^t \dot{p}(t') \cdot \mathcal{A}_n(p(t'))\, dt' = \int_{p_0}^{p(t)} \mathcal{A}_n(p) \cdot \, dp. \tag{2.1.27}$$

*Then, there exists a constant $\epsilon_0 > 0$ such that for all $0 < \epsilon \leq \epsilon_0$ the following holds. Let $\psi^\epsilon(x,t)$ be the unique solution of the initial value problem (2.1.1) with 'Bloch wavepacket' initial data:*

$$\begin{aligned} &i\epsilon\partial_t\psi^\epsilon = -\frac{1}{2}\epsilon^2\Delta_x\psi^\epsilon + V\left(\frac{x}{\epsilon}\right)\psi^\epsilon + W(x)\psi^\epsilon \\ &\psi^\epsilon(x,0) = \epsilon^{-d/4}e^{ip_0\cdot(x-q_0)/\epsilon}\left\{a_0\left(\frac{x-q_0}{\epsilon^{1/2}}\right)\chi_n\left(\frac{x}{\epsilon};p_0\right)\right. \\ &\left.+\epsilon^{1/2}\left[(-i\nabla_y)a_0\left(\frac{x-q_0}{\epsilon^{1/2}}\right)\cdot\nabla_p\chi_n\left(\frac{x}{\epsilon};p_0\right) + b_0\left(\frac{x-q_0}{\epsilon^{1/2}}\right)\chi_n\left(\frac{x}{\epsilon};p_0\right)\right]\right\}. \end{aligned} \tag{2.1.28}$$

*Then, for all $t \geq 0$ the solution evolves as a modulated 'Bloch wavepacket' plus a corrector $\eta^\epsilon(x,t)$:*

$$\begin{aligned} &\psi^\epsilon(x,t) = \epsilon^{-d/4}e^{iS(t)/\epsilon}e^{ip(t)\cdot(x-q(t))/\epsilon}e^{i\phi_B(t)}\left\{a\left(\frac{x-q(t)}{\epsilon^{1/2}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right)\right. \\ &\left.+\epsilon^{1/2}\left[(-i\nabla_y)a\left(\frac{x-q(t)}{\epsilon^{1/2}},t\right)\cdot\nabla_p\chi_n\left(\frac{x}{\epsilon};p(t)\right) + b\left(\frac{x-q(t)}{\epsilon^{1/2}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right)\right]\right\} \\ &+\eta^\epsilon(x,t) \end{aligned} \tag{2.1.29}$$

*where the corrector $\eta^\epsilon$ satisfies the following estimate:*

$$\|\eta^\epsilon(\cdot,t)\|_{L^2(\mathbb{R}^d)} \leq C\epsilon e^{ct}. \tag{2.1.30}$$

*Here, $c > 0, C > 0$ are constants independent of $\epsilon, t$. It follows that:*

$$\sup_{t\in[0,\tilde{C}\ln 1/\epsilon]} \|\eta^\epsilon(\cdot,t)\|_{L^2(\mathbb{R}^d)} = o(\epsilon^{1/2}) \tag{2.1.31}$$

*where $\tilde{C}$ is any constant satisfying $\tilde{C} < \frac{1}{2c}$.*

**Remark 2.1.4.** *We include the pre-factor $\epsilon^{-d/4}$ throughout so that the $L^2_x(\mathbb{R}^d)$ norm of $\psi^\epsilon(x,t)$ is of order 1 as $\epsilon \downarrow 0$.*

**Remark 2.1.5.** *We have improved the error bound of Carles and Sparber [61] from $C\epsilon^{1/2}e^{ct}$ to $C\epsilon e^{ct}$ by including correction terms in the asymptotic expansion proportional to $\epsilon^{1/2}$. Note that we must also assume that the initial data is well-prepared up to terms proportional to $\epsilon^{1/2}$ (2.1.28). By keeping more terms in the expansion we may produce approximations where the corrector can* *be bounded by $C\epsilon^{N/2}e^{ct}$ for any positive integer $N$. The only changes in the proof are that we include corrections to the initial data proportional to $\epsilon^{N/2}$, and that Assumption 2.1.2 is replaced by $\sum_{|\alpha|=1,2,\ldots,N+2}|\partial_x^\alpha W(x)| \in L^\infty(\mathbb{R}^d)$.*

**Remark 2.1.6.** *Keeping terms proportional to $\epsilon^{1/2}$ in the expansion will allow us to calculate corrections to the dynamics of physical observables proportional to $\epsilon$; see Theorem 2.1.2 and Section 2.4.*

**Remark 2.1.7.** *The time-scale of validity of the approximation (2.1.29), $t \sim \ln 1/\epsilon$, is known as 'Ehrenfest time'. Without additional assumptions this is known to be the general limit of validity of wavepacket, or coherent state, approximations. Note that including higher order terms (proportional to powers of $\epsilon^{1/2}$) in the approximation does not extend the time-scale of validity. Under further assumptions on the classical dynamics, coherent state approximations have been shown to be valid over the longer time-scale $t = o(1/\sqrt{\epsilon})$; see Refs. [64; 66] for further discussion.*

**Remark 2.1.8.** *For a discussion of Berry's phase, connection, and curvature, and gauge independence in the setting of a two-by-two matrix example, see Appendix A.7. We compute the Berry curvature in a 'non-separable' Schrödinger example and for Maxwell's equations in free space in Sections 2.7.1 and 2.7.2 respectively.*

There exists a family of time-dependent Gaussian explicit solutions of the envelope equation (2.1.22). Consider (2.1.22) with initial data:

$$a_0(y) = \frac{N}{[\det A_0]^{1/2}} \exp\left(i\frac{1}{2}y \cdot B_0 A_0^{-1} y\right) . \tag{2.1.32}$$

Here, $N \in \mathbb{C}$ is an arbitrary non-zero constant, and $A_0, B_0$ are $d \times d$ complex matrices satisfying:

$$\begin{aligned} A_0^T B_0 - B_0^T A_0 &= 0 \\ \overline{A_0^T} B_0 - \overline{B_0^T} A_0 &= 2iI. \end{aligned} \tag{2.1.33}$$

**Remark 2.1.9.** *The conditions (2.1.33) imply:*

1. *The matrices $B_0, A_0$ are invertible*

2. *The matrix $B_0 A_0^{-1}$ is complex symmetric: $(B_0 A_0^{-1})^T = B_0 A_0^{-1}$*

*3. The imaginary part of the matrix $B_0 A_0^{-1}$ is symmetric, positive definite, and satisfies:*

$$Im\ B_0 A_0^{-1} = (A_0 \overline{A_0^T})^{-1} \tag{2.1.34}$$

*and are equivalent to the condition that the matrix:*

$$Y := \begin{pmatrix} Re\ A_0 & Im\ A_0 \\ Re\ B_0 & Im\ B_0 \end{pmatrix} \text{ is symplectic: } Y^T J Y = J \text{ where } J := \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \tag{2.1.35}$$

*The proofs of (1)-(3) are given in Refs. [38; 36; 24].*

Note that it follows from assertion (3) of Remark 2.1.9 that $a_0(y)$ (2.1.32) satisfies $|a_0(y)| \leq Ce^{-c|y|^2}$ for constants $C > 0, c > 0$. We have then that:

**Proposition 2.1.1** (Gaussian wavepackets)**.** *The initial value problem (2.1.22) with initial data $a_0(y)$ given by (2.1.32) has the unique solution for all $t \geq 0$:*

$$a(y,t) = \frac{N}{[\det A(t)]^{1/2}} \exp\left( i \frac{1}{2} y \cdot B(t) A^{-1}(t) y \right). \tag{2.1.36}$$

*Here, the complex matrices $A(t), B(t)$ satisfy:*

$$\begin{aligned} &\dot{A}(t) = D_p^2 E_n(p(t)) B(t), \quad \dot{B}(t) = -D_q^2 W(q(t)) A(t), \\ &A(0) = A_0, B(0) = B_0. \end{aligned} \tag{2.1.37}$$

*Moreover, for all $t \geq 0$, the matrices $A(t), B(t)$ satisfy (2.1.33) with $A_0$ replaced by $A(t)$ and $B_0$ replaced by $B(t)$. Thus (see Remark 2.1.9), $|a(y,t)| \leq C(t)e^{-c(t)|y|^2}$ where $C(t) > 0, c(t) > 0$ for all $t \geq 0$. More generally, we may construct a basis of $L^2(\mathbb{R}^d)$ of solutions of the envelope equation (2.1.22), consisting of products of Gaussians with polynomials, known as the 'semiclassical wavepacket' basis [38; 36; 24].*

**Remark 2.1.10.** *Our convention for the complex matrices $A, B$ follows that introduced in Ref. [24], with $A, B$ standing for $Q, P$ in Ref. [24] respectively. Note that our convention is not to be confused with that introduced in Ref. [36]; our choice of $B$ corresponds to $iB$ in Ref. [36].*

### 2.1.4 Dynamics of observables associated with the asymptotic solution

We now deduce consequences for the physical observables associated with the solution $\psi^\epsilon(x,t)$ of (2.1.28), using the asymptotic form (2.1.29). Denote the solution of (2.1.28) through order $\epsilon^{1/2}$ by:

$$\begin{aligned}\tilde{\psi}^\epsilon(y,z,t) &:= \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} e^{i\phi_B(t)} \Big\{ a(y,t)\chi_n(z;p(t)) \\ &+\epsilon^{1/2} \Big[ (-i\nabla_y) a(y,t) \cdot \nabla_p \chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t)) \Big] \Big\}.\end{aligned} \tag{2.1.38}$$

Thus:

$$\psi^\epsilon(x,t) = \tilde{\psi}^\epsilon(y,z,t)\Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} + \eta^\epsilon(x,t). \tag{2.1.39}$$

where $\eta^\epsilon$ is the corrector which satisfies the bound (2.1.30). Define the physical observables:

$$\begin{aligned}\mathcal{Q}^\epsilon(t) &:= \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} x \left| \tilde{\psi}^\epsilon(y,z,t) \right|^2_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} \, \mathrm{d}x \\ \mathcal{P}^\epsilon(t) &:= \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} \overline{\tilde{\psi}^\epsilon(y,z,t)} \left( -i\epsilon^{1/2}\nabla_y \right) \tilde{\psi}^\epsilon(y,z,t) \Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} \, \mathrm{d}x.\end{aligned} \tag{2.1.40}$$

where $\mathcal{N}^\epsilon(t)$ is the normalization factor:

$$\mathcal{N}^\epsilon(t) = \int_{\mathbb{R}^d} \left| \tilde{\psi}^\epsilon(y,z,t) \right|^2_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} \, \mathrm{d}x. \tag{2.1.41}$$

We will refer to $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$ as the center of mass and average quasi-momentum of the wavepacket. We will see (Theorem 2.1.2): $\mathcal{Q}^\epsilon(t) = q(t) + o(1), \mathcal{P}^\epsilon(t) = p(t) + o(1)$ up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$.

**Remark 2.1.11.** *In the uniform background case $V = 0$, solutions of (2.1.13) are independent of $z$: $\chi_n(z;p) = 1$ for all $p \in \mathcal{B}$. The asymptotic solution (2.1.38) obtained in this case is therefore independent of $z$, and our definition of $\mathcal{P}^\epsilon(t)$ reduces to the usually defined momentum observable:*

$$\int_{\mathbb{R}^d} \overline{\psi^\epsilon(x,t)} (-i\epsilon\nabla_x) \psi^\epsilon(x,t) \, dx. \tag{2.1.42}$$

*In the periodic background case $V \neq 0$, $\mathcal{P}^\epsilon$ (2.1.40) corresponds to the quasi-momentum and may be measured in experiments [16].*

Let $a^\epsilon(y,t)$ satisfy the equation of a quantum harmonic oscillator, with parametric forcing defined by $(\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t))$:

$$\begin{aligned}& i\partial_t a^\epsilon = \mathscr{H}^\epsilon(t) a^\epsilon; \quad \mathscr{H}^\epsilon(t) := -\frac{1}{2}\nabla_y \cdot D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t)) \nabla_y + \frac{1}{2} y \cdot D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) y \\ & a^\epsilon(y,0) = a_0(y).\end{aligned} \tag{2.1.43}$$

Note that we have replaced dependence on $(q(t), p(t))$ in equation (2.1.22) with dependence on $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$.

For simplicity of presentation of the following theorem we assume that:

$$\begin{aligned} &\langle a_0(y) | \, y a_0(y) \rangle_{L^2_y(\mathbb{R}^d)} = \langle a_0(y) | \, (-i\nabla_y) a_0(y) \rangle_{L^2_y(\mathbb{R}^d)} = 0 \\ &\| a_0(y) \|_{L^2_y(\mathbb{R}^d)} = 1. \end{aligned} \tag{2.1.44}$$

The result holds for general $a_0(y) \in \mathcal{S}(\mathbb{R}^d)$; see Section 2.4.

**Theorem 2.1.2.** *Let $\tilde{\psi}^\epsilon(y, z, t)$ denote the asymptotic solution (2.1.38) including corrections proportional to $\epsilon^{1/2}$. Let $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$ denote the observables (2.1.40). Then, there exists an $\epsilon_0 > 0$ such that for all $0 < \epsilon \leq \epsilon_0$, and for all $t \in [0, \tilde{C}' \ln 1/\epsilon]$ where $\tilde{C}' > 0$ is a constant independent of $t, \epsilon$:*

1. *$\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$ satisfy:*

$$\begin{aligned} \mathcal{Q}^\epsilon(t) &= q(t) + \epsilon \left[ \langle b(y,t) | \, y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | \, y b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] + \epsilon \mathcal{A}_n(p(t)) + o(\epsilon) \\ \mathcal{P}^\epsilon(t) &= p(t) + \epsilon \left[ \langle b(y,t) | \, (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | \, (-i\nabla_y) b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] + o(\epsilon) \end{aligned} \tag{2.1.45}$$

*where $\mathcal{A}_n(p)$ is the nth band Berry connection (2.1.26), and $a(y,t), b(y,t)$ satisfy (2.1.22) and (2.1.24) respectively.*

2. *Let $a^\epsilon(y,t)$ satisfy (2.1.43). Then:*

$$\begin{aligned} \dot{\mathcal{Q}}^\epsilon_\alpha(t) &= \partial_{\mathcal{P}^\epsilon_\alpha} E_n(\mathcal{P}^\epsilon(t)) - \epsilon \dot{\mathcal{P}}^\epsilon_\beta(t) \mathcal{F}_{n,\alpha\beta}(\mathcal{P}^\epsilon(t)) \\ &+ \epsilon \frac{1}{2} \partial_{\mathcal{P}^\epsilon_\alpha} \left\langle \nabla_y a^\epsilon(y,t) \right| \cdot D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t)) \nabla_y a^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} + o(\epsilon) \\ \dot{\mathcal{P}}^\epsilon_\alpha(t) &= -\partial_{\mathcal{Q}^\epsilon_\alpha} W(\mathcal{Q}^\epsilon(t)) \\ &- \epsilon \frac{1}{2} \partial_{\mathcal{Q}^\epsilon_\alpha} \left\langle y a^\epsilon(y,t) \right| \cdot D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) y a^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} + o(\epsilon). \end{aligned} \tag{2.1.46}$$

*Here, $\mathcal{F}_{n,\alpha\beta}(\mathcal{P}^\epsilon(t))$ denotes the Berry curvature of the nth band:*

$$\mathcal{F}_{n,\alpha\beta}(\mathcal{P}^\epsilon) := \partial_{\mathcal{P}^\epsilon_\alpha} \mathcal{A}_{n,\beta}(\mathcal{P}^\epsilon) - \partial_{\mathcal{P}^\epsilon_\beta} \mathcal{A}_{n,\alpha}(\mathcal{P}^\epsilon) \tag{2.1.47}$$

*where $\mathcal{A}_n(\mathcal{P}^\epsilon)$ is the nth band Berry connection (2.1.26). When $d = 3$ the anomalous velocity $-\dot{\mathcal{P}}^\epsilon_\beta(t) \mathcal{F}_{n,\alpha\beta}(\mathcal{P}^\epsilon(t))$ may be re-written using the cross product as in (2.1.3); see Remark 2.1.12.*

3. *After dropping the terms of $o(\epsilon)$ in (2.1.46), equations (2.1.46), (2.1.43) form a closed, coupled 'particle-field' system for $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t), a^\epsilon(y,t)$.*

4. *Let*

$$\begin{aligned} \mathscr{Q}^\epsilon(t) &:= \mathcal{Q}^\epsilon(t) - \epsilon \mathcal{A}_n(\mathcal{P}^\epsilon(t)) \\ \mathscr{P}^\epsilon(t) &:= \mathcal{P}^\epsilon(t). \end{aligned} \tag{2.1.48}$$

*Let $\mathfrak{a}^\epsilon(y,t)$ denote the solution of (2.1.43) with co-efficients evaluated at $\mathscr{Q}^\epsilon(t), \mathscr{P}^\epsilon(t)$ rather than $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$.*

*Then, after dropping terms of $o(\epsilon)$, $\mathscr{Q}^\epsilon(t), \mathscr{P}^\epsilon(t), \mathfrak{a}^\epsilon(y,t)$ satisfy a closed, coupled 'particle-field' system which is expressible as an $\epsilon$-dependent Hamiltonian system:*

$$\begin{aligned} &\dot{\mathscr{Q}}^\epsilon = \nabla_{\mathscr{P}^\epsilon} \mathcal{H}^\epsilon, \dot{\mathscr{P}}^\epsilon = -\nabla_{\mathscr{Q}^\epsilon} \mathcal{H}^\epsilon \\ &i\partial_t \mathfrak{a}^\epsilon = \frac{\delta \mathcal{H}^\epsilon}{\delta \overline{\mathfrak{a}^\epsilon}} \end{aligned} \tag{2.1.49}$$

*with Hamiltonian:*

$$\begin{aligned} &\mathcal{H}^\epsilon(\mathscr{P}^\epsilon, \mathscr{Q}^\epsilon, \overline{\mathfrak{a}^\epsilon}, \mathfrak{a}^\epsilon) := E_n(\mathscr{P}^\epsilon) + W(\mathscr{Q}^\epsilon) + \epsilon \nabla_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) \cdot \mathcal{A}_n(\mathscr{P}^\epsilon) \\ &+ \epsilon \frac{1}{2} \left\langle \nabla_y \mathfrak{a}^\epsilon \right| \cdot D^2_{\mathscr{P}^\epsilon} E_n(\mathscr{P}^\epsilon) \nabla_y \mathfrak{a}^\epsilon \right\rangle_{L^2_y(\mathbb{R}^d)} + \epsilon \frac{1}{2} \left\langle y \mathfrak{a}^\epsilon \right| \cdot D^2_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) y \mathfrak{a}^\epsilon \right\rangle_{L^2_y(\mathbb{R}^d)} \end{aligned} \tag{2.1.50}$$

**Remark 2.1.12.** *In three spatial dimensions ($d = 3$) the anomalous velocity may be re-written using the cross product:*

$$\begin{aligned} -\dot{\mathcal{P}}^\epsilon_\beta(t) \mathcal{F}_{n,\alpha\beta}(\mathcal{P}^\epsilon(t)) &= -\dot{\mathcal{P}}^\epsilon_\beta(t) \left( \partial_{\mathcal{P}^\epsilon_\alpha} \mathcal{A}_{n,\beta}(\mathcal{P}^\epsilon(t)) - \partial_{\mathcal{P}^\epsilon_\beta} \mathcal{A}_{n,\alpha}(\mathcal{P}^\epsilon(t)) \right) \\ &= -(\delta_{\alpha\gamma}\delta_{\beta\phi} - \delta_{\alpha\phi}\delta_{\beta\gamma}) \dot{\mathcal{P}}^\epsilon_\beta(t) \partial_{\mathcal{P}^\epsilon_\gamma} \mathcal{A}_{n,\phi}(\mathcal{P}^\epsilon(t)) \\ &= -\varepsilon_{\eta\alpha\beta}\varepsilon_{\eta\gamma\phi} \dot{\mathcal{P}}^\epsilon_\beta(t) \partial_{\mathcal{P}^\epsilon_\gamma} \mathcal{A}_{n,\phi}(\mathcal{P}^\epsilon(t)) \\ &= -\left( \dot{\mathcal{P}}^\epsilon(t) \times \nabla_{\mathcal{P}^\epsilon} \times \mathcal{A}_n(\mathcal{P}^\epsilon(t)) \right)_\alpha . \end{aligned} \tag{2.1.51}$$

*Here, $\varepsilon$ and $\delta$ are the Levi-Civita and Kronecker delta symbols respectively and each equality follows from well-known properties of these symbols; see Section 2.1.6 (2.1.71)-(2.1.74). In this case the curl of the Berry connection: $\nabla_{\mathcal{P}^\epsilon} \times \mathcal{A}_n(\mathcal{P}^\epsilon)$ is often referred to as the Berry curvature, see for example [23].*

**Remark 2.1.13.** *Equations (2.1.46) agree with those derived elsewhere (for example (3.5)-(3.6) of Ref. [76]) up to the terms which depend on the wavepacket envelope $a^\epsilon$. The change of variables (2.1.48) was introduced in Ref. [23] to transform between the Hamiltonian system for the characteristics of a 'corrected' eikonal ((4.9)-(4.10) in that work) and a gauge-invariant system ((4.11)-(4.12) in that work).*

**Corollary 2.1.1.**

1. *Choose initial data $a_0(y)$ of the form* (2.1.32)-(2.1.33) *with $N = \pi^{-d/4}$ so that $\|a_0(y)\|_{L^2_y} = 1$. Then, $a^\epsilon(y,t)$, the solution of the initial value problem* (2.1.43), *is given by:*

$$a^\epsilon(y,t) = \frac{N}{[\det A^\epsilon(t)]^{1/2}} \exp\left( i\frac{1}{2} y \cdot B^\epsilon(t) A^{\epsilon-1}(t) y \right) , \tag{2.1.52}$$

*where $A^\epsilon(t), B^\epsilon(t)$ satisfy:*

$$\begin{aligned} &\dot{A}^\epsilon(t) = D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t)) B^\epsilon(t), \quad \dot{B}^\epsilon(t) = -D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) A^\epsilon(t), \\ &A^\epsilon(0) = A_0, B^\epsilon(0) = B_0. \end{aligned} \tag{2.1.53}$$

2. *After the change of variables (2.1.48), the full coupled system governing $(\mathscr{Q}^\epsilon, \mathscr{P}^\epsilon, A^\epsilon(t), B^\epsilon(t))$ governed by (2.1.46) (with $o(\epsilon)$ terms dropped) and (2.1.53), is expressible as a Hamiltonian system:*

$$\begin{aligned} &\dot{\mathscr{Q}}^\epsilon = \nabla_{\mathscr{P}^\epsilon} \mathcal{H}^\epsilon, \dot{\mathscr{P}}^\epsilon = -\nabla_{\mathscr{Q}^\epsilon} \mathcal{H}^\epsilon \\ &\dot{A}^\epsilon(t) = 4\frac{\partial \mathcal{H}^\epsilon}{\partial \overline{B^\epsilon}}, \dot{B}^\epsilon(t) = -4\frac{\partial \mathcal{H}^\epsilon}{\partial \overline{A^\epsilon}} \end{aligned} \tag{2.1.54}$$

*with Hamiltonian:*

$$\begin{aligned} \mathcal{H}^\epsilon(\mathscr{P}^\epsilon, \mathscr{Q}^\epsilon, \overline{A^\epsilon}, A^\epsilon, \overline{B^\epsilon}, B^\epsilon) &:= E_n(\mathscr{P}^\epsilon) + W(\mathscr{Q}^\epsilon) + \epsilon \nabla_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) \cdot \mathcal{A}_n(\mathscr{P}^\epsilon) \\ &+ \epsilon \frac{1}{4} Tr\left[ (\overline{B^\epsilon})^T D^2_{\mathcal{P}^\epsilon} E_n(\mathscr{P}^\epsilon) B^\epsilon \right] + \epsilon \frac{1}{4} Tr\left[ (\overline{A^\epsilon})^T D^2_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) A^\epsilon \right]. \end{aligned} \tag{2.1.55}$$

**Remark 2.1.14.** *In the special case where the periodic background potential $V = 0$ the Bloch band dispersion function $E_n(\mathscr{P}^\epsilon)$ reduces to the 'free' dispersion relation $\frac{1}{2}(\mathscr{P}^\epsilon)^2$ and the Hamiltonian (2.1.55) takes on the simple form:*

$$\begin{aligned} \mathcal{H}^\epsilon(\mathscr{P}^\epsilon, \mathscr{Q}^\epsilon, \overline{A^\epsilon}, A^\epsilon, \overline{B^\epsilon}, B^\epsilon) &:= \frac{1}{2}(\mathscr{P}^\epsilon)^2 + W(\mathscr{Q}^\epsilon) \\ &+ \epsilon \frac{1}{4} Tr\left[ (\overline{A^\epsilon})^T D^2_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) A^\epsilon \right] + \epsilon \frac{1}{4} Tr\left[ (\overline{B^\epsilon})^T B^\epsilon \right]. \end{aligned} \tag{2.1.56}$$

*The system (2.1.54), with Hamiltonian* $\mathcal{H}^\epsilon$ *given by (2.1.56) has been derived by other methods: see Proposition 4.4 and equations (32b)-(32c) of Ref. [55]. It was shown furthermore in Ref. [56] that corrections to the dynamics of* $\mathscr{Q}^\epsilon, \mathscr{P}^\epsilon$ *proportional to* $\epsilon$ *due to 'field-particle' coupling to the* $A^\epsilon, B^\epsilon$ *system can lead to qualitatively different dynamical behavior. In particular, the coupling may destabilize periodic orbits of the unperturbed (*$\epsilon = 0$*) system; see Section 9 of Ref. [56].*

**Remark 2.1.15.** *In Remark 2.1.7 we commented that the general timescale of validity of our results is up to 'Ehrenfest time'* $t \sim \ln 1/\epsilon$*, and that under further assumptions on the classical dynamics we expect that this time-scale may be extended up to* $t = o(1/\sqrt{\epsilon})$*. Note that the Berry curvature terms and the new 'field-particle' coupling terms occur at the same order in* $\epsilon$*. It is an interesting question to determine their impact on the dynamics for* $t$ *greater than the 'Ehrenfest time'.*

### 2.1.5 Discussion of results, relation to previous work

The $\epsilon \downarrow 0$ limit of (2.1.1) has been studied by other methods. For example, by space-adiabatic perturbation theory [57; 58; 72; 70], and by studying the propagation of Wigner functions associated to the solution of (2.1.1) [51; 4; 10]. The Wigner function approach is notable in that it has been used to study the propagation of wavepacket solutions of (2.1.1) through band crossings [48; 32]. It was shown in Ref. [23] that the anomalous velocity due to Berry curvature can be derived by a multiscale WKB-like ansatz by studying the characteristic equations of a corrected eikonal equation. The Hamiltonian structure of equations (2.1.46) without field-particle coupling terms was studied in Ref. [22]

The effective system (2.1.46), in particular the 'particle-field' coupling that we derive, is original to this work. Such coupled 'particle-field' models arise naturally in many settings where a coherent structure interacts with a linear or nonlinear wave-field; see, for example Ref. [74] and references therein.

The results detailed in Section 3.2 generalize to the case where the potential has the more general form $U\left(\frac{x}{\epsilon}, x\right)$ where $U$ is periodic in its first argument:

$$U(z + v, x) = U(z, x) \text{ for all } z, x \in \mathbb{R}^d, v \in \Lambda. \tag{2.1.57}$$

If $U(z, x)$ is not expressible as the sum of a periodic potential $V(z)$ and a smooth potential $W(x)$ we will say that $U$ is 'non-separable'. In this case we must work with an $x$-dependent Bloch eigenvalue problem:

$$\begin{aligned}
&H(p,x)\chi_n(z;p,x) = E_n(p,x)\chi_n(z;p,x) \\
&\chi_n(z+v;p,x) = \chi_n(z;p,x) \text{ for all } z,x \in \mathbb{R}^d, v \in \Lambda \\
&H(p,x) := \frac{1}{2}(p - i\nabla_z)^2 + U(z,x).
\end{aligned} \tag{2.1.58}$$

For details, see Section 2.5. Related problems were considered in Refs. [43; 65]. An interesting example of a potential of this type is that of a domain wall modulated honeycomb lattice potential, which was shown to support 'topologically protected' edge states in Ref. [26].

### 2.1.6 Notation and conventions

- Where necessary to avoid ambiguity we will use index notation, making the standard convention that repeated indices are summed over from 1 to $d$ where $d$ is the spatial dimension. Thus, in the expression:

$$\partial_{p_\alpha}\partial_{p_\beta} f(p)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})g(y), \tag{2.1.59}$$

  it is understood that we are summing over $\alpha \in \{1,...,d\}, \beta \in \{1,...,d\}$.

- Where there is no danger of confusion we will use the standard conventions:

$$v_\beta w_\beta = v \cdot w, v_\beta v_\beta = v \cdot v \tag{2.1.60}$$

- $\Delta_x = \nabla_x^2$ denotes the $d-$dimensional Laplacian

- $D_x^2$ denotes the $d-$dimensional Hessian matrix with respect to $x$

- We will adopt multi-index notation where appropriate so that:

$$\sum_{|\alpha|=l} |\partial_x^\alpha f(x)| \in L^\infty(\mathbb{R}^d) \tag{2.1.61}$$

  means all derivatives of order $l$ of $f(x)$ are uniformly bounded.

- It will be useful to introduce the energy spaces for every $l \in \mathbb{N}$:

$$\Sigma^l(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) : \|f\|_{\Sigma^l} := \sum_{|\alpha|+|\beta|\leq l} \|y^\alpha(-i\partial_y)^\beta f(y)\|_{L^2_y} < \infty, \right\} \tag{2.1.62}$$

- The space of Schwartz functions $\mathcal{S}(\mathbb{R}^d)$ is the space of functions defined as:

$$\mathcal{S}(\mathbb{R}^d) := \cap_{l \in \mathbb{N}} \Sigma^l(\mathbb{R}^d). \tag{2.1.63}$$

- We will refer throughout to the space of $L^2$-integrable functions which are periodic on the lattice $\Lambda$:

$$L^2_{per} := \left\{ f \in L^2_{loc}(\mathbb{R}^d) : \text{ for all } z \in \mathbb{R}^d, v \in \Lambda, f(z+v) = f(z) \right\}. \tag{2.1.64}$$

- We will write a fundamental period cell in $\mathbb{R}^d$ of the lattice $\Lambda$ as $\Omega$.

- We will make use of the Sobolev norms on a fundamental period cell $\Omega$ for integers $s \geq 0$:

$$\|f(z)\|_{H^s_z} := \sum_{|j| \leq s} \|(\partial_z)^j f(z)\|_{L^2_z}. \tag{2.1.65}$$

- It will also be useful to introduce the 'shifted' Sobolev norms, for arbitrary $p \in \mathbb{R}^d$:

$$\|f(z)\|_{H^s_{z,p}} := \sum_{|j| \leq s} \|(p - i\partial_z)^j f(z)\|_{L^2_z} \tag{2.1.66}$$

- Define the dual lattice to $\Lambda$:

$$\Lambda^* := \left\{ b \in \mathbb{R}^d : \exists v \in \Lambda : b \cdot v = 2\pi n, n \in \mathbb{Z} \right\} \tag{2.1.67}$$

- We will refer to a fundamental cell in $\mathbb{R}^d_p$ of the dual lattice $\Lambda^*$ as the Brillouin zone, or $\mathcal{B}$

- We make the standard convention for the $L^2$-inner product:

$$\langle f | g \rangle_{L^2(\mathcal{D})} := \int_{\mathcal{D}} \overline{f(x)} g(x) \, \mathrm{d}x \tag{2.1.68}$$

- We will make the conventions:

$$\begin{aligned} &f^\epsilon(x,t) = O(\epsilon^K e^{ct}) \iff \exists c > 0, C > 0, \text{ independent of } t, \epsilon \text{ such that } \|f^\epsilon(x,t)\|_{L^2_x} \leq C\epsilon^K e^{ct} \\ &g^\epsilon(t) = O(\epsilon^K e^{ct}) \iff \exists c > 0, C > 0, \text{ independent of } t, \epsilon \text{ such that } |g^\epsilon(t)| \leq C\epsilon^K e^{ct} \end{aligned} \tag{2.1.69}$$

- Let $A$ be a complex matrix. Then we will write $A^T$ for its transpose, $\overline{A}$ for its complex conjugate, and $\mathrm{Tr}A$ for its trace. Using index notation:

$$(A_{\alpha\beta})^T := A_{\beta\alpha}, \quad (\overline{A})_{\alpha\beta} := \overline{A_{\alpha\beta}}, \quad \mathrm{Tr}A := A_{\alpha\alpha} \tag{2.1.70}$$

- The Kronecker delta $\delta_{\alpha\beta}$ is defined:

$$\delta_{\alpha\beta} = \begin{cases} +1 & \text{when } \alpha = \beta \\ 0 & \text{when } \alpha \neq \beta \end{cases} \tag{2.1.71}$$

- In dimension $d = 3$, the Levi-Civita symbol $\varepsilon_{\alpha\beta\gamma}$ is defined:

$$\varepsilon_{\alpha\beta\gamma} := \begin{cases} +1 & \text{when } (\alpha,\beta,\gamma) \in \{(1,2,3),(2,3,1),(3,1,2)\} \\ -1 & \text{when } (\alpha,\beta,\gamma) \in \{(1,3,2),(2,3,1),(3,2,1)\} \\ 0 & \text{when } \alpha = \beta, \beta = \gamma, \text{ or } \gamma = \alpha \end{cases} \tag{2.1.72}$$

  and satisfies the identities:

$$\begin{aligned} &\varepsilon_{\alpha\beta\gamma} = \varepsilon_{\beta\gamma\alpha} = \varepsilon_{\gamma\alpha\beta} \\ &\varepsilon_{\phi\alpha\beta}\varepsilon_{\phi\gamma\phi} = \delta_{\alpha\gamma}\delta_{\beta\phi} - \delta_{\beta\gamma}\delta_{\alpha\phi}. \end{aligned} \tag{2.1.73}$$

  The cross product of 3-vectors $v, w$ may then be written:

$$(v \times w)_\alpha = \epsilon_{\alpha\beta\gamma} v_\beta w_\gamma \tag{2.1.74}$$

## 2.2 Summary of relevant Floquet-Bloch theory

In this section we recall the spectral theory of the operator:

$$H := -\frac{1}{2}\Delta_z + V(z). \tag{2.2.1}$$

where $V$ is periodic with respect to the lattice $\Lambda$ [46; 63]. For $p \in \mathbb{R}^d$, define the spaces of $p-$pseudo-periodic $L^2$ functions as follows:

$$L^2_p := \left\{ f \in L^2_{loc} : f(z+v) = e^{ip\cdot v} f(z) \text{ for all } z \in \mathbb{R}^d, v \in \Lambda \right\}. \tag{2.2.2}$$

Let $\Lambda^*$ denote the lattice dual to $\Lambda$:

$$\Lambda^* := \left\{ b \in \mathbb{R}^d : \exists v \in \Lambda : v \cdot b = 2\pi n, n \in \mathbb{Z} \right\} \tag{2.2.3}$$

since the $p-$pseudo-periodic boundary condition is invariant under $p \to p + b$ where $b \in \Lambda^*$, the dual lattice to $\Lambda$, it is natural to restrict to a fundamental cell, $\mathcal{B}$.

We now consider the family of eigenvalue problems depending on the parameter $p \in \mathcal{B}$:

$$\begin{aligned} &H\Phi(z;p) = E(p)\Phi(z;p) \\ &\Phi(z+v;p) = e^{ip\cdot v}\Phi(z;p) \text{ for all } z \in \mathbb{R}^d, v \in \Lambda \end{aligned} \tag{2.2.4}$$

We can also define the space $L^2_{loc}$ functions which are periodic with respect to the lattice:

$$L^2_{per} := \left\{ f(z) \in L^2_{loc}(\mathbb{R}^d) : \forall v \in \Lambda, f(z+v) = f(z) \right\}. \tag{2.2.5}$$

Then solving the eigenvalue problem (2.2.4) is equivalent via $\Phi(z;p) = e^{ip\cdot z}\chi(z;p)$ to solving the family of eigenvalue problems:

$$\begin{aligned} &H(p)\chi(z;p) = E(p)\chi(z;p), \\ &\chi(z+v;p) = \chi(z;p) \text{ for all } z \in \mathbb{R}^d, v \in \Lambda \\ &H(p) = \frac{1}{2}\left(p - i\nabla_z\right)^2 + V(z) \end{aligned} \tag{2.2.6}$$

For fixed $p$, the operator $H(p)$ with periodic boundary conditions is self-adjoint and has compact resolvent. So, for each $n \in \mathbb{N}$, there exists an eigenpair $E_n(p), \chi_n(z;p)$. The eigenvalues are real and can be ordered with multiplicity:

$$E_1(p) \le E_2(p) \le ... \le E_{n-1}(p) \le E_n(p) \le E_{n+1}(p) \le ... \tag{2.2.7}$$

and the set of normalized eigenfunctions $\{\chi_n(z;p) : n \in \mathbb{N}\}$ is complete in $L^2_{per}$. The set of Floquet-Bloch waves $\left\{\Phi_n(z;p) = e^{ipz}\chi_n(z;p) : n \in \mathbb{N}, p \in \mathcal{B}\right\}$ are complete in $L^2(\mathbb{R}^d)$:

$$g \in L^2(\mathbb{R}^d) \implies g(x) = \sum_{n\ge1} \int_{\mathbb{B}} \tilde{g}_n(p)\Phi_n(x;p)\,\mathrm{d}p, \text{ where } \tilde{g}_n(p) := \langle\, \Phi_n(\cdot;p) |\, g(\cdot)\rangle_{L^2(\mathbb{R}^d)} \tag{2.2.8}$$

where the sum converges in $L^2$. The $L^2(\mathbb{R}^d)$ spectrum of the operator (2.2.1) is obtained by taking the union of the closed real intervals swept out as $p$ varies over the Brillouin zone $\mathcal{B}$:

$$\sigma(H)_{L^2(\mathbb{R}^d)} = \cup_{n\in\mathbb{R}}\overline{\{E_n(p) : p \in \mathcal{B}\}} \tag{2.2.9}$$

Our results require sufficient regularity of the maps:

$$E_n : \mathcal{B} \to \mathbb{R}, \qquad p \mapsto E_n(p) \tag{2.2.10}$$

$$\chi_n : \mathcal{B} \to L^2_{per}, \qquad p \mapsto \chi_n(z;p) \tag{2.2.11}$$

**Definition 2.2.1.** *We will call an eigenvalue band $E_n(p)$ of the problem (2.2.6)* isolated *at a point $p \in \mathcal{B}$ if:*

$$\inf_{m \neq n} |E_m(p) - E_n(p)| > 0. \tag{2.2.12}$$

We have in this case:

**Theorem 2.2.1** (Smoothness of isolated bands)**.** *Let $E_n(p), \chi_n(z;p)$ satisfy the eigenvalue problem (2.2.6). Let the band $E_n(p)$ be isolated at a point $p_0$ in the sense of Definition 2.2.1. Then the maps (2.2.10) are smooth in a neighborhood of the point $p_0$.*

When bands are not isolated we have the following situation:

**Definition 2.2.2.** *Let $E_m(p), E_n(p) : m, n \in \mathbb{N}, m \neq n$ be eigenvalue bands of the eigenvalue problem (2.2.6). If $p^* \in \mathcal{B}$ is such that:*

$$E_m(p^*) = E_n(p^*), \tag{2.2.13}$$

*we will say that the bands $E_n(p)$ and $E_m(p)$ have a* band crossing *at $p^*$.*

In a neighborhood of a crossing, the band functions $E_n(p), E_m(p)$ are only Lipschitz continuous, and the eigenfunction maps $p \mapsto \chi_n(z;p), \chi_m(z;p)$ may be discontinuous [46]. This loss of regularity occurs at conical degeneracies, which appear, for example, in the band structure of honeycomb lattice potentials [28; 29], and in the dispersion surfaces of plane waves for homogeneous anisotropic media [6]. An in depth study of conical crossings which appear in the study of the Born-Oppenheimer approximation of molecular dynamics was given in Ref. [37].

It will be convenient to extend the maps $p \mapsto E_n(p), \chi_n(z;p)$ to maps on all of $\mathbb{R}^d$. Let $p \in \mathcal{B}$, and let $b \in \Lambda^*$ denote a reciprocal lattice vector. Then we have that:

$$\begin{aligned} &H(p+b)\left(e^{-ib\cdot z}\chi_n(z;p)\right) = e^{-ib\cdot z}H(p)\chi_n(z;p) \\ &\quad = e^{-ib\cdot z}E_n(p)\chi_n(z;p) = E_n(p)\left(e^{-ib\cdot z}\chi_n(z;p)\right) \\ &\text{for all } v \in \Lambda,\ e^{-ib\cdot(z+v)}\chi_n(z+v;p) \\ &\quad = e^{-ib\cdot v}e^{-ib\cdot z}\chi_n(z;p) = e^{-ib\cdot z}\chi_n(z;p), \end{aligned} \tag{2.2.14}$$

so that if $\chi_n(z;p)$ satisfies (2.2.6) with eigenvalue $E_n(p)$, then $e^{-ib\cdot z}\chi_n(z;p)$ satisfies (2.2.6) with $p$ replaced by $p+b$, with the same eigenvalue. It then follows that the map $p \mapsto E_n(p)$ extends to a periodic function with respect to the reciprocal lattice $\Lambda^*$. If the eigenvalue $E_n(p)$ is simple, then: (up to a constant phase shift) $\chi_n(z;p+b) = e^{-ib\cdot z}\chi_n(z;p)$.

## 2.3 Proof of Theorem 2.1.1 by multiscale analysis

### 2.3.1 Derivation of asymptotic solution (2.1.29) via multiscale expansion

Following Hagedorn [36; 37], and Carles and Sparber [61], we seek a solution of (2.1.1) of the form:

$$\psi^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} f^\epsilon(y,z,t)\Big|_{z=\frac{x}{\epsilon},y=\frac{x-q(t)}{\epsilon^{1/2}}} + \eta^\epsilon(x,t). \tag{2.3.1}$$

Substituting (2.3.1) into (2.1.1) gives an inhomogeneous time-dependent Schrödinger equation for $\eta^\epsilon(x,t)$, with a source term $r^\epsilon(x,t)$ which depends on $S(t), q(t), p(t)$, and $f^\epsilon(y,z,t)$:

$$\begin{aligned} i\epsilon\partial_t \eta^\epsilon(x,t) &= \left[ -\frac{\epsilon^2}{2}\Delta_x + V\left(\frac{x}{\epsilon}\right) + W(x) \right] \eta^\epsilon(x,t) + r^\epsilon[S,q,p,f^\epsilon](x,t) \\ \eta^\epsilon(x,0) &= \eta_0^\epsilon[S,q,p,f^\epsilon](x) = \psi^\epsilon(x,0) - \epsilon^{-d/4} e^{iS(0)/\epsilon} e^{ip(0)\cdot y/\epsilon^{1/2}} f^\epsilon(z,y,0)\Big|_{z=\frac{x}{\epsilon},y=\frac{x-q(0)}{\epsilon^{1/2}}} \end{aligned} \tag{2.3.2}$$

The idea behind the proof of Theorem 2.1.1 is to choose the functions $S(t), q(t), p(t)$, and $f^\epsilon(y,z,t)$ so that:

$$\begin{aligned} r^\epsilon[S,q,p,f^\epsilon](x,t) &= O(\epsilon^2) \\ \eta_0^\epsilon[S,q,p,f^\epsilon](x) &= O(\epsilon) \end{aligned} \tag{2.3.3}$$

We will derive $S(t), q(t), p(t), f^\epsilon(y,z,t)$ by a systematic formal analysis. This is the content of Sections 2.3.1.1, 2.3.1.2, 2.3.1.3. Proving rigorous bounds on the residual will be the content of Section 2.3.2. The bound (2.1.30) on $\eta^\epsilon(x,t)$ will then follow from applying the standard a priori $L^2$ bound for solutions of the time-dependent inhomogeneous Schrödinger equation.

Before starting on the formal asymptotic analysis, we note some exact manipulations which will ease calculations below. The residual $r^\epsilon(x,t)$ has the explicit form:

$$\begin{aligned} r^\epsilon(x,t) &= \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} \Bigg\{ \epsilon \left[ \frac{1}{2}(-i\nabla_y)^2 - i\partial_t \right] \\ &+ \epsilon^{1/2} \left[ (p(t) - i\nabla_z)\cdot(-i\nabla_y) - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y \right] \\ &+ \left[ \dot{S}(t) - \dot{q}(t)p(t) + \frac{1}{2}(p(t) - i\nabla_z)^2 + V(z) + W(q(t) + \epsilon^{1/2}y) \right] \Bigg\} f^\epsilon(y,z,t)\Big|_{z=\frac{x}{\epsilon},y=\frac{x-q(t)}{\epsilon^{1/2}}} \end{aligned} \tag{2.3.4}$$

Since $W$ is assumed smooth, we can replace $W(q(t)+\epsilon^{1/2}y)$ by its Taylor series expansion in $\epsilon^{1/2}y$:

$$\begin{aligned} W(q(t) + \epsilon^{1/2}y) &= W(q(t)) + \epsilon^{1/2}\nabla_q W(q(t))\cdot y + \epsilon\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta} W(q(t)) y_\alpha y_\beta \\ &+ \epsilon^{3/2}\frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma + \epsilon^2 \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t) + \tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma y_\delta. \end{aligned} \tag{2.3.5}$$

We expand $f^\epsilon(y,z,t)$ as a formal power series:

$$f^\epsilon(y,z,t) = f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + ... \tag{2.3.6}$$

and assume that for all $j \in \{0,1,2,...\}$ the $f^j(y,z,t)$ are periodic with respect to the lattice in $z$ and have sufficient smoothness and decay in $y$:

$$\begin{aligned} &\text{for all } v \in \Lambda, f^j(y,z+v,t) = f^j(y,z,t) \\ &f^j(y,z,t) \in \Sigma_y^{R-j}(\mathbb{R}^d). \end{aligned} \tag{2.3.7}$$

The $\Sigma^l$-spaces are defined in (2.1.62). $R > 0$ is a fixed positive integer which we will take as large as required. Recall the notation:

$$H(p) := \frac{1}{2}(p - i\nabla_z)^2 + V(z). \tag{2.3.8}$$

Substituting (2.3.5) and (2.3.6) then gives:

$$\begin{aligned} r^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} \Bigg\{ \epsilon^2 \left[ \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma y_\delta \right] \\ + \epsilon^{3/2}\left[\frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma\right] + \epsilon\left[\frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta} W(q(t)) y_\alpha y_\beta - i\partial_t\right] \\ + \epsilon^{1/2}\left[(p(t) - i\nabla_z)\cdot(-i\nabla_y) + \nabla_q W(q(t))\cdot y - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y\right] \\ + \left[\dot{S}(t) - \dot{q}(t)\cdot p(t) + H(p(t))\right]\Bigg\} \left\{ f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + ... \right\}\Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} \end{aligned} \tag{2.3.9}$$

In order to prove Theorem 2.1.1 it will be sufficient to choose the $f^j(y,z,t), j \in \{0,...,3\}$ so that terms of orders $\epsilon^{j/2}, j \in \{0,...,3\}$ vanish. With this choice of $f^j, j \in \{0,...,3\}$ we will then prove rigorously in Section 2.3.2 that $r^\epsilon(x,t)$ can be bounded by $C\epsilon^2 e^{ct}$ for constants $c > 0, C > 0$ independent of $\epsilon, t$. There will then be no loss of accuracy in the approximation by taking $f^j(y,z,t) = 0, j \geq 4$.

#### 2.3.1.1 Analysis of leading order terms

Recall that we assume each $f^j, j \in \{0,1,2,...\}$ to be periodic with respect to the lattice $\Lambda$ in $z$ (2.3.7). Collecting terms of order 1 in (2.3.9) and setting equal to zero therefore gives the following self-adjoint elliptic eigenvalue problem in $z$:

$$\begin{aligned} &H(p(t))f^0(y,z,t) = \left[-\dot{S}(t) + \dot{q}(t)\cdot p(t)\right] f^0(y,z,t) \\ &\text{for all } v \in \Lambda, f^0(y,z+v,t) = f^0(y,z,t) \\ &f^0(y,z,t) \in \Sigma_y^R(\mathbb{R}^d) \end{aligned} \tag{2.3.10}$$

Under Assumption 2.1.1, $E_n(p(t))$ is a simple eigenvalue with eigenfunction $\chi_n(z;p(t))$ for all $t \geq 0$. Projecting equation (2.3.10) onto the subspace of:

$$L^2_{per} := \left\{ f \in L^2_{loc}(\mathbb{R}^d) : \forall v \in \Lambda, f(z+v) = f(z) \right\}. \tag{2.3.11}$$

spanned by $\chi_n(z;p(t))$ implies:

$$\dot{S}(t) = \dot{q}(t)\cdot p(t) - E_n(p(t)) \tag{2.3.12}$$

which, after matching with the initial data (2.1.28), implies (2.1.21). Equation (2.3.10) then becomes:

$$\begin{aligned} &\left[H(p(t)) - E_n(p(t))\right] f^0(y,z,t) = 0 \\ &\text{for all } v \in \Lambda, f^0(y,z+v,t) = f^0(y,z,t) \\ &f^0(y,z,t) \in \Sigma_y^R(\mathbb{R}^d) \end{aligned} \tag{2.3.13}$$

which has the general solution:

$$f^0(y,z,t) = a^0(y,t)\chi_n(z;p(t)). \tag{2.3.14}$$

where $a^0(y,t)$ is an arbitrary function in $\Sigma_y^R(\mathbb{R}^d)$, to be fixed at higher order in the expansion.

#### 2.3.1.2 Analysis of order $\epsilon^{1/2}$ terms

Collecting terms of order $\epsilon^{1/2}$ in (2.3.9), substituting the form of $\dot{S}(t)$ (2.3.12), and setting equal to zero gives the following inhomogeneous self-adjoint elliptic equation in $z$ for $f^1(y,z,t)$:

$$\begin{aligned} &\left[H(p(t)) - E_n(p(t))\right] f^1(y,z,t) = \xi^1(y,z,t) \\ &\text{for all } z \in \Lambda, f^1(y,z+v,t) = f^1(y,z,t);\ f^1(y,z,t) \in \Sigma_y^{R-1}(\mathbb{R}^d) \\ &\xi^1 := -\left[(p(t) - i\nabla_z)\cdot(-i\nabla_y) + \nabla_q W(q(t))\cdot y - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y\right] f^0(y,z,t). \end{aligned} \tag{2.3.15}$$

Before solving (2.3.15) we remark on our general strategy for solving equations of this type.

**Remark 2.3.1.** *Collecting terms of orders $\epsilon^{j/2}$ for each $j \in \{1, 2, ...\}$ and setting equal to zero, we obtain inhomogeneous self-adjoint elliptic equations of the form:*

$$\begin{aligned} &[H(p(t)) - E_n(p(t))]\, f^j(y,z,t) = \xi^j[f^0, f^1, ..., f^{j-1}](y,z,t) \\ &\text{for all } z \in \Lambda, f^j(y, z+v, t) = f^j(y,z,t);\ f^j(y,z,t) \in \Sigma_y^{R-j}(\mathbb{R}^d) \end{aligned} \tag{2.3.16}$$

*Our strategy for solving (2.3.16) will be the same for each $j$. Under Assumption 2.1.1, the eigenvalue $E_n(p(t))$ is simple with eigenfunction $\chi_n(z;p(t))$ for all $t \geq 0$. By the Fredholm alternative, equation (2.3.16) is solvable if and only if:*

$$\text{for all } t \geq 0, \left\langle \chi_n(z;p(t)) \middle| \, \xi^j(y,z,t) \right\rangle_{L^2_z(\Omega)} = 0. \tag{2.3.17}$$

*We will first use identities derived in Appendix A.1 from the eigenvalue equation:*

$$[H(p) - E_n(p)]\chi_n(z;p) = 0 \tag{2.3.18}$$

*to write $\xi^j(y,z,t)$ as a sum:*

$$\xi^j(y,z,t) = \tilde{\xi}^j(y,z,t) + [H(p(t)) - E_n(p(t))]\, u^j(y,z,t) \tag{2.3.19}$$

*Note that by self-adjointness of $H(p(t)) - E_n(p(t))$, condition (2.3.17) is equivalent to the same condition with $\xi^j(y,z,t)$ replaced by $\tilde{\xi}^j(y,z,t)$:*

$$\text{for all } t \geq 0, \left\langle \chi_n(z;p(t)) \middle| \, \tilde{\xi}^j(y,z,t) \right\rangle_{L^2_z(\Omega)} = 0. \tag{2.3.20}$$

*For $f \in L^2_{per}$, define:*

$$P_n^{\perp}(p) f(z) := f(z) - \langle \chi_n(z;p) | \, f(z) \rangle_{L^2_z(\Omega)} \, \chi_n(z;p) \tag{2.3.21}$$

*to be the projection onto the orthogonal complement of the subspace of $L^2_{per}$ spanned by $\chi_n(z;p(t))$. Then, assuming (2.3.20) is satisfied, the general solution of (2.3.16) is:*

$$f^j(y,z,t) = a^j(y,t)\chi_n(z;p(t)) + u^j(y,z,t) + [H(p(t)) - E_n(p(t))]^{-1} P_n^{\perp}(p(t))\tilde{\xi}^j(y,z,t). \tag{2.3.22}$$

*Note that we have again made use of Assumption 2.1.1 to ensure that the operator $[H(p(t)) - E_n(p(t))]^{-1} P_n^{\perp}(p(t)) : L^2_{per} \to L^2_{per}$ is bounded for all $t \geq 0$. When $j = 1$, condition (2.3.20) may be enforced by choosing $\dot{q}(t), \dot{p}(t)$ to satisfy (2.1.19). For $j \geq 2$, enforcing the constraint (2.3.20) leads to evolution equations for $a^{j-2}(y,t)$.*

We will give the proof of the following Lemma at the end of this section:

**Lemma 2.3.1.** *$\xi^1(y,z,t)$, defined in (2.3.15), satisfies:*

$$\xi^1(y,z,t) = \tilde{\xi}^1(y,z,t) + \left[H(p(t)) - E_n(p(t))\right] u^1(y,z,t) \tag{2.3.23}$$

*where:*

$$\begin{aligned} &\tilde{\xi}^1(y,z,t) := \\ &-\left[(\nabla_p E_n(p(t)) - \dot{q}(t)) \cdot (-i\nabla_y) a^0(y,t) + (\nabla_q W(q(t)) + \dot{p}(t)) \cdot y a^0(y,t)\right] \chi_n(z;p(t)) \\ &u^1(y,z,t) := (-i\nabla_y) a^0(y,t) \cdot \nabla_p \chi_n(z;p(t)) \end{aligned} \tag{2.3.24}$$

The solvability condition of (2.3.15), given by (2.3.20) with $j = 1$ on $\tilde{\xi}^1(y,z,t)$ (2.3.24) is then equivalent to:

$$(\nabla_p E_n(p(t)) - \dot{q}(t)) \cdot (-i\nabla_y) a^0(y,t) + (\nabla_q W(q(t)) + \dot{p}(t)) \cdot y a^0(y,t) = 0 \tag{2.3.25}$$

which we can satisfy by choosing $(q(t), p(t))$ to evolve as the Hamiltonian flow of the $n$th Bloch band Hamiltonian $\mathcal{H}_n(q,p) = E_n(p) + W(q)$:

$$\dot{q}(t) = \nabla_p E_n(p(t)), \dot{p}(t) = -\nabla_q W(q(t)). \tag{2.3.26}$$

Taking $q(0), p(0) = q_0, p_0$ to match with the initial data (2.1.28) implies (2.1.19).

The general solution of (2.3.15) is given by taking $j = 1$ in (2.3.22), where $u^1, \tilde{\xi}^1$ are given by (2.3.24). With the choice (2.3.26) for $\dot{q}(t), \dot{p}(t)$ we have that $\tilde{\xi}^1 = 0$ for all $t \geq 0$ so that the general solution reduces to:

$$f^1(y,z,t) = a^1(y,t)\chi_n(z;p(t)) + (-i\nabla_y) a^0(y,t) \cdot \nabla_p \chi_n(z;p(t)) \tag{2.3.27}$$

where $a^1(y,t)$ is an arbitrary function in $\Sigma_y^{R-1}(\mathbb{R}^d)$ to be fixed at higher order in the expansion. Note that since $a^0(y,t) \in \Sigma_y^R(\mathbb{R}^d)$, this ensures that $f^1(y,z,t) \in \Sigma_y^{R-1}(\mathbb{R}^d)$ as required.

*Proof of Lemma 2.3.1.* By Assumption 2.1.1, $E_n(p)$ is smooth in a neighborhood of $p(t)$. By adding and subtracting $\nabla_p E_n(p(t)) \cdot (-i\nabla_y) f^0(y,z,t)$, $\xi^1(y,z,t)$ is equal to:

$$\begin{aligned} \xi^1(y,z,t) = &-\left[((p(t) - i\nabla_z) - \nabla_p E_n(p(t))) \cdot (-i\nabla_y)\right] f^0(y,z,t) \\ &-\left[(\nabla_p E_n(p(t)) - \dot{q}(t)) \cdot (-i\nabla_y)\right] f^0(y,z,t) - \left[(\nabla_q W(q(t)) + \dot{p}(t)) \cdot y\right] f^0(y,z,t) \end{aligned} \tag{2.3.28}$$

Substituting the explicit form of $f^0(y,z,t)$ (2.3.14) into (2.3.28) we have:

$$\begin{aligned}\xi^1(y,z,t) &= -(-i\nabla_y)a^0(y,t)\cdot[(p(t)-i\nabla_z)-\nabla_p E_n(p(t))]\,\chi_n(z;p(t)) \\ &- (-i\nabla_y)a^0(y,t)\cdot[\nabla_p E_n(p(t))-\dot{q}(t)]\,\chi_n(z;p(t)) - y a^0(y,t)\cdot[\nabla_q W(q(t))+\dot{p}(t)]\,\chi_n(z;p(t)).\end{aligned} \tag{2.3.29}$$

(2.3.24) then follows immediately from identity (A.1.2). □

#### 2.3.1.3 Analysis of order $\epsilon$ and $\epsilon^{3/2}$ terms (summary)

It is possible to continue the procedure outlined in Remark 2.3.1 to any order in $\epsilon^{1/2}$. In Appendices A.2 and A.3 we show the details of how to continue the procedure in order to cancel terms in the expansion of orders $\epsilon$ and $\epsilon^{3/2}$. In particular, we derive the evolution equations of the amplitudes $a^0(y,t), a^1(y,t)$ and show that:

$$a^0(y,t) = a(y,t)e^{i\phi_B(t)},\, a^1(y,t) = b(y,t)e^{i\phi_B(t)} \tag{2.3.30}$$

where $a(y,t), b(y,t), \phi_B(t)$ satisfy equations (2.1.22), (2.1.24), and (2.1.27) respectively.

### 2.3.2 Proof of estimate (2.1.30) for the corrector $\eta$

Let:

$$f_3^\epsilon(y,z,t) := f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + \epsilon f^2(y,z,t) + \epsilon^{3/2} f^3(y,z,t) \tag{2.3.31}$$

Where the $f^0, f^1, f^2, f^3$ are given by (2.3.14), (2.3.27), (A.2.5), (A.3.5) respectively, and define:

$$\psi_3^\epsilon(x,t) := \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} f_3^\epsilon(y,z,t)\Big|_{z=\frac{x}{\epsilon},\, y=\frac{x-q(t)}{\epsilon^{1/2}}} \tag{2.3.32}$$

Let $\psi^\epsilon(x,t)$ denote the exact solution of the initial value problem (2.1.28). From the manipulations of the previous Section, we have that $\eta_3^\epsilon(x,t) := \psi^\epsilon(x,t) - \psi_3^\epsilon(x,t)$ satisfies:

$$\begin{aligned}&i\epsilon\partial_t \eta_3^\epsilon(x,t) = \left[-\frac{\epsilon^2}{2}\Delta_x + V\left(\frac{x}{\epsilon}\right) + W(x)\right]\eta_3^\epsilon(x,t) + r_3^\epsilon(x,t) \\ &\eta_3^\epsilon(x,0) = \eta_{3,0}^\epsilon(x)\end{aligned} \tag{2.3.33}$$

where $r_3^\epsilon(x,t)$ is given by:

$$
\begin{aligned}
r_3^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} \Big\{ & \epsilon^2 \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma y_\delta \\
& \cdot \Big( f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + \epsilon f^2(y,z,t) + \epsilon^{3/2} f^3(y,z,t) \Big) \\
& + \epsilon^2 \left[ \frac{1}{6} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma \right] \Big( f^1(y,z,t) + \epsilon^{1/2} f^2(y,z,t) + \epsilon f^3(y,z,t) \Big) \\
& + \epsilon^2 \left[ -i\partial_t + \frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2} \partial_{q_\alpha}\partial_{q_\beta} W(q(t)) y_\alpha y_\beta \right] \Big( f^2(y,z,t) + \epsilon^{1/2} f^3(y,z,t) \Big) \\
& + \epsilon^2 \Big[ ((p(t) - i\nabla_z) - \nabla_p E_n(p(t))) \cdot (-i\nabla_y) \Big] f^3(y,z,t) \Big\} \Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}}
\end{aligned}
\tag{2.3.34}
$$

And $\eta_{3,0}^\epsilon(x)$ is given by:

$$
\eta_{3,0}^\epsilon(x) = -\,\epsilon^{-d/4} e^{ip_0\cdot y/\epsilon^{1/2}} \left\{ \epsilon \left[ f^2(z,y,0) + \epsilon^{1/2} f^3(z,y,0) \right] \right\} \Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q_0}{\epsilon^{1/2}}} \tag{2.3.35}
$$

Since the $f^j(y,z,t), j \in \{0,...,3\}$ are periodic with respect to the lattice $\Lambda$, we will follow Carles and Sparber [61] and bound the above expressions in the uniform norm in $z$ and the $L^2$ norm in $y$:

$$
\begin{aligned}
& \|r_3^\epsilon(x,t)\|_{L^2_x} \leq \\
& = \Big\| \epsilon^2 \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma y_\delta \\
& \cdot \Big( f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + \epsilon f^2(y,z,t) + \epsilon^{3/2} f^3(y,z,t) \Big) \\
& + \epsilon^2 \left[ \frac{1}{6} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma \right] \Big( f^1(y,z,t) + \epsilon^{1/2} f^2(y,z,t) + \epsilon f^3(y,z,t) \Big) \\
& + \epsilon^2 \left[ -i\partial_t + \frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2} \partial_{q_\alpha}\partial_{q_\beta} W(q(t)) y_\alpha y_\beta \right] \Big( f^2(y,z,t) + \epsilon^{1/2} f^3(y,z,t) \Big) \\
& + \epsilon^2 \Big[ ((p(t) - i\nabla_z) - \nabla_p E_n(p(t))) \cdot (-i\nabla_y) \Big] f^3(y,z,t) \Big\|_{L^\infty_z, L^2_y} \\
& \|\eta_3^\epsilon(x,0)\|_{L^2_x} \leq \left\| \epsilon \left[ f^2(z,y,0) + \epsilon^{1/2} f^3(z,y,0) \right] \right\|_{L^\infty_z, L^2_y}
\end{aligned}
\tag{2.3.36}
$$

where we have used the fact that:

$$
\left\| \epsilon^{-d/4} f\left( \frac{x-q(t)}{\epsilon^{1/2}} \right) \right\|_{L^2_x} = \|f(y)\|_{L^2_y}. \tag{2.3.37}
$$

We show how to bound the first term in (2.3.36). Bounding the other terms is similar, although care must be taken in bounding terms in $L^\infty_z$, see Appendix A.4. Let:

$$
\mathcal{I}(t) := \epsilon^2 \left\| \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma y_\delta f^0(y,z,t) \right\|_{L^\infty_z, L^2_y} \tag{2.3.38}
$$

where $f^0(y,z,t) = a^0(y,t)\chi_n(z;p(t))$ (2.3.14). By Assumption 2.1.2, $\sum_{|\alpha|=4} |\partial_x^\alpha W(x)| \in L^\infty(\mathbb{R}^d)$:

$$\mathcal{I}(t) \leq \epsilon^2 \frac{1}{4!} \left\| \sum_{|\alpha|=4} |\partial_x^\alpha W(x)| \right\|_{L^\infty(\mathbb{R}^d)} \sum_{|\alpha|=4} \|y^\alpha a(y,t)\chi_n(z;p(t))\|_{L^\infty_z, L^2_y} \tag{2.3.39}$$

Recall Assumption 2.1.1. Define:

$$S_n := \{p \in \mathbb{R}^d : \inf_{m \neq n} |E_m(p) - E_n(p)| \geq M\}, \tag{2.3.40}$$

so that for all $t \in [0,\infty)$, $p(t) \in S_n$. For each fixed $p \in S_n$, by elliptic regularity, $\chi_n(z;p)$ is smooth in $z$ so that $\|\chi_n(z;p)\|_{L^\infty_z} < \infty$. Using compactness of the Brillouin zone $\mathcal{B}$ and smoothness of $\chi_n(z;p)$ for $p \in S_n$ we have that:

$$\sup_{p \in \mathcal{B} \cap S_n} \|\chi_n(z;p)\|_{L^\infty_z} < \infty. \tag{2.3.41}$$

Recall that for any reciprocal lattice vector $b \in \Lambda^*$, $\chi_n(z;p+b) = e^{-ib\cdot z}\chi_n(z;p)$. It then follows that:

$$\text{for all } b \in \Lambda^*, \quad \|\chi_n(z;p+b)\|_{L^\infty_z} = \|\chi_n(z;p)\|_{L^\infty_z} \tag{2.3.42}$$

It then follows from combining (2.3.41) and (2.3.42) that:

$$\sup_{p \in S_n} \|\chi_n(z;p)\|_{L^\infty_z} < \infty. \tag{2.3.43}$$

In Appendix A.4 we show how to bound all $z$-dependence in $r_3^\epsilon(x,t)$ (2.3.34) uniformly in $p \in S_n$ in a similar way.

We have therefore that (2.3.39):

$$\mathcal{I}(t) \leq \epsilon^2 \frac{1}{4!} \left\| \sum_{|\alpha|=4} |\partial_x^\alpha W(x)| \right\|_{L^\infty(\mathbb{R}^d)} \sup_{p \in S_n} \|\chi_n(z;p)\|_{L^\infty_z} \sum_{|\alpha|=4} \|y^\alpha a(y,t)\|_{L^2_y} \tag{2.3.44}$$

We see that to complete the bound, we require a bound on the 4th moments of $a(y,t)$, which solves the Schrödinger equation with time-dependent co-efficients:

$$\begin{aligned} i\partial_t a(y,t) &= \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a(y,t) \\ a(y,0) &= a_0(y) \end{aligned} \tag{2.3.45}$$

Following Carles and Sparber [61] we first define, for any $l \in \mathbb{N}$, the spaces:

$$\Sigma^l(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) : \|f\|_{\Sigma^l} := \sum_{|\alpha|+|\beta| \leq l} \|y^\alpha(-i\partial_y)^\beta f(y)\|_{L^2_y} < \infty, \right\} \tag{2.3.46}$$

We then require the following Lemma due to Kitada [45]:

**Lemma 2.3.2** (Existence of unitary solution operator for the envelope equation)**.** *Let* $u_0 \in L^2(\mathbb{R}^d)$*, and* $\eta_{\alpha\beta}(t), \zeta_{\alpha\beta}(t)$ *be real-valued, symmetric, continuous, and uniformly bounded in* $t$*. Then the equation:*

$$\begin{aligned} i\partial_t u &= \frac{1}{2}\eta_{\alpha\beta}(t)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})u + \frac{1}{2}\zeta_{\alpha\beta}(t)y_\alpha y_\beta u \\ u(y,0) &= u_0(y) \end{aligned} \tag{2.3.47}$$

*has a unique solution* $u \in C([0,\infty); L^2(\mathbb{R}^d))$*. It satisfies:*

$$\|u(\cdot,t)\|_{L^2(\mathbb{R}^d)} = \|u_0(\cdot)\|_{L^2(\mathbb{R}^d)} \tag{2.3.48}$$

*Moreover, if* $u_0 \in \Sigma^l(\mathbb{R}^d)$*, then* $u \in C([0,\infty); \Sigma^l(\mathbb{R}^d))$*.*

We seek quantitative bounds on $\|u(\cdot,t)\|_{\Sigma^l(\mathbb{R}^d)}$ for $l \geq 1$. For simplicity, we consider in detail the case $l = 1$. Recall (2.1.23):

$$\mathscr{H}(t) := \frac{1}{2}\eta_{\alpha\beta}(t)(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\zeta_{\alpha\beta}(t)y_\alpha y_\beta \tag{2.3.49}$$

and let $u_0(y) \in \mathcal{S}(\mathbb{R}^d)$ so that $\forall l \geq 0$, the solution of (2.3.47), $u(y,t) \in C([0,\infty); \Sigma^l(\mathbb{R}^d))$. Then $(-i\partial_{y_\alpha})u(y,t) \in \mathcal{S}(\mathbb{R})$ solves:

$$\begin{aligned} i\partial_t(-i\partial_{y_\alpha})u &= \mathscr{H}(t)(-i\partial_{y_\alpha})u + [(-i\partial_{y_\alpha}), \mathscr{H}(t)]u \\ (-i\partial_{y_\alpha})u(y,0) &= (-i\partial_{y_\alpha})u_0(y) \end{aligned} \tag{2.3.50}$$

We can solve this equation using Duhamel's formula and the solution operator of equation (2.3.47). It follows that:

$$\|(-i\partial_{y_\alpha})u(y,t)\|_{L^2_y} \leq \|(-i\partial_{y_\alpha})u(y,0)\|_{L^2_y} + \int_0^t \|[(-i\partial_{y_\alpha}), \mathscr{H}(s)]u(y,s)\|_{L^2_y}\,\mathrm{d}s \tag{2.3.51}$$

Since $\zeta_{\alpha\beta}(t)$ is symmetric, the commutator is given explicitly by:

$$[(-i\partial_{y_\alpha}), \mathscr{H}(s)] = (-i)\zeta_{\alpha\beta}(t)y_\beta \tag{2.3.52}$$

So that:

$$\|(-i\partial_{y_\alpha})u(y,t)\|_{L^2_y} \leq \|(-i\partial_{y_\alpha})u_0(y)\|_{L^2_y} + \int_0^t |\zeta_{\alpha\beta}(t)|\|y_\beta u(y,s)\|_{L^2_y}\,\mathrm{d}s \tag{2.3.53}$$

By an identical reasoning we can derive a similar bound on $y_\alpha u(y,t)$:

$$\|y_\alpha u(y,t)\|_{L^2_y} \leq \|y_\alpha u_0(y)\|_{L^2_y} + \int_0^t |\eta_{\alpha\beta}(s)|\|(-i\partial_{y_\beta})u(y,s)\|_{L^2_y}\,\mathrm{d}s \tag{2.3.54}$$

Adding inequalities (2.3.53) and (2.3.54) gives:

$$\|u(\cdot,t)\|_{\Sigma^1} \leq \|u_0(\cdot)\|_{\Sigma^1} + 2\int_0^t \max_{\alpha,\beta \in \{1,\dots,d\}} \{|\eta_{\alpha\beta}(s)|, |\zeta_{\alpha\beta}(s)|\} \|u(\cdot,s)\|_{\Sigma^1} \, \mathrm{d}s \tag{2.3.55}$$

Using the following version of Gronwall's inequality:

**Lemma 2.3.3** (Gronwall's inequality)**.** *Let $v(t)$ satisfy the inequality:*

$$v(t) \leq a(t) + \int_0^t b(s)v(s) \, ds \tag{2.3.56}$$

*where $b(t)$ is non-negative and $a(t)$ is non-decreasing. Then:*

$$v(t) \leq a(t) \exp\left(\int_0^t b(s) \, ds\right) \tag{2.3.57}$$

We have that:

$$\|u(\cdot,t)\|_{\Sigma^1} \leq \|u_0(\cdot)\|_{\Sigma^1} e^{2\int_0^t \max_{\alpha,\beta\in\{1,\dots,d\}} \left\{|\eta_{\alpha\beta}(s)|,|\zeta_{\alpha\beta}(s)|\right\} \mathrm{d}s} \tag{2.3.58}$$

More generally, we have for any $l \geq 0$ that there exists a constant $C_l > 0$ such that:

$$\|u(\cdot,t)\|_{\Sigma^l} \leq \|u_0(\cdot)\|_{\Sigma^l} e^{C_l \int_0^t \max_{\alpha,\beta\in\{1,\dots,d\}} \left\{|\eta_{\alpha\beta}(s)|,|\zeta_{\alpha\beta}(s)|\right\} \mathrm{d}s} \tag{2.3.59}$$

We have proved the following:

**Lemma 2.3.4** (Bound on solutions of (2.3.47) in the spaces $\Sigma^l(\mathbb{R}^d)$)**.** *Let the time-dependent coefficients $\eta_{\alpha\beta}(t), \zeta_{\alpha\beta}(t)$ be real-valued, symmetric, continuous, and uniformly bounded in $t$. Let $u_0(y) \in \Sigma^l(\mathbb{R}^d)$. Then, by Lemma 2.3.2, there exists a unique solution $u(y,t) \in C([0,\infty);\Sigma^l(\mathbb{R}^d))$. For each integer $l \geq 0$, there exists a constant $C_l > 0$ such that this solution satisfies:*

$$\|u(\cdot,t)\|_{\Sigma^l(\mathbb{R}^d)} \leq \|u_0(\cdot)\|_{\Sigma^l} e^{C_l \int_0^t \max_{\alpha,\beta\in\{1,\dots,d\}} \left\{|\eta_{\alpha\beta}(s)|,|\zeta_{\alpha\beta}(s)|\right\} ds} \tag{2.3.60}$$

Since the map $p \mapsto E_n(p)$ is $\mathcal{B}$-periodic and smooth for all $p \in S_n$, we have that under Assumption 2.1.1, $\sup_{t\in[0,\infty)} \max_{\alpha,\beta\in\{1,\dots,d\}} |\partial_{p_\alpha}\partial_{p_\beta} E_n(p(t))| < \infty$. Under Assumption 2.1.2 we have that $\sup_{t\in[0,\infty)} \max_{\alpha,\beta\in\{1,\dots,d\}} |\partial_{q_\alpha}\partial_{q_\beta} W(q(t))| < \infty$. Since $\partial_{p_\alpha}\partial_{p_\beta} E_n(p(t)), \partial_{q_\alpha}\partial_{q_\beta} W(q(t))$ are clearly real-valued, symmetric, and continuous in $t$ we have that Lemma 2.3.4 applies to solutions of (2.3.45). Since $a_0(y) \in \mathcal{S}(\mathbb{R}^d)$ by assumption we have that for any integer $l \geq 0$:

$$\begin{aligned} &\|a(y,t)\|_{\Sigma^l(\mathbb{R}^d)} \leq \|a_0(y)\|_{\Sigma^l(\mathbb{R}^d)} \\ &\cdot \exp\left( C_l \max_{\alpha,\beta\in\{1,\dots,d\}} \sup_{s\in[0,\infty)} \left\{ |\partial_{p_\alpha}\partial_{p_\beta} E_n(p(s))|, |\partial_{q_\alpha}\partial_{q_\beta} W(q(s))| \right\} t \right). \end{aligned} \tag{2.3.61}$$

**Remark 2.3.2.** *Terms which depend on $b(y,t)$ rather than $a(y,t)$ may be dealt with similarly, by an application of Duhamel's formula and a Gronwall inequality.*

We have therefore that:

$$\begin{aligned}&\epsilon^2 \left\| \int_0^1 \frac{(\tau-1)^4}{4!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}\partial_{q_\delta} W(q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau y_\alpha y_\beta y_\gamma y_\delta a(y,t)\chi_n(z;p(t)) \right\|_{L^\infty_z, L^2_y} \\ &\leq c_1 \epsilon^2 e^{c_2 t}\end{aligned} \tag{2.3.62}$$

where:

$$\begin{aligned} c_1 &:= \frac{1}{4!} \left\| \sum_{|\alpha|=4} |\partial_x^\alpha W(x)| \right\|_{L^\infty_x(\mathbb{R}^d)} \sup_{p\in S_n} \|\chi_n(z;p)\|_{L^\infty_z} \|a_0(y)\|_{\Sigma^4_y(\mathbb{R}^d)} \\ c_2 &:= C_l \max_{\alpha,\beta\in\{1,\dots,d\}} \sup_{s\in[0,\infty)} \left\{ |\partial_{p_\alpha}\partial_{p_\beta} E_n(p(s))|, |\partial_{q_\alpha}\partial_{q_\beta} W(q(s))| \right\} \end{aligned} \tag{2.3.63}$$

are constants independent of $t,\epsilon$.

We conclude that there exist constants $C_1, C_2, C_3 > 0$, independent of $t,\epsilon$ such that:

$$\begin{aligned} &\|\eta^\epsilon_{3,0}(x)\|_{L^2_x} \leq C_1 \epsilon \\ &\|r^\epsilon_3(x,t)\|_{L^2_x} \leq C_2 e^{C_3 t}\epsilon^2 \end{aligned} \tag{2.3.64}$$

The bound (2.1.30) then follows from the basic a priori $L^2$ bound for solutions of the linear time-dependent Schrödinger equation:

**Lemma 2.3.5.** *Let $\psi(x,t)$ be the unique solution of:*

$$\begin{aligned} i\partial_t \psi &= H\psi + f \\ \psi(x,0) &= \psi_0(x) \end{aligned} \tag{2.3.65}$$

*where $H$ is a self-adjoint operator. Then:*

$$\|\psi(\cdot,t)\|_{L^2(\mathbb{R}^d)} \leq \|\psi_0(\cdot)\|_{L^2(\mathbb{R}^d)} + \int_0^t \|f(\cdot,t')\|_{L^2(\mathbb{R}^d)}\,dt' \tag{2.3.66}$$

*when $f=0$, we have:*

$$\|\psi(\cdot,t)\|_{L^2(\mathbb{R}^d)} = \|\psi_0(\cdot)\|_{L^2(\mathbb{R}^d)} \tag{2.3.67}$$

Applying Lemma 2.3.5 to equation (2.3.33) then gives the bound on $\eta^\epsilon_3(x,t)$:

$$\begin{aligned} \|\eta^\epsilon_3(x,t)\|_{L^2_x} &\leq \|\eta^\epsilon_3(x,0)\|_{L^2_x} + \frac{1}{\epsilon}\int_0^t \|r^\epsilon_3(x,t')\|_{L^2_x}\,\mathrm{d}t' \\ &\leq C_1\epsilon + \frac{1}{\epsilon}\int_0^t C_2 e^{C_3 t'}\epsilon^2\,\mathrm{d}t' \\ &\leq Ce^{Ct}\epsilon \end{aligned} \tag{2.3.68}$$

where $C$ is a constant independent of $\epsilon, t$. This completes the proof of Theorem 2.1.1.

## 2.4 Proof of Theorem 2.1.2 on dynamics of physical observables

Let $\psi^\epsilon(x,t)$ be the solution of (2.1.28). By Theorem 2.1.1 we have that this solution has the form:

$$\psi^\epsilon(x,t) = \tilde{\psi}^\epsilon(y,z,t)\Big|_{y=\frac{x-q(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon}} + \eta^\epsilon(x,t) \tag{2.4.1}$$

where:

$$\begin{aligned}\tilde{\psi}^\epsilon(y,z,t) &:= \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} e^{i\phi_B(t)} \Big\{ a(y,t)\chi_n(z;p(t)) \\ &+\epsilon^{1/2}\Big[(-i\nabla_y)a(y,t)\cdot\nabla_p\chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t))\Big]\Big\}\end{aligned} \tag{2.4.2}$$

In this section we compute the dynamics of the physical observables:

$$\begin{aligned}\mathcal{Q}^\epsilon(t) &:= \frac{1}{\mathcal{N}^\epsilon(t)}\int_{\mathbb{R}^d} x\left|\tilde{\psi}^\epsilon(y,z,t)\right|^2_{z=\frac{x}{\epsilon},y=\frac{x-q(t)}{\epsilon^{1/2}}}\,\mathrm{d}x \\ \mathcal{P}^\epsilon(t) &:= \frac{1}{\mathcal{N}^\epsilon(t)}\int_{\mathbb{R}^d}\overline{\tilde{\psi}^\epsilon(y,z,t)}\left(-i\epsilon^{1/2}\nabla_y\right)\tilde{\psi}^\epsilon(y,z,t)\Big|_{z=\frac{x}{\epsilon},y=\frac{x-q(t)}{\epsilon^{1/2}}}\,\mathrm{d}x\end{aligned} \tag{2.4.3}$$

where:

$$\mathcal{N}^\epsilon(t) = \int_{\mathbb{R}^d}\left|\tilde{\psi}^\epsilon(y,z,t)\right|^2_{z=\frac{x}{\epsilon},y=\frac{x-q(t)}{\epsilon^{1/2}}}\,\mathrm{d}x \tag{2.4.4}$$

**Remark 2.4.1.** *Throughout this section we will employ a short-hand notation:*

$$\begin{aligned}&f^\epsilon(x,t) = O(\epsilon^K e^{ct}) \iff \exists c>0, C>0 \text{ independent of } t,\epsilon \text{ such that } \|f^\epsilon(x,t)\|_{L^2_x} \le C\epsilon^K e^{ct} \\ &g^\epsilon(t) = O(\epsilon^K e^{ct}) \iff \exists c>0, C>0 \text{ independent of } t,\epsilon \text{ such that } |g^\epsilon(t)| \le C\epsilon^K e^{ct}\end{aligned} \tag{2.4.5}$$

We will use the following Lemma which is a mild generalization of that found in Ref. [8] (as Lemma 4.2):

**Lemma 2.4.1.** *Let $f \in \mathcal{S}(\mathbb{R}^d)$, $g$ smooth and periodic with respect to the lattice $\Lambda$, $s \in \mathbb{R}$ a constant, and $\delta > 0$ an arbitrary positive parameter. Then for any positive integer $N > 0$:*

$$\int_{\mathbb{R}^d} f(x)\, g\left(\frac{x}{\delta}+\frac{s}{\delta^2}\right)\, dx = \left(\int_{\mathbb{R}^d} f(x)\, dx\right)\left(\int_\Omega g(z)\, dz\right) + O(\delta^N). \tag{2.4.6}$$

For the proof, see Appendix A.5.

### 2.4.1 Asymptotic expansion and dynamics of $\mathcal{N}^\epsilon(t)$

By changing variables in the integral (2.4.4), we have that:

$$\mathcal{N}^\epsilon(t) = \epsilon^{d/2} \int_{\mathbb{R}^d} \left| \tilde{\psi}^\epsilon(y,z,t) \right|^2_{z=\frac{y}{\epsilon^{1/2}}+\frac{q(t)}{\epsilon}} \, \mathrm{d}y. \tag{2.4.7}$$

Substituting (2.4.2) into (2.4.7) gives:

$$= \int_{\mathbb{R}^d} \left\{ \overline{a(y,t)\chi_n(z;p(t)) + \epsilon^{1/2}\left[(-i\nabla_y)a(y,t)\cdot\nabla_p\chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t))\right]} \right\}$$
$$\left\{ a(y,t)\chi_n(z;p(t)) + \epsilon^{1/2}\left[(-i\nabla_y)a(y,t)\cdot\nabla_p\chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t))\right] \right\}\Big|_{z=\frac{y}{\epsilon^{1/2}}+\frac{q(t)}{\epsilon}} \, \mathrm{d}y. \tag{2.4.8}$$

We expand the product in the integral and apply Lemma 2.4.1 term by term with $s = q(t), \delta = \epsilon^{1/2}$. Since the $\chi_n$ are assumed normalized: for all $t \in [0,\infty)$ $\|\chi_n(\cdot;p(t))\|_{L^2(\Omega)} = 1$, we have:

$$\begin{aligned} \mathcal{N}^\epsilon(t) &= \|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} \\ &+ \epsilon^{1/2}\Big[\langle (-i\nabla_y)a(y,t) |\, a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \cdot \langle \nabla_p\chi_n(z;p(t)) |\, \chi_n(z;p(t))\rangle_{L^2_z(\Omega)} \\ &+ \langle a(y,t) |\, (-i\nabla_y)a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \cdot \langle \chi_n(z;p(t)) |\, \nabla_p\chi_n(z;p(t))\rangle_{L^2_z(\Omega)} \\ &+ \langle b(y,t) |\, a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) |\, b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\Big] + O(\epsilon e^{ct}). \end{aligned} \tag{2.4.9}$$

**Remark 2.4.2.** *In (2.4.9) we have made explicit all terms through order $\epsilon^{1/2}$. To justify the error bound, consider that the remaining terms may be bounded by $\mathcal{C}(t)\epsilon$ where $\mathcal{C}(t)$ depends on $\Sigma^{l_1}_y$-norms of $a(y,t), b(y,t)$ and $L^2_z$-norms of $\partial_p^{l_2}\chi_n(z;p(t))$ where $l_1, l_2$ are positive integers. By an identical reasoning to that given in Section 2.3.2 we have that $\mathcal{C}(t)$ may be bounded by $Ce^{ct}$ where $c > 0, C > 0$ are constants independent of $\epsilon, t$. Error terms of this type will arise throughout the following discussion and will be treated similarly.*

Under Assumption 2.1.1, in a neighborhood of the curve $p(t) \in \mathcal{B}$, the mapping $p \mapsto \chi_n(z;p)$ is smooth. Hence, we may differentiate the normalization condition: $\|\chi_n(\cdot;p)\|^2_{L^2(\Omega)} = 1$ with respect to $p$ and evaluate along the curve $p(t)$ to obtain the identity:

$$\langle \chi_n(z;p(t)) |\, \nabla_p\chi_n(z;p(t))\rangle_{L^2_z(\Omega)} + \langle \nabla_p\chi_n(z;p(t)) |\, \chi_n(z;p(t))\rangle_{L^2_z(\Omega)} = 0 \tag{2.4.10}$$

It follows from this, and the fact that $(-i\nabla_y)$ is symmetric with respect to the $L^2_y$-inner product, that:

$$\begin{aligned} &\langle (-i\nabla_y) a(y,t) |\, a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \cdot \langle \nabla_p \chi_n(z;p(t)) |\, \chi_n(z;p(t)) \rangle_{L^2_z(\Omega)} \\ &+ \langle a(y,t) |\, (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \cdot \langle \chi_n(z;p(t)) |\, \nabla_p \chi_n(z;p(t)) \rangle_{L^2_z(\Omega)} = 0 \end{aligned} \tag{2.4.11}$$

so that (2.4.9) reduces to:

$$\mathcal{N}^\epsilon(t) = \|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} + \epsilon^{1/2} \left[ \langle b(y,t) |\, a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) |\, b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] + O(\epsilon e^{ct}). \tag{2.4.12}$$

From $L^2$-norm conservation for solutions of (2.1.22), we have that $\|a(y,t)\|_{L^2_y} = \|a_0(y)\|_{L^2_y}$. In Appendix A.6 we calculate (A.6.17):

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[ \langle b(y,t) |\, a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) |\, b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] = 0, \tag{2.4.13}$$

so that:

$$\dot{\mathcal{N}}^\epsilon(t) = O(\epsilon e^{Ct}) \tag{2.4.14}$$

Integrating in time then gives:

$$\begin{aligned} \mathcal{N}^\epsilon(t) &= \mathcal{N}^\epsilon(0) + O(\epsilon e^{ct}) \\ &= \|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)} + \epsilon^{1/2} \left[ \langle b_0(y) |\, a_0(y) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a_0(y) |\, b_0(y) \rangle_{L^2_y(\mathbb{R}^d)} \right] + O(\epsilon e^{ct}). \end{aligned} \tag{2.4.15}$$

### 2.4.2 Asymptotic expansion of $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$; proof of assertion (1) of Theorem 2.1.2

Changing variables in the integrals (2.4.3) and using the identity:

$$x = q(t) + \epsilon^{1/2} y \Big|_{y = \frac{x - q(t)}{\epsilon^{1/2}}} \tag{2.4.16}$$

we have:

$$\begin{aligned} \mathcal{Q}^\epsilon(t) &= q(t) + \epsilon^{1/2+d/2} \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} y \left| \tilde{\psi}^\epsilon(y,z,t) \right|^2_{z = \frac{q(t)}{\epsilon} + \frac{y}{\epsilon^{1/2}}} \, \mathrm{d}y \\ \mathcal{P}^\epsilon(t) &= \epsilon^{1/2+d/2} \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} \overline{\tilde{\psi}^\epsilon(y,z,t)} \, (-i\nabla_y) \, \tilde{\psi}^\epsilon(y,z,t) \Big|_{z = \frac{q(t)}{\epsilon} + \frac{y}{\epsilon^{1/2}}} \, \mathrm{d}y. \end{aligned} \tag{2.4.17}$$

Substituting (2.4.2) into (2.4.17) we have, for each $\alpha \in \{1, ..., d\}$:

$$\mathcal{Q}^\epsilon_\alpha(t) = q_\alpha(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} y_\alpha \Big| a(y,t)\chi_n(z;p(t)) + \epsilon^{1/2} \left[ (-i\partial_{y_\beta}) a(y,t) \partial_{p_\beta} \chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t)) \right] \Big|^2_{z = \frac{q(t)}{\epsilon} + \frac{y}{\epsilon^{1/2}}} \, \mathrm{d}y$$

$$\mathcal{P}^\epsilon_\alpha(t) = p_\alpha(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \int_{\mathbb{R}^d} \overline{a(y,t)\chi_n(z;p(t)) + \epsilon^{1/2} \left[ (-i\partial_{y_\beta}) a(y,t) \partial_{p_\beta} \chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t)) \right]} (-i\partial_{y_\alpha}) \Big( a(y,t)\chi_n(z;p(t)) + \epsilon^{1/2} \left[ (-i\partial_{y_\beta}) a(y,t) \partial_{p_\beta} \chi_n(z;p(t)) + b(y,t)\chi_n(z;p(t)) \right] \Big) \Big|_{z = \frac{q(t)}{\epsilon} + \frac{y}{\epsilon^{1/2}}} \, \mathrm{d}y \tag{2.4.18}$$

Expanding all products and applying Lemma 2.4.1 term by term in (2.4.18) we obtain:

$$\begin{aligned}
\mathcal{Q}^\epsilon_\alpha(t) &= q_\alpha(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \langle a(y,t) | \, y_\alpha a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \Big[ \langle b(y,t) | \, y_\alpha a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | \, y_\alpha b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \big\langle (-i\partial_{y_\beta}) a(y,t) \big| \, y_\alpha a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \partial_{p_\beta} \chi_n(z;p(t)) \big| \, \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \\
&+ \big\langle y_\alpha a(y,t) | \, (-i\partial_{y_\beta}) a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \chi_n(z;p(t)) | \, \partial_{p_\beta} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \Big] \\
&+ O(\epsilon^{3/2} e^{ct}) \\
\mathcal{P}^\epsilon_\alpha(t) &= p_\alpha(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \langle a(y,t) | \, (-i\partial_{y_\alpha}) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \Big[ \langle b(y,t) | \, (-i\partial_{y_\alpha}) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | \, (-i\partial_{y_\alpha}) b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \Big] \\
&+ O(\epsilon^{3/2} e^{ct}).
\end{aligned} \tag{2.4.19}$$

Here, terms of higher order than $\epsilon$ are bounded by a similar reasoning to that given in Section 2.3.2 (Remark 2.4.2). Using the identity (2.4.10) and the fact that $(-i\nabla_y)$ is self-adjoint we have that:

$$\begin{aligned}
&\big\langle (-i\partial_{y_\beta}) a(y,t) \big| \, y_\alpha a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \partial_{p_\beta} \chi_n(z;p(t)) \big| \, \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \\
&+ \big\langle y_\alpha a(y,t) | \, (-i\partial_{y_\beta}) a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \chi_n(z;p(t)) | \, \partial_{p_\beta} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \\
&= \big\langle a(y,t) | \, [y_\alpha, (-i\partial_{y_\beta})] a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \chi_n(z;p(t)) | \, \partial_{p_\beta} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)}
\end{aligned} \tag{2.4.20}$$

where $[y_\alpha, (-i\partial_{y_\beta})] := y_\alpha(-i\partial_{y_\beta}) - (-i\partial_{y_\beta})y_\alpha$ is the commutator. Since $[y_\alpha, (-i\partial_{y_\beta})] = i\delta_{\alpha\beta}$ We have that:

$$\begin{aligned} &\left\langle a(y,t) \right| [y_\alpha, (-i\partial_{y_\beta})] a(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \left\langle \chi_n(z;p(t)) \right| \partial_{p_\beta} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \\ &= i \|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} \left\langle \chi_n(z;p(t)) \right| \partial_{p_\alpha} \chi_n(z;p(t)) \rangle_{L^2_z(\Omega)} . \end{aligned} \tag{2.4.21}$$

Using $L^2$-norm conservation for solutions of (2.1.22), we have that for all $t \geq 0$, $\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} = \|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)}$. Using (2.4.15), we have that $\|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)} = \mathcal{N}^\epsilon(t) + O(\epsilon^{1/2} e^{ct})$ (2.4.12). We have proved that:

$$\begin{aligned} &i \|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} \left\langle \chi_n(z;p(t)) \right| \nabla_p \chi_n(z;p(t)) \rangle_{L^2_z(\Omega)} \\ &= \mathcal{N}^\epsilon(t) \mathcal{A}_n(p(t)) + O(\epsilon^{1/2} e^{ct}) \end{aligned} \tag{2.4.22}$$

where the last equality holds by the definition of the $n$-th band Berry connection (2.1.26). We have proved that:

$$\begin{aligned} &\mathcal{Q}^\epsilon(t) = q(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \left\langle a(y,t) \right| y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\ &+ \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \left[ \left\langle b(y,t) \right| y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| y b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \\ &+ \epsilon \mathcal{A}_n(p(t)) + O(\epsilon^{3/2} e^{ct}) \\ &\mathcal{P}^\epsilon(t) = p(t) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \left\langle a(y,t) \right| (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\ &+ \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \left[ \left\langle b(y,t) \right| (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| (-i\nabla_y) b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \\ &+ O(\epsilon^{3/2} e^{ct}). \end{aligned} \tag{2.4.23}$$

### 2.4.3 Computation of dynamics of $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$; proof of assertion (2) of Theorem 2.1.2

Differentiating both sides of (2.4.23) with respect to time and using $\dot{\mathcal{N}}^\epsilon(t) = O(\epsilon e^{ct})$ (2.4.14) gives:

$$\begin{aligned}
&\dot{\mathcal{Q}}^\epsilon_\alpha(t) = \dot{q}_\alpha(t) + \epsilon^{1/2}\frac{1}{\mathcal{N}^\epsilon(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle a(y,t)\right|y_\alpha a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \\
&+\epsilon\frac{1}{\mathcal{N}^\epsilon(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left[\left\langle b(y,t)\right|y_\alpha a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|y_\alpha b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&+\epsilon\dot{p}_\beta(t)\partial_{p_\beta}\mathcal{A}_{n,\alpha}(p(t)) + O(\epsilon^{3/2}e^{ct}) \\
&\dot{\mathcal{P}}^\epsilon_\alpha(t) = \dot{p}_\alpha(t) + \epsilon^{1/2}\frac{1}{\mathcal{N}^\epsilon(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle a(y,t)\right|(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \\
&+\epsilon\frac{1}{\mathcal{N}^\epsilon(t)}\frac{\mathrm{d}}{\mathrm{d}t}\left[\left\langle b(y,t)\right|(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|(-i\partial_{y_\alpha})b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&+O(\epsilon^{3/2}e^{ct})
\end{aligned} \tag{2.4.24}$$

Recall that $(q(t), p(t))$ satisfy the classical system (2.1.19). In Appendix A.6 we calculate (A.6.13):

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left\langle a(y,t)\right|y_\alpha a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} = \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\left\langle a(y,t)\right|(-i\partial_{y_\beta})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \\
&\frac{\mathrm{d}}{\mathrm{d}t}\left\langle a(y,t)\right|(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} = -\partial_{q_\alpha}\partial_{q_\beta}W(q(t))\left\langle a(y,t)\right|y_\beta a(y,t)\rangle_{L^2_y(\mathbb{R}^d)}
\end{aligned} \tag{2.4.25}$$

and (A.6.18):

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left[\left\langle b(y,t)\right|y_\alpha a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|y_\alpha b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&= \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\left[\left\langle b(y,t)\right|(-i\partial_{y_\beta})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|(-i\partial_{y_\beta})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&+\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))\left\langle a(y,t)\right|(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \\
&+\partial_{q_\beta}W(q(t))\partial_{p_\alpha}\mathcal{A}_{n,\beta}(p(t))\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} \\
&\frac{\mathrm{d}}{\mathrm{d}t}\left[\left\langle b(y,t)\right|(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|(-i\partial_{y_\alpha})b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&= -\partial_{q_\alpha}\partial_{q_\beta}W(q(t))\left[\left\langle b(y,t)\right|y_\beta a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t)\right|y_\beta a(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&-\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))\left\langle a(y,t)\right|y_\beta y_\gamma a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} - \partial_{q_\alpha}\partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)}
\end{aligned} \tag{2.4.26}$$

Substituting these expressions into (2.4.24) and using $\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} = \mathcal{N}^\epsilon(t) + O(\epsilon^{1/2} e^{ct})$ (2.4.9) we have:

$$\begin{aligned}
&\dot{\mathcal{Q}}^\epsilon_\alpha(t) = \partial_{p_\alpha} E_n(p(t)) + \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{p_\alpha}\partial_{p_\beta} E_n(p(t)) \left\langle a(y,t) \right| (-i\partial_{y_\beta}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{p_\alpha}\partial_{p_\beta} E_n(p(t)) \left[ \left\langle b(y,t) \right| (-i\partial_{y_\beta}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| (-i\partial_{y_\beta}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \right] \\
&+ \epsilon \frac{1}{2} \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma} E_n(p(t)) \left\langle a(y,t) \right| (-i\partial_{y_\beta})(-i\partial_{y_\gamma}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \epsilon \partial_{q_\beta} W(q(t)) \partial_{p_\alpha} \mathcal{A}_{n,\beta}(p(t)) - \epsilon \partial_{q_\beta} W(q(t)) \partial_{p_\beta} \mathcal{A}_{n,\alpha}(p(t)) + O(\epsilon^{3/2} e^{ct}) \\
&\dot{\mathcal{P}}^\epsilon_\alpha(t) = -\partial_{q_\alpha} W(q(t)) - \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{q_\alpha}\partial_{q_\beta} W(q(t)) \left\langle a(y,t) \right| y_\beta a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{q_\alpha}\partial_{q_\beta} W(q(t)) \left[ \left\langle b(y,t) \right| y_\beta a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle b(y,t) \right| y_\beta a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \right] \\
&- \epsilon \frac{1}{2} \frac{1}{\mathcal{N}^\epsilon(t)} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) \left\langle a(y,t) \right| y_\beta y_\gamma a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \epsilon \partial_{q_\alpha}\partial_{q_\beta} W(q(t)) \mathcal{A}_{n,\beta}(p(t)) + O(\epsilon^{3/2} e^{ct})
\end{aligned} \tag{2.4.27}$$

Equation (2.4.23) gives expressions for $q(t), p(t)$ in terms of $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$:

$$\begin{aligned}
&q_\alpha(t) = \mathcal{Q}^\epsilon_\alpha(t) - \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \left\langle a(y,t) \right| y_\alpha a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \left[ \left\langle b(y,t) \right| y_\alpha a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| y_\alpha b(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \right] - \epsilon \mathcal{A}_{n,\alpha}(p(t)) + O(\epsilon^{3/2} e^{ct}) \\
&p_\alpha(t) = \mathcal{P}^\epsilon_\alpha(t) - \epsilon^{1/2} \frac{1}{\mathcal{N}^\epsilon(t)} \left\langle a(y,t) \right| (-i\partial_{y_\alpha}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \epsilon \frac{1}{\mathcal{N}^\epsilon(t)} \left[ \left\langle b(y,t) \right| (-i\partial_{y_\alpha}) a(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| (-i\partial_{y_\alpha}) b(y,t) \left.\right\rangle_{L^2_y(\mathbb{R}^d)} \right] + O(\epsilon^{3/2} e^{ct})
\end{aligned} \tag{2.4.28}$$

Substituting these expressions into (2.4.27), Taylor-expanding in $\epsilon^{1/2}$, and again using $\mathcal{N}^\epsilon(t) = \|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)} + O(\epsilon^{1/2} e^{ct})$ (2.4.9) then gives:

$$
\begin{aligned}
&\dot{\mathcal{Q}}^\epsilon_\alpha(t) = \partial_{\mathcal{P}^\epsilon_\alpha} E_n(\mathcal{P}^\epsilon(t)) \\
&+ \epsilon \frac{1}{2} \partial_{\mathcal{P}^\epsilon_\alpha} \partial_{\mathcal{P}^\epsilon_\beta} \partial_{\mathcal{P}^\epsilon_\gamma} E_n(\mathcal{P}^\epsilon(t)) \left[ \frac{1}{\|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)}} \left\langle a(y,t) \right| (-i\partial_{y_\beta})(-i\partial_{y_\gamma}) a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \left. \frac{1}{\|a_0(y)\|^4_{L^2_y(\mathbb{R}^d)}} \left\langle a(y,t) \right| (-i\partial_{y_\beta}) a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \left\langle a(y,t) \right| (-i\partial_{y_\gamma}) a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \Big] \\
&+ \epsilon \partial_{\mathcal{Q}^\epsilon_\gamma} W(\mathcal{Q}^\epsilon(t)) \mathcal{F}_{n,\alpha\gamma}(\mathcal{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct}) \\
&\dot{\mathcal{P}}^\epsilon_\alpha(t) = -\partial_{\mathcal{Q}^\epsilon_\alpha} W(\mathcal{Q}^\epsilon(t)) - \epsilon \frac{1}{2} \partial_{\mathcal{Q}^\epsilon_\alpha} \partial_{\mathcal{Q}^\epsilon_\beta} \partial_{\mathcal{Q}^\epsilon_\gamma} W(\mathcal{Q}^\epsilon(t)) \left[ \frac{1}{\|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)}} \left\langle a(y,t) \right| y_\beta y_\gamma a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \left. \frac{1}{\|a_0(y)\|^4_{L^2_y(\mathbb{R}^d)}} \left\langle a(y,t) \right| y_\beta a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \left\langle a(y,t) \right| y_\gamma a(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \Big] + O(\epsilon^{3/2} e^{ct}).
\end{aligned}
\tag{2.4.29}
$$

where $\mathcal{F}_{n,\alpha\gamma}(\mathcal{P}^\epsilon) := \partial_{\mathcal{P}^\epsilon_\alpha} \mathcal{A}_{n,\gamma}(\mathcal{P}^\epsilon) - \partial_{\mathcal{P}^\epsilon_\beta} \mathcal{A}_{n,\alpha}(\mathcal{P}^\epsilon)$ is the $n$th band Berry curvature (2.1.47). Note that the system (2.4.29) is not closed: $a(y,t)$ satisfies an equation parametrically forced by $q(t), p(t)$ (2.1.22). Recall the definition of $a^\epsilon(y,t)$ (2.1.43) as the solution of (2.1.22) with co-efficients evaluated at $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$:

$$
\begin{aligned}
&i\partial_t a^\epsilon(y,t) = \frac{1}{2} \partial_{\mathcal{P}^\epsilon_\alpha} \partial_{\mathcal{P}^\epsilon_\beta} E_n(\mathcal{P}^\epsilon(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta}) a^\epsilon(y,t) + \frac{1}{2} \partial_{\mathcal{Q}^\epsilon_\alpha} \partial_{\mathcal{Q}^\epsilon_\beta} W(\mathcal{Q}^\epsilon(t)) y_\alpha y_\beta a^\epsilon(y,t) \\
&a^\epsilon(y,0) = a_0(y),
\end{aligned}
\tag{2.4.30}
$$

Recall the definition of the $\Sigma^l$ norms (2.3.46). If we can show that $\|a^\epsilon(y,t) - a(y,t)\|_{\Sigma^l_y(\mathbb{R}^d)} = O(\epsilon^{1/2} e^{ct})$ for each positive integer $l$, then we may replace $a(y,t)$ by $a^\epsilon(y,t)$ everywhere in (2.4.29) and, after dropping error terms, we will have obtained a closed system for $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t), a^\epsilon(y,t)$. Let:

$$
\begin{aligned}
&\mathscr{H}^\epsilon(t) := \frac{1}{2} \partial_{\mathcal{P}^\epsilon_\alpha} \partial_{\mathcal{P}^\epsilon_\beta} E_n(\mathcal{P}^\epsilon(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2} \partial_{\mathcal{Q}^\epsilon_\alpha} \partial_{\mathcal{Q}^\epsilon_\beta} W(q(t)) y_\alpha y_\beta, \\
&\mathscr{H}(t) := \frac{1}{2} \partial_{p_\alpha} \partial_{p_\beta} E_n(p(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2} \partial_{q_\alpha} \partial_{q_\beta} W(q(t)) y_\alpha y_\beta
\end{aligned}
\tag{2.4.31}
$$

then $a^\epsilon(y,t) - a(y,t)$ satisfies:

$$
\begin{aligned}
&i\partial_t \left( a^\epsilon(y,t) - a(y,t) \right) = \mathscr{H}^\epsilon(t) a^\epsilon(y,t) - \mathscr{H}(t) a(y,t) \\
&= \mathscr{H}^\epsilon(t) \left( a^\epsilon(y,t) - a(y,t) \right) + \left( \mathscr{H}^\epsilon(t) - \mathscr{H}(t) \right) a(y,t) \\
&a^\epsilon(y,0) - a(y,0) = 0
\end{aligned}
\tag{2.4.32}
$$

Using the fact that $\mathscr{H}^\epsilon(t)$ is self-adjoint on $L^2_y(\mathbb{R}^d)$ for each $t$, it follows from (2.4.32) that:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\|a^\epsilon(y,t)-a(y,t)\|^2_{L^2_y(\mathbb{R}^d)}\\ &= i\left\langle \left(\mathscr{H}^\epsilon(t)-\mathscr{H}(t)\right)a(y,t)\right| a^\epsilon(y,t)-a(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\\ &\quad - i\left\langle a^\epsilon(y,t)-a(y,t)\right|\left(\mathscr{H}^\epsilon(t)-\mathscr{H}(t)\right)a(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\end{aligned} \tag{2.4.33}$$

By the Cauchy-Schwarz inequality:

$$\leq 2\|a^\epsilon(y,t)-a(y,t)\|_{L^2_y(\mathbb{R}^d)}\|\left(\mathscr{H}^\epsilon(t)-\mathscr{H}(t)\right)a(y,t)\|_{L^2_y(\mathbb{R}^d)} \tag{2.4.34}$$

It then follows that:

$$\|a^\epsilon(y,t)-a(y,t)\|_{L^2_y(\mathbb{R}^d)} \leq \int_0^t \|\left(\mathscr{H}^\epsilon(s)-\mathscr{H}(s)\right)a(y,s)\|_{L^2_y(\mathbb{R}^d)}\,\mathrm{d}s. \tag{2.4.35}$$

Using the precise forms of $\mathscr{H}^\epsilon(t), \mathscr{H}(t)$ we have:

$$\begin{aligned}&\|a^\epsilon(y,t)-a(y,t)\|_{L^2_y(\mathbb{R}^d)} \leq \int_0^t\\ &\sup_{s\in[0,\infty),\alpha,\beta\in\{1,\dots,d\}}\Big(|\partial_{\mathcal{P}^\epsilon_\alpha}\partial_{\mathcal{P}^\epsilon_\beta}E_n(\mathcal{P}^\epsilon(s))-\partial_{p_\alpha}\partial_{p_\beta}E_n(p(s))|+|\partial_{\mathcal{Q}^\epsilon_\alpha}\partial_{\mathcal{Q}^\epsilon_\beta}W(\mathcal{Q}^\epsilon(s))-\partial_{q_\alpha}\partial_{q_\beta}W(q(s))|\Big)\\ &\|a(y,s)\|_{\Sigma^2_y(\mathbb{R}^d)}\,\mathrm{d}s\end{aligned} \tag{2.4.36}$$

where $\Sigma^2_y(\mathbb{R}^d)$ is the norm defined in (2.3.46). Recall that $|\mathcal{Q}^\epsilon(t)-q(t)|+|\mathcal{P}^\epsilon(t)-p(t)| = O(\epsilon^{1/2}e^{ct})$ (2.4.23). It follows from compactness of the Brillouin zone and Assumptions 2.1.1 and 2.1.2 that there exists a uniform bound in $t$ on third derivatives of $E_n(p), W(q)$ for all $p$ along the line segments connecting $p(t)$ and $\mathcal{P}^\epsilon(t)$, and all $q$ along the line segments connecting $q(t)$ and $\mathcal{Q}^\epsilon(t)$. We may therefore conclude from the mean-value theorem that there exist constants $c>0, C>0$ independent of $\epsilon, t$ such that:

$$\|a^\epsilon(y,t)-a(y,t)\|_{L^2_y(\mathbb{R}^d)} \leq C\epsilon^{1/2}\int_0^t e^{cs}\|a(y,s)\|_{\Sigma^2_y(\mathbb{R}^d)}\,\mathrm{d}s. \tag{2.4.37}$$

We now use the a priori bounds on the $\Sigma^l_y(\mathbb{R}^d)$-norms of $a(y,t)$ for each $l\in\mathbb{N}$ (Lemma 2.3.4) to see that:

$$\|a^\epsilon(y,t)-a(y,t)\|_{L^2_y(\mathbb{R}^d)} \leq \epsilon^{1/2}C'e^{c't}. \tag{2.4.38}$$

for some constants $c' > 0, C' > 0$ independent of $\epsilon, t$. By a similar argument, we see that for any integer $l \geq 0$ there exist a constants $c_l' > 0, C_l' > 0$ such that:

$$\|a^\epsilon(y,t) - a(y,t)\|_{\Sigma_y^l(\mathbb{R}^d)} \leq \epsilon^{1/2} C_l' e^{c_l' t}. \tag{2.4.39}$$

It then follows that we may replace $a(y,t)$ by $a^\epsilon(y,t)$ everywhere in (2.4.29), generating further errors which are $O(\epsilon^{3/2} e^{ct})$ to derive:

$$\begin{aligned}
&\dot{\mathcal{Q}}_\alpha^\epsilon(t) = \partial_{\mathcal{P}_\alpha^\epsilon} E_n(\mathcal{P}^\epsilon(t)) \\
&+ \epsilon \frac{1}{2} \partial_{\mathcal{P}_\alpha^\epsilon} \partial_{\mathcal{P}_\beta^\epsilon} \partial_{\mathcal{P}_\gamma^\epsilon} E_n(\mathcal{P}^\epsilon(t)) \left[ \frac{1}{\|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)}} \left\langle a^\epsilon(y,t) \right| (-i\partial_{y_\beta})(-i\partial_{y_\gamma}) a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \left. \frac{1}{\|a_0(y)\|^4_{L^2_y(\mathbb{R}^d)}} \left\langle a^\epsilon(y,t) \right| (-i\partial_{y_\beta}) a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \left\langle a^\epsilon(y,t) \right| (-i\partial_{y_\gamma}) a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \Big] \\
&+ \epsilon \partial_{\mathcal{Q}_\gamma^\epsilon} W(\mathcal{Q}^\epsilon(t)) \mathcal{F}_{n,\alpha\gamma}(\mathcal{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct}) \\
&\dot{\mathcal{P}}_\alpha^\epsilon(t) = -\partial_{\mathcal{Q}_\alpha^\epsilon} W(\mathcal{Q}^\epsilon(t)) - \epsilon \frac{1}{2} \partial_{\mathcal{Q}_\alpha^\epsilon} \partial_{\mathcal{Q}_\beta^\epsilon} \partial_{\mathcal{Q}_\gamma^\epsilon} W(\mathcal{Q}^\epsilon(t)) \left[ \frac{1}{\|a_0(y)\|^2_{L^2_y(\mathbb{R}^d)}} \left\langle a^\epsilon(y,t) \right| y_\beta y_\gamma a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \left. \frac{1}{\|a_0(y)\|^4_{L^2_y(\mathbb{R}^d)}} \left\langle a^\epsilon(y,t) \right| y_\beta a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \left\langle a^\epsilon(y,t) \right| y_\gamma a^\epsilon(y,t) \right\rangle_{L^2_y(\mathbb{R}^d)} \Big] + O(\epsilon^{3/2} e^{ct}).
\end{aligned} \tag{2.4.40}$$

### 2.4.4 Hamiltonian structure of dynamics of $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$; proof of assertion (3) of Theorem 2.1.2

Following Ref. [23], we introduce the new variables (2.1.48):

$$\begin{aligned}
&\mathscr{Q}^\epsilon(t) := \mathcal{Q}^\epsilon(t) - \epsilon \mathcal{A}_n(\mathcal{P}^\epsilon(t)) \\
&\mathscr{P}^\epsilon(t) := \mathcal{P}^\epsilon(t).
\end{aligned} \tag{2.4.41}$$

Let $\mathfrak{a}^\epsilon(y,t)$ denote the solution of (2.1.43) with co-efficients evaluated at $\mathscr{Q}^\epsilon(t), \mathscr{P}^\epsilon(t)$ rather than $\mathcal{Q}^\epsilon(t), \mathcal{P}^\epsilon(t)$, with initial data normalized in $L^2_y(\mathbb{R}^d)$:

$$\begin{aligned}
&i\partial_t \mathfrak{a}^\epsilon(y,t) = \frac{1}{2} \partial_{\mathscr{P}_\alpha^\epsilon} \partial_{\mathscr{P}_\beta^\epsilon} E_n(\mathscr{P}^\epsilon(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta}) \mathfrak{a}^\epsilon(y,t) + \frac{1}{2} \partial_{\mathscr{Q}_\alpha^\epsilon} \partial_{\mathscr{Q}_\beta^\epsilon} W(\mathscr{Q}^\epsilon(t)) y_\alpha y_\beta \mathfrak{a}^\epsilon(y,t) \\
&\mathfrak{a}^\epsilon(y,0) = \frac{a_0(y)}{\|a_0(y)\|_{L^2_y(\mathbb{R}^d)}}.
\end{aligned} \tag{2.4.42}$$

Since $\mathscr{Q}^\epsilon(t) - \mathcal{Q}^\epsilon(t) = O(\epsilon e^{ct})$, $\mathscr{P}^\epsilon(t) = \mathcal{P}^\epsilon(t)$, by a similar argument to that given in the previous section we have that for each integer $l \geq 0$:

$$\left\| \frac{a^\epsilon(y,t)}{\|a_0(y)\|_{L^2_y(\mathbb{R}^d)}} - \mathfrak{a}^\epsilon(y,t) \right\|_{\Sigma^l_y(\mathbb{R}^d)} = O(\epsilon e^{ct}). \tag{2.4.43}$$

Differentiating (2.4.41), using equations (2.4.40) for $\dot{\mathcal{Q}}^\epsilon(t), \dot{\mathcal{P}}^\epsilon(t)$, and using (2.4.43) to replace $\frac{a^\epsilon(y,t)}{\|a_0(y)\|_{L^2_y(\mathbb{R}^d)}}$ with $\mathfrak{a}^\epsilon(y,t)$ everywhere we obtain:

$$\begin{aligned}
&\dot{\mathscr{Q}}^\epsilon_\alpha(t) = \partial_{\mathscr{P}^\epsilon_\alpha} E_n(\mathscr{P}^\epsilon(t)) + \epsilon \frac{1}{2} \partial_{\mathscr{P}^\epsilon_\alpha} \partial_{\mathscr{P}_\beta} \partial_{\mathscr{P}^\epsilon_\gamma} E_n(\mathscr{P}^\epsilon(t)) \Big[ \big\langle \mathfrak{a}^\epsilon(y,t) \big| (-i\partial_{y_\beta})(-i\partial_{y_\gamma}) \mathfrak{a}^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \big\langle \mathfrak{a}^\epsilon(y,t) \big| (-i\partial_{y_\beta}) \mathfrak{a}^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \big\langle \mathfrak{a}^\epsilon(y,t) \big| (-i\partial_{y_\gamma}) \mathfrak{a}^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} \Big] \\
&+ \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon(t)) \partial_{\mathscr{P}^\epsilon_\beta} \mathcal{A}_{n,\alpha}(\mathscr{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct}) \\
&\dot{\mathscr{P}}^\epsilon_\alpha(t) = -\partial_{\mathscr{Q}^\epsilon_\alpha} W(\mathscr{Q}^\epsilon(t)) - \epsilon \frac{1}{2} \partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} \partial_{\mathscr{Q}^\epsilon_\gamma} W(\mathscr{Q}^\epsilon(t)) \Big[ \langle \mathfrak{a}^\epsilon(y,t) | \, y_\beta y_\gamma \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\
&- \langle \mathfrak{a}^\epsilon(y,t) | \, y_\beta \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \langle \mathfrak{a}^\epsilon(y,t) | \, y_\gamma \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \Big] \\
&- \partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon(t)) \mathcal{A}_{n,\beta}(\mathscr{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct}).
\end{aligned} \tag{2.4.44}$$

Note that, up to error terms, equations (2.4.44) (2.4.42) constitute a closed system for $\mathscr{Q}^\epsilon(t)$, $\mathscr{P}^\epsilon(t)$, $\mathfrak{a}^\epsilon(y,t)$.

We now show that this system may be derived from a Hamiltonian. Let:

$$\begin{aligned}
\mu^\epsilon(t) &:= \langle \mathfrak{a}^\epsilon(y,t) | \, y \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\
\lambda^\epsilon(t) &:= \langle \mathfrak{a}^\epsilon(y,t) | \, (-i\nabla_y) \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} .
\end{aligned} \tag{2.4.45}$$

Then, we may write (2.4.44) as:

$$\begin{aligned}
&\dot{\mathscr{Q}}^\epsilon_\alpha(t) = \partial_{\mathscr{P}^\epsilon_\alpha} E_n(\mathscr{P}^\epsilon(t)) \\
&+ \epsilon \frac{1}{2} \partial_{\mathscr{P}^\epsilon_\alpha} \partial_{\mathscr{P}_\beta} \partial_{\mathscr{P}^\epsilon_\gamma} E_n(\mathscr{P}^\epsilon(t)) \Big[ \big\langle \mathfrak{a}^\epsilon(y,t) \big| (-i\partial_{y_\beta})(-i\partial_{y_\gamma}) \mathfrak{a}^\epsilon(y,t) \big\rangle_{L^2_y(\mathbb{R}^d)} - \lambda^\epsilon_\beta(t) \lambda^\epsilon_\gamma(t) \Big] \\
&+ \epsilon \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon(t)) \partial_{\mathscr{P}^\epsilon_\beta} \mathcal{A}_{n,\alpha}(\mathscr{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct}) \\
&\dot{\mathscr{P}}^\epsilon_\alpha(t) = -\partial_{\mathscr{Q}^\epsilon_\alpha} W(\mathscr{Q}^\epsilon(t)) - \epsilon \frac{1}{2} \partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} \partial_{\mathscr{Q}^\epsilon_\gamma} W(\mathscr{Q}^\epsilon(t)) \Big[ \langle \mathfrak{a}^\epsilon(y,t) | \, y_\beta y_\gamma \mathfrak{a}^\epsilon(y,t) \rangle_{L^2_y(\mathbb{R}^d)} - \mu^\epsilon_\alpha(t) \mu^\epsilon_\beta(t) \Big] \\
&- \epsilon \partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon(t)) \mathcal{A}_{n,\beta}(\mathscr{P}^\epsilon(t)) + O(\epsilon^{3/2} e^{ct})
\end{aligned} \tag{2.4.46}$$

By an identical calculation to that given in Appendix A.6 (A.6.13) (A.6.14), we have that:

$$\begin{aligned} \dot{\mu}^\epsilon_\alpha(t) &= \partial_{\mathscr{P}^\epsilon_\alpha} \partial_{\mathscr{P}^\epsilon_\beta} E_n(\mathscr{P}^\epsilon(t)) \lambda^\epsilon_\beta(t) \\ \dot{\lambda}^\epsilon_\alpha(t) &= -\partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon(t)) \mu^\epsilon_\beta(t). \end{aligned} \tag{2.4.47}$$

Let:

$$\begin{aligned} &\mathcal{H}^\epsilon(\mathscr{Q}^\epsilon, \mathscr{P}^\epsilon, \overline{\mathfrak{a}^\epsilon}, \mathfrak{a}^\epsilon, \mu^\epsilon, \lambda^\epsilon) := E_n(\mathscr{P}^\epsilon) + \epsilon W(\mathscr{Q}^\epsilon) + \epsilon \nabla_{\mathscr{Q}^\epsilon} W(\mathscr{Q}^\epsilon) \cdot \mathcal{A}_n(\mathscr{P}^\epsilon) \\ &+ \epsilon \frac{1}{2} \partial_{\mathscr{P}^\epsilon_\alpha} \partial_{\mathscr{P}^\epsilon_\beta} E_n(\mathscr{P}^\epsilon) \left[ \left\langle \partial_{y_\alpha} a^\epsilon \middle| \partial_{y_\beta} a^\epsilon \right\rangle_{L^2_y(\mathbb{R}^d)} - \lambda^\epsilon_\alpha \lambda^\epsilon_\beta \right] \\ &+ \epsilon \frac{1}{2} \partial_{\mathscr{Q}^\epsilon_\alpha} \partial_{\mathscr{Q}^\epsilon_\beta} W(\mathscr{Q}^\epsilon) \left[ \left\langle y_\alpha a^\epsilon \middle| y_\beta a^\epsilon \right\rangle_{L^2_y(\mathbb{R}^d)} - \mu^\epsilon_\alpha \mu^\epsilon_\beta \right] \end{aligned} \tag{2.4.48}$$

Then we may write the closed system (2.4.42), (2.4.47), (2.4.46) as:

$$\begin{aligned} &\dot{\mathscr{Q}}^\epsilon = \nabla_{\mathscr{P}^\epsilon} \mathcal{H}^\epsilon(\mathscr{P}^\epsilon), \dot{\mathscr{P}}^\epsilon = -\nabla_{\mathscr{Q}^\epsilon} \mathcal{H}^\epsilon(\mathscr{Q}^\epsilon), \\ &i\partial_t \mathfrak{a}^\epsilon = \frac{\delta \mathcal{H}^\epsilon}{\delta \overline{\mathfrak{a}^\epsilon}}, \dot{\mu}^\epsilon(t) = -\nabla_{\lambda^\epsilon} \mathcal{H}^\epsilon, \dot{\lambda}^\epsilon(t) = \nabla_{\mu^\epsilon} \mathcal{H}^\epsilon. \end{aligned} \tag{2.4.49}$$

The precise statements (1),(2),(3) of Theorem 2.1.2 follow from the following observations. The errors in equations (2.4.23), (2.4.40), (2.4.46) may each be bounded by $\epsilon^{3/2} C_1 e^{c_1 t}$, $\epsilon^{3/2} C_2 e^{c_2 t}$, $\epsilon^{3/2} C_3 e^{c_3 t}$ for positive constants $c_j, C_j$, $j \in \{1, 2, 3\}$. Define:

$$c' := \max_{j \in \{1,2,3\}} c_j, \; C' := \max_{j \in \{1,2,3\}} C_j. \tag{2.4.50}$$

Then all of these errors may be bounded by $\epsilon^{3/2} C' e^{c' t}$. It follows that these terms are $o(\epsilon)$ for all $t \in [0, \tilde{C}' \ln 1/\epsilon]$ where $\tilde{C}'$ is any constant such that $\tilde{C}' < \frac{1}{2c'}$. Next, in Appendix A.6 (A.6.13) (A.6.14) we show that $\langle a_0(y) | \, y a_0(y) \rangle_{L^2_y(\mathbb{R}^d)} = \langle a_0(y) | \, (-i\nabla_y) a_0(y) \rangle_{L^2_y(\mathbb{R}^d)} = 0$ implies that for all $t \geq 0$ $\langle a(y,t) | \, y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} = \langle a(y,t) | \, (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} = 0$. Imposing the constraints (2.1.44), then, the simplified expressions (2.1.45) (2.1.46) follow from (2.4.23), (2.4.40) respectively. We are also justified in ignoring the $\lambda^\epsilon, \mu^\epsilon$ degrees of freedom in (2.4.48) (2.4.49) since for all $t \geq 0$, $\lambda^\epsilon(t) = \mu^\epsilon(t) = 0$. In this way we obtain the simplified Hamiltonian system (2.1.49) (2.1.50).

## 2.5 Semiclassical wavepacket asymptotic solutions when the potential is 'non-separable'

In this section we consider the following *generalization* of equation (2.1.1) for $\psi^\epsilon(x,t) : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}$:

$$
\begin{aligned}
i\epsilon\partial_t \psi^\epsilon &= -\frac{1}{2}\epsilon^2 \Delta_x \psi^\epsilon + U\left(\frac{x}{\epsilon}, x\right)\psi^\epsilon \\
\psi^\epsilon(x,0) &= \psi_0^\epsilon(x).
\end{aligned}
\tag{2.5.1}
$$

We assume that $U(z,x)$ is *periodic* in its first argument with respect to some $d$-dimensional lattice $\Lambda$ for each fixed value of the second:

$$
U(z+v,x) = U(z,x) \text{ for all } z,x \in \mathbb{R}^d, v \in \Lambda, \tag{2.5.2}
$$

and that $U(z,x)$ is a *smooth* function of both $z$ and $x$. We show how to construct semiclassical wavepacket asymptotic solutions of (2.5.1) which approximate exact solutions up to error of $o(1)$ up to 'Ehrenfest time'. We will not go through the details of calculating corrections to the asymptotic solution proportional to $\epsilon^{1/2}$ and then computing the dynamics of observables associated to this solution including corrections proportional to $\epsilon$ as we did in sections 2.1-2.4 for the special case of (2.5.1) where $U$ is 'separable': $U(z,x) = V(z) + W(x)$. A similar analysis would be possible in this setting, although we expect that the system derived in this way would be complicated and difficult to interpret.

The model (2.5.1) (and generalizations of (2.5.1) where $U$ is time-dependent and non-zero magnetic fields are present) was studied by E, Lu, and Yang [23] through a multi-scale WKB-type expansion. They showed how Berry curvature associated to the appropriate Bloch eigenvalue problem in this case (2.5.3) enters into the characteristic equations of an '$\epsilon$-corrected' eikonal equation (see Section 5 of that paper). In Section 2.7 we derive the form of the Berry curvature for an example potential $U(z,x)$ related to that which appears in a model of a system displaying robust 'edge' states [27].

Consider the family of self-adjoint eigenvalue problems parameterized by real parameters $q, p \in$

$\mathbb{R}^d \times \mathbb{R}^d$:

$$\begin{aligned} &H(q,p)\chi(z;q,p) = E(q,p)\chi(z;q,p) \\ &\chi(z;q,p) = \chi(z;q,p) \text{ for all } z,q,p \in \mathbb{R}^d, v \in \Lambda \\ &H(q,p) := \frac{1}{2}(p - i\nabla_z)^2 + U(z,q). \end{aligned} \tag{2.5.3}$$

Just as in the separable case (2.1.13), there is no loss in restricting our attention to $p \in \mathcal{B}$, a fundamental cell of the reciprocal lattice $\Lambda^*$. For fixed $q$ and $p$, the spectrum of (2.5.3) is real and discrete and the eigenvalues can be ordered with multiplicity:

$$E_1(q,p) \leq E_2(q,p) \leq ... \leq E_n(q,p) \leq ... \tag{2.5.4}$$

and the associated normalized eigenfunctions $\chi_n(z;q,p)$ are a basis of the space:

$$L^2_{per} := \left\{ f \in L^2_{loc} : f(z+v) = f(z) \text{ for all } v \in \Lambda, z \in \mathbb{R}^d \right\}. \tag{2.5.5}$$

Varying $q$ and $p$, we again obtain band functions: $(q,p) \mapsto E_n(q,p)$. If a band $E_n(q,p)$ is *isolated* at some $q_0, p_0 \in \mathcal{B} \times \mathbb{R}^d$:

$$\inf_{m \neq n} |E_m(q_0,p_0) - E_n(q_0,p_0)| > 0 \tag{2.5.6}$$

then a Lyapunov-Schmidt reduction argument shows that the maps $(q,p) \mapsto E_n(q,p)$, $\chi_n(z;q,p)$ are smooth in a neighborhood of $q_0, p_0$ (cf. Definition 2.2.1, Theorem 2.2.1). The natural generalization of the 'isolated band' Assumption 2.1.1 to this setting is the following:

**Assumption 2.5.1** (Uniformly isolated band assumption)**.** *Let $E_n(q,p)$ denote an eigenvalue band function of the periodic Schrödinger operator* (2.5.3)*. Assume that $(q_0,p_0) \in \mathbb{R}^d \times \mathbb{R}^d$ are such that the flow generated by the classical Hamiltonian $\mathcal{H}_n(q,p) := E_n(q,p)$:*

$$\begin{aligned} &\dot{q}(t) = \nabla_p E_n(q(t),p(t)), \quad \dot{p}(t) = -\nabla_q E_n(q(t),p(t)) \\ &q(0), p(0) = q_0, p_0 \end{aligned} \tag{2.5.7}$$

*has a unique smooth solution $(q(t),p(t)) \in \mathbb{R}^d \times \mathbb{R}^d$, $\forall t \geq 0$, and that there exists a constant $M > 0$ such that:*

$$\inf_{m \neq n} |E_m(q(t),p(t)) - E_n(q(t),p(t))| > M \textit{ for all } t \geq 0. \tag{2.5.8}$$

*That is, the $n$th spectral band is uniformly isolated along the trajectory $(q(t),p(t))$ for all $t \geq 0$.*

The appropriate generalization of Assumption 2.1.2 to this setting is the following:

**Assumption 2.5.2.** $\sum_{|\alpha|=1,2,3} |\partial_x^\alpha U(z,x)| \in L^\infty(\Omega \times \mathbb{R}^d)$.

We have then the following result on the propagation of semiclassical wavepacket solutions of (2.5.1) up to errors of $o(1)$ over the Ehrenfest time-scale. Our result may be viewed as a direct generalization of Theorem 1.7 of Carles and Sparber [61] to this setting:

**Theorem 2.5.1.** *Let Assumptions 2.5.1 and 2.5.2 hold. Let $a_0(y), b_0(y) \in \mathcal{S}(\mathbb{R}^d)$. Let $S(t)$ denote the classical action along the path $(q(t), p(t))$:*

$$S(t) = \int_0^t p(t') \cdot \nabla_p E_n(q(t'), p(t')) - E_n(q(t'), p(t'))\, dt'. \tag{2.5.9}$$

*Let $a(y,t)$ satisfy:*

$$\begin{aligned} i\partial_t a(y,t) &= \mathscr{H}(t) a(y,t) \\ a(y,0) &= a_0(y), \end{aligned} \tag{2.5.10}$$

*where:*

$$\begin{aligned} \mathscr{H}(t) :=& \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta} E_n(q(t),p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta} E_n(q(t),p(t)) y_\alpha y_\beta \\ &+ \frac{1}{2}\partial_{p_\alpha}\partial_{q_\beta} E_n(q(t),p(t)) \left[(-i\partial_{y_\alpha}) y_\beta + y_\beta(-i\partial_{y_\alpha})\right] \\ &+ \operatorname{Im} \left\langle \nabla_q \chi_n(\cdot; q(t),p(t)) \right| \left[H(q(t),p(t)) - E_n(q(t),p(t))\right] \cdot \nabla_p \chi_n(\cdot; q(t),p(t)) \rangle_{L^2_z(\Omega)} . \end{aligned} \tag{2.5.11}$$

*Let $\mathcal{A}_q(q,p), \mathcal{A}_p(q,p)$ denote the nth band Berry connections with respect to $q$ and $p$ respectively:*

$$\mathcal{A}_q(q,p) := i \left\langle \chi_n(\cdot;q,p) \right| \nabla_q \chi_n(\cdot;q,p) \rangle_{L^2_z(\Omega)}, \quad \mathcal{A}_q(q,p) := i \left\langle \chi_n(\cdot;q,p) \right| \nabla_q \chi_n(\cdot;q,p) \rangle_{L^2_z(\Omega)} \tag{2.5.12}$$

*Let $\phi_B(t)$ denote the Berry phase associated with transport of $\chi_n(z;q,p)$ along the path $q(t), p(t) \in \mathbb{R}^d \times \mathcal{B}$ given by:*

$$\begin{aligned} \phi_B(t) &= \int_0^t \dot{q}(t') \cdot \mathcal{A}_q(q(t'),p(t')) + \dot{p}(t') \cdot \mathcal{A}_p(q(t'),p(t'))\, dt' \\ &= \int_{(q_0,p_0)}^{(q(t),p(t))} \mathcal{A}_q(q,p) \cdot\, dq + \mathcal{A}_p(q,p) \cdot\, dp. \end{aligned} \tag{2.5.13}$$

*Then, there exists a constant $\epsilon_0 > 0$ such that for all $0 < \epsilon < \epsilon_0$ the following holds. Let $\psi^\epsilon(x,t)$ be the unique solution of the initial value problem* (2.5.1) *with 'Bloch wavepacket' initial data:*

$$\begin{aligned} i\epsilon\partial_t\psi^\epsilon &= -\frac{1}{2}\epsilon^2\Delta_x\psi^\epsilon + U\left(\frac{x}{\epsilon}, x\right)\psi^\epsilon \\ \psi^\epsilon(x,0) &= \epsilon^{-d/4}e^{ip_0\cdot[x-q_0]/\epsilon}a_0\left(\frac{x-q_0}{\epsilon^{1/2}}\right)\chi_n\left(\frac{x}{\epsilon};q_0,p_0\right). \end{aligned} \tag{2.5.14}$$

*Then for all $t \geq 0$ the solution evolves as a modulated 'Bloch wavepacket' plus a corrector $\eta^\epsilon(x,t)$:*

$$\begin{aligned} \psi^\epsilon(x,t) = \epsilon^{-d/4}e^{iS(t)/\epsilon}e^{ip(t)\cdot[x-q(t)]/\epsilon}e^{i\phi_B(t)}a\left(\frac{x-q(t)}{\epsilon^{1/2}},t\right)\chi_n\left(\frac{x}{\epsilon};q(t),p(t)\right) \\ + \eta^\epsilon(x,t) \end{aligned} \tag{2.5.15}$$

*where the corrector $\eta^\epsilon$ satisfies the estimate:*

$$\|\eta^\epsilon(\cdot,t)\|_{L^2(\mathbb{R}^d)} \leq C\epsilon^{1/2}e^{ct}. \tag{2.5.16}$$

*Here, $c > 0$, $C > 0$ are constants independent of $\epsilon, t$. It follows that:*

$$\sup_{t\in[0,\tilde{C}\ln 1/\epsilon]} \|\eta^\epsilon(\cdot,t)\|_{L^2(\mathbb{R}^d)} = o(1) \tag{2.5.17}$$

*where $\tilde{C}$ is any constant satisfying $\tilde{C} < \frac{1}{2c}$.*

**Remark 2.5.1.** *The term:*

$$\text{Im}\left\langle \nabla_q\chi_n(\cdot;q(t),p(t))\right| [H(q(t),p(t)) - E_n(q(t),p(t))]\cdot\nabla_p\chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} \tag{2.5.18}$$

*contributes an overall phase shift to the solution $a(y,t)$ of* (2.5.11)*. This term has been derived elsewhere and interpreted as a 'correction to the wavepacket energy'. See, for example, (2.18) of [71] and (6.8) of [76].*

**Remark 2.5.2.** *For a discussion of Berry's phase, connection, and curvature, and gauge independence in the setting of a two-by-two matrix example, see Appendix A.7. We compute the Berry curvature in a 'non-separable' Schrödinger example and for Maxwell's equations in free space in Sections 2.7.1 and 2.7.2 respectively.*

Equations (2.5.7), (2.5.9), (2.5.11) and (2.5.13) may be derived by a formal multiscale analysis, which we present in the following section. The proof of the bound (2.5.16) is sufficiently similar to the separable case (Section 2.3.2) that we omit it.

### 2.5.1 Derivation of the asymptotic solution (2.5.15) via multiscale expansion

We seek a solution of (2.5.1) of the form:

$$\psi^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} f^\epsilon(y,z,t)\Big|_{y=\frac{x-q(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}} + \eta^\epsilon(x,t). \tag{2.5.19}$$

Substituting (2.5.19) into (2.5.1) gives an inhomogeneous time-dependent Schrödinger equation for $\eta^\epsilon(x,t)$, with a source term $r^\epsilon(x,t)$ which depends on $S(t), q(t), p(t)$, and $f^\epsilon(y,z,t)$:

$$\begin{aligned} i\epsilon\partial_t \eta^\epsilon &= \left[ -\frac{\epsilon^2}{2}\Delta_x + U\left(\frac{x}{\epsilon}, x\right)\right]\eta^\epsilon + r^\epsilon[S,q,p,f^\epsilon] \\ \eta^\epsilon(x,0) &= \psi^\epsilon(x,0) - \epsilon^{-d/4} e^{iS(0)/\epsilon} e^{ip(0)\cdot y/\epsilon^{1/2}} f^\epsilon(y,z,0)\Big|_{y=\frac{x-q_0}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}}. \end{aligned} \tag{2.5.20}$$

The source term $r^\epsilon(x,t)$ has the explicit form:

$$\begin{aligned} r^\epsilon(x,t) &= \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} \Bigg\{ \epsilon \left[\frac{1}{2}(-i\nabla_y)^2 - i\partial_t\right] \\ &+ \epsilon^{1/2}\left[(p(t) - i\nabla_z)\cdot(-i\nabla_y) - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y\right] \\ &+ \left[\dot{S}(t) - \dot{q}(t)p(t) + \frac{1}{2}(p(t) - i\nabla_z)^2 + U(z, q(t) + \epsilon^{1/2}y)\right]\Bigg\} f^\epsilon(y,z,t)\Bigg|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}} \end{aligned} \tag{2.5.21}$$

Since $U$ is assumed smooth, we can replace $U(z, q(t)+\epsilon^{1/2}y)$ by its Taylor series expansion in $\epsilon^{1/2}y$:

$$\begin{aligned} U(z, q(t) + \epsilon^{1/2}y) &= U(z,q(t)) + \epsilon^{1/2}\nabla_q U(z,q(t))\cdot y + \epsilon\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta \\ &+ \epsilon^{3/2}\int_0^1 \frac{(\tau-1)^3}{3!}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}U(z, q(t)+\tau\epsilon^{1/2}y)\,\mathrm{d}\tau\, y_\alpha y_\beta y_\gamma \end{aligned} \tag{2.5.22}$$

We expand $f^\epsilon(y,z,t)$ as a formal power series:

$$f^\epsilon(y,z,t) = f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + ... \tag{2.5.23}$$

and assume that for all $j \in \{0,1,2,...\}$ the $f^j(y,z,t)$ are periodic with respect to the lattice in $z$ and have sufficient smoothness and decay in $y$:

$$\begin{aligned} &\text{for all } v \in \Lambda, f^j(y, z+v, t) = f^j(y,z,t) \\ &f^j(y,z,t) \in \Sigma_y^{R-j}(\mathbb{R}^d). \end{aligned} \tag{2.5.24}$$

The $\Sigma^l$-spaces are defined in (2.1.62). Here, $R > 0$ is a fixed positive integer which we will take as large as required. Recall the notation (2.5.3):

$$H(q,p) := \frac{1}{2}(p - i\nabla_z)^2 + U(z,q). \tag{2.5.25}$$

Substituting (2.5.22) and (2.5.23) then gives:

$$
\begin{aligned}
r^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)\cdot y/\epsilon^{1/2}} \Bigg\{ \epsilon^{3/2} \left[ \int_0^1 \frac{(\tau-1)^3}{3!} \partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} U(z, q(t) + \tau\epsilon^{1/2} y) \, \mathrm{d}\tau y_\alpha y_\beta y_\gamma \right] \\
+ \epsilon \left[ \frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta} U(z, q(t)) y_\alpha y_\beta - i\partial_t \right] \\
+ \epsilon^{1/2} \left[ (p(t) - i\nabla_z)\cdot(-i\nabla_y) + \nabla_q U(z,q(t))\cdot y - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y \right] \\
+ \left[ \dot{S}(t) - \dot{q}(t)\cdot p(t) + H(q(t),p(t)) \right] \Bigg\} \left\{ f^0(y,z,t) + \epsilon^{1/2} f^1(y,z,t) + ... \right\} \Big|_{z=\frac{x}{\epsilon}, y=\frac{x-q(t)}{\epsilon^{1/2}}}.
\end{aligned}
\tag{2.5.26}
$$

In order to prove Theorem 2.5.1 it is sufficient to choose the $f^j(y,z,t), j \in \{0,...,2\}$ so that terms of orders $\epsilon^{j/2}, j \in \{0,...,2\}$ vanish. There is then no loss of accuracy in the approximation by taking $f^j(y,z,t) = 0$, $j \geq 3$.

#### 2.5.1.1 Analysis of leading order terms

Recall that we assume each $f^j, j \in \{0,1,2,...\}$ to be *periodic* with respect to the lattice $\Lambda$ in $z$ (2.5.24). Collecting terms of order 1 in (2.5.26) and setting equal to zero therefore gives the following self-adjoint elliptic eigenvalue problem in $z$:

$$
\begin{aligned}
& H(q(t),p(t)) f^0(y,z,t) = \left[ -\dot{S}(t) + \dot{q}(t)\cdot p(t) \right] f^0(y,z,t), \\
& \text{for all } v \in \Lambda,\ f^0(y,z+v,t) = f^0(y,z,t), \\
& f^0(y,z,t) \in \Sigma^R_y(\mathbb{R}^d).
\end{aligned}
\tag{2.5.27}
$$

Under Assumption 2.5.1, $E_n(q(t),p(t))$ is a simple eigenvalue for all $t \geq 0$. Projecting (2.5.27) onto the subspace of $L^2_{per}$ spanned by $\chi_n(z;q(t),p(t))$ implies:

$$
\dot{S}(t) = \dot{q}(t)\cdot p(t) - E_n(q(t),p(t)) \tag{2.5.28}
$$

which, after matching with the initial data (2.5.20), implies (2.5.9). Equation (2.5.27) then becomes:

$$
\begin{aligned}
& \left[ H(q(t),p(t)) - E_n(q(t),p(t)) \right] f^0(y,z,t) = 0, \\
& \text{for all } v \in \Lambda,\ f^0(y,z+v,t) = f^0(y,z,t), \\
& f^0(y,z,t) \in \Sigma^R_y(\mathbb{R}^d)
\end{aligned}
\tag{2.5.29}
$$

which has the general solution:

$$f^0(y,z,t) = a^0(y,t)\chi_n(z;q(t),p(t)), \tag{2.5.30}$$

where $a^0(y,t)$ is an arbitrary function in $\Sigma_y^R(\mathbb{R}^d)$ to be fixed at higher order in the expansion.

#### 2.5.1.2 Analysis of order $\epsilon^{1/2}$ terms

Collecting terms of order $\epsilon^{1/2}$ in (2.5.26), substituting the form of $\dot{S}(t)$ (2.5.9), and setting equal to zero gives the following inhomogeneous self-adjoint elliptic equation in $z$ for $f^1(y,z,t)$:

$$\begin{aligned} &[H(q(t),p(t)) - E_n(q(t),p(t))]\, f^1(y,z,t) = \xi^1(y,z,t), \\ &\text{for all } z \in \Lambda, f^1(y,z+v,t) = f^1(y,z,t);\; f^1(y,z,t) \in \Sigma_y^{R-1}(\mathbb{R}^d), \\ &\xi^1 := -\left[(p(t) - i\nabla_z)\cdot(-i\nabla_y) + \nabla_q U(z,q(t))\cdot y - \dot{q}(t)\cdot(-i\nabla_y) + \dot{p}(t)\cdot y\right] f^0(y,z,t). \end{aligned} \tag{2.5.31}$$

We now follow the same general strategy followed in the separable case (see Remark 2.3.1) to solve (2.5.31). We first observe that by differentiating (2.5.3) with respect to $q, p$ we derive the identities:

$$\begin{aligned} &[H(q(t),p(t)) - E_n(q(t),p(t))]\nabla_p\chi_n(z;q(t),p(t)) = \\ &-\left[(p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))\right]\chi_n(z;q(t),p(t)) \\ &[H(q(t),p(t)) - E_n(q(t),p(t))]\nabla_q\chi_n(z;q(t),p(t)) = \\ &-\left[\partial_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))\right]\chi_n(z;q(t),p(t)), \end{aligned} \tag{2.5.32}$$

which generalize identities (A.1.2) to this setting. Using (2.5.32) and the form of $f^0(y,z,t)$ (2.5.30) we may write:

$$\xi^1(y,z,t) = \tilde{\xi}^1(y,z,t) + [H(q(t),p(t)) - E_n(q(t),p(t))]u^1(y,z,t) \tag{2.5.33}$$

where:

$$\begin{aligned} \tilde{\xi}^1(y,z,t) = &-\big[(\nabla_p E_n(q(t),p(t)) - \dot{q}(t))\cdot(-i\nabla_y)a^0(y,t) \\ &+(\nabla_q E_n(q(t),p(t)) + \dot{p}(t))\cdot y a^0(y,t)\big]\,\chi_n(z;q(t),p(t)) \\ u^1(y,z,t) = &(-i\nabla_y)a^0(y,t)\cdot\nabla_p\chi_n(z;q(t),p(t)) + y a^0(y,t)\cdot\nabla_q\chi_n(z;q(t),p(t)). \end{aligned} \tag{2.5.34}$$

The solvability condition of (2.5.31) is then equivalent to:

$$(\nabla_p E_n(q(t),p(t)) - \dot{q}(t))\cdot(-i\nabla_y)a^0(y,t) + (\nabla_q E_n(q(t),p(t)) + \dot{p}(t))\cdot y a^0(y,t) = 0 \tag{2.5.35}$$

which we can satisfy by choosing $q(t)$, $p(t)$ to evolve along the Hamiltonian flow of the $n$th Bloch band Hamiltonian $\mathcal{H}_n(q,p) = E_n(q,p)$:

$$\dot{q}(t) = \nabla_p E_n(q(t),p(t)), \quad \dot{p}(t) = -\nabla_q E_n(q(t),p(t)). \tag{2.5.36}$$

Taking $q(0), p(0) = q_0, p_0$ to match with the initial data (2.5.20) implies (2.5.7). With the choice (2.5.36) for $\dot{q}(t)$, $\dot{p}(t)$, $\tilde{\xi}(y,z,t) = 0$ for all $t \geq 0$. We may therefore solve (2.5.31) by taking:

$$\begin{aligned} f^1(y,z,t) &= a^1(y,t)\chi_n(z;q(t),p(t)) \\ &\quad + (-i\nabla_y)a^0(y,t)\cdot\nabla_p\chi_n(z;q(t),p(t)) + ya^0(y,t)\cdot\nabla_q\chi_n(z;q(t),p(t)) \end{aligned} \tag{2.5.37}$$

where $a^1(y,t)$ is an arbitrary function in $\Sigma_y^{R-1}(\mathbb{R}^d)$ to be fixed at higher order in the expansion. Note that since $a^0(y,t) \in \Sigma_y^R(\mathbb{R}^d)$, this ensures that $f^1(y,z,t) \in \Sigma_y^{R-1}(\mathbb{R}^d)$ as required.

#### 2.5.1.3 Analysis of order $\epsilon$ terms

Equating terms of order $\epsilon$ in (2.5.26), using equations (2.5.9) and (2.5.7), and then setting equal to zero gives the following inhomogeneous self-adjoint elliptic equation in $z$ for $f^2(y,z,t)$:

$$\begin{aligned} &[H(q(t),p(t)) - E_n(q(t),p(t))]f^2(y,z,t) = \xi^2(y,z,t), \\ &\text{for all } z\in\Lambda,\ f^2(y,z+v,t) = f^2(y,z,t); f^2(y,z,t)\in\Sigma_y^{R-2}(\mathbb{R}^d), \\ &\xi^2(y,z,t) := -\left[\frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta - i\partial_t\right] f^0(y,z,t) \\ &+ \left[-((p(t)-i\nabla_z) - \nabla_p E_n(q(t),p(t)))\cdot(-i\nabla_y) - (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t)))\cdot y\right] f^1(y,z,t). \end{aligned} \tag{2.5.38}$$

Again following the strategy of Remark 2.3.1, we first record the following generalizations of (A.1.3) which result from taking second derivatives of (2.5.3) with respect to $q$ and $p$:

$$\begin{aligned} &[\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(q,p)]\chi_n(z;q,p) + [(p-i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q,p)]\partial_{p_\beta}\chi_n(z;q,p) \\ &[(p-i\partial_z)_\beta - \partial_{p_\beta}E_n(q,p)]\partial_{p_\alpha}\chi_n(z;q,p) + [H(q,p)-E_n(q,p)]\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;q,p) = 0 \end{aligned} \tag{2.5.39}$$

$$\begin{aligned} &[\partial_{q_\alpha}\partial_{q_\beta}U(z,q) - \partial_{q_\alpha}\partial_{q_\beta}E_n(q,p)]\chi_n(z;q,p) + [\partial_{q_\alpha}U(z,q) - \partial_{q_\alpha}E_n(q,p)]\partial_{q_\beta}\chi_n(z;q,p) \\ &[\partial_{q_\beta}U(z,q) - \partial_{q_\beta}E_n(q,p)]\partial_{q_\alpha}\chi_n(z;q,p) + [H(q,p)-E_n(q,p)]\partial_{q_\alpha}\partial_{q_\beta}\chi_n(z;q,p) = 0 \end{aligned} \tag{2.5.40}$$

$$\begin{aligned} &[-\partial_{p_\alpha}\partial_{q_\beta}E_n(q,p)]\chi_n(z;q,p) + [(p-i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q,p)]\partial_{q_\beta}\chi_n(z;q,p) \\ &[\partial_{q_\beta}U(z,q) - \partial_{q_\beta}E_n(q,p)]\partial_{p_\alpha}\chi_n(z;q,p) + [H(q,p)-E_n(q,p)]\partial_{p_\alpha}\partial_{q_\beta}\chi_n(z;q,p) = 0. \end{aligned} \tag{2.5.41}$$

We now work to manipulate $\xi^2(y,z,t)$ into the form:

$$\xi^2(y,z,t) = \tilde{\xi}^2(y,z,t) + [H(q(t),p(t)) - E_n(q(t),p(t))]u^2(y,z,t), \tag{2.5.42}$$

where $\tilde{\xi}^2(y,z,t)$ and $u^2(y,z,t)$ are functions to be determined. We start by substituting the forms of $f^0(y,z,t)$ (2.5.30) and $f^1(y,z,t)$ (2.5.37) into the expression for $\xi^2(y,z,t)$ (2.5.38):

$$\begin{aligned}
\xi^2(y,z,t) = &- \left[\frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta - i\partial_t\right] \cdot \left[a^0(y,t)\chi_n(z;q(t),p(t))\right] \\
&+ [-((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))) \cdot (-i\nabla_y) - (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))) \cdot y] \\
&\cdot \left[a^1(y,t)\chi_n(z;q(t),p(t)) + (-i\nabla_y)a^0(y,t) \cdot \nabla_p\chi_n(z;q(t),p(t)) + ya^0(y,t) \cdot \nabla_q\chi_n(z;q(t),p(t))\right].
\end{aligned} \tag{2.5.43}$$

We now observe that the terms depending on $a^1(y,t)$ in (2.5.43) have an identical form to the terms depending on $a^0(y,t)$ which appeared in (2.5.31). An identical manipulation using the identities (2.5.32) therefore gives:

$$\begin{aligned}
&[-((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))) \cdot (-i\nabla_y) - (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))) \cdot y] \\
&\cdot \left[a^1(y,t)\chi_n(z;q(t),p(t))\right] \\
&= [H(q(t),p(t)) - E_n(q(t),p(t))] \cdot \\
&\left[(-i\nabla_y)a^1(y,t) \cdot \nabla_p\chi_n(z;q(t),p(t)) + ya^1(y,t) \cdot \nabla_q\chi_n(z;q(t),p(t))\right].
\end{aligned} \tag{2.5.44}$$

All remaining terms in (2.5.43) may be written as the sum of terms $T_1 + T_2$, where:

$$\begin{aligned}
T_1 &:= - \left[\frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta - i\partial_t\right] \cdot \left[a^0(y,t)\chi_n(z;q(t),p(t))\right] \\
T_2 &:= [-((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))) \cdot (-i\nabla_y) - (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))) \cdot y] \\
&\quad \cdot \left[(-i\nabla_y)a^0(y,t) \cdot \nabla_p\chi_n(z;q(t),p(t)) + ya^0(y,t) \cdot \nabla_q\chi_n(z;q(t),p(t))\right].
\end{aligned} \tag{2.5.45}$$

Using (2.5.7), we have that:

$$\begin{aligned}
T_1 = &- \left[\frac{1}{2}(-i\nabla_y)^2 a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta a^0(y,t) - i\partial_t a^0(y,t)\right]\chi_n(z;q(t),p(t)) \\
&+ i\nabla_p E_n(q(t),p(t))a^0(y,t) \cdot \nabla_p\chi_n(z;q(t),p(t)) \\
&- i\nabla_q E_n(q(t),p(t))a^0(y,t) \cdot \nabla_q\chi_n(z;q(t),p(t)).
\end{aligned} \tag{2.5.46}$$

Terms $T_2$ may be written out as follows:

$$\begin{aligned}
&T_2 = T_{21} + T_{22} + T_{23} \\
&T_{21} := -(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q(t),p(t)))\partial_{p_\beta}\chi_n(z;q(t),p(t)) \\
&T_{22} := -(-i\partial_{y_\alpha})y_\beta a^0(y,t)((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q(t),p(t)))\partial_{q_\beta}\chi_n(z;q(t),p(t)) \\
&\qquad - y_\alpha(-i\partial_{y_\beta})a^0(y,t)(\partial_{q_\alpha}U(z,q(t)) - \partial_{q_\alpha}E_n(q(t),p(t)))\partial_{p_\beta}\chi_n(z;q(t),p(t)) \\
&T_{23} := -y_\alpha y_\beta a^0(y,t)(\partial_{q_\alpha}U(z,q(t)) - \partial_{q_\alpha}E_n(q(t),p(t)))\partial_{q_\beta}\chi_n(z;q(t),p(t)).
\end{aligned} \tag{2.5.47}$$

Using (2.5.39) and (2.5.40) respectively we have that:

$$\begin{aligned}
T_{21} =& \frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(q(t),p(t))\right)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ [H(q(t),p(t)) - E_n(q(t),p(t))]\left[\frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;q(t),p(t))\right],
\end{aligned} \tag{2.5.48}$$

and:

$$\begin{aligned}
T_{23} =& \frac{1}{2}\left(\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t)) - \partial_{q_\alpha}\partial_{q_\beta}E_n(q(t),p(t))\right)y_\alpha y_\beta a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ [H(q(t),p(t)) - E_n(q(t),p(t))]\left[\frac{1}{2}y_\alpha y_\beta a^0(y,t)\partial_{q_\alpha}\partial_{q_\beta}\chi_n(z;q(t),p(t))\right].
\end{aligned} \tag{2.5.49}$$

We simplify $T_{22}$ as follows. First, we observe that:

$$\begin{aligned}
(-i\partial_{y_\alpha})y_\beta &= \frac{1}{2}(-i\partial_{y_\alpha})y_\beta + \frac{1}{2}y_\beta(-i\partial_{y_\alpha}) - i\delta_{\alpha\beta} \\
y_\alpha(-i\partial_{y_\beta}) &= \frac{1}{2}y_\alpha(-i\partial_{y_\beta}) + \frac{1}{2}(-i\partial_{y_\beta})y_\alpha + i\delta_{\alpha\beta}.
\end{aligned} \tag{2.5.50}$$

Hence, we can write $T_{22}$ as:

$$\begin{aligned}
T_{22} = &-\frac{1}{2}(-i\partial_{y_\alpha})y_\beta a^0(y,t)((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q(t),p(t)))\partial_{q_\beta}\chi_n(z;q(t),p(t)) \\
&-\frac{1}{2}y_\beta(-i\partial_{y_\alpha})a^0(y,t)((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(q(t),p(t)))\partial_{q_\beta}\chi_n(z;q(t),p(t)) \\
&+ia^0(y,t)\frac{1}{2}((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t)))\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&-\frac{1}{2}y_\alpha(-i\partial_{y_\beta})a^0(y,t)(\partial_{q_\alpha}U(z,q(t)) - \partial_{q_\alpha}E_n(q(t),p(t)))\partial_{p_\beta}\chi_n(z;q(t),p(t)) \\
&-\frac{1}{2}(-i\partial_{y_\beta})y_\alpha a^0(y,t)(\partial_{q_\alpha}U(z,q(t)) - \partial_{q_\alpha}E_n(q(t),p(t)))\partial_{p_\beta}\chi_n(z;q(t),p(t)) \\
&-ia^0(y,t)\frac{1}{2}(\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t)))\cdot\nabla_p\chi_n(z;q(t),p(t)).
\end{aligned} \tag{2.5.51}$$

We now make use of (2.5.41) to conclude that:

$$
\begin{aligned}
T_{22} = &- \frac{1}{2}\partial_{p_\alpha}\partial_{q_\beta}E_n(q(t),p(t))(-i\partial_{y_\alpha})y_\beta a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ [H(q(t),p(t)) - E_n(q(t),p(t))]\left[\frac{1}{2}(-i\partial_{y_\alpha})y_\beta a^0(y,t)\partial_{p_\alpha}\partial_{q_\beta}\chi_n(z;q(t),p(t))\right] \\
&- \frac{1}{2}\partial_{q_\alpha}\partial_{p_\beta}E_n(q(t),p(t))y_\alpha(-i\partial_{y_\beta})a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ [H(q(t),p(t)) - E_n(q(t),p(t))]\left[\frac{1}{2}y_\alpha(-i\partial_{y_\beta})a^0(y,t)\partial_{q_\alpha}\partial_{p_\beta}\chi_n(z;q(t),p(t))\right] \\
&+ ia^0(y,t)\frac{1}{2}((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t)))\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&- ia^0(y,t)\frac{1}{2}(\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t)))\cdot\nabla_p\chi_n(z;q(t),p(t)).
\end{aligned}
\tag{2.5.52}
$$

Putting together (2.5.46), (2.5.47), (2.5.48), (2.5.49), and (2.5.52) we have that:

$$
\xi^2(y,z,t) = \tilde{\xi}^2(y,z,t) + [H(q(t),p(t)) - E_n(q(t),p(t))]u^2(y,z,t), \tag{2.5.53}
$$

where:

$$
\begin{aligned}
u^2(y,z,t) = &(-i\nabla_y)a^1(y,t)\cdot\nabla_p\chi_n(z;q(t),p(t)) + ya^1(y,t)\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&+ \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;q(t),p(t)) + \frac{1}{2}(-i\partial_{y_\alpha})y_\beta a^0(y,t)\partial_{p_\alpha}\partial_{q_\beta}\chi_n(z;q(t),p(t)) \\
&+ \frac{1}{2}y_\alpha(-i\partial_{y_\beta})a^0(y,t)\partial_{q_\alpha}\partial_{p_\beta}\chi_n(z;q(t),p(t)) + \frac{1}{2}y_\alpha y_\beta a^0(y,t)\partial_{q_\alpha}\partial_{q_\beta}\chi_n(z;q(t),p(t)),
\end{aligned}
\tag{2.5.54}
$$

and:

$$
\begin{aligned}
\tilde{\xi}^2(y,z,t) = &-\left[\frac{1}{2}(-i\nabla_y)^2a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t))y_\alpha y_\beta a^0(y,t) - i\partial_t a^0(y,t)\right]\chi_n(z;q(t),p(t)) \\
&+ i\nabla_p E_n(q(t),p(t))a^0(y,t)\cdot\nabla_p\chi_n(z;q(t),p(t)) - i\nabla_q E_n(q(t),p(t))a^0(y,t)\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&+ \frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(q(t),p(t))\right)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ \frac{1}{2}\left(\partial_{q_\alpha}\partial_{q_\beta}U(z,q(t)) - \partial_{q_\alpha}\partial_{q_\beta}E_n(q(t),p(t))\right)y_\alpha y_\beta a^0(y,t)\chi_n(z;q(t),p(t)) \\
&+ ia^0(y,t)\frac{1}{2}((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t)))\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&- ia^0(y,t)\frac{1}{2}(\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t)))\cdot\nabla_p\chi_n(z;q(t),p(t)).
\end{aligned}
\tag{2.5.55}
$$

Taking note of some exact cancellations and re-arranging gives:

$$\begin{aligned}
\tilde{\xi}^2(y,z,t) = &- \Bigg[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(q(t),p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}E_n(q(t),p(t))y_\alpha y_\beta a^0(y,t) \\
&+ \frac{1}{2}\partial_{p_\alpha}\partial_{q_\beta}E_n(q(t),p(t))(-i\partial_{y_\alpha})y_\beta a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{p_\beta}E_n(q(t),p(t))y_\alpha(-i\partial_{y_\beta})a^0(y,t) \\
&- i\partial_t a^0(y,t)\Bigg]\chi_n(z;q(t),p(t)) \\
&+ i\nabla_p E_n(q(t),p(t))a^0(y,t)\cdot\nabla_p\chi_n(z;q(t),p(t)) - i\nabla_q E_n(q(t),p(t))a^0(y,t)\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&+ ia^0(y,t)\frac{1}{2}((p(t)-i\nabla_z)-\nabla_p E_n(q(t),p(t)))\cdot\nabla_q\chi_n(z;q(t),p(t)) \\
&- ia^0(y,t)\frac{1}{2}(\nabla_q U(z,q(t))-\nabla_q E_n(q(t),p(t)))\cdot\nabla_p\chi_n(z;q(t),p(t)).
\end{aligned} \tag{2.5.56}$$

By Assumption 2.5.1, equation (2.5.38) is solvable for $f^2(y,z,t)$ under the condition that the projection of $\xi^2(y,z,t)$ onto the subspace of $L^2_{per}$ spanned by $\chi_n(z;q(t),p(t))$ vanishes. By self-adjointness of $H(q(t),p(t))$ and from the decomposition of $\xi^2(y,z,t)$ displayed in (2.5.53), this condition is equivalent to the condition that the projection of $\tilde{\xi}^2(y,z,t)$ given by (2.5.56) onto the subspace of $L^2_{per}$ spanned by $\chi_n(z;q(t),p(t))$ vanishes. This condition is equivalent to requiring that $a^0(y,t)$ satisfies the following Schrödinger equation for all $t \geq 0$:

$$\begin{aligned}
i\partial_t a^0(y,t) = &\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(q(t),p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}E_n(q(t),p(t))y_\alpha y_\beta a^0(y,t) \\
&+ \frac{1}{2}\partial_{p_\alpha}\partial_{q_\beta}E_n(q(t),p(t))(-i\partial_{y_\alpha})y_\beta a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{p_\beta}E_n(q(t),p(t))y_\alpha(-i\partial_{y_\beta})a^0(y,t) \\
&- \nabla_p E_n(q(t),p(t))\cdot\mathcal{A}_q(q(t),p(t))a^0(y,t) + \nabla_q E_n(q(t),p(t))\cdot\mathcal{A}_p(q(t),p(t))a^0(y,t) \\
&+ \frac{1}{2}i\left\langle\chi_n(\cdot;q(t),p(t))\right|(\nabla_q U(z,q(t))-\nabla_q E_n(q(t),p(t)))\cdot\nabla_p\chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)}a^0(y,t) \\
&- \frac{1}{2}i\left\langle\chi_n(\cdot;q(t),p(t))\right|((p(t)-i\nabla_z)-\nabla_p E_n(q(t),p(t)))\cdot\nabla_q\chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)}a^0(y,t).
\end{aligned} \tag{2.5.57}$$

Here, $\mathcal{A}_q(q,p)$ and $\mathcal{A}_p(q,p)$ are the Berry connections with respect to $q$, $p$ defined by (2.5.12). The last two terms in (2.5.57) may be simplified using self-adjointness of $H(q,p)$ as follows:

$$\begin{aligned}
&\frac{1}{2}i\left\langle \chi_n(\cdot;q(t),p(t))\right| (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))) \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&- \frac{1}{2}i\left\langle \chi_n(\cdot;q(t),p(t))\right| ((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))) \cdot \nabla_q \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&= \frac{1}{2}i\left\langle (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t)))\, \chi_n(\cdot;q(t),p(t))\right| \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&- \frac{1}{2}i\left\langle ((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t)))\, \chi_n(\cdot;q(t),p(t))\right| \cdot \nabla_q \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&= -\frac{1}{2}i\left\langle [H(q(t),p(t)) - E_n(q(t),p(t))]\, \nabla_q \chi_n(\cdot;q(t),p(t))\right| \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&+ \frac{1}{2}i\left\langle [H(q(t),p(t)) - E_n(q(t),p(t))]\, \nabla_p \chi_n(\cdot;q(t),p(t))\right| \cdot \nabla_q \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&= -\frac{1}{2}i\left\langle \nabla_q \chi_n(\cdot;q(t),p(t))\right| [H(q(t),p(t)) - E_n(q(t),p(t))] \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t) \\
&+ \frac{1}{2}i\left\langle \nabla_p \chi_n(\cdot;q(t),p(t))\right| [H(q(t),p(t)) - E_n(q(t),p(t))] \cdot \nabla_q \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t),
\end{aligned} \tag{2.5.58}$$

where the second-to-last equality in (2.5.58) follows from (2.5.32). By self-adjointness of $H(q,p)$, the final expression in (2.5.58) has the form:

$$\frac{1}{2}i(\overline{z} - z) = \operatorname{Im} z, \tag{2.5.59}$$

where:

$$z := \left\langle \nabla_q \chi_n(\cdot;q(t),p(t))\right| [H(q(t),p(t)) - E_n(q(t),p(t))] \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)}. \tag{2.5.60}$$

Hence (2.5.57) may be written in the compact form:

$$\begin{aligned}
i\partial_t a^0(y,t) &= \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta} E_n(q(t),p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta} E_n(q(t),p(t)) y_\alpha y_\beta a^0(y,t) \\
&+ \frac{1}{2}\partial_{p_\alpha}\partial_{q_\beta} E_n(q(t),p(t)) \left[(-i\partial_{y_\alpha}) y_\beta + y_\beta(-i\partial_{y_\alpha})\right] a^0(y,t) \\
&- \nabla_p E_n(q(t),p(t)) \cdot \mathcal{A}_q(q(t),p(t)) a^0(y,t) + \nabla_q E_n(q(t),p(t)) \cdot \mathcal{A}_p(q(t),p(t)) a^0(y,t) \\
&+ \operatorname{Im} \left\langle \nabla_q \chi_n(\cdot;q(t),p(t))\right| [H(q(t),p(t)) - E_n(q(t),p(t))] \cdot \nabla_p \chi_n(\cdot;q(t),p(t))\rangle_{L^2_z(\Omega)} a^0(y,t).
\end{aligned} \tag{2.5.61}$$

Equations (2.5.11) and (2.5.13) now follow from substituting $a^0(y,t) = e^{i\phi_B(t)}a(y,t)$ into (2.5.61) and matching with the initial data (2.5.20). Equation (2.5.38) now has the unique solution:

$$
\begin{aligned}
&f^2(y,z,t) = u^2(y,z,t) \\
&+ i\nabla_p E_n(q(t),p(t))a^0(y,t) \cdot [H(q(t),p(t)) - E_n(q(t),p(t))]^{-1} P^\perp(q(t),p(t)) \nabla_p \chi_n(z;q(t),p(t)) \\
&- i\nabla_q E_n(q(t),p(t))a^0(y,t) \cdot [H(q(t),p(t)) - E_n(q(t),p(t))]^{-1} P^\perp(q(t),p(t)) \nabla_q \chi_n(z;q(t),p(t)) \\
&+ ia^0(y,t)\frac{1}{2}[H(q(t),p(t)) - E_n(q(t),p(t))]^{-1} P^\perp(q(t),p(t)) \\
&\qquad\qquad \cdot ((p(t) - i\nabla_z) - \nabla_p E_n(q(t),p(t))) \cdot \nabla_q \chi_n(z;q(t),p(t)) \\
&- ia^0(y,t)\frac{1}{2}[H(q(t),p(t)) - E_n(q(t),p(t))]^{-1} P^\perp(q(t),p(t)) \\
&\qquad\qquad \cdot (\nabla_q U(z,q(t)) - \nabla_q E_n(q(t),p(t))) \cdot \nabla_p \chi_n(z;q(t),p(t)).
\end{aligned}
\tag{2.5.62}
$$

Here, $u^2(y,z,t)$ is defined by (2.5.54) and $P^\perp(q(t),p(t))$ denotes the projection operator on $L^2_{per}$ onto the orthogonal complement of the subspace spanned by $\chi_n(z;q(t),p(t))$. Invertability of the operator $[H(q(t),p(t)) - E_n(q(t),p(t))]$ on $P^\perp(q(t),p(t))L^2_{per}$ for all $t \geq 0$ is guaranteed by Assumption 2.5.1. Theorem 2.5.1 now follows from an identical analysis to that given in Section 2.3.2.

## 2.6 Semiclassical wavepacket solutions of Maxwell's equations

We now discuss how the above theory (Sections 2.1-2.5) may be adapted to the setting where the Schrödinger equations (2.1.1) or (2.5.1) are replaced by a time-dependent Maxwell system. Consider the following system of equations for the electromagnetic fields $E^\delta(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^3, H^\delta(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^3$ in matter depending on a small parameter $\delta \ll 1$:

$$
\partial_t \begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = \begin{pmatrix} 0 & \nabla\times \\ -\nabla\times & 0 \end{pmatrix} \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix}, \qquad \nabla \cdot \begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = 0 \tag{2.6.1}
$$

together with the *constitutive relations*:

$$
\begin{pmatrix} D^\delta(x,t) \\ B^\delta(x,t) \end{pmatrix} = \begin{pmatrix} \varepsilon\left(\frac{x}{\delta},x\right) & \chi^\dagger\left(\frac{x}{\delta},x\right) \\ \chi\left(\frac{x}{\delta},x\right) & \mu\left(\frac{x}{\delta},x\right) \end{pmatrix} \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix}. \tag{2.6.2}
$$

Here, we assume that each entry in the matrix of constitutive relations is smooth in both arguments and periodic with respect to a lattice $\Lambda$ in its first argument, and such that the matrix as a whole is positive-definite and Hermitian at each value of $x \in \mathbb{R}^3$. Note that when studying Maxwell's equations it is convenient to label the small parameter $\delta$ rather than $\epsilon$ to avoid confusion with the dielectric tensor $\varepsilon$.

The essential observations that will allow us to adapt the theory developed above for Schrödinger's equation are the following:

**Remark 2.6.1** (Schrödinger structure of Maxwell's equations and conservation of weighted norm)**.** *Let:*

$$\Psi^\delta(x,t) := \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix}, \tag{2.6.3}$$

*so that $\Psi^\delta(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^6$. Substituting* (2.6.3) *into* (2.6.1) *and using positive-definiteness of the matrix* (2.6.2) *we see that we can write the Maxwell system* (2.6.1) *as a Schrödinger equation for $\Psi^\delta(x,t)$:*

$$i\partial_t \Psi^\delta(x,t) = \mathcal{H}^\delta(-i\nabla, x)\Psi^\delta(x,t) \tag{2.6.4}$$

*where:*

$$\mathcal{H}^\delta(-i\nabla, x) := \begin{pmatrix} \varepsilon\left(\frac{x}{\delta}, x\right) & \chi^\dagger\left(\frac{x}{\delta}, x\right) \\ \chi\left(\frac{x}{\delta}, x\right) & \mu\left(\frac{x}{\delta}, x\right) \end{pmatrix}^{-1} \begin{pmatrix} 0 & i\nabla\times \\ -i\nabla\times & 0 \end{pmatrix}. \tag{2.6.5}$$

*Now, let $\Phi(x), \Theta(x) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}^6$ be arbitrary functions and define the weighted, $\delta$-dependent inner product:*

$$\langle \Phi | \Theta \rangle^\delta := \int_{\mathbb{R}^3} \overline{\Phi(x)} \cdot \begin{pmatrix} \varepsilon\left(\frac{x}{\delta}, x\right) & \chi^\dagger\left(\frac{x}{\delta}, x\right) \\ \chi\left(\frac{x}{\delta}, x\right) & \mu\left(\frac{x}{\delta}, x\right) \end{pmatrix} \begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix} \Theta(x)\, dx. \tag{2.6.6}$$

*Then, by assumption on the elements of* (2.6.2)*, the operator $\mathcal{H}^\delta(-i\nabla, x)$ defined by* (2.6.5) *is* symmetric *with respect to $\langle | \rangle^\delta$. It follows that the norm (induced by this inner product) of solutions of* (2.6.4) *is conserved: if $\Psi^\delta(x,t)$ solves* (2.6.4) *for all $t \geq 0$, then:*

$$\frac{d}{dt}\left\langle \Psi^\delta(\cdot,t) \middle| \Psi^\delta(\cdot,t) \right\rangle^\delta = 0. \tag{2.6.7}$$

*The conservation law* (2.6.7) *is precisely what is needed to prove convergence (as $\delta \downarrow 0$) of the asymptotic semiclassical wavepacket solutions (in the norm induced by the inner product* (2.6.6)*).*

The appropriate Bloch eigenvalue problem (cf. (2.1.13) and (2.5.3)) in this setting is the following:

$$\begin{aligned} & H(q,p)X(z;q,p) = E(q,p)X(z;q,p), \\ & \text{for all } v \in \Lambda,\ X(z+v;q,p) = X(z;q,p), \\ & H(q,p) := \begin{pmatrix} \varepsilon\,(z,q) & \chi^\dagger\,(z,q) \\ \chi\,(z,q) & \mu\,(z,q) \end{pmatrix}^{-1} \begin{pmatrix} 0 & -(p-i\nabla_z)\times \\ (p-i\nabla_z)\times & 0 \end{pmatrix}. \end{aligned} \tag{2.6.8}$$

Just as before (cf. (2.1.13) and (2.5.3)), the operator (2.6.8) is self-adjoint (with respect to the inner product 2.6.6 with discrete real eigenvalues which may be ordered with multiplicity:

$$E_1(q,p) \leq E_2(q,p) \leq ... \leq E_n(q,p) \leq ... \tag{2.6.9}$$

which vary smoothly in $q$ and $p$ along with their associated eigenfunctions $X(z;q,p)$ away from band degeneracies (cf. Theorem 2.2.1). We expect that there exist solutions of the system (2.6.1)-(2.6.2) satisfying:

$$\begin{pmatrix} E^\delta(x,t) \\ H^\delta(x,t) \end{pmatrix} = \delta^{-3/4} e^{iS(t)/\delta} e^{ip(t)\cdot(x-q(t))/\delta} a\left(\frac{x-q(t)}{\delta^{1/2}}, t\right) X_n\left(\frac{x}{\delta}; q(t), p(t)\right) + o(1), \tag{2.6.10}$$

where $X_n(z;p,q)$ satisfies (2.6.8) and the band $E_n(q,p)$ is *isolated* along the trajectory $q(t), p(t)$, up to 'Ehrenfest time' $t \sim \ln 1/\delta$ (cf. Theorems 2.1.1 and 2.5.1) for appropriate evolution of $S(t)$, $q(t)$, $p(t)$, $a(y,t)$. To fully generalize the theory displayed in Sections 2.1-2.5 to this setting is the subject of ongoing work.

The $\delta \downarrow 0$ limit of the system (2.6.1)-(2.6.2) was studied by De Nittis and Lein [53; 54]. By proving an Egorov theorem, they are able to describe the evolution of observables associated to solutions of (2.6.1)-(2.6.2) up to and including terms proportional to $\delta$. These terms again depend on the Bloch band's Berry curvature.

Interestingly, Berry curvature corrections to the dynamics of wavepacket solutions of the Maxwell system (2.6.1)-(2.6.2) have been derived even when all entries in the matrix of constitutive relations (2.6.2) are *independent of the periodic scale.* This is in contrast to the Schrödinger case. In the Schrödinger cases (2.1.1) and (2.5.1), if the periodic background is trivial, i.e. $U(z,x)$ is actually *independent* of $z$, then the associated Bloch functions $\chi_n(z;q,p)$ are also trivial: for all $n, q, p$, we may take $\chi_n(z;q,p) = 1$. In particular, the correction to the equations of motion of observables associated to the wavepacket solution due to Berry curvature (see (2.1.3), for example) is always zero. These corrections are responsible for the *spin Hall effect of light* which has been experimentally observed [7; 77]. We give a derivation of Berry curvature for eigenfunctions of (2.6.8) in 'free space' in Section 2.7.2.

Light propagation in a so-called *biaxial crystal* is described by (2.6.1)-(2.6.2) with $\chi\left(\frac{x}{\epsilon}, x\right) = 0$, $\mu\left(\frac{x}{\epsilon}, x\right) = 1$, and $\varepsilon\left(\frac{x}{\epsilon}, x\right) = \varepsilon$ where $\varepsilon$ is a constant Hermitian matrix with 3 real distinct eigenvalues. Such media exhibit conical intersections in their dispersion surfaces (which correspond to the eigenvalue bands of (2.6.8)). These intersection points are responsible for the phenomenon of *conical diffraction* [6]. It would be interesting to understand the dynamics due to Berry curvature in the case where the medium is 'strained' so that the matrix $\varepsilon$ varies across the medium: $\varepsilon \to \varepsilon(x)$. We expect the Berry curvature-induced dynamics to be non-trivial in this case because of the presence of multiple degeneracies: along the 'optic axis' the dispersion surfaces are two-fold degenerate, and at the origin of parameter space the dispersion surfaces are three-fold degenerate (in Section 2.7.2 we consider the simplest case, where $\varepsilon(x)$ is a scalar function multiplying the identity matrix).

## 2.7 Examples of systems with non-zero Berry curvature

### 2.7.1 Berry curvature near to a domain wall 'edge' modulation of a honeycomb structure

In this section we consider the eigenvalue problem (2.5.3) when $d = 2$ and:

$$U(z, x) = V_{h,e}(z) + \kappa(\mathfrak{K} \cdot x) V_{h,o}(z) . \tag{2.7.1}$$

Here, $V_{h,e}$ is a smooth honeycomb lattice potential in the sense of Definition 2.1 of [28]. It was demonstrated in [27] that Schrödinger's operator with a closely-related potential to (2.7.1) supports robust 'edge' states. $V_{h,e}(z)$ therefore has the periodicity of a honeycomb lattice $\Lambda_h$:

$$\forall v \in \Lambda_h, V_{h,e}(z + v) = V_{h,e}(z), \tag{2.7.2}$$

is even:

$$V_{h,e}(-z) = V_{h,e}(z) \tag{2.7.3}$$

and is invariant under rotation by $2\pi/3$:

$$V_{h,e}(R^* z) = V_{h,e}(z) \tag{2.7.4}$$

where $R^*$ denotes the counter-clockwise rotation matrix by $2\pi/3$. $V_{h,o}(z)$ is assumed smooth, has the periodicity of the lattice, and is odd:

$$V_{h,o}(-z) = -V_{h,o}(z). \tag{2.7.5}$$

Let $v_1, v_2$ denote primitive lattice vectors of $\Lambda$ so that:

$$\Lambda_h = \mathbb{Z}v_1 \oplus \mathbb{Z}v_2 \tag{2.7.6}$$

and $k_1, k_2$ denote primitive lattice vectors of the dual space $\Lambda^*$ so that:

$$\begin{aligned} &k_\alpha \cdot v_\beta = \delta_{\alpha\beta} \\ &\Lambda_h^* = \mathbb{Z}k_1 \oplus \mathbb{Z}k_2 \end{aligned} \tag{2.7.7}$$

We define an edge in the structure, following [26], by fixing real constants $a_1, b_1$ and setting:

$$\begin{aligned} &\mathfrak{v}_1 = a_1 v_1 + b_1 v_2 \\ &\mathfrak{v}_2 = a_2 v_1 + b_2 v_2 \end{aligned} \tag{2.7.8}$$

where $a_1 b_2 - a_2 b_1 = 1$ so that $\mathbb{Z}v_1 \oplus \mathbb{Z}v_2 = \mathbb{Z}\mathfrak{v}_1 \oplus \mathbb{Z}\mathfrak{v}_2 = \Lambda_h$. We have the dual lattice vectors:

$$\begin{aligned} &\mathfrak{K}_1 = b_2 k_1 - a_2 k_2 \\ &\mathfrak{K}_2 = -b_1 k_1 + a_1 k_2 \end{aligned} \tag{2.7.9}$$

so that:

$$\begin{aligned} &\mathfrak{K}_\alpha \cdot \mathfrak{v}_\beta = \delta_{\alpha\beta} \\ &\Lambda_h^* = \mathbb{Z}\mathfrak{K}_1 \oplus \mathbb{Z}\mathfrak{K}_2. \end{aligned} \tag{2.7.10}$$

The 'domain wall' function $\kappa(\zeta)$ is assumed smooth and satisfies:

$$\kappa(0) = 0, \kappa'(0) > 0, \lim_{\zeta \to \infty} \kappa(\zeta) =: \kappa_\infty > 0, \lim_{\zeta \to -\infty} \kappa(\zeta) =: \kappa_{-\infty} < 0 \tag{2.7.11}$$

For example, we may take $\kappa(\zeta) = \tanh(\zeta)$. The eigenvalue problem (2.5.3) takes the form:

$$\begin{aligned} &H(p,q)\chi(z;p,q) = E(p,q)\chi(z;p,q) \\ &\forall v \in \Lambda_h,\ \chi(z+v;p,q) = \chi(z;p,q) \\ &H(p,q) := \frac{1}{2}(p - i\nabla_z)^2 + V_{h,e}(z) + \kappa(\mathfrak{K}\cdot q)V_{h,o}(z)\,. \end{aligned} \tag{2.7.12}$$

Taking $\mathfrak{K}_2 \cdot q = 0$ in (2.7.12) gives:

$$\begin{aligned} &H(p,0)\chi(z;p,0) = E(p,0)\chi(z;p,0) \\ &\forall v \in \Lambda_h,\ \chi(z+v;p,0) = \chi(z;p,0) \\ &H(p,0) := \frac{1}{2}(p - i\nabla_z)^2 + V_{h,e}(z). \end{aligned} \tag{2.7.13}$$

which is the Bloch eigenvalue problem for a honeycomb lattice potential, as studied in [28]. In that paper (see Theorem 5.1) it was shown that for generic honeycomb lattice potentials $V_{h,e}(z)$ there exist conical singularities in the dispersion surface of the operator $H(p,0)$. They occur at every vertex of the Brillouin zone. After symmetry reduction, there are essentially two distinct vertices of $\mathcal{B}$, known as the $K$ and $K'$ points. The $K$ and $K'$ points are related by:

$$K' = -K. \tag{2.7.14}$$

Let $E_{\pm}(p,0)$ denote eigenvalue bands which are degenerate at the quasi-momentum $k = K$ with energy $E^*$:

$$E_{\pm}(K,0) = E^* \tag{2.7.15}$$

And let:

$$\begin{aligned} &\chi_1(z;K,0), \chi_2(z;K,0) := \overline{\chi_1(-z;K,0)} \\ &\forall v \in \Lambda_h, j \in \{1,2\}, \chi_j(z+v;K,0) = \chi_j(z;K,0) \end{aligned} \tag{2.7.16}$$

denote the basis of the degenerate $E^*$-eigenspace introduced in [28]. It was shown in that paper that generically this degeneracy is lifted for $p - K \neq 0$ and $|p - K|$ small enough. Moreover, the eigenvalue splitting is conical:

$$E_{\pm}(p,0) = E^* \pm |\lambda||p-K| + O(|p-K|^2). \tag{2.7.17}$$

where $\lambda$ is a complex constant which depends on the degenerate eigenfunctions (2.7.16) and is non-zero for generic $V_{h,o}$.

#### 2.7.1.1 Derivation of local character of eigenvalue bands

We now study the behavior of the eigenvalue bands $E_{\pm}(p,q)$ for small $p-K, q$ by a formal degenerate perturbation theory about the point $(K,0)$ and energy $E^*$. The argument we present may be made rigorous by *Lyapunov-Schmidt reduction* (see the Appendices of [25] for examples of these techniques). Let:

$$\begin{aligned} p' &:= p - K \\ q_2 &:= \mathfrak{K}_2 \cdot q \end{aligned} \tag{2.7.18}$$

then we can re-write (2.7.12) as:

$$\begin{aligned} &H(K+p', q_2)\chi(z; K+p', q_2) = E(K+p', q_2)\chi(z; K+p', q_2) \\ &\forall v \in \Lambda_h, \chi(z+v; K+p', q_2) = \chi(z; K+p', q_2) \\ &H(K+p', q_2) := \frac{1}{2}(K+p'-i\nabla_z)^2 + V_{h,e}(z) + \kappa(q_2)V_{h,o}(z). \end{aligned} \tag{2.7.19}$$

Expanding the eigenvalue problem (2.7.19) in $p'$ and $q_2$ using smoothness of $\kappa(\zeta)$ we have:

$$\begin{aligned} &\left[H(K,0) + p' \cdot (K - i\nabla_z) + q_2 \partial_\zeta \kappa(0) V_{h,o}(z) + O({p'}^2, q_2^2)\right] \chi(z; K+p', q_2) \\ &= E(K+p', q_2)\chi(z; K+p', q_2) \end{aligned} \tag{2.7.20}$$

we seek a solution of (2.7.20) of the form:

$$\begin{aligned} E(K+p', q_2) &= E^* + E'(p', q_2) \\ \chi(z; K+p', q_2) &= \chi(z; K, 0) + \chi'(z; p', q_2) \end{aligned} \tag{2.7.21}$$

where:

$$\begin{aligned} &\left\langle \chi_1(\cdot; K, 0) \middle| \chi'(\cdot; p', q_2) \right\rangle_{L^2_z(\Omega)} = \left\langle \chi_2(\cdot; K, 0) \middle| \chi'(\cdot; p', q_2) \right\rangle_{L^2_z(\Omega)} = 0 \\ &\chi(z; K, 0) = \alpha(p', q_2)\chi_1(z; K, 0) + \beta(p', q_2)\chi_2(z; K, 0) \end{aligned} \tag{2.7.22}$$

where $\alpha(p', q_2), \beta(p', q_2)$ are functions to be determined, and $\chi'(z; p', q_2)$ has the periodicity of the lattice:

$$\forall v \in \Lambda_h, \chi'(z+v; p', q_2) = \chi'(z; p', q_2). \tag{2.7.23}$$

Here and in the remainder of this section $\Omega$ refers to a fundamental cell of the honeycomb lattice. Substituting (2.7.21) into (2.7.20) gives:

$$\begin{aligned} &[H(K,0) - E^*]\, \chi'(z; p', q_2) = \\ &- \left[p' \cdot (K - i\nabla_z) + q_2 \partial_\zeta \kappa(0) V_{h,o}(z) - E'(p', q_2)\right] \left[\alpha(p', q_2)\chi_1(z; K, 0) + \beta(p', q_2)\chi_2(z; K, 0)\right] \\ &+ \text{higher order terms in } p', q_2. \end{aligned} \tag{2.7.24}$$

Ignoring higher order terms, equation (2.7.24) is uniquely solvable for $\chi'(z;p',q_2)$ if and only if the projection of the right-hand side onto the null space of $[H(K,0)-E^*]$ is zero:

$$Q_{\parallel}\left\{ \left[p'\cdot(K-i\nabla_z)+q_2\partial_\zeta\kappa(0)V_{h,o}(z)-E'(p',q_2)\right]\left[\alpha(p',q_2)\chi_1(z;K,0)+\beta(p',q_2)\chi_2(z;K,0)\right]\right\}$$
$$=0, \tag{2.7.25}$$

where:

$$Q_{\parallel}f(z):=\sum_{j\in\{1,2\}}\langle\chi_j(z;K,0)|\,f(z)\rangle_{L^2_z(\Omega)}\,\chi_j(z;K,0). \tag{2.7.26}$$

Equation (2.7.25) can be written as a matrix equation for $E'(p',q_2),\alpha(p',q_2),\beta(p',q_2)$:

$$\mathcal{M}(E',p',q_2)\begin{pmatrix}\alpha(p',q_2)\\ \beta(p',q_2)\end{pmatrix}=0 \tag{2.7.27}$$

where:

$$\mathcal{M}(E',p',q_2):=$$
$$\begin{pmatrix} p'\cdot\langle\chi_1(z;K,0)|\,(K-i\nabla_z)\chi_1(z;K,0)\rangle_{L^2_z(\Omega)}+\partial_\zeta\kappa(0)q_2\,\langle\chi_1(z;K,0)|\,V_{h,o}(z)\chi_1(z;K,0)\rangle_{L^2_z(\Omega)}-E' & p'\cdot\langle\chi_1(z;K,0)|\,(K-i\nabla_z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)}+\partial_\zeta\kappa(0)q_2\,\langle\chi_1(z;K,0)|\,V_{h,o}(z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)} \\ p'\cdot\langle\chi_1(z;K,0)|\,(K-i\nabla_z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)}+\partial_\zeta\kappa(0)q_2\,\langle\chi_1(z;K,0)|\,V_{h,o}(z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)} & p'\cdot\langle\chi_2(z;K,0)|\,(K-i\nabla_z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)}+\partial_\zeta\kappa(0)q_2\,\langle\chi_2(z;K,0)|\,V_{h,o}(z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)}-E' \end{pmatrix} \tag{2.7.28}$$

We can use symmetries to simplify the matrix (2.7.28). Let:

$$p'_j:=v_j\cdot p'. \tag{2.7.29}$$

From Proposition 4.2 of [29] we have that:

$$\begin{aligned} &j\in\{1,2\},p'\cdot\langle\chi_j(z;K,0)|\,(K-i\nabla_z)\chi_j(z;K,0)\rangle_{L^2_z(\Omega)}=0\\ &\langle\chi_1(z;K,0)|\,(K-i\nabla_z)\chi_2(z;K,0)\rangle_{L^2_z(\Omega)}=\overline{\langle\chi_2(z;K,0)|\,(K-i\nabla_z)\chi_1(z;K,0)\rangle_{L^2_z(\Omega)}}\\ &=\overline{\lambda_\sharp}(p'_1+ip'_2)\end{aligned} \tag{2.7.30}$$

where $\lambda_\sharp \in \mathbb{C}$ is a complex constant which is non-zero for generic honeycomb lattice potentials $V_{h,e}(z)$. From Proposition 6.2 of [26] we have that:

$$\begin{aligned} &\langle \chi_1(z;K,0) | V_{h,o}(z) \chi_2(z;K,0) \rangle_{L^2_z(\Omega)} = \langle \chi_2(z;K,0) | V_{h,o}(z) \chi_1(z;K,0) \rangle_{L^2_z(\Omega)} = 0 \\ &\langle \chi_1(z;K,0) | V_{h,o}(z) \chi_1(z;K,0) \rangle_{L^2_z(\Omega)} = - \langle \chi_2(z;K,0) | V_{h,o}(z) \chi_2(z;K,0) \rangle_{L^2_z(\Omega)} \\ &=: \theta_\sharp. \end{aligned} \tag{2.7.31}$$

Here, $\theta_\sharp$ is a real constant which is non-zero for generic $V_{h,e}$ and $V_{h,o}$. We have, therefore, that the matrix (2.7.28) takes the form:

$$\mathcal{M}(p',q_2) = \begin{pmatrix} \partial_\zeta \kappa(0) \theta_\sharp q_2 - E' & \overline{\lambda_\sharp}(p'_1 + i p'_2) \\ \lambda_\sharp (p'_1 - i p'_2) & -\partial_\zeta \kappa(0) \theta_\sharp q_2 - E' \end{pmatrix}. \tag{2.7.32}$$

Solving the matrix problem (2.7.27) we have that the local character of the dispersion surface $E(K + p', q_2)$ is conical:

$$\begin{aligned} &E_\pm(p'_1,p'_2,q_2) = E^* \pm ((\partial_\zeta \kappa(0) \theta_\sharp q_2)^2 + (|\lambda_\sharp| p'_1)^2 + (|\lambda_\sharp| p'_2)^2)^{1/2} + o(|q_2|,|p'_1|,|p'_2|) \\ &\chi_\pm(z;p'_1,p'_2,q_2) = \alpha_\pm(p'_1,p'_2,q_2)\chi_1(z;K,0) + \beta_\pm(p'_1,p'_2,q_2)\chi_2(z;K,0) + o(1) \end{aligned} \tag{2.7.33}$$

where $\alpha_\pm, \beta_\pm$ solve:

$$\begin{aligned} &\begin{pmatrix} \partial_\zeta \kappa(0) \theta_\sharp q_2 & \overline{\lambda_\sharp}(p'_1 + i p'_2) \\ \lambda_\sharp (p'_1 - i p'_2) & -\partial_\zeta \kappa(0) \theta_\sharp q_2 \end{pmatrix} \begin{pmatrix} \alpha_\pm(p',q) \\ \beta_\pm(p',q) \end{pmatrix} \\ &= \pm((\partial_\zeta \kappa(0) \theta_\sharp q_2)^2 + (|\lambda_\sharp| p'_1)^2 + (|\lambda_\sharp| p'_2)^2)^{1/2} \begin{pmatrix} \alpha_\pm(p',q) \\ \beta_\pm(p',q) \end{pmatrix}. \end{aligned} \tag{2.7.34}$$

#### 2.7.1.2 Direct derivation of Berry curvature of eigenspaces of the matrix problem (2.7.34)

To ease notation, let:

$$\theta := \partial_\zeta \kappa(0) \theta_\sharp, \quad \lambda := \lambda_\sharp. \tag{2.7.35}$$

In this section we compute the Berry curvature of the $\pm \left( (\theta q_2)^2 + (|\lambda| p'_1)^2 + (|\lambda| p'_2)^2 \right)^{1/2}$-eigenspaces of the matrix eigenvalue problem:

$$\begin{pmatrix} \theta q_2 & \overline{\lambda}(p'_1 + i p'_2) \\ \lambda(p'_1 - i p'_2) & -\theta q_2 \end{pmatrix} \begin{pmatrix} \alpha_\pm(p',q) \\ \beta_\pm(p',q) \end{pmatrix} = \pm \left( (\theta q_2)^2 + (|\lambda| p'_1)^2 + (|\lambda| p'_2)^2 \right)^{1/2} \begin{pmatrix} \alpha_\pm(p',q) \\ \beta_\pm(p',q) \end{pmatrix}. \tag{2.7.36}$$

where $\theta, \lambda$ are real and imaginary constants, respectively. The matrix (2.7.36) has been well-studied as the prototype of a self-adjoint operator displaying a conical crossing in its eigenvalue bands. For another route to calculating the Berry curvature in this case see, for example, [5]. We can simplify greatly the study of this problem by changing variables. First, we decompose $\overline{\lambda}$ as follows:

$$\overline{\lambda} = |\lambda| e^{i\mu}. \tag{2.7.37}$$

Then, we change variables to spherical polar co-ordinates $\rho, \phi, \tilde{\phi}$:

$$\begin{aligned} \rho(p_1', p_2', q_2) &= ((|\lambda| p_1')^2 + (|\lambda| p_2')^2 + (\theta q_2)^2)^{1/2} \\ \phi(p_1', p_2') &= \arctan\left(\frac{p_2'}{p_1'}\right) + \mu \\ \tilde{\phi}(p_1', p_2', q_2) &= \arctan\left(\frac{((|\lambda| p_1')^2 + (|\lambda| p_2')^2)^{1/2}}{\theta q_2}\right) \end{aligned} \tag{2.7.38}$$

so that:

$$\begin{aligned} |\lambda| p_1' &= \rho \sin\tilde{\phi} \cos(\phi - \mu) \\ |\lambda| p_2' &= \rho \sin\tilde{\phi} \sin(\phi - \mu) \\ \theta q_2 &= \rho \cos\tilde{\phi} \end{aligned} \tag{2.7.39}$$

and the eigenvalue problem (2.7.36) becomes:

$$\begin{pmatrix} \cos\tilde{\phi} & e^{i\phi}\sin\tilde{\phi} \\ e^{-i\phi}\sin\tilde{\phi} & -\cos\tilde{\phi} \end{pmatrix} \begin{pmatrix} \alpha_\pm(\tilde{\phi}, \phi) \\ \beta_\pm(\tilde{\phi}, \phi) \end{pmatrix} = \pm \begin{pmatrix} \alpha_\pm(\tilde{\phi}, \phi) \\ \beta_\pm(\tilde{\phi}, \phi) \end{pmatrix} \tag{2.7.40}$$

which has the solution for all $\phi \in [0, 2\pi), \tilde{\phi} \in [0, \pi)$:

$$\begin{pmatrix} \alpha_+(\tilde{\phi}, \phi) \\ \beta_+(\tilde{\phi}, \phi) \end{pmatrix} = \begin{pmatrix} e^{i\phi/2}\cos(\tilde{\phi}/2) \\ e^{-i\phi/2}\sin(\tilde{\phi}/2) \end{pmatrix}, \begin{pmatrix} \alpha_-(\tilde{\phi}, \phi) \\ \beta_-(\tilde{\phi}, \phi) \end{pmatrix} = \begin{pmatrix} -e^{i\phi/2}\sin(\tilde{\phi}/2) \\ e^{-i\phi/2}\cos(\tilde{\phi}/2) \end{pmatrix}. \tag{2.7.41}$$

The normalized eigenvectors (2.7.41) are clearly unique only up to a phase, or *gauge*. The choice of gauge (2.7.41) turns out to simplify calculations in the present case. For a general discussion of these issues, see Appendix A.7. Our final result (2.7.49) is manifestly gauge-invariant. We record at this point:

$$\begin{aligned} &\partial_{p_1'}\rho = |\lambda|\sin\tilde{\phi}\cos(\phi-\mu), \partial_{p_2'}\rho = |\lambda|\sin\tilde{\phi}\sin(\phi-\mu), \partial_{q_2}\rho = \theta\cos\tilde{\phi} \\ &\partial_{p_1'}\phi = -\frac{|\lambda|\sin(\phi-\mu)}{\rho\sin\tilde{\phi}}, \partial_{p_2'}\phi = \frac{|\lambda|\cos(\phi-\mu)}{\rho\sin\tilde{\phi}}, \partial_{q_2}\phi = 0 \\ &\partial_{p_1'}\tilde{\phi} = \frac{|\lambda|\cos\tilde{\phi}\cos(\phi-\mu)}{\rho}, \partial_{p_2'}\tilde{\phi} = \frac{|\lambda|\cos\tilde{\phi}\sin(\phi-\mu)}{\rho}, \partial_{q_2}\tilde{\phi} = -\frac{\theta\sin\tilde{\phi}}{\rho} \end{aligned} \tag{2.7.42}$$

which implies that:

$$\partial_{p_1'} \begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix} = \frac{1}{2}\left(\frac{|\lambda|\cos\tilde\phi\cos(\phi-\mu)}{\rho}\right)\begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix}$$
$$+\frac{1}{2}\left(-\frac{|\lambda|\sin(\phi-\mu)}{\rho\sin\tilde\phi}\right)\begin{pmatrix} ie^{i\phi/2}\cos(\tilde\phi/2) \\ -ie^{-i\phi/2}\sin(\tilde\phi/2) \end{pmatrix}$$
$$\partial_{p_2'} \begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix} = \frac{1}{2}\left(\frac{|\lambda|\cos\tilde\phi\sin(\phi-\mu)}{\rho}\right)\begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix}$$
$$+\frac{1}{2}\left(\frac{|\lambda|\cos(\phi-\mu)}{\rho\sin\tilde\phi}\right)\begin{pmatrix} ie^{i\phi/2}\cos(\tilde\phi/2) \\ -ie^{-i\phi/2}\sin(\tilde\phi/2) \end{pmatrix}$$
$$\partial_{q_2} \begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix} = \frac{1}{2}\left(-\frac{\theta\sin\tilde\phi}{\rho}\right)\begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix}$$
$$\partial_{p_1'} \begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix} = -\frac{1}{2}\left(\frac{|\lambda|\cos\tilde\phi\cos(\phi-\mu)}{\rho}\right)\begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix} \tag{2.7.43}$$
$$+\frac{1}{2}\left(-\frac{|\lambda|\sin(\phi-\mu)}{\rho\sin\tilde\phi}\right)\begin{pmatrix} -ie^{i\phi/2}\sin(\tilde\phi/2) \\ -ie^{-i\phi/2}\cos(\tilde\phi/2) \end{pmatrix}$$
$$\partial_{p_2'} \begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix} = -\frac{1}{2}\left(\frac{|\lambda|\cos\tilde\phi\sin(\phi-\mu)}{\rho}\right)\begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix}$$
$$+\frac{1}{2}\left(\frac{|\lambda|\cos(\phi-\mu)}{\rho\sin\tilde\phi}\right)\begin{pmatrix} -ie^{i\phi/2}\sin(\tilde\phi/2) \\ -ie^{-i\phi/2}\cos(\tilde\phi/2) \end{pmatrix}$$

$$\partial_{q_2} \begin{pmatrix} \alpha_-(\tilde\phi,\phi) \\ \beta_-(\tilde\phi,\phi) \end{pmatrix} = -\frac{1}{2}\left(-\frac{\theta\sin\tilde\phi}{\rho}\right)\begin{pmatrix} \alpha_+(\tilde\phi,\phi) \\ \beta_+(\tilde\phi,\phi) \end{pmatrix}.$$

Using the identity:

$$\cos^2(\tilde\phi/2) - \sin^2(\tilde\phi/2) = \cos(\tilde\phi) \tag{2.7.44}$$

we have that the Berry connections with respect to variation of each parameter satisfy:

$$\begin{aligned}\mathcal{A}_{\pm,p_1'} &:= \left\langle \begin{pmatrix}\alpha_\pm(\tilde\phi,\phi)\\ \beta_\pm(\tilde\phi,\phi)\end{pmatrix} \middle| \partial_{p_1'}\begin{pmatrix}\alpha_\pm(\tilde\phi,\phi)\\ \beta_\pm(\tilde\phi,\phi)\end{pmatrix}\right\rangle = \pm\frac{|\lambda|\sin(\phi-\mu)\cos\tilde\phi}{2\rho\sin\tilde\phi}\\ \mathcal{A}_{\pm,p_2'} &:= \left\langle \begin{pmatrix}\alpha_\pm(\tilde\phi,\phi)\\ \beta_\pm(\tilde\phi,\phi)\end{pmatrix} \middle| \partial_{p_2'}\begin{pmatrix}\alpha_\pm(\tilde\phi,\phi)\\ \beta_\pm(\tilde\phi,\phi)\end{pmatrix}\right\rangle = \mp\frac{|\lambda|\cos(\phi-\mu)\cos\tilde\phi}{2\rho\sin\tilde\phi} \qquad (2.7.45)\\ \mathcal{A}_{\pm,q_2} &:= \left\langle \begin{pmatrix}\alpha_\pm(\tilde\phi,\phi)\\ \beta_\pm(\tilde\phi,\phi)\end{pmatrix} \middle| \partial_{q_2}\begin{pmatrix}\alpha_+(\tilde\phi,\phi)\\ \beta_+(\tilde\phi,\phi)\end{pmatrix}\right\rangle = 0.\end{aligned}$$

Here, $\langle|\rangle$ refers to the standard $\mathbb{C}^2$-inner product. We have then that:

$$\begin{aligned}\partial_{p_1'}\mathcal{A}_{\pm,p_2'} &= \pm\frac{|\lambda|^2}{2\rho^2}\left(\cos\tilde\phi\cos^2(\phi-\mu)+\frac{\cos^2(\phi-\mu)\cos\tilde\phi-\sin^2(\phi-\mu)\cos\tilde\phi}{\sin^2\tilde\phi}\right)\\ \partial_{p_2'}\mathcal{A}_{\pm,p_1'} &= \pm\frac{|\lambda|^2}{2\rho^2}\left(-\cos\tilde\phi\sin^2(\phi-\mu)+\frac{\cos^2(\phi-\mu)\cos\tilde\phi-\sin^2(\phi-\mu)\cos\tilde\phi}{\sin^2\tilde\phi}\right)\\ \partial_{p_2'}\mathcal{A}_{\pm,q_2} &= 0 \qquad (2.7.46)\\ \partial_{q_2}\mathcal{A}_{\pm,p_2'} &= \mp\frac{|\lambda|\theta}{2\rho^2}\sin\tilde\phi\cos(\phi-\mu)\\ \partial_{q_2}\mathcal{A}_{\pm,p_1'} &= \pm\frac{|\lambda|\theta}{2\rho^2}\sin\tilde\phi\sin(\phi-\mu)\\ \partial_{p_1'}\mathcal{A}_{\pm,q_2} &= 0\end{aligned}$$

From which it follows that the Berry curvatures satisfy:

$$\begin{aligned}\partial_{p_2'}\mathcal{A}_{\pm,q_2}-\partial_{q_2}\mathcal{A}_{\pm,p_2'} &= \pm\frac{|\lambda|\theta\cos(\phi-\mu)\sin\tilde\phi}{2\rho^2} = \pm\frac{|\lambda|^2\theta}{2\rho^3}p_1'\\ \partial_{q_2}\mathcal{A}_{\pm,p_1'}-\partial_{p_1'}\mathcal{A}_{\pm,q_2} &= \pm\frac{|\lambda|\theta\sin(\phi-\mu)\sin\tilde\phi}{2\rho^2} = \pm\frac{|\lambda|^2\theta}{2\rho^3}p_2' \qquad (2.7.47)\\ \partial_{p_1'}\mathcal{A}_{\pm,p_2'}-\partial_{p_2'}\mathcal{A}_{\pm,p_1'} &= \pm\frac{|\lambda|^2}{2\rho^2}\cos\tilde\phi = \pm\frac{|\lambda|^2\theta}{2\rho^3}q_2.\end{aligned}$$

We may write the result (2.7.47) compactly as follows. Define the vectors:

$$\mathfrak{p} := \begin{pmatrix}|\lambda|p_1'\\ |\lambda|p_2'\\ \theta q_2\end{pmatrix}, \mathcal{A}_{\pm,\mathfrak{p}} := \begin{pmatrix}\mathcal{A}_{\pm,|\lambda|p_1'}\\ \mathcal{A}_{\pm,|\lambda|p_2'}\\ \mathcal{A}_{\pm,\theta q_2}\end{pmatrix}. \qquad (2.7.48)$$

Then (2.7.47) is equivalent to:

$$\nabla_{\mathfrak{p}}\times\mathcal{A}_{\pm,\mathfrak{p}} = \pm\frac{\mathfrak{p}}{2|\mathfrak{p}|^3}. \qquad (2.7.49)$$

Hence the Berry curvature takes the form of a *monopole* at $p_1' = p_2' = 0, q_2 = 0$, where the eigenvalue bands of (2.7.19) are 2-fold degenerate.

### 2.7.2 Berry curvature due to degeneracy of polarization condition when wave-vector is zero

In free space:

$$\varepsilon\left(\frac{x}{\epsilon}, x\right) = \mu\left(\frac{x}{\epsilon}, x\right) = 1, \text{ and } \chi\left(\frac{x}{\epsilon}, x\right) = 0. \tag{2.7.50}$$

The Maxwell-Bloch eigenvalue problem (2.6.8) then reduces to:

$$\begin{pmatrix} 0 & -p\times \\ p\times & 0 \end{pmatrix} X(p) = E(p)X(p). \tag{2.7.51}$$

For any fixed $p \in \mathbb{R}^3$, we may choose a real orthonormal basis $\{\hat{p}, \hat{v}(p), \hat{w}(p)\}$ of $\mathbb{R}^3$ (here, $\hat{p} := p/|p|$) with the property that:

$$\hat{p} \times \hat{v}(p) = \hat{w}(p). \tag{2.7.52}$$

$\hat{v}(p)$, $\hat{w}(p)$ are clearly unique *up to a rotation*. Given $\hat{v}(p)$ and $\hat{w}(p)$ which satisfy (2.7.52), the vectors $\hat{v}_\theta(p)$ and $\hat{w}_\theta(p)$ defined by:

$$\begin{pmatrix} \hat{v}_\theta(p) \\ \hat{w}_\theta(p) \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \hat{v}(p) \\ \hat{w}(p) \end{pmatrix} \tag{2.7.53}$$

will also satisfy (2.7.52) for any $\theta \in [0, 2\pi)$. We can now solve (2.7.51) exactly. There are precisely 3 eigenvalues: $|p|, -|p|$, and 0. The $|p|$-eigenspace and $-|p|$-eigenspace are spanned by, respectively:

$$\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{v}(p) \\ \hat{w}(p) \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{w}(p) \\ -\hat{v}(p) \end{pmatrix} \right\}, \qquad \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{w}(p) \\ \hat{v}(p) \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} -\hat{v}(p) \\ \hat{w}(p) \end{pmatrix} \right\}. \tag{2.7.54}$$

The 0-eigenspace is spanned by:

$$\left\{ \begin{pmatrix} \hat{p} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{p} \end{pmatrix} \right\}. \tag{2.7.55}$$

We now restrict our attention to the $|p|$-eigenspace. The $-|p|$-eigenspace is similar, while the 0-eigenspace turns out to be physically unimportant because of the 'divergence-free' condition of Maxwell's equations in free space.

We may simplify calculations (the Berry connections with respect to this basis will turn out to be *diagonal* (2.7.63)) considerably by changing basis to that of *circular polarizations*:

$$\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{v}(p) \\ \hat{w}(p) \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{w}(p) \\ -\hat{v}(p) \end{pmatrix} \right\} \mapsto \left\{ \frac{1}{2} \begin{pmatrix} \hat{v}(p) + i\hat{w}(p) \\ \hat{w}(p) - i\hat{v}(p) \end{pmatrix}, \frac{1}{2} \begin{pmatrix} \hat{v}(p) - i\hat{w}(p) \\ \hat{w}(p) + i\hat{v}(p) \end{pmatrix} \right\}. \tag{2.7.56}$$

We define:

$$e_+(p) := \frac{1}{2} \begin{pmatrix} \hat{v}(p) + i\hat{w}(p) \\ \hat{w}(p) - i\hat{v}(p) \end{pmatrix}, \quad e_-(p) := \frac{1}{2} \begin{pmatrix} \hat{v}(p) - i\hat{w}(p) \\ \hat{w}(p) + i\hat{v}(p) \end{pmatrix}. \tag{2.7.57}$$

The *rotational* freedom in the choice of $\hat{v}(p)$ and $\hat{w}(p)$ corresponds to a *phase* freedom in the choice of $e_+(p), e_-(p)$:

$$e_{\pm,\theta}(p) := \frac{1}{2} \begin{pmatrix} \hat{v}_\theta(p) \pm i\hat{w}_\theta(p) \\ \hat{w}_\theta(p) \mp i\hat{v}_\theta(p) \end{pmatrix} = e^{\pm i\theta} \frac{1}{2} \begin{pmatrix} \hat{v}(p) \pm i\hat{w}(p) \\ \hat{w}(p) \mp i\hat{v}(p) \end{pmatrix} = e^{\pm i\theta} e_\pm(p). \tag{2.7.58}$$

In order to compute the Berry connections and curvatures associated with transport of $e_+(p), e_-(p)$ (2.7.57), we must compute the derivatives $\nabla_p e_+(p)$ and $\nabla_p e_-(p)$. In order to compute these quantities, we fix an orthonormal right-handed basis of $\mathbb{R}^3$ and then write $\hat{p}$, $\hat{v}(p)$ and $\hat{w}(p)$ as vectors with respect to this basis using spherical polar co-ordinates:

$$\begin{aligned} \hat{p} &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\ \hat{v} &= (-\sin\phi, \cos\phi, 0) \\ \hat{w} &= (-\cos\theta\cos\phi, -\cos\theta\sin\phi, \sin\theta) \end{aligned} \tag{2.7.59}$$

The gradient operator $\nabla_p$ in spherical polar co-ordinates takes the form:

$$\nabla_p = \hat{p}\partial_{|p|} + \hat{\theta}\frac{1}{|p|}\partial_\theta + \hat{\phi}\frac{1}{|p|\sin\theta}\partial_\phi, \tag{2.7.60}$$

where $\hat{\theta}, \hat{\phi}$ denote unit vectors pointing in the directions of varying $\theta, \phi$. Hence:

$$\begin{aligned} \nabla_p \hat{v} &= \left( \hat{\phi}\frac{-\cos\phi}{|p|\sin\theta}, \hat{\phi}\frac{-\sin\phi}{|p|\sin\theta}, 0 \right) \\ \nabla_p \hat{w} &= \left( \hat{\theta}\frac{\sin\theta\cos\phi}{|p|} + \hat{\phi}\frac{\cos\theta\sin\phi}{|p|\sin\theta}, \hat{\theta}\frac{\sin\theta\sin\phi}{|p|} + \hat{\phi}\frac{-\cos\theta\cos\phi}{|p|\sin\theta}, \hat{\theta}\frac{\cos\theta}{|p|} \right). \end{aligned} \tag{2.7.61}$$

We compute from (2.7.61) that:

$$\begin{aligned} &\langle \hat{v} | \nabla_p \hat{v} \rangle = \langle \hat{w} | \nabla_p \hat{w} \rangle = 0, \\ &\langle \hat{v} | \nabla_p \hat{w} \rangle = -\frac{1}{|p|\tan\theta}\hat{\phi}, \quad \langle \hat{w} | \nabla_p \hat{v} \rangle = \frac{1}{|p|\tan\theta}\hat{\phi} \end{aligned} \tag{2.7.62}$$

where $\langle | \rangle$ refers to the standard inner product on $\mathbb{R}^3$. We therefore have that the Berry connections with respect to the basis of circular polarizations (2.7.57) have the form:

$$\begin{aligned} &i \langle e_- | \nabla_p e_+ \rangle = i \langle e_+ | \nabla_p e_- \rangle = 0, \\ &i \langle e_+ | \nabla_p e_+ \rangle = \frac{1}{|p| \tan\theta} \hat{\phi}, \quad i \langle e_- | \nabla_p e_- \rangle = -\frac{1}{|p| \tan\theta} \hat{\phi}. \end{aligned} \tag{2.7.63}$$

The Berry curvatures associated with $e_+(p)$ and $e_-(p)$ can now be computed using the curl operator in spherical polar co-ordinates as follows:

$$\begin{aligned} \mathcal{F}_\sigma(p) &:= \nabla_p \times i \langle e_\sigma(p) | \nabla_p e_\sigma(p) \rangle \\ &= -\sigma \frac{\hat{p}}{|p|^2}, \qquad \sigma = \pm. \end{aligned} \tag{2.7.64}$$

The Berry curvature has the form of a *monopole* at $p = 0$, the point in parameter space at which the eigenvalue 0 of (2.7.51) is no longer *two*-fold degenerate but *six*-fold degenerate.

# Chapter 3

# Dynamics at a one-dimensional band crossing

*The research described in this chapter is joint with M. I. Weinstein.*

## 3.1 Introduction

In this work we study the non-dimensionalized, semi-classically scaled, time-dependent Schrödinger equation for $\psi^\epsilon(x,t) : \mathbb{R} \times [0, \infty) \to \mathbb{C}$:

$$\begin{aligned} &i\epsilon\partial_t\psi^\epsilon = -\frac{1}{2}\epsilon^2\partial_x^2\psi^\epsilon + V\left(\frac{x}{\epsilon}\right)\psi^\epsilon + W(x)\psi^\epsilon \ \equiv \ H^\epsilon \ \psi^\epsilon \\ &\psi^\epsilon(x,0) = \psi_0^\epsilon(x). \end{aligned} \tag{3.1.1}$$

Here, $\epsilon$ is a positive real parameter which we assume to be small. We assume throughout that the function $V$ is smooth and 1-periodic so that:

$$V(z+1) = V(z) \text{ for all } z \in \mathbb{R}, \tag{3.1.2}$$

and that $W$ is smooth with all derivatives uniformly bounded (this assumption may be relaxed; see Remark 1.2 of [73]). Equation (3.1.1) is the independent-particle approximation in condensed matter physics [3] for the dynamics of an electron in a crystal described by periodic potential $V$, under the influence of an external electric field generated by a 'slowly varying' potential $W$.

Let $E_n$ denote the $n$th Bloch band dispersion function of the periodic operator $-\frac{1}{2}\partial_z^2 + V(z)$. It is known that [61; 73] for any uniformly *isolated*, or non-degenerate, band $E_n$ (see Figure 3.1) there

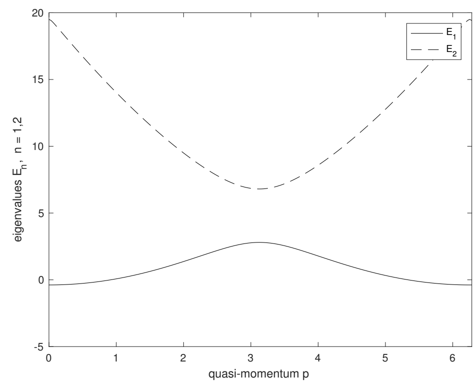



Figure 3.1: Plot of the two lowest Bloch band dispersion functions $E_1(p), E_2(p)$ when the 1-periodic potential is given by $V(z) = 4\cos(2\pi z)$. Note that both bands are *isolated* from each other and all other bands: for all $p \in [0, 2\pi]$, $G(E_2(p)) > 0$ and $G(E_1(p)) > 0$ where $G(E_n(p))$ is the spectral band gap function (3.2.8). Consequently, the maps $p \mapsto E_1(p), E_2(p)$ are smooth.

exists a family of explicit asymptotic solutions of (3.1.1) known as semiclassical wavepackets which, for any fixed positive integer $N$, approximate exact solutions up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$ up to errors of order $\epsilon^N$ in $L^2_x$. The center of mass and average quasi-momentum of these solutions evolve (up to errors of $o(1)$) along classical trajectories generated by the 'Bloch band' Hamiltonian $\mathcal{H}_n := E_n(p) + W(q)$. We refer to such an asymptotic solution as a *wavepacket associated with the band* $E_n$. The 'Ehrenfest' time-scale of validity of the asymptotics is known to be the general limit of applicability of wavepacket, or coherent state, approximations [66]. These results generalize to $d$-dimensional analogs of (3.1.1) [73; 61].

In this work we consider the following question concerning the dynamics of wave-packets in a situation where two Bloch bands are not isolated:

**Problem 1.** *Consider equation (3.1.1) with initial conditions given by a wavepacket associated with a band $E_n$ which is then driven by the external potential $W$ through a point in phase space where the Bloch band $E_n$ is degenerate, i.e. intersects with an adjacent band; see Figure 3.2. How are the dynamics different from the isolated band case?*

More precisely, suppose that two bands $E_n(p), E_{n+1}(p)$ (WLOG, $E_{n-1}$ is similar) touch at a quasi-momentum $p^*$ in the Brillouin zone, but are otherwise non-degenerate in a neighborhood of $p^*$ (see Figure 3.2 ). Then, we study a wavepacket associated with the band $E_n$ initially localized in phase

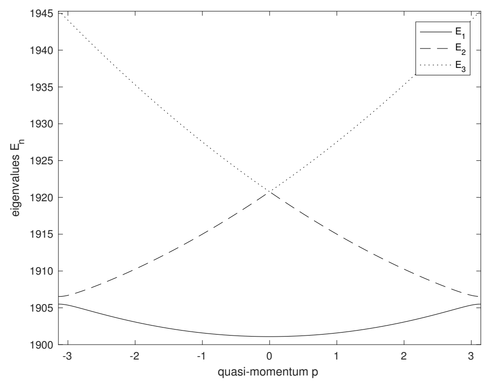



Figure 3.2: Plot of the three lowest Bloch band dispersion functions when $V(z) = \wp_{1/2,i\omega'}(z + i\omega')$, the 'one-gap' potential (see Example 1), with $\omega' = .8$. The band $E_1(p)$ is isolated over the whole Brillouin zone $[-\pi, \pi]$, but the bands $E_2(p), E_3(p)$ are *degenerate* at $p = 0$. For this choice of potential, for *all* integers $n \geq 2$ the band $E_n(p)$ is degenerate with the band $E_{n+1}(p)$ at either $p = 0$ or $p = \pi$, hence 'one gap'.

space on a classical trajectory $(q(t), p(t))$ generated by $\mathcal{H}_n$ which encounters the crossing after some finite time $t^*$: for some $t^* > 0$, $\lim_{t \uparrow t^*} p(t) = p^*$.

Our results can be roughly stated as follows; we give a more precise statement in Section 3.2. Assume that an "incident" wavepacket is *driven* through the crossing so that $\lim_{t \uparrow t^*} \dot{p}(t) = \lim_{t \uparrow t^*} \partial_q W(q(t)) \neq 0$. For a precise set up, see the Band Crossing Scenario (Property 3). Then:

1. **Quantifying the breakdown of the 'single-band' description as $t \uparrow t^*$; Theorem 3.3.2**: Fix any positive integer, $N$. For $t \ll t^*$, the solution of (3.1.1) can be represented as a wavepacket associated with the band $E_n$ with errors which are $O((\sqrt{\epsilon})^N)$ in $L^2(\mathbb{R})$. As $t \uparrow t^*$, this 'single-band' description fails to capture the dynamics of the PDE to any order in $\sqrt{\epsilon}$ higher than order $(\sqrt{\epsilon})^0 = 1$, since it does not incorporate an excited wave associated with the band $E_{n+1}$ whose norm grows to be of the order $\sqrt{\epsilon}$ as $t$ approaches $t^*$ on the non-adiabatic time-scale $s = (t - t^*)/\sqrt{\epsilon}$.

2. **Coupling of degenerate bands and excitation of a reflected wave-packet; Theorem 3.3.3:** For $t \sim t^*$ and for $t \gg t^*$ the solution of (3.1.1) is well-approximated by the sum of two semiclassical wavepackets: a "transmitted" wavepacket associated with the band $E_{n+1}$ with $L^2$-norm proportional to 1 and a "reflected" wavepacket associated with the band

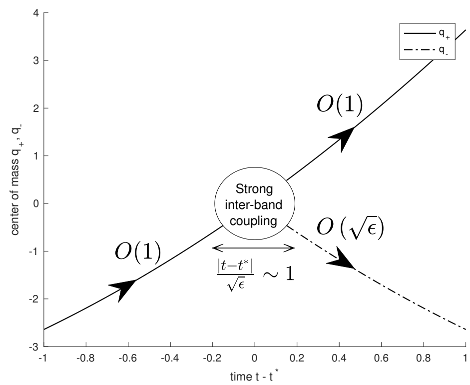



Figure 3.3: Plot of position of center of mass against time of the "incident/transmitted" wavepacket $q_+(t)$ and the "excited/reflected" wavepacket $q_-(t)$, which satisfy (3.3.16) and (3.3.35) respectively, for $t$ near to $t^*$. As $t$ approaches $t^*$ such that the expected quasi-momentum of the incident wavepacket is *degenerate* ($p_+(t^*) = p^*$ where $E_+(p^*) = E_-(p^*)$) inter-band coupling, which occurs over the emergent non-adiabatic time-scale $s := \frac{t-t^*}{\sqrt{\epsilon}}$, is non-negligible and leads to the excitation of the second wavepacket. The size in $L^2_x$ of the "excited" wavepacket is smaller than that of the "incident" wavepacket by a factor of $\sqrt{\epsilon}$ and proportional to the "coupling coefficient" $\langle \chi_-(\cdot;p^*) | \, \partial_p \chi_+(\cdot;p^*) \rangle$. Here $E_\pm(p), \chi_\pm(z;p)$ refer to the *smooth continuations* of the band eigenpairs $E_n(p), E_{n+1}(p), \chi_n(z;p), \chi_{n+1}(z;p)$ through the crossing (see Property 2 and Figure 3.4). Such continuations always exist at one-dimensional band crossings (Theorem 3.3.1).

> $E_n$ with $L^2$-norm proportional to $\sqrt{\epsilon}$ (Figure 3.3). The size of the error terms is $o(\sqrt{\epsilon})$ in $L^2(\mathbb{R})$. The expansion is constructed via a rigorous matched-asymptotic analysis in which the "transmitted" and a "reflected" wave-packets evolve on an additional emergent non-adiabatic time-scale $s = \frac{t-t^*}{\sqrt{\epsilon}}$.

Our proof of Theorem 3.3.2 relies on the existence of *smooth continuations* of the Bloch band dispersion functions $E_n, E_{n+1}$ through the crossing point $p^*$; see Property 2 and Figure 3.4. Such continuations exist in one spatial dimension; the details are presented in Theorem 3.3.1. Our proof does not readily generalize to cases where no such continuation exists; for example at 'conical', or 'Dirac' points which occur in dimensions $d \geq 2$ [28; 29]. The dynamics of semiclassical wavepackets at such crossings was studied in the context of the Born-Oppenheimer approximation of molecular dynamics by Hagedorn [37]. Adapting his methods to the present context is the subject of ongoing

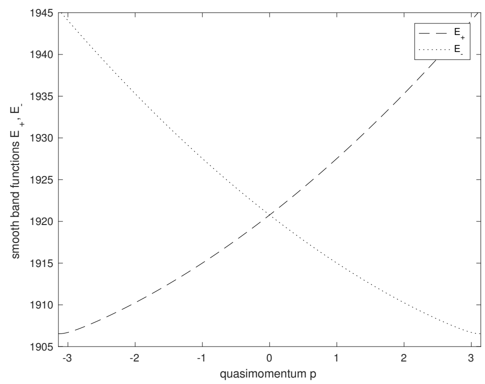



Figure 3.4: Plot of the maps $E_+(p), E_-(p)$ defined by (3.3.3) with $n = 2$ and where $E_2(p), E_3(p)$ are the second and third lowest Bloch band dispersion functions when $V(z) = \wp_{1/2,i\omega'}(z + i\omega')$, the 'one-gap' potential with $\omega' = .8$. The lowest three Bloch bands of this potential are shown in Figure 3.2.

work.

Quantum dynamics at eigenvalue band crossings was studied by Landau [47], and Zener [78] in the 1930s. A discussion of these phenomena from the perspective of normal forms and microlocal analysis was given by Colin de Verdiere et al. [17]. The propagation of Wigner measures through crossings in the context of the Born-Oppenheimer approximation has been well studied by Fermanian-Kammerer and others [30; 31; 49; 33; 12; 32; 13]. A model of the dynamics at a 'conical' Bloch band degeneracy was derived in [35]. So-called 'avoided' crossings are also of considerable interest: see, for example, [34] and references therein.

### 3.1.1 Notation

- It will be useful to introduce the energy spaces for every $l \in \mathbb{N}$:

$$\Sigma^l(\mathbb{R}) := \left\{ f \in L^2(\mathbb{R}) : \|f\|_{\Sigma^l} := \sum_{|\alpha|+|\beta| \leq l} \|y^\alpha (-i\partial_y)^\beta f(y)\|_{L^2_y} < \infty, \right\} \tag{3.1.3}$$

- The space of Schwartz functions $\mathcal{S}(\mathbb{R})$ is the space of functions defined as:

$$\mathcal{S}(\mathbb{R}) := \cap_{l \in \mathbb{N}} \Sigma^l(\mathbb{R}). \tag{3.1.4}$$

- We will refer throughout to the space of $L^2$-integrable functions which are $1-$periodic:

$$L^2_{per} := \left\{ f \in L^2_{loc}(\mathbb{R}) : f(z+1) = f(z) \text{ at almost every } z \in \mathbb{R} \right\}. \tag{3.1.5}$$

- For functions of period 1, the Brillouin zone $\mathcal{B}$ may be chosen to be any real interval of length $2\pi$. Since the band degeneracy we consider occurs at quasi-momentum $p^* = \pi$, we fix $\mathcal{B} := [0, 2\pi]$.

- We make the standard conventions for the $L^2$-inner product and induced norm:

$$\langle f | g \rangle_{L^2(\mathcal{D})} := \int_{\mathcal{D}} \overline{f(x)} g(x) \, \mathrm{d}x, \quad \|f\|_{L^2(\mathcal{D})} := \langle f | f \rangle^{1/2}_{L^2(\mathcal{D})} \tag{3.1.6}$$

  For brevity, when $\mathcal{D} = \mathbb{R}$ we omit the domain of integration:

$$\langle f | g \rangle_{L^2} := \int_{\mathbb{R}} \overline{f(x)} g(x) \, \mathrm{d}x, \quad \|f\|_{L^2} := \langle f | f \rangle^{1/2}_{L^2}, \tag{3.1.7}$$

  and when $\mathcal{D} = [0, 1]$ we omit all subscripts:

$$\langle f | g \rangle := \int_{[0,1]} \overline{f(x)} g(x) \, \mathrm{d}x, \quad \|f\| := \langle f | f \rangle^{1/2}, \tag{3.1.8}$$

**Acknowledgements**

The authors wish to thank George Hagedorn, Jianfeng Lu, and Christof Sparber for stimulating discussions. This research was supported in part by National Science Foundation Grant Nos. DMS-1412560 and Simons Foundation Math + X Investigator Award No. 376319 (Michael I. Weinstein).

## 3.2 Review of Floquet-Bloch theory and the isolated band theory of wavepackets

### 3.2.1 Floquet-Bloch theory

In order to state our results we require some background on the spectral theory of the Schrödinger operator:

$$H := -\frac{1}{2} \partial_z^2 + V(z) \tag{3.2.1}$$

where $V$ is 1-periodic (see [46; 63] for proofs and details). Consider the family of self-adjoint eigenvalue problems parameterized by the real parameter $p$:

$$\begin{aligned} &H\Phi(z;p) = E(p)\Phi(z;p) \\ &\Phi(z+1;p) = e^{ip}\Phi(z;p) \text{ for all } z \in \mathbb{R}. \end{aligned} \tag{3.2.2}$$

Because of the explicit $2\pi$-periodicity of the boundary condition, there is no loss of generality in restricting our attention to $p \in \mathcal{B}$, where $\mathcal{B}$ is any real interval of length $2\pi$. $\mathcal{B}$ is usually fixed to be $[-\pi, \pi]$ or $[0, 2\pi]$ and referred to as the Brillouin zone. The eigenvalue problem (3.2.2) is equivalent (by the transformation $\Phi(z;p) = e^{ipz}\chi(z;p)$) to the family of self-adjoint eigenvalue problems with 1-periodic boundary conditions:

$$\begin{aligned} &H(p)\chi(z;p) = E(p)\chi(z;p) \\ &\chi(z+1;p) = \chi(z;p) \text{ for all } z \in \mathbb{R} \\ &H(p) := \frac{1}{2}(p - i\partial_z)^2 + V(z). \end{aligned} \tag{3.2.3}$$

For fixed $p$, the spectrum of the operator (3.2.3) is real and discrete and the eigenvalues can be ordered with multiplicity:

$$E_1(p) \leq E_2(p) \leq ... \leq E_n(p) \leq ... \tag{3.2.4}$$

and the associated normalized eigenfunctions of (3.2.3) $\chi_n(z;p)$ are a basis of the space:

$$L^2_{per} := \left\{ f \in L^2_{loc} : f(z+1) = f(z) \text{ at almost every } z \in \mathbb{R} \right\} \tag{3.2.5}$$

The maps $p \mapsto E_n(p)$, for $p$ varying over $\mathcal{B}$, are known as the spectral band functions and their graphs are called the dispersion curves of $H$. The set of all dispersion surfaces as $p$ varies over $\mathcal{B}$ is called the band structure of $H$ (3.2.1). Any function in $L^2(\mathbb{R})$ may be expressed as a superposition of *Bloch waves*:

$$\left\{ \Phi_n(z;p) = e^{ipz}\chi_n(z;p) : n \in \mathbb{N}, p \in \mathcal{B} \right\}. \tag{3.2.6}$$

Moreover, the $L^2$-spectrum of the operator (3.2.1) is the union of the real intervals swept out by the spectral band functions $E_n(p)$:

$$\sigma(H)_{L^2(\mathbb{R}^d)} = \cup_{n \in \mathbb{R}} \left\{ E_n(p) : p \in \mathcal{B} \right\}. \tag{3.2.7}$$

We define a measure of the spectral gap or separation at quasimomentum $p \in \mathcal{B}$ between $E_n$ and all other spectral band functions satisfying (3.2.3):

$$G(E_n(p)) := \min_{m \neq n} |E_n(p) - E_m(p)|. \tag{3.2.8}$$

We make the following definitions:

**Definition 3.2.1.** *Let $E_n(p)$ denote an eigenvalue band of either of the equivalent eigenvalue problems* (3.2.2), (3.2.3) *and let $\tilde{p} \in \mathcal{B}$. If:*

$$G(E_n(\tilde{p})) > 0, \tag{3.2.9}$$

*then we will say that $E_n(p)$ is* isolated *at $\tilde{p}$. If:*

$$G(E_n(\tilde{p})) = 0, \tag{3.2.10}$$

*then we will say that $E_n(p)$ is involved in a* Bloch band degeneracy.

### 3.2.2 Isolated band theory

**Property 1** (Isolated Band Property)**.** *Let $E_n$ denote a band dispersion function satisfying (3.2.3) for $p \in \mathcal{B}$. Let $t_0 < t_1 \leq \infty$ and $q_0, p_0 \in \mathbb{R} \times \mathcal{B}$ be such that the equations of motion of the classical Hamiltonian $\mathcal{H}_n(p, q) := E_n(p) + W(q)$:*

$$\begin{aligned} \dot{q}(t) &= \partial_p E_n(p(t)), & \dot{p}(t) &= -\partial_q W(q(t)) \\ q(t_0) &= q_0 & p(t_0) &= p_0 \end{aligned} \tag{3.2.11}$$

*have a unique smooth solution $(q(t), p(t))$ for $t \in [t_0, t_1)$ such that $E_n$ is isolated along the trajectory $(q(t), p(t))$ for $t \in [t_0, t_1)$; i.e:*

$$M(t_0, t_1) := \inf_{t \in [t_0, t_1)} G(E_n(p(t))) > 0, \tag{3.2.12}$$

*where $G(E_n(p))$ is defined by (3.2.8).*

For arbitrary constant $S_0 \in \mathbb{R}$ we let $S(t)$ denote the classical action along the path $(q(t), p(t))$:

$$S(t) = S_0 + \int_{t_0}^{t} p(t')\partial_p E_n(p(t')) - E_n(p(t')) - W(q(t'))\, \mathrm{d}t' \tag{3.2.13}$$

For arbitrary $a_0^0(y) \in \mathcal{S}(\mathbb{R})$, let $a^0(y,t)$ denote the unique solution of Schrödinger's equation with a time-dependent harmonic oscillator Hamiltonian depending on the classical trajectory $(q(t), p(t))$ with initial data specified at $t_0$ by $a_0^0(y)$:

$$\begin{aligned} & i\partial_t a^0(y,t) = \mathscr{H}(t) a^0(y,t), \\ & \mathscr{H}(t) := \frac{1}{2}\partial_p^2 E_n(p(t))(-i\partial_y)^2 + \frac{1}{2}\partial_q^2 W(q(t)) y^2 + \partial_q W(q(t)) \mathcal{A}_n(p(t)), \\ & a^0(y,t_0) = a_0^0(y). \end{aligned} \tag{3.2.14}$$

Here, $p \in \mathcal{B} \mapsto \mathcal{A}_n(p)$ denotes the $n$-th band Berry connection (see Section 3.1.1 for conventions regarding inner products and norms):

$$\mathcal{A}_n(p) := i \left\langle \chi_n(\cdot;p)) \right| \partial_p \chi_n(\cdot;p) \rangle . \tag{3.2.15}$$

Since the $\chi_n(z;p)$ are assumed normalized:

$$\text{for all } p \in \mathbb{R}, \ \|\chi_n(\cdot,p)\| = 1, \tag{3.2.16}$$

it follows that $\mathcal{A}_n(p)$ is real-valued. The term $\partial_q W(q(t))\mathcal{A}_n(p(t))$ in (3.2.14) therefore leads to an overall phase shift in the solution of (3.2.14) known as Berry's phase.

**Remark 3.2.1.** *For any path $p(t)$ through parameter space it is possible to choose phases of the eigenfunctions $\chi_n(z;p)$ in such a way that the Berry connection* (3.2.15) *is zero when evaluated along the curve $p(t)$ for all $t$. This choice is known as the* adiabatic gauge*. See Proposition 3.1 of [37], for example.*

We now state a mild refinement of the result of Carles-Sparber [61] which we find more directly applicable:

**Theorem 3.2.1** (Order 1 wave-packet)**.** *Let $(q(t), p(t))$ denote the classical trajectory generated by the Hamiltonian $\mathcal{H}_n(p,q) = E_n(p) + W(q)$, where $p \mapsto E_n(p)$ denotes the $n^{th}$ spectral band function for the periodic Schrödinger operator $-\frac{1}{2}\partial_z^2 + V(z)$. Assume that band $E_n$ satisfies the Isolated Band Property 1 along the trajectory $(q(t), p(t))$ for $t \in [t_0, t_1)$, i.e. $M(t_0,t_1) > 0$; see* (3.2.12)*.*

*Let $S(t)$ be as in* (3.2.13) *and $a^0(y,t)$ be the unique solution of* (3.2.14) *with initial data $a_0^0(y) \in \mathcal{S}(\mathbb{R})$.*

*Then, for sufficiently small $\epsilon > 0$ the following holds. Let $\psi^\epsilon(x,t)$ denote the unique solution of the initial value problem (3.1.1) with approximate 'Bloch wavepacket' initial data given at $t = t_0$:*

$$\begin{aligned} &i\epsilon\partial_t\psi^\epsilon = H^\epsilon\psi^\epsilon \\ &\psi^\epsilon(x,t_0) = \epsilon^{-1/4}e^{iS_0/\epsilon}e^{ip_0(x-q_0)/\epsilon}a_0^0\left(\frac{x-q_0}{\sqrt{\epsilon}}\right)\chi_n\left(\frac{x}{\epsilon};p_0\right). \end{aligned} \tag{3.2.17}$$

*For $t \in [t_0, t_1)$, the solution evolves as a modulated 'Bloch wavepacket' plus a corrector $\eta^\epsilon(x,t)$:*

$$\psi^\epsilon(x,t) = \epsilon^{-1/4}e^{iS(t)/\epsilon}e^{ip(t)(x-q(t))/\epsilon}a^0\left(\frac{x-q(t)}{\sqrt{\epsilon}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right) + \eta^\epsilon(x,t) \tag{3.2.18}$$

*where the leading order term is of order 1 in $L^2(\mathbb{R})$ and the corrector $\eta^\epsilon$ satisfies:*

$$\|\eta^\epsilon(\cdot,t)\|_{L^2} \leq Ce^{c(t-t_0)}\sqrt{\epsilon}, \qquad t_0 \leq t < t_1. \tag{3.2.19}$$

*The constants $C > 0, c > 0$ depend on $M(t_0,t_1)$ and the initial data specified at $t_0$, are independent of $\epsilon$ and do not depend otherwise on $t_0$ and $t_1$. Moreover, $C \uparrow \infty$ as $M(t_0,t_1) \downarrow 0$.*

*In particular, if $M(t_0,\infty) > 0$ then*

$$\sup_{t\in[t_0,\tilde{C}\ln 1/\epsilon]} \|\eta^\epsilon(\cdot,t)\|_{L^2} = o(1), \tag{3.2.20}$$

*where $\tilde{C}$ is any constant such that $\tilde{C} < \frac{1}{2c}$.*

**Remark 3.2.2.** *The timescale $t \sim \ln 1/\epsilon$ is known as 'Ehrenfest time' and is known to be the general limit of applicability of wavepacket, or coherent state, approximations (see [66] and references therein).*

It is convenient at this point to introduce a short-hand notation for the leading order ($O(1)$ in $L^2$) 'Bloch wavepacket' asymptotic solution associated with the band $E_n$ with centering along the classical trajectory $(q(t),p(t))$ and envelope function $a^0(y,t)$ (3.2.18):

$$\begin{aligned} &\mathrm{WP}^{0,\epsilon}[S(t),q(t),p(t),a^0(y,t),\chi_n(z;p(t))](x,t) := \\ &\epsilon^{-1/4}e^{iS(t)/\epsilon}e^{ip(t)(x-q(t))/\epsilon}a^0\left(\frac{x-q(t)}{\sqrt{\epsilon}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right). \end{aligned} \tag{3.2.21}$$

In our analysis we require a refinement of Theorem 1.1 of [73] where it was demonstrated how to compute corrections to the asymptotic solution (3.2.18) in order to improve the error bound (3.2.19) by a factor of $\sqrt{\epsilon}$.

For any $a^1_0(y) \in \mathcal{S}(\mathbb{R})$, let $a^1(y,t)$ denote the unique solution of the following inhomogeneous Schrödinger equation with initial data specified at $t_0$ by $a^1_0(y)$ *driven* by the solution $a^0(y,t)$ of (3.2.14):

$$\begin{aligned}
&i\partial_t a^1(y,t) = \mathscr{H}(t)a^1(y,t) + \mathscr{I}(t)a^0(y,t),\\
&\mathscr{I}(t) := \frac{1}{6}\partial_p^3 E_n(p(t))(-i\partial_y)^3 + \frac{1}{6}\partial_q^3 W(q(t))y^3\\
&+\partial_q W(q(t))\partial_p \mathcal{A}_n(p(t))(-i\partial_y) + \partial_q^2 W(q(t))\mathcal{A}_n(p(t))y,\\
&a^1(y,t_0) = a^1_0(y).
\end{aligned} \tag{3.2.22}$$

Again, $\mathcal{A}_n(p)$ denotes the Berry connection, displayed in (3.2.15). We next introduce a convenient short-hand notation for the 'Bloch wavepacket' asymptotic solution associated with the band $E_n$ with a first-order correction to $\mathrm{WP}^{0,\epsilon}$ in (3.2.21):

$$\begin{aligned}
&\mathrm{WP}^{1,\epsilon}[S(t),q(t),p(t),a^0(y,t),a^1(y,t),\chi_n(z;p(t))](x,t) :=\\
&\epsilon^{-1/4}e^{iS(t)/\epsilon}e^{ip(t)(x-q(t))/\epsilon}\left\{a^0\left(\frac{x-q(t)}{\sqrt{\epsilon}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right)\right.\\
&\left.+\sqrt{\epsilon}\left[a^1\left(\frac{x-q(t)}{\sqrt{\epsilon}},t\right)\chi_n\left(\frac{x}{\epsilon};p(t)\right)+(-i\partial_y)a^0\left(\frac{x-q(t)}{\sqrt{\epsilon}},t\right)\partial_p\chi_n\left(\frac{x}{\epsilon};p(t)\right)\right]\right\}.
\end{aligned} \tag{3.2.23}$$

Then, we have the following mild generalization of the result of Theorem 1.1 in [73]:

**Theorem 3.2.2** (Order 1 wave-packet with order $\sqrt{\epsilon}$ correction)**.** *Assume the same setting as in Theorem 3.2.1, in particular that the Isolated Band Property 1 holds along the trajectory* $(p(t),q(t))$ *of the classical Hamiltonian* $\mathcal{H}_n = E_n(p) + W(q)$ *for* $t \in [t_0,t_1)$*, where* $t_0 < t_1 \le \infty$*. Let* $a^0_0(y)$ *and* $a^1_0(y) \in \mathcal{S}(\mathbb{R})$*. Let* $S(t)$ *be as in (3.2.13) with initial action* $S(0) = S_0 \in \mathbb{R}$*. Let* $a^0(y,t)$ *as in (3.2.14) and* $a^1(y,t)$ *be as in* (3.2.22)*.*

*Then, for sufficiently small* $\epsilon > 0$*, we have that the unique solution* $\psi^\epsilon(x,t)$ *of the initial value problem (3.1.1) with approximate 'Bloch wavepacket' initial data with corrections proportional to* $\sqrt{\epsilon}$ *given at* $t = t_0$*:*

$$\begin{aligned}
&i\epsilon\partial_t\psi^\epsilon = H^\epsilon\psi^\epsilon\\
&\psi^\epsilon(x,t_0) = \mathrm{WP}^{1,\epsilon}[S_0,q_0,p_0,a^0_0(y),a^1_0(y),\chi_n(z;p_0)](x) + O_{L^2_x}(\epsilon)
\end{aligned} \tag{3.2.24}$$

*evolves as a modulated 'Bloch wavepacket' plus a corrector* $\eta^\epsilon(x,t)$*:*

$$\psi^\epsilon(x,t) = \mathrm{WP}^{1,\epsilon}[S(t),q(t),p(t),a^0(y,t),a^1(y,t),\chi_n(z;p(t))](x,t) + \eta^\epsilon(x,t) \tag{3.2.25}$$

*where the corrector $\eta^\epsilon$ satisfies, for $t \in [t_0, t_1)$, the bound:*

$$\|\eta^\epsilon(\cdot, t)\|_{L^2} \leq Ce^{ct}\epsilon \tag{3.2.26}$$

*where the constants $C > 0, c > 0$ are as stated in Theorem 3.2.1.*

*Furthermore, it follows that if $M(t_0, \infty) > 0$, then we have the following error bound on the Ehrenfest time-scale:*

$$\sup_{t \in [0, \tilde{C} \ln 1/\epsilon]} \|\eta^\epsilon(\cdot, t)\|_{L^2} = o(\sqrt{\epsilon}), \tag{3.2.27}$$

*where $\tilde{C}$ is any constant such that $\tilde{C} < \frac{1}{2c}$, cf.* (3.2.20).

**Remark 3.2.3.** *By a natural extension of the methods of [61] and [73] one may derive, for any integer $k \geq 0$, 'kth-order Bloch wavepacket' approximate solutions:*

$$\mathrm{WP}^{k,\epsilon}[S(t), q(t), p(t), a^0(y, t), a^1(y, t), a^2(y, t), ..., \chi_n(z; p(t))](x, t) \tag{3.2.28}$$

*such that the exact solution $\psi^\epsilon(x, t)$ of* (3.1.1) *with 'k-th order Bloch wavepacket' initial data:*

$$\psi_0^\epsilon(x) = \mathrm{WP}^{k,\epsilon}[S_0, q_0, p_0, a_0^0(y), a_0^1(y), a_0^2(y), ..., \chi_n(z; p_0)](x) \tag{3.2.29}$$

*satisfies:*

$$\begin{aligned} &\psi^\epsilon(x, t) = \\ &\mathrm{WP}^{k,\epsilon}[S(t), q(t), p(t), a^0(y, t), a^1(y, t), a^2(y, t), ..., \chi_n(z; p(t))](x, t) + o_{L^2_x}(\epsilon^{k/2}) \end{aligned} \tag{3.2.30}$$

*up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$. Note that each function $\mathrm{WP}^{k,\epsilon}[...](x, t)$ depends on $k+1$ envelope functions $a^0(y, t), a^1(y, t), a^2(y, t), ...$ each of which satisfies a suitable Schrödinger equation driven by the $k$ previously defined envelope functions. Hence $a^2(y, t)$ satisfies a Schrödinger equation driven by $a^0(y, t)$ and $a^1(y, t)$ and so on.*

## 3.3 Statement of results on dynamics at band crossings

### 3.3.1 Linear band crossings

We next give a precise discussion of the character of one-dimensional band crossings. The following property describes a *linear band crossing*, illustrated in Figures 3.2 and 3.4. In Theorem 3.3.1 we assert that Bloch band degeneracies in one dimension are of this type:

**Property 2** (Linear band crossing)**.** *Let $E_n(p), E_{n+1}(p)$ denote two spectral band functions satisfying* (3.2.3) *for $p \in \mathcal{B}$, and let $p^*$, $U$ denote a point and open interval respectively with $p^* \in U \subset \mathcal{B}$ such that:*

(A1) *The bands $E_n$ and $E_{n+1}$ are degenerate at $p^*$, and this degeneracy is unique in $U$:*

$$\begin{aligned} &E_n(p^*) = E_{n+1}(p^*) \\ &\text{if } \tilde{p}^* \in U \text{ and } E_n(\tilde{p}^*) = E_{n+1}(\tilde{p}^*), \text{ then } \tilde{p}^* = p^*. \end{aligned} \tag{3.3.1}$$

(A2) *The bands $E_{n+1}, E_n$ are uniformly isolated from the rest of the spectrum for all $p \in U$, i.e. there exists a positive constant $M > 0$ such that:*

$$\min_{p \in \overline{U}} \min_{m \notin \{n, n+1\}} \{|E_m(p) - E_{n+1}(p)|, |E_n(p) - E_m(p)|\} \geq M > 0 \tag{3.3.2}$$

(A3) *The maps:*

$$\begin{aligned} p \mapsto (E_+(p), \chi_+(z;p)) &:= \begin{cases} (E_n(p), \chi_n(z;p)) & \text{for } p \in U \text{ and } p < p^* \\ (E_{n+1}(p), \chi_{n+1}(z;p)) & \text{for } p \in U \text{ and } p \geq p^* \end{cases} \\ p \mapsto (E_-(p), \chi_-(z;p)) &:= \begin{cases} (E_{n+1}(p), \chi_{n+1}(z;p)) & \text{for } p \in U \text{ and } p < p^* \\ (E_n(p), \chi_n(z;p)) & \text{for } p \in U \text{ and } p \geq p^* \end{cases} \end{aligned} \tag{3.3.3}$$

*are smooth for all $p \in U$.*

(A4) *The bands $E_+, E_-$ satisfy $\partial_p E_+(p^*) > 0$, $\partial_p E_-(p^*) < 0$ and in particular:*

$$\partial_p E_+(p^*) - \partial_p E_-(p^*) = 2\partial_p E_+(p^*) > 0. \tag{3.3.4}$$

**Caveat Lector!** *In* (3.3.3)*, the notation $+$ and $-$ refers to the sign of the* derivative *of the smooth band functions at the crossing point: $\partial_p E_+(p^*) > 0, \partial_p E_-(p^*) < 0$. This is not to be confused with an ordering of the bands themselves. Indeed, with our conventions we have:*

$$\text{for } p \in U \text{ and } p < p^*\text{: } E_+(p) = E_n(p) < E_{n+1}(p) = E_-(p). \tag{3.3.5}$$

It is useful to view the functions $E_+(p), E_-(p)$ as *smooth continuations* of the band functions $E_n(p), E_{n+1}(p)$ from the interval $\{p \in U : p \leq p^*\}$ to the interval $\{p \in U : p > p^*\}$. We will refer to any crossing satisfying Property 2 as a *linear crossing.* In one spatial dimension, *all* band crossings are linear. Moreover, crossings can only occur at 0 or $\pi$ (modulo $2\pi$):

**Theorem 3.3.1.** *Let $E_n(p), E_{n+1}(p)$ denote spectral band functions satisfying* (3.2.3) *for $p \in \mathcal{B}$, and let $p^* \in \mathcal{B}$ be such that: $E_n(p^*) = E_{n+1}(p^*)$. Then:*

1. *$p^* = 0$ or $\pi$ (modulo $2\pi$).*
2. *There exists an open interval $U$ containing $p^*$ such that hypotheses (A1)-(A4) of Property 2 hold.*

The proof of Theorem 3.3.1 is given in Appendix B.1.

**Corollary 3.3.1.** *Let $E_n(p), E_{n+1}(p)$ denote spectral band functions in one dimension which cross at some $p^* \in \mathcal{B}$. Let $P_{\pm}^{\perp}(p)$ denote the projection onto the orthogonal complement in $L^2_{per}$ of the functions $\chi_+(z;p), \chi_-(z;p)$, defined for $p \in U$ by* (3.3.3)*. Then:*

$$\|(H(p) - E_\sigma(p))^{-1} P_{\pm}^{\perp}(p)\|_{L^2_{per} \to H^2_{per}} \leq \frac{1}{M}, \qquad \sigma = \pm,\ p \in \overline{U}. \tag{3.3.6}$$

*where $M > 0$ is the constant appearing in* (3.3.2)*.*

The bound (3.3.6) follows immediately from (3.3.2). When we consider the dynamics of wavepackets associated with $E_n(p)$ or $E_{n+1}(p)$ and spectrally localized close to $p^*$, the gap condition (3.3.2) and Corollary 3.3.1 will allow us to bound contributions to the solution from all bands other than $E_n(p)$ and $E_{n+1}(p)$ uniformly through the crossing time, see Appendix D of [73] for details.

**Remark 3.3.1.** *Theorem 3.3.1 does not generalize to spatial dimensions larger than one. Indeed, at so-called 'conical' or 'Dirac' points, which occur in the spectral band structure of two-dimensional periodic Schrödinger operators with* honeycomb lattice *symmetry, the local band structure is the union of Lipschitz surfaces [28; 29] and the map $p \mapsto \chi_n(z;p)$ from the Brillouin zone to the Bloch eigenfunctions is discontinuous [29].*

### 3.3.2 Examples of potentials with linear band crossings

**Example 1** (Weierstrass elliptic functions)**.** *Let $\omega_1, \omega_3 \in \mathbb{C}$ with* $\text{Im}\,(\omega_3/\omega_1) \neq 0$. *Define $\wp_{\omega_1,\omega_3}(z)$, the* Weierstrass elliptic function with periods $2\omega_1, 2\omega_3$ *by:*

$$\wp_{\omega_1,\omega_3}(z) := \frac{1}{z^2} + \sum_{\substack{(m,n)\in\mathbb{Z}\times\mathbb{Z},\\(m,n)\neq(0,0)}} \frac{1}{(z - 2m\omega_1 - 2n\omega_3)^2} - \frac{1}{(2m\omega_1 + 2n\omega_3)^2}. \tag{3.3.7}$$

*The function $\wp_{\omega_1,\omega_3}(z)$ is doubly-periodic and even:*

$$\begin{aligned}&\wp_{\omega_1,\omega_3}(z+2\omega_1) = \wp_{\omega_1,\omega_3}(z+2\omega_3) = \wp_{\omega_1,\omega_3}(z)\\ &\wp_{\omega_1,\omega_3}(-z) = \wp_{\omega_1,\omega_3}(z),\end{aligned} \tag{3.3.8}$$

*and has poles of degree two at the points $\Omega_{m,n} = 2m\omega_1 + 2n\omega_3$ for all $(m,n) \in \mathbb{Z} \times \mathbb{Z}$. If $\omega_1 = \omega$, $\omega_3 = i\omega'$ with $\omega, \omega' \in \mathbb{R}$ and $\omega > 0$, then $\wp_{\omega,i\omega'}(z)$ is real for $z$ such that* $\mathrm{Re}\, z \in \{0,\omega\}$ *or* $\mathrm{Im}\, z \in \{0,\omega'\}$ *by the symmetries* (3.3.8)*. Now fix $\omega = 1/2$, and define for any $\omega' \in \mathbb{R}$ with $\omega' \neq 0$ and positive integer $m$:*

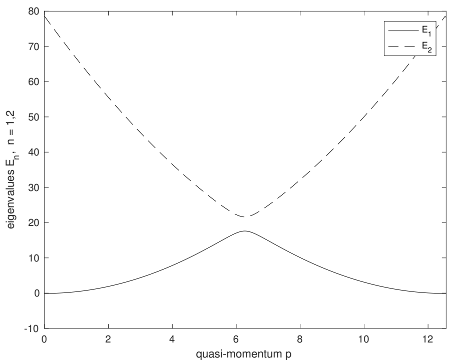
$$V(z) := \frac{m(m+1)}{2}\wp_{1/2,i\omega'}(z+i\omega'). \tag{3.3.9}$$

*Then for $z \in \mathbb{R}$, $V(z)$ is a real, smooth, 1-periodic function.*

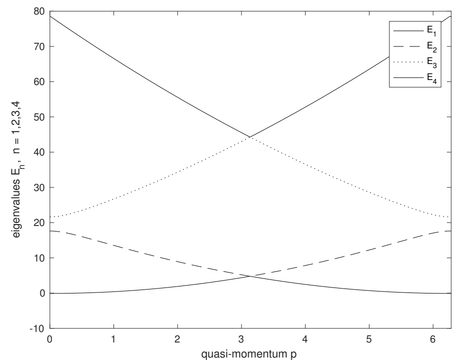
*The $m$ lowest Bloch band dispersion functions defined by* (3.2.3) *for this potential are non-degenerate for all $p \in \mathcal{B}$, but for* every *$n > m$, the band $E_n(p)$ has a linear crossing with the band $E_{n+1}(p)$ at $p = 0$ or $p = \pi$ [50]. Such potentials are known as 'm-gap' potentials since the* $L^2(\mathbb{R})$ *spectrum of the operator $-\frac{1}{2}\partial_z^2 + V(z)$ in this case consists of $m+1$ real intervals with $m$ 'gaps' between them. Indeed,* all *'m-gap' potentials, for positive integers $m$, must be elliptic functions [41]. Any Weierstrass elliptic function may be written in terms of Jacobi elliptic functions; for more detail see [9; 75; 14; 1; 59].*

*The lowest three bands of a 'one-gap' potential are shown in Figure 3.2. The smooth bands at the linear crossing between the second and third bands defined by* (3.3.3)*, whose existence is ensured by Theorem 3.3.1, are shown in Figure 3.4.*

**Example 2** (Trivial band crossings)**.** *Every Bloch band of any* 1*-periodic function which has minimal period* 1/2 *will be degenerate. To see this, let $V(z)$ be* 1/2*-periodic. We may plot the band structure of the operator $-\frac{1}{2}\partial_z^2 + V(z)$ with respect to the natural $4\pi$-periodic Brillouin zone, which we take for concreteness to be* $[0, 4\pi]$*. Now, we may also treat $V(z)$ as a 1-periodic potential and plot its band structure with respect to the $2\pi$-periodic Brillouin zone* $[0, 2\pi]$*. But it is clear that any eigenpair of the* 1/2*-periodic eigenvalue problem will also be an eigenpair of the* 1*-periodic eigenvalue problem. Hence the band structure of the 1-periodic operator is nothing but the band structure of the 1/2-periodic operator 'folded over' onto the shorter interval. More precisely, eigenvalues of the 1/2-periodic operator with quasi-momentum $p \in [2\pi, 4\pi]$ will be eigenvalues of the 1-periodic operator with quasi-momentum $p - 2\pi$. For an example, see Figure 3.5. We will refer to such*




(a)




(b)

Figure 3.5: Lowest Bloch bands when $V(z) = 4\cos(4\pi z)$, viewed as a 1/2-periodic potential and plotted over the natural Brillouin zone in this case $[0, 4\pi]$ (a) and viewed as a 1-periodic potential and plotted over $[0, 2\pi]$ (b). When $V(z)$ is viewed as a 1-periodic potential, *every* Bloch band is degenerate at $p = \pi$.

*crossings as "trivial", since they may be removed by a proper choice of Brillouin zone. The wave "excited" at such crossings is zero: see Remark 3.3.5 and Appendix B.2.*

### 3.3.3 Band crossing dynamics

We now make precise the scenario of a wavepacket whose quasi-momentum is driven by the external potential $W$ towards a quasi-momentum $p^* \in \mathcal{B}$ at which there is a linear band crossing; see Property 2.

**Property 3** (Band Crossing Scenario)**.** *Let $E_n, E_{n+1}$ denote spectral band functions associated with the eigenvalue problem (3.2.3) for $p \in \mathcal{B}$ which have a linear crossing in the sense of Property 2 at $p^*$. Let $q_0, p_0 \in \mathbb{R} \times \mathcal{B}$ be such that $G(E_n(p_0)) > 0$ (i.e. the band $E_n(p)$ is* isolated *at $p_0$: recall the definition of the spectral gap function $G$ (3.2.8)). We assume the existence of a positive constant $t^* > 0$ such that the equations of motion of the classical Hamiltonian $\mathcal{H}_n(q, p) := E_n(p) + W(q)$:*

$$\dot{q}(t) = \partial_p E_n(p(t)) \qquad \dot{p}(t) = -\partial_q W(q(t)) \tag{3.3.10}$$
$$q(0) = q_0 \qquad p(0) = p_0$$

*have a unique smooth solution $(q(t), p(t)) \subset \mathbb{R} \times \mathcal{B}$ for all $t \in [0, t^*)$ such that the Bloch band function $E_n$ is isolated when evaluated at $p(t)$ for every $t \in [0, t^*)$:*

$$\text{for all } t \in [0, t^*),\ G(E_n(p(t))) > 0 \text{ and } \lim_{t \uparrow t^*} p(t) = p^*. \tag{3.3.11}$$

*Let $q^*$ denote the limit: $\lim_{t\uparrow t^*} q(t)$. We assume that the wavepacket is 'driven' towards the crossing in the following sense:*

$$\lim_{t \uparrow t^*} \dot{p}(t) = -\partial_q W(q^*) > 0. \tag{3.3.12}$$

**Remark 3.3.2.** *We choose the sign of $-\partial_q W(q^*)$ in* (3.3.12) *to be positive without loss of generality. Note that it follows from* (3.3.12) *that for $t < t^*$ with $|t - t^*|$ sufficiently small, $p(t) < p^*$: i.e. the wave-packet quasi-momentum approaches $p^*$ 'from the left'. As a consequence the 'smooth extension' of the map $t \mapsto E_n(p(t))$ for $t \geq t^*$ makes use of $E_+(p(t))$ rather than $E_-(p(t))$; see Proposition 3.3.1.*

We aim to describe the solution of the PDE (3.1.1) with 'Bloch wavepacket' initial data of the form:

$$\psi^\epsilon(x, 0) = \mathrm{WP}^{1,\epsilon}[S_0, q_0, p_0, a_0^0(y), a_0^1(y), \chi_n(z; p_0)](x)\ ; \tag{3.3.13}$$

see (3.2.23). Here, $a_0^0, a_0^1 \in \mathcal{S}(\mathbb{R})$ and $S_0 \in \mathbb{R}$ in the Band Crossing Scenario (Property 3) up to errors of $o_{L^2}(\sqrt{\epsilon})$ for $t$ up to and greater than the crossing time $t^*$.

Note that for $t < t^*$, (3.3.11) implies that Property 1 holds with $t_0 = 0$ and $t_1 = t$. By Theorem 3.2.2 the solution $\psi^\epsilon(x, t)$ of (3.1.1) satisfies, for fixed $t$ and $\epsilon \downarrow 0$:

$$\psi^\epsilon(x, t) = \mathrm{WP}^{1,\epsilon}[S(t), q(t), p(t), a^0(y, t), a^1(y, t), \chi_n(z; p(t))](x, t) + O_{L^2}(\epsilon) \tag{3.3.14}$$

where $q(t), p(t), S(t), a^0(y, t), a^1(y, t)$ are as in (3.3.10), (3.2.13), (3.2.14), and (3.2.22) respectively.

Two difficulties arise in estimating error term in the solution $\psi^\epsilon(x, t)$ of (3.1.1) for $t \geq t^*$:

**Difficulty 1.** *The functions $q(t)$, $p(t)$, $S(t)$, $a^0(y, t)$, $a^1(y, t)$, $\chi_n(z; p(t))$, and $\partial_p \chi_n(z; p(t))$, and therefore the function:*

$$\mathrm{WP}^{1,\epsilon}[S(t), q(t), p(t), a^0(y, t), a^1(y, t), \chi_n(z; p(t))](x, t), \tag{3.3.15}$$

*are not well-defined at $t = t^*$ since the band function $E_n(p)$ and its associated eigenfunctions $\chi_n(z; p)$ are not smooth in $p$ at $p^*$.*

**Difficulty 2.** *The $L^2_x$-norm of the error in the approximation* (3.3.14) *depends directly on the inverse of the spectral gap function $G(E_n(p(t)))$, which blows up as $t \uparrow t^*$ since $|G(E_n(p(t)))| \sim |E_{n+1}(p(t)) - E_n(p(t))| \downarrow 0$.*

We return to Difficulty 2 below: see Theorem 3.3.2 and Corollary 3.3.2.

### 3.3.4 Resolution of Difficulty 1; Smooth Continuation of Bands

Difficulty 1 may be overcome by making proper use of the smooth band functions $E_+, E_-$; see (3.3.3) in Property 2, Theorem 3.3.1 and Figure 3.4. The following proposition shows how in the Band Crossing Scenario (Property 3), we may extend the map $[0, t^*) \to \mathbb{R} \times \mathcal{B}, t \mapsto (q(t), p(t))$ to a smooth map over an interval $[0, T]$ with $T > t^*$ using the smooth band function $E_+$:

**Proposition 3.3.1.** *Assume the Band Crossing Scenario (Property 3) with crossing occurring for $t = t^*$. Then for sufficiently small positive $\delta$ with $0 < \delta < t^*$, the equations of motion of the classical Hamiltonian $\mathcal{H}_+(q, p) := E_+(p) + W(q)$ with data specified at $t^*$:*

$$\begin{aligned} &\dot{q}_+(t) = \partial_p E_+(p_+(t)), && \dot{p}_+(t) = -\partial_q W(q_+(t)) \\ &q_+(t^*) = q^* && p_+(t^*) = p^* \end{aligned} \tag{3.3.16}$$

*have a unique smooth solution $(q_+(t), p_+(t)) \subset \mathbb{R} \times U$ over the interval $t \in [t^* - \delta, t^* + \delta]$ which satisfies:*

$$\text{for all } t \in [t^* - \delta, t^*),\ q(t) = q_+(t),\ p(t) = p_+(t). \tag{3.3.17}$$

*Furthermore, for sufficiently small $T \geq t^* + \delta > 0$, there exists a solution $(q_{n+1}(t), p_{n+1}(t)) \subset \mathbb{R} \times \mathcal{B}$ of the equations of motion of the classical Hamiltonian $\mathcal{H}_{n+1}(q, p) := E_{n+1}(p) + W(q)$ over the interval $t \in (t^*, T]$ satisfying the limits:*

$$\begin{aligned} &\dot{q}_{n+1}(t) = \partial_p E_{n+1}(p_{n+1}(t)) && \dot{p}_{n+1}(t) = -\partial_q W(q_{n+1}(t)) \\ &\lim_{t \downarrow t^*} q_{n+1}(t) = q^* && \lim_{t \downarrow t^*} p_{n+1}(t) = p^* \end{aligned} \tag{3.3.18}$$

*such that $G(E_{n+1}(p_{n+1}(t))) > 0$ for all $t \in (t^*, T]$. This solution satisfies:*

$$\text{for all } t \in (t^*, t^* + \delta],\ q_+(t) = q_{n+1}(t),\ p_+(t) = p_{n+1}(t). \tag{3.3.19}$$

*It follows from* (3.3.17) *and* (3.3.19) *that the map:*

$$t \mapsto (\mathfrak{q}_+(t), \mathfrak{p}_+(t)) := \begin{cases} (q(t), p(t)) & \text{for } t \in [0, t^* - \delta] \\ (q_+(t), p_+(t)) & \text{for } t \in [t^* - \delta, t^* + \delta] \\ (q_{n+1}(t), p_{n+1}(t)) & \text{for } t \in [t^* + \delta, T] \end{cases} \tag{3.3.20}$$

*is smooth as a map* $[0, T] \to \mathbb{R} \times \mathcal{B}$.

*Proof.* The potential $W$ is smooth by assumption, the band functions $E_n, E_{n+1}$ are smooth everywhere away from $p^*$, and the band function $E_+$ is smooth in $U$, a neighborhood of $p^*$. The proposition then follows easily from existence and uniqueness for solutions of ODEs with smooth coefficients. □

Corresponding to the smooth extension $t \mapsto (\mathfrak{q}_+(t), \mathfrak{p}_+(t))$ we may define the smooth extension of $\chi_n(z; p(t))$ through the crossing:

$$t \mapsto \mathfrak{X}_+(z; \mathfrak{p}_+(t)) := \begin{cases} \chi_n(z; p(t)) & \text{for } t \in [0, t^* - \delta] \\ \chi_+(z; p_+(t)) & \text{for } t \in [t^* - \delta, t^* + \delta] \\ \chi_{n+1}(z; p_{n+1}(t)) & \text{for } t \in [t^* + \delta, T] \end{cases}. \tag{3.3.21}$$

Finally, using the smooth maps $t \mapsto (\mathfrak{q}_+(t), \mathfrak{p}_+(t))$ and $t \mapsto \mathfrak{X}_+(z; \mathfrak{p}_+(t))$, we introduce smooth extensions of the functions $a^0(y,t)$, $a^1(y,t)$, and $S(t)$ over the whole interval $t \in [0, T]$ as follows:

**Definition 3.3.1** (Smooth extensions of $a^0(y,t)$, $a^1(y,t)$, and $S(t)$)**.** *Let:*

$$S^* := \lim_{t \uparrow t^*} S(t), \;\; a^{0,*}(y) := \lim_{t \uparrow t^*} a^0(y,t), \;\text{ and } a^{1,*}(y) := \lim_{t \uparrow t^*} a^1(y,t). \tag{3.3.22}$$

*Then let* $S_+(t)$, $a^0_+(y,t)$, *and* $a^1_+(y,t)$ *be defined for* $t \in [t^* - \delta, t^* + \delta]$ *by* (3.2.13), (3.2.14), *and* (3.2.22) *with* $t_0 = t^*$, *and where all dependence on* $p(t)$, $q(t)$, $E_n(p(t))$, $\chi_n(z; p(t))$, *and* $W(q(t))$ *replaced by dependence on* $p_+(t), q_+(t)$, $E_+(p_+(t))$, $\chi_+(z; p_+(t))$, *and* $W(q_+(t))$ *respectively, and:*

$$S_0 = S^*, \;\; a^0_0(y) = a^{0,*}(y), \;\text{ and } a^1_0(y) = a^{1,*}(y). \tag{3.3.23}$$

*Then let* $S_{n+1}(t)$, $a^0_{n+1}(y,t)$, $a^1_{n+1}(y,t)$ *be defined for* $t \in (t^*, T]$ *by equations* (3.2.13), (3.2.14), *and* (3.2.22), *replacing dependence on* $p(t)$, $q(t)$, $E_n(p(t))$, $\chi_n(z; p(t))$, *and* $W(q(t))$ *by dependence on* $p_{n+1}(t), q_{n+1}(t)$, $E_{n+1}(p_{n+1}(t))$, $\chi_{n+1}(z; p_{n+1}(t))$, *and* $W(q_{n+1}(t))$ *and the limits:*

$$\lim_{t \downarrow t^*} S_{n+1}(t) = S^*, \;\; \lim_{t \downarrow t^*} a_{n+1}(y,t) = a^{0,*}(y), \;\text{ and } \lim_{t \downarrow t^*} a^1(y,t) = a^{1,*}(y). \tag{3.3.24}$$

*We denote by* $\mathfrak{S}_+(t)$, $\mathfrak{a}_+^0(y,t)$, *and* $\mathfrak{a}_+^1(y,t)$ *smooth maps defined over the whole interval* $t \in [0,T]$ *defined analogously to* (3.3.20) *so that, for example:*

$$t \mapsto \mathfrak{a}_+^0(y,t) := \begin{cases} a^0(y,t) & \text{for } t \in [0, t^* - \delta] \\ a_+^0(y,t) & \text{for } t \in [t^* - \delta, t^* + \delta] \\ a_{n+1}^0(y,t) & \text{for } t \in [t^* + \delta, T] \end{cases} . \tag{3.3.25}$$

We now define a *first-order wavepacket smoothly continued through the crossing*, an expression which is smooth for all $t \in [0,T]$ by (recall the definition of $\text{WP}^{1,\epsilon}$ (3.2.23)):

$$\text{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}_+^0(y,t), \mathfrak{a}_+^1(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](x,t) :=$$
$$\begin{cases} \text{WP}^{1,\epsilon}[S(t), q(t), p(t), a^0(y,t), a^1(y,t), \chi_n(z; p(t))](x,t) & \text{for } t \in [0, t^* - \delta] \\ \text{WP}^{1,\epsilon}[S_+(t), q_+(t), p_+(t), a_+^0(y,t), a_+^1(y,t), \chi_+(z; p(t))](x,t) & \text{for } t \in [t^* - \delta, t^* + \delta] \\ \text{WP}^{1,\epsilon}[S_{n+1}(t), q_{n+1}(t), p_{n+1}(t), a_{n+1}^0(y,t), a_{n+1}^1(y,t), \chi_{n+1}(z; p(t))](x,t) & \text{for } t \in [t^* + \delta, T] \end{cases} . \tag{3.3.26}$$

**Remark 3.3.3.** *Note that by construction,* (3.3.26) *is a wavepacket associated with the band* $E_n$ *for* $t \in [0, t^* - \delta]$, *a wavepacket associated with the band* $E_{n+1}$ *for* $t \in [t^* + \delta, T]$, *and a wavepacket associated with the 'smooth transition'* $E_+$ *for* $t \in [t^* - \delta, t^* + \delta]$.

### 3.3.5 Resolution of Difficulty 2; Incorporation of the second band and a new, fast / non-adiabatic, time-scale

We first present a result which quantifies, through a blow-up rate of the error bound, the breakdown of the single band approximation (3.3.14) as $t \uparrow t^*$:

**Theorem 3.3.2.** *Assume the Band Crossing Scenario (Property 3). Assume* $a_0^0(y)$ *and* $a_0^1(y) \in \mathcal{S}(\mathbb{R})$ *and let* $\psi^\epsilon(x,t)$ *denote the unique solution of (3.1.1) with 'Bloch wavepacket' initial data:*

$$\psi^\epsilon(x,0) = \text{WP}_n^{1,\epsilon}[S_0, q_0, p_0, a_0^0(y), a_0^1(y), \chi_n(z; p_0)](x). \tag{3.3.27}$$

*Then for* $t \in [0, t^*)$, $\psi^\epsilon(x,t)$ *satisfies:*

$$\psi^\epsilon(x,t) = \text{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}_+^0(y,t), \mathfrak{a}_+^1(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](x) + \eta^\epsilon(x,t) \tag{3.3.28}$$

*where* $\mathrm{WP}_+^{1,\epsilon}(x,t)$ *is given by (3.3.26). Moreover, the corrector* $\eta^\epsilon(x,t)$ *satisfies the following bound for* $0 < t < t^*$*, which blows up as* $t \uparrow t^*$*:*

$$\begin{aligned}\|\eta^\epsilon(\cdot,t)\|_{L^2} \leq C\,|\langle \chi_-(\cdot;p^*)|\,\partial_p\chi_+(\cdot;p^*)\rangle| \left(\frac{\epsilon}{|t-t^*|} + \frac{\epsilon^{3/2}}{|t-t^*|^2}\right) \\ + O\left(\epsilon, \epsilon^{3/2}\ln|t-t^*|, \frac{\epsilon^{3/2}}{|t-t^*|}\right)\end{aligned} \tag{3.3.29}$$

*The constants in* (3.3.29) *(explicit and implied) are independent of* $t, \epsilon$ *and are finite as long as:* $\partial_p E_+(p^*) - \partial_p E_-(p^*) = 2\partial_p E_+(p^*) > 0$ *and* $\partial_q W(q^*) \neq 0$*.*

Theorem 3.3.2 is proved in Section 3.4 and Appendix B.3.

**Remark 3.3.4.** *The manner in which the nonzero constants* $\partial_p E_+(p^*) - \partial_p E_-(p^*) = 2\partial_p E_+(p^*)$ *and* $\partial_q W(q^*)$ *play a role in the bound* (3.3.29) *is seen in* (3.4.22) *and* (B.3.6)*.*

Theorem 3.3.2 shows that the single band ansatz, even when smoothly continued through the linear band crossing, fails to give a good approximation (error of size $o_{L^2_x}(\sqrt{\epsilon})$) to the solution $\psi^\epsilon(x,t)$ of equation (3.1.1) for small $|t-t^*|$. Furthermore, since the dominant terms in the bound (3.3.29), $\sqrt{\epsilon} \times (\sqrt{\epsilon}/|t-t^*|), \sqrt{\epsilon} \times (\sqrt{\epsilon}/|t-t^*|)^2$, are proportional to

$$\langle \chi_-(\cdot;p^*)|\,\partial_p\chi_+(\cdot;p^*)\rangle\,, \tag{3.3.30}$$

we see that the failure of the single band wave-packet approximation is due to contributions to the solution from the other band participating in the linear crossing, $p \mapsto E_-(p)$, growing to be of size $\sim \sqrt{\epsilon}$ when:

$$|t-t^*| \sim \sqrt{\epsilon}. \tag{3.3.31}$$

**Remark 3.3.5.** *At "trivial" crossings, which occur when the potential* $V(z)$ *has minimal period* 1/2 *(recall Example 2), the "inter-band coupling coefficient"* (3.3.30) *is zero (see Appendix B.2). It follows that the amplitude of the wave associated with the other band involved in the crossing "excited" (Theorem 3.3.3) at the crossing is also zero. This is consistent with the observation that the crossing may be removed by making the proper choice of Brillouin zone.*

The following Corollary of Theorem 3.3.2 precisely characterizes the time interval of validity of the single band ansatz:

**Corollary 3.3.2.** *Let $t = t^* - \epsilon^\xi$. Then, for small enough $\epsilon > 0$, (3.3.29) implies that the corrector function $\eta^\epsilon(x,t)$ which appears in* (3.3.28) *satisfies:*

$$\sup_{t \in [0, t^* - \epsilon^\xi]} \|\eta^\epsilon(\cdot, t)\|_{L^2} \leq C\epsilon^{1-\xi} \tag{3.3.32}$$

*where $C > 0$ is a constant independent of $\epsilon, \xi, t$. In particular, if $0 < \xi < 1/2$, then:*

$$\sup_{t \in [0, t^* - \epsilon^\xi]} \|\eta^\epsilon(\cdot, t)\|_{L^2} = o(\sqrt{\epsilon}). \tag{3.3.33}$$

*It follows that $\eta^\epsilon(x,t)$ is negligible in $L^2(\mathbb{R})$ compared with* $\mathrm{WP}^{1,\epsilon}$ *in the expansion* (3.3.28) *for $t \in [0, t^* - \epsilon^\xi]$.*

In order to describe the solution for $t \sim t^*$ and $t \geq t^*$, it is necessary to make a more general ansatz for the solution which accounts for the excitation of a wave associated with the other band involved in the crossing over the time-scale:

$$s := \frac{t - t^*}{\sqrt{\epsilon}}. \tag{3.3.34}$$

The following proposition, which is analogous to Proposition 3.3.1, is required to construct this excited wave:

**Proposition 3.3.2.** *Assume the Band Crossing Scenario (Property 3). Then for sufficiently small positive $\delta'$ the equations of motion of the classical Hamiltonian $\mathcal{H}_-(q,p) := E_-(p) + W(q)$ with data specified at $t^*$:*

$$\dot{q}_-(t) = \partial_p E_-(p_-(t)) \qquad \dot{p}_-(t) = -\partial_q W(q_-(t)) \tag{3.3.35}$$

$$q_-(t^*) = q^* \qquad p_-(t^*) = p^* \tag{3.3.36}$$

*have a unique smooth solution $(q_-(t), p_-(t)) \subset \mathbb{R} \times U$ over the interval $t \in [t^* - \delta', t^* + \delta']$. Furthermore, for sufficiently small $T' \geq t^* + \delta' > 0$, there exists a solution $(q_n(t), p_n(t)) \subset \mathbb{R} \times \mathcal{B}$ of the equations of motion of the classical Hamiltonian $\mathcal{H}_n(q,p) := E_n(p) + W(q)$ over the interval $t \in (t^*, T']$ satisfying the limits:*

$$\dot{q}_n(t) = \partial_p E_n(p_n(t)) \qquad \dot{p}_n(t) = -\partial_q W(q_n(t)) \tag{3.3.37}$$

$$\lim_{t \downarrow t^*} q_n(t) = q^* \qquad \lim_{t \downarrow t^*} p_n(t) = p^*$$

*such that* $G(E_n(p_n(t))) > 0$ *for all* $t \in (t^*, T']$. *This solution satisfies:*

$$\text{for all } t \in (t^*, t^* + \delta'],\ q_-(t) = q_n(t),\ p_-(t) = p_n(t). \tag{3.3.38}$$

*It follows from* (3.3.38) *that the map:*

$$(\mathfrak{q}_-(t), \mathfrak{p}_-(t)) := \begin{cases} (q_-(t), p_-(t)) & \text{for } t \in [t^* - \delta', t^* + \delta'] \\ (q_n(t), p_n(t)) & \text{for } t \in [t^* + \delta', T]. \end{cases} \tag{3.3.39}$$

*is smooth over the interval* $t \in [t^* - \delta', T']$.

We again define, as in (3.3.21):

$$t \mapsto \mathfrak{X}_-(z; \mathfrak{p}_-(t)) := \begin{cases} \chi_-(z; p_-(t)) & \text{for } t \in [t^* - \delta', t^* + \delta'] \\ \chi_n(z; p_n(t)) & \text{for } t \in [t^* + \delta', T'] \end{cases}. \tag{3.3.40}$$

The precise form of the wave "excited" at the crossing time is derived from a rigorous multi-scale analysis on the emergent nonadiabatic time-scale (3.3.34) (see Section 3.5.1). The following definition is the result of this calculation:

**Definition 3.3.2** (Parameters of the excited wave-packet)**.** *We let* $S_-(t)$ *and* $a^0_-(y,t)$ *be defined for* $t \in [t^* - \delta', t^* + \delta']$ *by* (3.2.13) *and* (3.2.14) *with* $t_0 = t^*$, *in which all dependence on* $p(t)$, $q(t)$, $E_n(p(t))$, $\chi_n(z; p(t))$, *and* $W(q(t))$ *replaced by dependence on* $p_-(t), q_-(t)$, $E_-(p_-(t))$, $\chi_-(z; p_-(t))$, *and* $W(q_-(t))$ *respectively.*

*Moreover,* $S_0 = S^*$ *and the initial data for* $a^0_-(y,t)$, *generated by the incoming '+ band' wave-packet is given by:*

$$\begin{aligned} a^0_-(y, t^*) = \ & \partial_q W(q^*) \times \langle \chi_-(\cdot; p^*) | \, \partial_p \chi_+(\cdot; p^*) \rangle \\ & \times \int_{-\infty}^{\infty} e^{i[\partial_q W(q^*)][\partial_p E_+(p^*) - \partial_p E_-(p^*)]\tau^2/2} \times a^{0,*}(y - [\partial_p E_+(p^*) - \partial_p E_-(p^*)]\tau) \, \mathrm{d}\tau \end{aligned} \tag{3.3.41}$$

*The definitions of* $S^*$ *and* $\lim_{t \uparrow t^*} a^0(y,t) = a^{0,*}(y)$ *are given in* (3.3.22).

*Recall that* $\partial_q W(q^*)$ *is assumed to be non-zero (see* (3.3.12)*) and that* $\partial_p E_+(p^*) - \partial_p E_-(p^*) = 2\partial_p E_+(p^*)$ *is always nonzero at band crossings (Theorem 3.3.1, Property 2 (A4)) and hence the integral in* (3.3.41) *is well-defined since* $a^{0,*}(y)$ *is localized. We then define* $S_n(t)$, $a^0_n(y,t)$ *for*

*$t \in (t^*, T']$ by replacing dependence on $p(t)$, $q(t)$, $E_n(p(t))$, $\chi_n(z; p(t))$, and $W(q(t))$ by dependence on $p_n(t), q_n(t)$, $E_n(p_n(t))$, $\chi_n(z; p_n(t))$, and $W(q_n(t))$ respectively, and by the limits:*

$$\lim_{t \downarrow t^*} S_n(t) = S^*, \ \lim_{t \downarrow t^*} a_n^0(y,t) = a^{0,*}(y). \tag{3.3.42}$$

*We denote by $\mathfrak{S}_-(t)$, $\mathfrak{a}_-^0(y,t)$ the smooth maps defined over the whole interval $t \in [t^* - \delta', T']$ in analogy with the definitions of $\mathfrak{S}_+(t)$ and $\mathfrak{a}_+(y,t)$ in Definition* (3.3.25).

We now define the wave-packet associated with the band $E_-$ which is "excited" at the crossing time $t^*$ by:

$$\begin{aligned} &\mathrm{WP}^{\epsilon,0}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}_-^0(y,t), \mathfrak{X}_-(z; \mathfrak{p}_-(t))](x,t) := \\ &:= \begin{cases} \mathrm{WP}^{\epsilon,0}[S_-(t), q_-(t), p_-(t), a_-^0(y,t), \chi_-(z; p(t))](x,t) & \text{for } t \in [t^* - \delta', t^* + \delta'] \\ \mathrm{WP}^{\epsilon,0}[S_n(t), q_n(t), p_n(t), a_n^0(y,t), \chi_n(z; p(t))](x,t) & \text{for } t \in [t^* + \delta', T] \end{cases}. \end{aligned} \tag{3.3.43}$$

### 3.3.6 The main theorem

Our main theorem is that a size 1 incoming wave-packet associated with the '+ band', when encountering a band-crossing, generates a size 1 'transmitted + band' wave-packet and a 'reflected − band' wave-packet of size $\sqrt{\epsilon}$. Moreover, when the wave-packet is in a neighborhood of the crossing, *i.e.* $t \approx t_*$ and hence $(p(t), q(t)) \approx (p_*, q_*)$, the detailed dynamics are non-adiabatic and are described by an ansatz incorporating wave-packets from both bands with envelopes varying on an additional fast scale. The precise statement is the following:

**Theorem 3.3.3.** *Assume the Band Crossing Scenario (Property 3) in which the crossing time, along the trajectory $(p(t), q(t))$ is $t = t_*$. Let $\xi, \xi'$ be fixed such that $3/8 < \xi' < \xi < 1/2$. Let $\tilde{T} > 0$, with $0 < t_* < \tilde{T}$, be sufficiently small that Propositions 3.3.1 and 3.3.2 hold with $T = \tilde{T}$ and $T' = \tilde{T}$ respectively.*

*Let $\psi^\epsilon(x,t)$ denote the unique solution of (3.1.1) with 'incident Bloch wavepacket' initial data (3.3.27), defined for $t \in [0, \tilde{T}]$.*

*Then, there exists an $\epsilon_0 > 0$ such that for all $0 < \epsilon < \epsilon_0$ the following holds.*

1. *For $t \in [0, t^* - \epsilon^\xi)$, $\psi^\epsilon(x,t)$ may be approximated up to errors of $o_{L^2_x}(\sqrt{\epsilon})$ by a single-band ansatz (see Theorem 3.3.2 and Corollary 3.3.2):*

$$\psi^\epsilon(x,t) = \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}_+^0(y,t), \mathfrak{a}_+^1(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](x,t) + o_{L^2_x}(\sqrt{\epsilon}). \tag{3.3.44}$$

2. *For $t \in (t^* + \epsilon^\xi, \tilde{T}]$, $\psi^\epsilon(x,t)$ is approximated up to errors of $o_{L^2_x}(\sqrt{\epsilon})$ by the sum of two Bloch wave-packets, one associated with each band involved in the crossing (recall Definition 3.3.2):*

$$\begin{aligned}\psi^\epsilon(x,t) &= \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z;\mathfrak{p}_+(t))](x,t) \\ &+ \sqrt{\epsilon}\, \mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}^0_-(y,t), \mathfrak{X}_-(z;\mathfrak{p}_-(t))](x,t) + o_{L^2_x}(\sqrt{\epsilon}).\end{aligned} \tag{3.3.45}$$

*Over the interval $t \in (t^* - \epsilon^{\xi'}, t^* + \epsilon^\xi)$, the solution $\psi^\epsilon(x,t)$ is expressible, with errors of size $o_{L^2_x}(\sqrt{\epsilon})$, by a superposition of wave-packets from both $+$ and $-$ bands, whose amplitudes vary on an additional (fast / non-adiabatic) time scale:*

$$s := \frac{t - t^*}{\sqrt{\epsilon}}. \tag{3.3.46}$$

*The detailed construction appears in Section 3.5.1.*

**Remark 3.3.6.** *The restriction to sufficiently small $\tilde{T} > 0$ in Theorem 3.3.3 is to ensure that neither the incident nor excited wavepacket encounter a second band crossing over the time interval $t \in [0, \tilde{T}]$. It is clear that this assumption may be relaxed and the analysis repeated each time a wavepacket is incident on a band crossing in order to obtain results valid over arbitrary finite time intervals, fixed independent of $\epsilon$.*

**Remark 3.3.7.** *By construction:*

$$\mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z;\mathfrak{p}_+(t))](x,t) \tag{3.3.47}$$

*is a wavepacket with $L^2_x$-norm proportional to 1 associated with the band $E_n$ for $t \in [0, t^* - \delta]$ and with $E_{n+1}$ for $t \in [t^* + \delta, \tilde{T}]$, and:*

$$\sqrt{\epsilon}\mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}^0_-(y,t), \mathfrak{X}_-(z;\mathfrak{p}_-(t))](x,t) \tag{3.3.48}$$

*is a wavepacket with $L^2_x$-norm proportional to $\sqrt{\epsilon}$ associated with the band $E_n$ for $t \in [t^* + \delta', \tilde{T}]$. Hence the statement of Theorem 3.3.3 is consistent with the description of our results given in Section 3.1.*

**Remark 3.3.8.** *To leading order in $\sqrt{\epsilon}$, the center of mass of the wavepacket 'excited' at the crossing is given by $\mathfrak{q}_-(t)$, which, for $t - t^*$ small enough, evolves according to (3.3.35). The center of mass of the* incoming *wavepacket is given by (again to leading order in $\sqrt{\epsilon}$) $\mathfrak{q}_+(t)$, which* *evolves (again for $t - t^*$ small enough) according to* (3.3.16). *Since* $\dot{\mathfrak{q}}_+(t^*) = \partial_p E_+(p^*) > 0$ *and* $\dot{\mathfrak{q}}_-(t^*) = \partial_p E_-(p^*) < 0$ *we have that the velocities of the centers of mass of each wavepacket have* opposite signs*: see Figure 3.3.*

**Remark 3.3.9.** *By dropping terms of $o(1)$ in $L^2_x$ in* (3.3.44), (3.3.45)*, and in the asymptotic solution which we construct for $t \in (t^* - \epsilon^{\xi'}, t^* + \epsilon^{\xi'})$, we have that, under the assumptions of Theorem 3.3.3, for all $t \in [0, \tilde{T}]$:*

$$\psi^\epsilon(x,t) = \mathrm{WP}^{0,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](x,t) + o_{L^2_x}(1). \tag{3.3.49}$$

## 3.4 Sketch of proof of Theorem 3.3.2 on blow-up of error in single-band approximation as $t$ approaches the crossing time $t^*$

### 3.4.1 Strategy for estimating the corrector

In this section we recall the simple Lemma which we use in the proofs of Theorem 3.3.2 and Theorem 3.3.3 to estimate the corrector to a wave-packet approximate solution. A similar strategy was followed in [61; 73]

**Lemma 3.4.1.** *For $0 < T \leq \infty$, let $\psi^\epsilon \in C^0([t_0, T); L^2(\mathbb{R}))$ denote the unique solution of the initial value problem* (3.1.1) *with initial data $\psi^\epsilon_0(x)$ given at $t = t_0$:*

$$\begin{aligned} i\epsilon\partial_t\psi^\epsilon &= H^\epsilon\psi^\epsilon \\ \psi^\epsilon(x,t_0) &= \psi^\epsilon_0(x) \ . \end{aligned} \tag{3.4.1}$$

*Furthermore, let $\psi^\epsilon_{app}(x,t) \in C^0([t_0,T); L^2(\mathbb{R}))$, $r^\epsilon(x,t)$ be such that:*

$$\begin{aligned} i\epsilon\partial_t\psi^\epsilon_{app} &= H^\epsilon\psi^\epsilon_{app} + r^\epsilon \\ \psi^\epsilon_{app}(x,t_0) &= \psi^\epsilon_{app,0}(x). \end{aligned} \tag{3.4.2}$$

*Introduce $\eta^\epsilon(x,t)$ defined by:*

$$\eta^\epsilon(x,t) := \psi^\epsilon(x,t) - \psi^\epsilon_{app}(x,t). \tag{3.4.3}$$

*Then,*

$$\|\eta^\epsilon(\cdot,t)\|_{L^2} \leq \|\psi^\epsilon_0(\cdot) - \psi^\epsilon_{app,0}(\cdot)\|_{L^2} + \frac{1}{\epsilon}\int_{t_0}^t \|r^\epsilon(\cdot,t')\|_{L^2}\,dt'. \tag{3.4.4}$$

**Remark 3.4.1.** *We shall apply Lemma 3.4.1 with $\psi^\epsilon_{app}(x,t)$ equal to an* approximate solution *of* (3.1.1) *and $r^\epsilon(x,t)$ equal to the* residual.

*Proof.* The function $\eta^\epsilon(x,t)$ satisfies the initial value problem:

$$\begin{aligned} i\epsilon\partial_t\eta^\epsilon &= H^\epsilon\eta^\epsilon + r^\epsilon \\ \psi^\epsilon_{app}(x,t_0) &= \psi^\epsilon_0(x) - \psi^\epsilon_{app,0}(x) \end{aligned} \tag{3.4.5}$$

Multiplying both sides of (3.4.5) by $\overline{\eta^\epsilon}$, taking the imaginary part yields and using self-adjointness of $H^\epsilon$ we obtain: $\epsilon\partial_t\|\eta^\epsilon\|^2_{L^2} = -i\left\langle \eta^\epsilon | \, r^\epsilon\right\rangle_{L^2} + i\left\langle r^\epsilon | \, \eta^\epsilon\right\rangle_{L^2}$. This implies, using the Cauchy-Schwarz inequality that $2\epsilon\|\eta^\epsilon\|_{L^2}\ \partial_t\|\eta^\epsilon\|_{L^2} \leq 2\|r^\epsilon\|_{L^2}\|\eta^\epsilon\|_{L^2}$. Cancelling common factors from both sides (note that the inequality is trivially true if $\|\eta^\epsilon\|_{L^2} = 0$) and integrating from $t_0$ to $t$ gives (3.4.4). □

We now estimate the error in the single-band approximation as $t \uparrow t^*$, as measured by the $L^2_x$-norm of the corrector function $\eta^\epsilon(x,t)$ which appears in (3.3.28). We start by recalling the strategy of the proof of Theorem 3.2.2; the proof of Theorem 3.2.1 is similar. Let $\psi^\epsilon(x,t)$ denote the exact solution of (3.1.1) with approximate 'Bloch wavepacket' initial data (3.2.24) specified at $t = t_0$. Then by Lemma 3.4.1, if we can find an approximate solution of (3.1.1), $\psi^\epsilon_{app}(x,t)$, such that (3.4.2) holds with:

$$\|\psi^\epsilon_0(\cdot) - \psi^\epsilon_{app,0}(\cdot)\|_{L^2} \leq C\epsilon \tag{3.4.6}$$

$$\text{and } \|r^\epsilon(\cdot,t)\|_{L^2} \leq Ce^{ct}\epsilon^2, \tag{3.4.7}$$

where the constants $C > 0, c > 0$ are independent of $\epsilon, t$, then it follows from (3.4.3) and (3.4.4) that:

$$\|\psi^\epsilon(\cdot,t) - \psi^\epsilon_{app}(\cdot,t)\|_{L^2} \leq C\epsilon e^{ct}. \tag{3.4.8}$$

If in addition we have that:

$$\|\psi^\epsilon_{app}(\cdot,t)\ -\ \mathrm{WP}^{1,\epsilon}[S(t),q(t),p(t),a^0(y,t),a^1(y,t),\chi_n(z;p(t))](\cdot,t)\|_{L^2} \leq Ce^{ct}\epsilon, \tag{3.4.9}$$

where $q(t), p(t)$ and so on are as in the statement of Theorem 3.2.2, then the conclusions of Theorem 3.2.2 follow immediately by the triangle inequality. The details of how to construct such a $\psi^\epsilon_{app}(x,t)$ were presented in [73].

Theorem 3.2.2 implies, in particular, that the solution $\psi^\epsilon(x,t)$ of (3.1.1) with initial data (3.3.27) as initial data satisfies:

$$\begin{aligned}&\text{for } t \in [0, t^* - \delta],\\ &\|\psi^\epsilon(\cdot,t) \ - \ \mathrm{WP}^{1,\epsilon}[S(t), q(t), p(t), a^0(y,t), a^1(y,t), \chi_n(z; p(t))](\cdot,t)\|_{L^2} = O_{L^2_x}(\epsilon).\end{aligned} \tag{3.4.10}$$

Due to the band crossing at $p^*$, the Isolated Band Property 1 does not hold as $t \uparrow t^*$. As a result the proof of Theorem 3.2.2 fails as follows:

1. As $t \uparrow t^*$, the $L^2_x$-norm of the residual $r^\epsilon(x,t)$ defined by (3.4.2), diverges.
2. The integral $\frac{1}{\epsilon}\int_0^t \|r^\epsilon(\cdot,t')\|_{L^2}\,\mathrm{d}t'$, and hence the bound (3.4.4) on the $L^2$-norm of the corrector function $\eta^\epsilon(x,t)$ diverges as $t \uparrow t^*$.

Theorem 3.3.2 is proved by analyzing the rates of blow-up of singular terms in $r^\epsilon(x,t)$ and then deducing the resulting rate of blow-up of the bound (3.4.4). In Section 3.4.2 explain the strategy by studying a representative term. We then sketch the general argument in Appendix B.3.

### 3.4.2 Estimation of representative term demonstrating blow-up as $t \uparrow t^*$

Let $t \in [t^* - \delta, t^*]$ where $\delta > 0$ is as in Proposition 3.3.1 so that:

$$\begin{aligned}&\mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](x,t)\\ &= \mathrm{WP}^{1,\epsilon}[S_+(t), q_+(t), p_+(t), a^0_+(y,t), a^1_+(y,t), \chi_+(z; p(t))](x,t)\end{aligned} \tag{3.4.11}$$

Here, $q_+(t), p_+(t)$ are as in (3.3.16), $S_+(t), a^0_+(y,t), a^1_+(y,t)$ are as in Definition 3.3.1, and $E_+(p)$, $\chi_+(z;p)$ are as in (3.3.3). The representative term which appears in the residual $r^\epsilon(x,t)$ (3.4.2) which we will consider is the following:

$$\begin{aligned}&R^\epsilon(x,t) := \epsilon^{-1/4} e^{i\phi^\epsilon_+(y,t)/\epsilon} \Big[\\ &\epsilon^2(-i\partial_t)\Big(-i\partial_q W(q_+(t)) a^0_+(y,t) \mathcal{R}_+(p_+(t)) P^\perp_+(p_+(t)) \partial_p \chi_+(z; p_+(t))\Big)\Big]\Big|_{y=\frac{x-q_+(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}}\\ &\text{where } \phi^\epsilon_+(y,t) := S_+(t) + \epsilon^{1/2} p_+(t) y\end{aligned} \tag{3.4.12}$$

Here, $P^\perp_+(p)$ denotes the projection operator onto the orthogonal complement of the subspace of $L^2_{per}$ spanned by $\chi_+(z;p)$, and:

$$\mathcal{R}_+(p) := (H(p) - E_+(p))^{-1} \tag{3.4.13}$$

denotes the resolvent operator where $H(p)$ is as in (3.2.3). Because of the band crossing at $p^*$, the operator $\mathcal{R}_+(p)P_+^\perp(p)$ is singular as $p \to p^*$ on the subspace of $L^2_{per}$ spanned by $\chi_-(z;p)$. The operator $\mathcal{R}_+(p)P_\pm^\perp(p)$ however, where $P_\pm^\perp(p)$ is defined as the projection onto the orthogonal complement of $\chi_+(z;p)$ and $\chi_-(z;p)$ in $L^2_{per}$ is regular for all $p \in U$ by (A2) of Property 2 (see Corollary 3.3.1).

We isolate the singular part of (3.4.12) as follows. Expressing $\partial_p\chi_+(z;p_+(t))$ in terms of its projections onto both $\chi_+(z;p_+(t))$ and $\chi_-(z;p_+(t))$, and their orthogonal complement, the range of $P_\pm^\perp(p_+(t))$, we have

$$\begin{aligned}\mathcal{R}_+(p_+(t))P_+^\perp(p_+(t))\partial_p\chi_+(z;p_+(t)) &= \mathcal{R}_+(p(t))P_\pm^\perp(p_+(t))\partial_p\chi_+(z;p_+(t)) \\ &+ (E_-(p_+(t)) - E_+(p_+(t)))^{-1}\left\langle \chi_-(\cdot;p_+(t)) \middle| \partial_p\chi_+(\cdot;p_+(t))\right\rangle \chi_-(z;p(t))\ .\end{aligned} \tag{3.4.14}$$

Since $p_+(t) \to p^*$ as $t \uparrow t_*$, $E_+(p^*) = E_-(p^*)$, the singular behavior is isolated in the latter term of (3.4.14). We decompose $R^\epsilon(x,t)$ into its corresponding regular and singular parts:

$$R^\epsilon(x,t) := R^\epsilon_{regular}(x,t) + R^\epsilon_{singular}(x,t) \tag{3.4.15}$$

where:

$$\begin{aligned}&R^\epsilon_{regular}(x,t) = \epsilon^{-1/4}e^{i\phi^\epsilon_+(y,t)/\epsilon}\Big[ \\ &\epsilon^2(-i\partial_t)\Big(-i\partial_q W(q_+(t))a^0_+(y,t)\mathcal{R}_+(p_+(t))P_\pm^\perp(p_+(t))\partial_p\chi_+(z;p_+(t))\Big)\Big]\Big|_{y=\frac{x-q_+(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon}} \\ &R^\epsilon_{singular}(x,t) = \epsilon^{-1/4}e^{i\phi^\epsilon_+(y,t)/\epsilon}\Big[\epsilon^2(-i\partial_t)\Big(-i\partial_q W(q_+(t))a^0_+(y,t) \\ &\times\ (E_-(p_+(t)) - E_+(p_+(t)))^{-1}\left\langle \chi_-(z;p_+(t)) \middle| \partial_p\chi_+(z;p_+(t))\right\rangle \chi_-(z;p_+(t))\Big)\Big]\Big|_{y=\frac{x-q_+(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon}}\ .\end{aligned} \tag{3.4.16}$$

It follows from the techniques detailed in [73] that:

$$R^\epsilon_{regular}(x,t) = O_{L^2_x}(\epsilon^2) \tag{3.4.17}$$

uniformly as $t \uparrow t^*$. On the other hand, $R^\epsilon_{singular}(x,t)$ is explicitly singular, since it depends on $(E_-(p_+(t)) - E_+(p_+(t)))^{-1}$ which is unbounded as $t \uparrow t^*$. The time derivative of $R^\epsilon_{singular}(x,t)$ yields two terms:

$$R^\epsilon_{singular}(x,t) = R^{1,\epsilon}_{singular}(x,t) + R^{2,\epsilon}_{singular}(x,t), \tag{3.4.18}$$

where:

$$\begin{aligned} R^{1,\epsilon}_{singular}(x,t) &:= \epsilon^{-1/4} e^{i\phi^\epsilon_+(y,t)/\epsilon} \Big[ \epsilon^2 (E_-(p_+(t)) - E_+(p_+(t)))^{-1} \\ &\times (-i\partial_t) \Big( - i\partial_q W(q_+(t)) a^0_+(y,t) \langle \chi_-(z;p_+(t)) | \, \partial_p \chi_+(z;p_+(t)) \rangle \, \chi_-(z;p_+(t)) \Big) \Big] \Big|_{y = \frac{x-q_+(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} \\ R^{2,\epsilon}_{singular}(x,t) &:= \epsilon^{-1/4} e^{i\phi^\epsilon_+(y,t)/\epsilon} \Big[ \epsilon^2 \partial_t \Big( (E_-(p_+(t)) - E_+(p_+(t)))^{-1} \Big) \\ &\times (-i) \Big( -i\partial_q W(q_+(t)) a^0_+(y,t) \langle \chi_-(z;p_+(t)) | \, \partial_p \chi_+(z;p_+(t)) \rangle \, \chi_-(z;p_+(t)) \Big) \Big] \Big|_{y = \frac{x-q_+(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} . \end{aligned} \tag{3.4.19}$$

We now concentrate on $R^{2,\epsilon}_{singular}(x,t)$ which will turn out to be the dominant term as $t \uparrow t^*$. We first evaluate the time-derivative:

$$\begin{aligned} &\partial_t \Big( (E_-(p_+(t)) - E_+(p_+(t)))^{-1} \Big) = \\ &\partial_q W(q_+(t)) (\partial_p E_-(p_+(t)) - \partial_p E_+(p_+(t))) \, (E_-(p_+(t)) - E_+(p_+(t)))^{-2} . \end{aligned} \tag{3.4.20}$$

We then follow [61; 73] in estimating $R^{2,\epsilon}_{singular}$ in $L^2_x$ by taking the $L^\infty$ norm of all $z$-dependence and the $L^2$-norm of all $y$ dependence:

$$\begin{aligned} \| R^{2,\epsilon}_{singular}(\cdot,t) \|_{L^2} &\leq \epsilon^2 |\partial_q W(q_+(t))|^2 \, |\partial_p E_-(p_+(t)) - \partial_p E_+(p_+(t))| \, |E_-(p_+(t)) - E_+(p_+(t))|^{-2} \\ &\times \| a^0_+(\cdot,t) \|_{L^2} \Big| \langle \chi_-(\cdot;p_+(t)) | \, \partial_p \chi_+(\cdot;p_+(t)) \rangle_{L^2[0,1]} \Big| \, \| \chi_+(\cdot,p_+(t)) \|_{L^\infty[0,1]} . \end{aligned} \tag{3.4.21}$$

Taylor-expanding in $t - t^*$, using the non-degeneracy conditions (3.3.4) and (3.3.12), we have that as $t \uparrow t^*$:

$$\begin{aligned} &\Big| (E_+(p_+(t)) - E_-(p_+(t)))^{-2} \Big| \leq \\ &\left| \frac{1}{\partial_q W(q^*) \, (\partial_p E_+(p^*) - \partial_p E_-(p^*))} \right|^2 \left( \frac{1}{|t-t^*|^2} \right) + O\left( \frac{1}{|t-t^*|} \right) . \end{aligned} \tag{3.4.22}$$

Substituting (3.4.22) into (3.4.21) and Taylor-expanding all other terms gives:

$$\begin{aligned} &\| R^{2,\epsilon}_{singular}(\cdot,t) \|_{L^2} \leq \\ &\left| \frac{\langle \chi_-(\cdot;p^*) | \, \partial_p \chi_+(\cdot;p^*) \rangle_{L^2[0,1]} \, \| a^0_+(\cdot,t^*) \|_{L^2} \| \chi_+(\cdot,p^*) \|_{L^\infty[0,1]}}{\partial_p E_-(p^*) - \partial_p E_+(p^*)} \right| \left( \frac{\epsilon^2}{|t-t^*|^2} \right) + O\left( \frac{\epsilon^2}{|t-t^*|} \right) \end{aligned} \tag{3.4.23}$$

Similar analysis shows that:

$$\| R^{1,\epsilon}_{singular}(\cdot,t) \|_{L^2} = O\left( \frac{\epsilon^2}{|t-t^*|} \right) . \tag{3.4.24}$$

Recall the relationship between the residual $r^\epsilon(x,t)$ and the bound on the solution error $\eta^\epsilon(x,t) := \psi^\epsilon(x,t) - \psi^\epsilon_{app}(x,t)$ (3.4.4). Putting everything ((3.4.15), (3.4.17), (3.4.23), and (3.4.24)) together, then integrating once in time and dividing by $\epsilon$, we see that the term contributed by $R^\epsilon(x,t)$ to the solution error $\eta^\epsilon(x,t)$ may be bounded by:

$$\begin{aligned}&\frac{1}{\epsilon}\int_0^t \|R^\epsilon(\cdot,t')\|_{L^2}\,\mathrm{d}t' \leq \\ &\left| \frac{\langle \chi_-(\cdot;p^*) | \, \partial_p \chi_+(\cdot;p^*)\rangle_{L^2[0,1]} \, \|a^0_+(\cdot,t^*)\|_{L^2} \|\chi_+(\cdot,p^*)\|_{L^\infty[0,1]}}{\partial_p E_-(p^*) - \partial_p E_+(p^*)} \right| \left( \frac{\epsilon}{|t-t^*|} \right) \\ &+ O\left(\epsilon, \epsilon \ln|t-t^*|\right).\end{aligned} \tag{3.4.25}$$

It follows that the right hand side of (3.4.25), which is the bound on the corrector to the wave-packet ansatz, is of the same size as the $O(\epsilon^{1/2})$ term in the wave-packet approximate solution for $|t - t_*| \sim \epsilon^{1/2}$.

## 3.5 Proof of Theorem 3.3.3 on coupled band dynamics when $t \sim t^*$

We now turn to the proof of Theorem 3.3.3, on the dynamics through the crossing time $t^*$. Theorem 3.3.2 and Corollary 3.3.2 give a description of the exact solution $\psi^\epsilon(x,t)$ of (3.1.1) with initial data given by (3.3.27) which is valid with errors of $o_{L^2_x}(\epsilon^{1/2})$ up to $t = t^* - \epsilon^\xi$ for any $\xi \in (0,1/2)$:

$$\begin{aligned}&\text{For all } t \in [0, t^* - \epsilon^\xi), \\ &\psi^\epsilon(x,t) = \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z;\mathfrak{p}_+(t))](x,t) + o_{L^2_x}(\epsilon^{1/2}).\end{aligned} \tag{3.5.1}$$

We seek to extend (3.5.1) to a description of $\psi^\epsilon(x,t)$ up to errors of $o_{L^2_x}(\epsilon^{1/2})$ over the entire interval $t \in [0, \tilde{T}]$ where $\tilde{T}$ is chosen such that Propositions 3.3.1 and 3.3.2 hold with $T = \tilde{T}$ and $T' = \tilde{T}$. We first claim that the proof of Theorem 3.3.3 may be reduced to (a) the construction of a function $\psi^\epsilon_{app,inner}(x,t)$ satisfying certain properties and (b) an application of Lemma 3.4.1:

**Proposition 3.5.1.** *Let $\xi, \xi' \in (0,1/2)$ be such that $\xi' < \xi$ so that $(t^* - \epsilon^\xi, t^* + \epsilon^\xi) \subset (t^* - \epsilon^{\xi'}, t^* + \epsilon^{\xi'})$. Assume (3.5.1) for an incoming wave-packet. Consider an approximate solution $\psi^\epsilon_{app,inner}(x,t)$ which satisfies the following three properties:*

(P1) *$\psi^\epsilon_{app,inner}(x,t)$ is equal to the single-band ansatz in the 'incoming' overlap region $t \in (t^* -$*

*$\epsilon^{\xi'}, t^* - \epsilon^{\xi})$ up to errors of $o(\epsilon^{1/2})$ in $L^2(\mathbb{R})$. That is,*

*for all $t \in (t^* - \epsilon^{\xi'}, t^* - \epsilon^{\xi})$,*

$$\left\| \psi^\epsilon_{app,inner}(\cdot, t) - \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](\cdot, t) \right\|_{L^2} = o(\epsilon^{1/2}), \tag{3.5.2}$$

(P2) *$\psi^\epsilon_{app,inner}(x,t)$ is an approximate solution to* (3.1.1) *$(i\epsilon\partial_t - H^\epsilon)\psi^\epsilon = 0$:*

$$i\epsilon\partial_t \psi^\epsilon_{app,inner} - H^\epsilon \psi^\epsilon_{app,inner} = r^\epsilon_{inner} \tag{3.5.3}$$

*with residual satisfying the bound:*

$$\frac{1}{\epsilon} \int_{t^* - \epsilon^{\xi'}}^{t^* + \epsilon^{\xi'}} \| r^\epsilon_{inner}(\cdot, t') \|_{L^2} \, dt' = o(\epsilon^{1/2}), \tag{3.5.4}$$

(P3) *$\psi^\epsilon_{app,inner}(x,t)$ matches the 'two-band' ansatz of* (3.3.45) *in the 'outgoing' overlap region $t \in (t^* + \epsilon^{\xi}, t^* + \epsilon^{\xi'})$ up to errors of $o(\epsilon^{1/2})$ in $L^2(\mathbb{R})$. That is,*

$$\begin{aligned} &\text{for all } t \in (t^* + \epsilon^{\xi}, t^* + \epsilon^{\xi'}), \\ &\Big\| \psi^\epsilon_{app,inner}(\cdot, t) - \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](\cdot, t) \\ &- \epsilon^{1/2} \mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}^0_-(y,t), \mathfrak{X}_-(z; \mathfrak{p}_-(t))](\cdot, t) \Big\|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.5}$$

*Then, under conditions (P1), (P2), and (P3), Theorem 3.3.3 holds.*

*Proof.* We apply Lemma 3.4.1 with $t_0 = t^* - \epsilon^{\xi'}$, $t_1 = t^* + \epsilon^{\xi'}$, $\psi^\epsilon_{app}(x,t) = \psi^\epsilon_{app,inner}(x,t)$, and $r^\epsilon(x,t) = r^\epsilon_{app,inner}(x,t)$. It then follows from (P1) and (P2) that:

$$\begin{aligned} &\text{For all } t \in (t^* - \epsilon^{\xi'}, t^* + \epsilon^{\xi'}), \\ &\| \psi^\epsilon(\cdot, t) - \psi^\epsilon_{app,inner}(\cdot, t) \|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.6}$$

Combining (3.5.6) with (P3), we have that:

$$\begin{aligned} &\text{For all } t \in (t^* + \epsilon^{\xi}, t^* + \epsilon^{\xi'}), \\ &\Big\| \psi^\epsilon(\cdot, t) - \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z; \mathfrak{p}_+(t))](\cdot, t) \\ &+ \epsilon^{1/2} \mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}^0_-(y,t), \mathfrak{X}_-(z; \mathfrak{p}_-(t))](x, t) \Big\|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.7}$$

We claim that the main statement (3.3.45) of Theorem 3.3.3 then follows from the isolated band theory. For any $\tilde{T}_0$ fixed independent of $\epsilon$ such that $t^* < \tilde{T}_0 < \tilde{T}$, the Isolated Band Property

1 holds for the bands $E_n(p)$ and $E_{n+1}(p)$ and trajectories $p_n(t)$ and $p_{n+1}(t)$ defined by (3.3.37), (3.3.18) with $t_0 = \tilde{T}_0, t_1 = \tilde{T}$. By linearity, the two-band wavepacket ansatz agrees (modulo errors of $o_{L^2_x}(\epsilon^{1/2})$) with the exact solution $\psi^\epsilon_{outgoing}(x,t)$ of the full equation (3.1.1) over the interval $t \in [\tilde{T}_0, \tilde{T}]$ with initial data given at $\tilde{T}_0$ by:

$$\begin{aligned} &\psi^\epsilon_{outgoing}(x,\tilde{T}_0) = \\ &\mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(\tilde{T}_0), \mathfrak{q}_+(\tilde{T}_0), \mathfrak{p}_+(\tilde{T}_0), \mathfrak{a}^0_+(y,\tilde{T}_0), \mathfrak{a}^1_+(y,\tilde{T}_0), \mathfrak{X}_+(z;\mathfrak{p}_+(\tilde{T}_0))](x,\tilde{T}_0) \\ &+ \epsilon^{1/2}\mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(\tilde{T}_0), \mathfrak{q}_-(\tilde{T}_0), \mathfrak{p}_-(\tilde{T}_0), \mathfrak{a}^0_-(y,\tilde{T}_0), \mathfrak{X}_-(z;\mathfrak{p}_-(\tilde{T}_0))](x,\tilde{T}_0). \end{aligned} \tag{3.5.8}$$

By performing the same analysis as in the proof of Theorem 3.3.2 backwards in time towards $t^*$, we have that:

$$\begin{aligned} &\text{For all } t \in (t^* + \epsilon^\xi, \tilde{T}], \\ &\Big\| \psi^\epsilon_{outgoing}(\cdot,t) - \mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z;\mathfrak{p}_+(t))](\cdot,t) \\ &+\epsilon^{1/2}\mathrm{WP}^{0,\epsilon}[\mathfrak{S}_-(t), \mathfrak{q}_-(t), \mathfrak{p}_-(t), \mathfrak{a}^0_-(y,t), \mathfrak{X}_-(z;\mathfrak{p}_-(t))](x,t) \Big\|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.9}$$

But now combining the triangle inequality with (3.5.7), we have that:

$$\begin{aligned} &\text{For all } t \in (t^* + \epsilon^\xi, t^* + \epsilon^{\xi'}), \\ &\left\| \psi^\epsilon(\cdot,t) - \psi^\epsilon_{outgoing}(\cdot,t) \right\|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.10}$$

Since $\psi^\epsilon(x,t)$ and $\psi^\epsilon_{outgoing}(x,t)$ are both exact solutions of (3.1.1), applying Lemma 3.4.1 one more time with $\psi^\epsilon_{app}(x,t) = \psi^\epsilon_{outgoing}(x,t)$ gives that:

$$\begin{aligned} &\text{For all } t \in (t^* + \epsilon^\xi, \tilde{T}], \\ &\left\| \psi^\epsilon(\cdot,t) - \psi^\epsilon_{outgoing}(\cdot,t) \right\|_{L^2} = o(\epsilon^{1/2}). \end{aligned} \tag{3.5.11}$$

The main statement of Theorem 3.3.3 (3.3.45) then follows from combining (3.5.11) and (3.5.9). □

This brings us to the core construction of the paper.

### 3.5.1 Derivation of $\psi^\epsilon_{app,inner}$ satisfying hypotheses of Proposition 3.5.1

We make the following ansatz for $\psi^\epsilon_{app,inner}(x,t)$, which incorporates both + and − bands, and a new 'fast' timescale:

$$s = \frac{t - t^*}{\epsilon^{1/2}}, \tag{3.5.12}$$

which was motivated by the preceding single-band analysis:

$$\psi^{\epsilon}_{app,inner}(x,t) = \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\}/\epsilon} f^{\epsilon}_{\sigma,inner}\left(y_\sigma, z, t, s\right)\Big|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}, s=\frac{t-t^*}{\epsilon^{1/2}}} . \quad (3.5.13)$$

The new time scale has been introduced in the envelope functions $f^{\epsilon}_{\sigma,inner}$. We take $(q_\sigma(t), p_\sigma(t))$, $\sigma = \pm$ as in (3.3.16) and (3.3.35), $S_\sigma(t), \sigma = \pm$, as in Definitions 3.3.1 and 3.3.2, and assume that $f^{\epsilon}_{\sigma,inner}(y_\sigma, z, t, s)$ may be expanded in powers of $\epsilon^{1/2}$:

$$f^{\epsilon}_{\sigma,inner}(y_\sigma, z, t, s) = f^{0}_{\sigma,inner}(y_\sigma, z, t, s) + \epsilon^{1/2} f^{1}_{\sigma,inner}(y_\sigma, z, t, s) + ... \quad (3.5.14)$$

Then, $\psi^{\epsilon}_{app,inner}$, given by (3.5.13), satisfies the non-homogeneous Schroedinger equation (3.5.3) with residual:

$$\begin{aligned} r^{\epsilon}_{inner}(x,t) &= \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\left\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon} \left\{ \epsilon^{3/2} \left[ y^3_\sigma \int_0^1 \frac{(\tau-1)^3}{3!} \partial^3_x W\left(q_\sigma(t) + \tau\epsilon^{1/2}y_\sigma\right) \mathrm{d}\tau \right] \right. \\ &+ \epsilon \left[ \frac{1}{2}(-i\partial_{y_\sigma})^2 + \frac{1}{2}\partial^2_x W(q_\sigma(t)) y^2_\sigma - i\partial_t \right] + \epsilon^{1/2} \left[ \left( p_\sigma(t) - i\partial_z - \partial_p E_\sigma(p_\sigma(t)) \right)(-i\partial_{y_\sigma}) - i\partial_s \right] \\ &+ \left. \left[ H(p_\sigma(t)) - E_\sigma(p_\sigma(t)) \right] \right\} \left\{ f^0_{\sigma,inner}(y_\sigma, z, t, s) + \epsilon^{1/2} f^1_{\sigma,inner}(y_\sigma, z, t, s) + ... \right\} \Big|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}, s=\frac{t-t^*}{\epsilon^{1/2}}} \\ &= r^{\epsilon}_{inner,0}(x,t) + \epsilon^{1/2} r^{\epsilon}_{inner,1}(x,t) + (\epsilon^{1/2})^2 r^{\epsilon}_{inner,2}(x,t) + \ldots + (\epsilon^{1/2})^m r^{\epsilon}_{inner,3}(x,t) + \ldots \end{aligned} \quad (3.5.15)$$

Here, $H(p) = -\frac{1}{2}(p - i\partial_z)^2 + V(z)$; see (3.2.3).

In the coming sections we construct the functions $f^{j}_{\sigma,inner}$ so that $\psi^{\epsilon}_{app,inner}(x,t)$ satisfies the properties (P1), (P2) and (P3) of Proposition 3.5.1.

#### 3.5.1.1 Terms in $r^{\epsilon}_{inner}$ with $L^2_x$ norm of order $\epsilon^0$

The terms with $L^2_x$ norm proportional to $\epsilon^0 = 1$ in (3.5.15) are of the form:

$$r^{\epsilon}_{inner,0}(x,t) = \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\left\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon} \left[ H(p_\sigma(t)) - E_\sigma(p_\sigma(t)) \right] f^0_{\sigma,inner}(y_\sigma, z, t, s) \Big|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}, s=\frac{t-t^*}{\epsilon^{1/2}}} . \quad (3.5.16)$$

We may set these two terms individually to zero by defining:

$$f^0_{\sigma,inner}(y_\sigma, z, t, s) = a^0_{\sigma,inner}(y_\sigma, t, s)\ \chi_\sigma(z; p_\sigma(t)), \quad \sigma = \pm \quad . \quad (3.5.17)$$

The functions $a^0_{\sigma,inner}(y_\sigma, t, s)$, $\sigma = \pm$ are left arbitrary for now and will be determined a later stage.

#### 3.5.1.2 Terms in $r^\epsilon_{inner}$ with $L^2_x$ norm of order $\epsilon^{1/2}$

The terms with $L^2_x$ norm proportional to $\epsilon^{1/2}$ in (3.5.15) are of the form $\epsilon^{1/2}$ times the following expression which is $O_{L^2}(1)$:

$$\begin{aligned} & r^\epsilon_{inner,1}(x,t) = \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\left\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon} \Bigg\{ \\ & \left[ \Big( p_\sigma(t) - i\partial_z - \partial_p E_\sigma(p_\sigma(t)) \Big) (-i\partial_{y_\sigma}) - i\partial_s \right] f^0_{\sigma,inner}(y_\sigma, z, t, s) \\ & + \Big[ H(p_\sigma(t)) - E_\sigma(p_\sigma(t)) \Big] f^1_{\sigma,inner}(y_\sigma, z, t, s) \Bigg\} \Bigg|_{y_\sigma = \frac{x-q_\sigma(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}, s=\frac{t-t^*}{\epsilon^{1/2}}} . \end{aligned} \tag{3.5.18}$$

**Proposition 3.5.2.** *Substituting the expression* (3.5.17) *for* $f^0_{\sigma,inner}(y_\sigma, z, t, s)$ *into* (3.5.18) *yields the following equivalent expression for* (3.5.18)*:*

$$\begin{aligned} & \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\left\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon} \Bigg\{ \Big[ H(p_\sigma(t)) - E_\sigma(p_\sigma(t)) \Big] \Big( f^1_{\sigma,inner}(y_\sigma, z, t, s) \\ & - (-i\partial_{y_\sigma}) a^0_{\sigma,inner}(y_\sigma, t, s) \partial_{p_\sigma} \chi_\sigma(z; p_\sigma(t)) \Big) - i\partial_s a^0_{\sigma,inner}(y_\sigma, s) \chi_\sigma(z; p_\sigma(t)) \Bigg\} \Bigg|_{y_\sigma = \frac{x-q_\sigma(t)}{\epsilon^{1/2}}, z=\frac{x}{\epsilon}, s=\frac{t-t^*}{\epsilon^{1/2}}} . \end{aligned} \tag{3.5.19}$$

*Proof.* Differentiating the eigenvalue problem (3.2.3) satisfied by $(E_\sigma, \chi_\sigma)$ with respect to $p$, we obtain the following pair of identities for $\sigma = \pm$:

$$\begin{aligned} & (p_\sigma(t) - i\partial_z - \partial_{p_\sigma} E_\sigma(p_\sigma(t)))\, \chi_\sigma(z; p_\sigma(t)) \\ & = -\,(H(p_\sigma(t)) - E_\sigma(p_\sigma(t)))\, \partial_p \chi_\sigma(z; p_\sigma(t)). \end{aligned} \tag{3.5.20}$$

Relation (3.5.19) now follows from substituting (3.5.17) into (3.5.18) and using (3.5.20). □

We may therefore set the expression in (3.5.18) equal to zero by setting each term in the sum individually to zero. To do this, we first take:

$$\partial_s a^0_{\sigma,inner}(y_\sigma, t, s) = 0, \qquad \sigma = \pm \quad . \tag{3.5.21}$$

We then require, for $\sigma \in \pm$, that $f^1_{\sigma,inner}(y_\sigma, z, t, s)$ satisfy:

$$\Big[ H(p_\sigma(t)) - E_\sigma(p_\sigma(t)) \Big] \Big( f^1_{\sigma,inner}(y_\sigma, z, t, s) - (-i\partial_{y_\sigma}) a^0_{\sigma,inner}(y_\sigma, t, s) \partial_{p_\sigma} \chi_\sigma(z; p_\sigma(t)) \Big) = 0 \tag{3.5.22}$$

Therefore, for $\sigma = \pm$,

$$f^1_{\sigma,inner}(y_\sigma, z, t, s) = a^1_{\sigma,inner}(y_\sigma, t, s)\chi_\sigma(z; p_\sigma(t)) + (-i\partial_{y_\sigma})a^0_{\sigma,inner}(y_\sigma, t)\partial_p\chi_\sigma(z; p_\sigma(t)), \quad (3.5.23)$$

where the functions $a^1_{\sigma,inner}(y_\sigma, t, s)$ are thus far arbitrary and to be determined.

#### 3.5.1.3 Terms in $r^\epsilon_{inner}$ with $L^2_x$ norm of order $\epsilon^1$

The terms in $r^\epsilon_{inner}$ with $L^2_x$ norm proportional to $\epsilon^1$ in (3.5.15) are of the form: $\epsilon$ times the following expression which is $O_{L^2}(1)$:

$$\begin{aligned} r^\epsilon_{inner,2}(x,t) = \epsilon^{-1/4} \sum_{\sigma=\pm} e^{i\left\{S_\sigma(t) + \epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon} \Bigg\{ \\ + \left[\frac{1}{2}(-i\partial_{y_\sigma})^2 + \frac{1}{2}\partial_x^2 W(q_\sigma(t))y_\sigma^2 - i\partial_t\right] f^0_{\sigma,inner}(y_\sigma, z, t, s) \\ + \left[\Big(p_\sigma(t) - i\partial_z - \partial_p E_\sigma(p_\sigma(t))\Big)(-i\partial_{y_\sigma}) - i\partial_s\right] f^1_{\sigma,inner}(y_\sigma, z, t, s) \\ + \Big[H(p_\sigma(t)) - E_\sigma(p_\sigma(t))\Big] f^2_{\sigma,inner}(y_\sigma, z, t, s)\Bigg\}\Bigg|_{y_\sigma = \frac{x - q_\sigma(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}, s = \frac{t-t^*}{\epsilon^{1/2}}}. \end{aligned} \quad (3.5.24)$$

Recall (Proposition 3.5.1, (P2)) that we must choose the $f^j_{\sigma,inner}$ in (3.5.15) such that:

$$\frac{1}{\epsilon}\int_{t^*-\epsilon^{\xi'}}^{t^*+\epsilon^{\xi'}} \|r^\epsilon_{inner}(\cdot, t')\|_{L^2}\,\mathrm{d}t' = o(\epsilon^{1/2}). \quad (3.5.25)$$

It follows that we need to choose the undetermined functions so that $r^\epsilon_{inner,2}(x,t)$ in (3.5.24) satisfies:

$$\int_{t^*-\epsilon^{\xi}}^{t^*+\epsilon^{\xi'}} \|r^\epsilon_{inner,2}(\cdot, t)\|_{L^2} = o(\epsilon^{1/2}). \quad (3.5.26)$$

In contrast to considerations at previous orders in $\epsilon^{1/2}$, we will not be able to satisfy (3.5.26) by choosing each summand of (3.5.24) to satisfy the smallness condition (3.5.26). To see this and to see how to proceed, we first simplify the expression (3.5.24) using the expressions for $f^0_{\sigma,inner}(y_\sigma, z, t, s)$ (3.5.17) and $f^1_{\sigma,inner}(y_\sigma, z, t, s)$ (3.5.23) derived above.

**Proposition 3.5.3.** *The expression* (3.5.24) *may be written in the following form:*

$$\begin{aligned}
&r^{\epsilon}_{inner,2}(x,t)\\
&= \epsilon^{-1/4}\sum_{\sigma=\pm} e^{i\left\{S_\sigma(t)+\epsilon^{1/2}p_\sigma(t)y_\sigma\right\}/\epsilon}\Bigg\{\Big[H(p_\sigma(t))-E_\sigma(p_\sigma(t))\Big]\Big(f^2_{\sigma,inner}(y_\sigma,z,t,s)\\
&-(-i\partial_{y_\sigma})a^1_{\sigma,inner}(y_\sigma,t,s)\partial_{p_\sigma}\chi_\sigma(z;p_\sigma(t))-\frac{1}{2}(-i\partial_{y_\sigma})^2 a^0_{\sigma,inner}(y_\sigma,t)\partial^2_{p_\sigma}\chi_\sigma(z;p_\sigma(t))\Big)\\
&-i\partial_s a^1_{\sigma,inner}(y_\sigma,t,s)\chi_\sigma(z;p_\sigma(t))-[\ i\partial_t-\ \mathscr{H}_\sigma(t)\ ]\ a^0_{\sigma,inner}(y_\sigma,t)\chi_\sigma(z;p_\sigma(t))\\
&+i\partial_{q_\sigma}W(q_\sigma(t))a^0_{\sigma,inner}(y_\sigma,t,s)\left\langle\chi_{-\sigma}(\cdot;p_\sigma(t))\right|\left.\partial_{p_\sigma}\chi_\sigma(\cdot;p_\sigma(t))\right\rangle\chi_{-\sigma}(z;p_\sigma(t))\\
&+i\partial_{q_\sigma}W(q_\sigma(t))a^0_{\sigma,inner}(y_\sigma,t,s)P^\perp_\pm(p_\sigma(t))\partial_{p_\sigma}\chi_\sigma(z;p_\sigma(t))\Bigg\}\Bigg|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon},s=\frac{t-t^*}{\epsilon^{1/2}}}.
\end{aligned}\tag{3.5.27}$$

*Here, we recall that* $H(p)=-\frac{1}{2}(p-i\partial_z)^2+V(z)$ *and* $\mathscr{H}_\sigma(t)$ *denotes the time-dependent harmonic oscillator Hamiltonian defined in* (3.2.14)*, where we replace* $p(t),q(t),E_n,\chi_n,y$*, respectively, by* $p_\sigma(t),q_\sigma(t),E_\sigma,\chi_\sigma,y_\sigma$*. Finally,* $P^\perp_\pm(p_\sigma(t))$ *denotes the orthogonal projection operator given by:*

$$P^\perp_\pm(p_\sigma(t))f(z):=f(z)-\sum_{\sigma'=\pm}\left\langle\chi_{\sigma'}(\cdot;p_\sigma(t))\right|\left.f(\cdot)\right\rangle\chi_{\sigma'}(z;p_\sigma(t)).\tag{3.5.28}$$

*Proof.* We begin with the identity, obtained by differentiating the eigenvalue problem (3.2.3), satisfied by the eigenpair $(E_\sigma,\chi_\sigma)$, *twice* with respect to $p$:

$$\begin{aligned}
&\frac{1}{2}\left(1-\partial_p^2E_\sigma(p_\sigma(t))\right)\chi_\sigma(z;p_\sigma(t))+\left(p_\sigma(t)-i\partial_z-\partial_{p_\sigma}E_\sigma(p_\sigma(t))\right)\partial_{p_\sigma}\chi_\sigma(z;p_\sigma(t))\\
&=-\frac{1}{2}\left(H(p_\sigma(t))-E_\sigma(p_\sigma(t))\right)\partial^2_{p_\sigma}\chi_\sigma(z;p_\sigma(t)),\qquad \sigma=\pm\ .
\end{aligned}\tag{3.5.29}$$

To obtain the expression (3.5.27), we first substitute expression (3.5.17) for $f^0_{\sigma,inner}$ and expression (3.5.23) for $f^1_{\sigma,inner}$ into (3.5.24). We then simplify using the identity (3.5.29) and the expansion of $\partial_{p_\sigma}\chi_\sigma(z;p_\sigma(t))$ in terms of its orthogonal components:

$$\begin{aligned}
&\partial_p\chi_\sigma(z;p_\sigma(t))=\\
&\sum_{\sigma'=\pm}\left\langle\chi_{\sigma'}(\cdot;p_\sigma(t))\right|\left.\partial_p\chi_\sigma(\cdot;p_\sigma(t))\right\rangle\chi_{\sigma'}(z;p_\sigma(t))+P^\perp_\pm(p_\sigma(t))\chi_\sigma(z;p_\sigma(t)).
\end{aligned}\tag{3.5.30}$$

□

By Proposition 3.5.3 the smallness condition (3.5.26) may be studied with the expression (3.5.27) in place of (3.5.24). We proceed in two steps.

(A) We first use certain degrees of freedom to eliminate 'in-band' contributions to (3.5.27).

(B) We will then be left with contributions which relate to the coupling of bands revealed in analysis of the breakdown of the single-band approximation.

*Step A:* We first choose $a^0_{\sigma,inner}(y_\sigma, t)$ so that:

$$i\partial_t a^0_{\sigma,inner}(y_\sigma, t) = \mathscr{H}_\sigma(t) a^0_{\sigma,inner}(y_\sigma, t), \qquad \sigma = \pm \ . \tag{3.5.31}$$

We also require that $z \mapsto f^2_{\sigma,inner}(y_\sigma, z, t, s)$ be a 1− periodic solution of:

$$\begin{aligned}&\Big[H(p_\sigma(t)) - E_\sigma(p_\sigma(t))\Big] \Big( f^2_{\sigma,inner}(y_\sigma, z, t, s) \\ &-(-i\partial_{y_\sigma}) a^1_{\sigma,inner}(y_\sigma, t, s)\partial_{p_\sigma}\chi_\sigma(z; p_\sigma(t)) - \frac{1}{2}(-i\partial_{y_\sigma})^2 a^0_{\sigma,inner}(y_\sigma, t)\partial^2_{p_\sigma}\chi_\sigma(z; p_\sigma(t))\Big) \\ &= -i\partial_{q_\sigma} W(q_\sigma(t)) a^0_{\sigma,inner}(y_\sigma, t, s) P^\perp_\pm(p_\sigma(t))\partial_{p_\sigma}\chi_\sigma(z; p_\sigma(t)) \ .\end{aligned} \tag{3.5.32}$$

Equation (3.5.32) is solvable, with a uniform bound in time on the inverse, for all $t$ near $t^*$ by Corollary 3.3.1. Hence we have for $\sigma = \pm$:

$$\begin{aligned}&f^2_{\sigma,inner}(y_\sigma, z, t, s) = a^2_{\sigma,inner}(y_\sigma, t, s)\chi_\sigma(z; p_\sigma(t)) \\ &+ (-i\partial_{y_\sigma}) a^1_{\sigma,inner}(y_\sigma, s, t)\partial_p\chi_\sigma(z; p_\sigma(t)) + \frac{1}{2}(-i\partial_{y_\sigma})^2 a^0_{\sigma,inner}(y_\sigma, t)\partial^2_p\chi_\sigma(z; p_\sigma(t)) \\ &- i\partial_q W(q_\sigma(t))\mathcal{R}_\sigma(p_\sigma(t)) P^\perp_\pm(p_\sigma(t))\partial_p\chi_\sigma(z; p_\sigma(t)).\end{aligned} \tag{3.5.33}$$

Here, $a^2_{\sigma,inner}(y_\sigma, t, s)$ is presently arbitrary and can be determined at higher order in $\epsilon^{1/2}$.

The initial data for equations (3.5.31) is fixed by the requirement that $\psi^\epsilon_{app,inner}$ satisfy (P1) of Proposition 3.5.1. By inspection of the incoming solution, we see that this is equivalent to requiring that:

$$\text{for } t \in (t^* - \epsilon^{\xi'}, t^* - \epsilon^{\xi}) : \ a^0_{+,inner}(y, t) = a^0_+(y, t) \text{ and } a_{-,inner}(y, t) = 0. \tag{3.5.34}$$

The only choice of initial data $a^0_{+,inner}(y, t^*)$, $a^0_{-,inner}(y, t^*)$ for (3.5.31) consistent with (3.5.34) are:

$$a^0_{+,inner}(y, t^*) = \lim_{t \uparrow t^*} a^0_+(y, t) \equiv a^{0,*}(y), \quad a^0_{-,inner}(y, t^*) = 0 \ .$$

Indeed, for all $t \in (t^* - \epsilon^{\xi'}, t^* + \epsilon^{\xi'})$:

$$a^0_{+,inner}(y_+, t) = a_+(y_+, t), \text{ and } a^0_{-,inner}(y_-, t) = 0. \tag{3.5.35}$$

The choices (3.5.31), (3.5.33), and (3.5.35) simplify (3.5.27) to:

$$r^{\epsilon}_{inner,2}(x,t) = \epsilon^{-1/4} e^{i\left\{S_+(t)+\epsilon^{1/2}p_+(t)y_+\right\}/\epsilon} \Big\{ -i\partial_s a^1_{+,inner}(y_+,t,s)\chi_+(z;p_+(t))$$
$$+i\partial_{q_+}W(q_+(t))a^0_{+,inner}(y_+,t,s)\left\langle \chi_-(\cdot;p_+(t))\right| \partial_{p_+}\chi_+(\cdot;p_+(t))\big\rangle \chi_-(z;p_+(t))\Big\} \tag{3.5.36}$$
$$\epsilon^{-1/4} e^{i\left\{S_-(t)+\epsilon^{1/2}p_-(t)y_-\right\}/\epsilon} \Big\{ -i\partial_s a^1_{-,inner}(y_-,t,s)\chi_-(z;p_-(t))\Big\}\Big|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon},s=\frac{t-t^*}{\epsilon^{1/2}}}.$$

We find that at this order in $\epsilon^{1/2}$ that there is no loss in taking

$$a^1_{+,inner}(y_+,t,s) = a^1_{+,inner}(y_+,s), \qquad a^1_{-,inner}(y_-,t,s) = a^1_{-,inner}(y_+,s),$$

independent of $t$. From (3.5.36) it is natural to set

$$\begin{aligned} &\partial_s a^1_{+,inner}(y_+,t,s) = 0 \\ &a^1_{+,inner}(y_+,0) = a^1_{+,inner,0}(y_+). \end{aligned} \tag{3.5.37}$$

and to choose $a^1_{-,inner}(y_+,s)$ to eliminate the projection of $r^{\epsilon}_{inner,2}(x,t)$ onto the vector $\chi_-(z;p_+(t))$.

The function $a^1_{+,inner,0}(y_+)$ is at this point arbitrary, it will be fixed below by enforcing (P1) of Proposition 3.5.1. Taking $a^1_{+,inner}(y_+,s)$ to satisfy (3.5.37) reduces (3.5.36) to the following:

$$r^{\epsilon}_{inner,2}(x,t) = \epsilon^{-1/4} e^{i\left\{S_+(t)+\epsilon^{1/2}p_+(t)y_+\right\}/\epsilon} \Big[$$
$$i\partial_q W(q_+(t))a_+(y_+,t)\left\langle \chi_-(\cdot;p_+(t))\right| \partial_p\chi_+(\cdot;p_+(t))\rangle \chi_-(z;p_+(t))] \tag{3.5.38}$$
$$+\epsilon^{-1/4} e^{i\left\{S_-(t)+\epsilon^{1/2}p_-(t)y_-\right\}/\epsilon} \left[-i\partial_s a^1_{-,inner}(y_-,s)\chi_-(z;p_-(t))\right]\Big|_{y_\sigma=\frac{x-q_\sigma(t)}{\epsilon^{1/2}},z=\frac{x}{\epsilon},s=\frac{t-t^*}{\epsilon^{1/2}}}.$$

We next determine the evolution of $a^1_{-,inner}(y_-,s)$ to satisfy the smallness condition (3.5.26). We find it useful at this point to re-express functions of $t$ and $y_+$ in terms of the variables $y_-$ and $s$ using the relations:

$$y_+ = y_- + \frac{q_-(t)-q_+(t)}{\epsilon^{1/2}}, \qquad t = t^* + \epsilon^{1/2}s. \tag{3.5.39}$$

This yields:

$$\begin{aligned}
&r^{\epsilon}_{inner,2}(x,t^*+\epsilon^{1/2}s)\\
&= \epsilon^{-1/4}e^{i\left\{S_+(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_+(t^*+\epsilon^{1/2}s)y_-+p_+(t^*+\epsilon^{1/2}s)(q_-(t^*+\epsilon^{1/2}s)-q_+(t^*+\epsilon^{1/2}s))\right\}/\epsilon}\Bigg[\\
&i\partial_q W(q_+(t^*+\epsilon^{1/2}s))a_+\left(y_-+\frac{q_-(t^*+\epsilon^{1/2}s)-q_+(t^*+\epsilon^{1/2}s)}{\epsilon^{1/2}},t^*+\epsilon^{1/2}s\right)\\
&\times\left\langle \chi_-(\cdot;p_+(t^*+\epsilon^{1/2}s))\middle|\,\partial_p\chi_+(\cdot;p_+(t^*+\epsilon^{1/2}s))\right\rangle\chi_-(z;p_+(t^*+\epsilon^{1/2}s))\Bigg]\\
&+\epsilon^{-1/4}e^{i\left\{S_-(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_-(t^*+\epsilon^{1/2}s)y_-\right\}/\epsilon}\Bigg[\\
&-i\partial_s a^1_{-,inner}(y_-,s)\chi_-(z;p_-(t^*+\epsilon^{1/2}s))\Bigg]\Bigg|_{y_-=\frac{x-q_-(t^*+\epsilon^{1/2}s)}{\epsilon^{1/2}},z=\frac{x}{\epsilon}}.
\end{aligned}\tag{3.5.40}$$

In terms of $s$, the condition (3.5.26) reads:

$$\int_{-\epsilon^{\xi'-1/2}}^{\epsilon^{\xi'-1/2}}\|r^{\epsilon}_{inner,2}(\cdot,t^*+\epsilon^{1/2}s)\|_{L^2}=o(1).\tag{3.5.41}$$

We proceed with the construction of $a^1_{-,inner}(y_-,s)$ by seeking the expression in $r^{\epsilon}_{inner,2}(x,t^*+\epsilon^{1/2}s)$ which, to leading order, will be balanced (indeed cancelled out by) the term proportional to $\partial_s a^1_{-,inner}(y_-,s)$, for $-\epsilon^{\xi'-1/2}<s<\epsilon^{\xi'-1/2}$ $(0<\xi'<1/2)$.

Thus we expand the expression for $r^{\epsilon}_{inner,2}(x,t^*+\epsilon^{1/2}s)$ in powers of $\epsilon^{1/2}s$, making use of the equations governing $(q_\pm(t),p_\pm(t))$ and $S_\pm(t)$ (3.3.16), (3.3.35), Definitions 3.3.1 and 3.3.2 to compute their derivatives. We first Taylor-expand the expression within square brackets in (3.5.40):

$$\begin{aligned}
&r^{\epsilon}_{inner,2}(x,t^*+\epsilon^{1/2}s)\\
&= \epsilon^{-1/4}e^{i\left\{S_+(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_+(t^*+\epsilon^{1/2}s)y_-+p_+(t^*+\epsilon^{1/2}s)(q_-(t^*+\epsilon^{1/2}s)-q_+(t^*+\epsilon^{1/2}s))\right\}/\epsilon}\Bigg[\\
&i\partial_q W(q^*)\ a_+\left(y_-+[\partial_p E_-(p^*)-\partial_p E_+(p^*)]s,t^*\right)\ \left\langle\chi_-(\cdot;p^*)\right|\partial_p\chi_+(\cdot;p^*)\rangle\,\chi_-(z;p^*)\Bigg]\\
&+\epsilon^{-1/4}e^{i\left\{S_-(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_-(t^*+\epsilon^{1/2}s)y_-\right\}/\epsilon}\left[-i\partial_s a^1_{-,inner}(y_-,s)\chi_-(z;p^*)\right]\Bigg|_{y_-=\frac{x-q_-(t^*+\epsilon^{1/2}s)}{\epsilon^{1/2}},z=\frac{x}{\epsilon}}\\
&+O_{L^2_x}(\epsilon^{1/2}s,\epsilon^{1/2}s^2).
\end{aligned}\tag{3.5.42}$$

Rearranging terms, we obtain:

$$
\begin{aligned}
& r^{\epsilon}_{inner,2}(x, t^* + \epsilon^{1/2} s) \\
&= \epsilon^{-1/4} e^{i\left\{S_-(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_-(t^*+\epsilon^{1/2}s)y_-\right\}/\epsilon} i\chi_-(z;p^*)\times \\
& \Big\{ e^{i\left\{S_+(t^*+\epsilon^{1/2}s)-S_-(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}(p_+(t^*+\epsilon^{1/2}s)-p_-(t^*+\epsilon^{1/2}s))y_-+p_+(t^*+\epsilon^{1/2}s)(q_-(t^*+\epsilon^{1/2}s)-q_+(t^*+\epsilon^{1/2}s))\right\}/\epsilon} \\
& \times \left[\partial_q W(q^*)\ a_+\left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s, t^*\right)\ \langle \chi_-(\cdot;p^*) |\, \partial_p \chi_+(\cdot;p^*)\rangle\right] \\
& -\partial_s a^1_{-,inner}(y_-, s) \Big\} \Bigg|_{y_- = \frac{x - q_-(t^*+\epsilon^{1/2}s)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} \\
& + O_{L^2_x}(\epsilon^{1/2} s, \epsilon^{1/2} s^2).
\end{aligned}
\tag{3.5.43}
$$

We next Taylor-expand the exponential:

$$
\begin{aligned}
& S_+(t^* + \epsilon^{1/2} s) - S_-(t^* + \epsilon^{1/2} s) \\
& = (\epsilon^{1/2} s) p^* (\partial_p E_+(p^*) - \partial_p E_-(p^*)) \\
& + \frac{1}{2}(\epsilon^{1/2} s)^2 \left(\partial_q W(q^*) p^* (\partial_p^2 E_-(p^*) - \partial_p^2 E_+(p^*)) + \partial_q W(q^*)(\partial_p E_-(p^*) - \partial_p E_+(p^*))\right) \\
& + O(\epsilon^{3/2} s^3) \\
& \epsilon^{1/2}(p_+(t^* + \epsilon^{1/2} s) - p_-(t^* + \epsilon^{1/2} s)) y_- \\
& = O(\epsilon^{3/2} s^2 y_-) \\
& p_+(t^* + \epsilon^{1/2} s)(q_-(t^* + \epsilon^{1/2} s) - q_+(t^* + \epsilon^{1/2} s)) \\
& = (\epsilon^{1/2} s)(p^*(\partial_p E_-(p^*) - \partial_p E_+(p^*))) \\
& + \frac{1}{2}(\epsilon^{1/2} s)^2 \left(-2\partial_q W(q^*)(\partial_p E_-(p^*) - \partial_p E_+(p^*)) + \partial_q W(q^*) p^* (\partial_p^2 E_+(p^*) - \partial_p^2 E_-(p^*))\right) \\
& + O(\epsilon^{3/2} s^3).
\end{aligned}
\tag{3.5.44}
$$

Substituting these expressions and using the fact that $a_+(y,t) \in \mathcal{S}(\mathbb{R})$ gives:

$$
\begin{aligned}
r^{\epsilon}_{inner,2}(x, t^* + \epsilon^{1/2} s) &= \epsilon^{-1/4} e^{i\left\{S_-(t^*+\epsilon^{1/2}s)+\epsilon^{1/2}p_-(t^*+\epsilon^{1/2}s)y_-\right\}/\epsilon} i\chi_-(z;p^*) \\
& \times \Big\{ e^{i\frac{1}{2}\partial_q W(q^*)(\partial_p E_+(p^*) - \partial_p E_-(p^*)) s^2} \\
& \times \Big[ \partial_q W(q^*)\ \langle \chi_-(\cdot;p^*) |\, \partial_p \chi_+(\cdot;p^*)\rangle\ a_+\left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s, t^*\right) \Big] \\
& -\partial_s a^1_{-,inner}(y_-, s) \Big\}\ + O_{L^2_x}(\epsilon^{1/2} s, \epsilon^{1/2} s^2, \epsilon^{1/2} s^3) \Big|_{y_- = \frac{x - q_-(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}, s = \frac{t - t^*}{\epsilon^{1/2}}}.
\end{aligned}
\tag{3.5.45}
$$

It follows that by taking $a^1_{-,inner}(y_-, s)$ to satisfy:

$$\begin{aligned} &\partial_s a^1_{-,inner}(y_-, s) = e^{i\frac{1}{2}\partial_q W(q^*)(\partial_p E_+(p^*) - \partial_p E_-(p^*))s^2} \\ &\times \partial_q W(q^*) a_+ \left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s, t^*\right) \langle \chi_-(\cdot; p^*) | \, \partial_p \chi_+(\cdot; p^*) \rangle \\ &a^1_{-,inner}(y_-, 0) = a^1_{-,inner,0}(y_-). \end{aligned} \tag{3.5.46}$$

We have that $\psi^\epsilon_{app,inner}(x,t)$ satisfies (3.5.41), and therefore (P2) of Proposition 3.5.1, provided $3/8 < \xi' < 1/2$. That is, for $3/8 < \xi' < 1/2$, we have

$$\int_{-\epsilon^{\xi'-1/2}}^{\epsilon^{\xi'-1/2}} \|O_{L^2_x}(\epsilon^{1/2}s, \epsilon^{1/2}s^2, \epsilon^{1/2}s^3)\|_{L^2_x} \, \mathrm{d}s = O(\epsilon^{2\xi'-1/2}, \epsilon^{3\xi'-1}, \epsilon^{4\xi-3/2}) \;=\; o(1) \;. \tag{3.5.47}$$

The initial data choices $a^1_{+,inner,0}(y_+)$ and $a^1_{-,inner,0}(y_-)$ are forced by the requirement that $\psi^\epsilon_{app,inner}(x,t)$ satisfies the matching condition (P1) of Proposition 3.5.1. Since these terms appear at order $\epsilon^{1/2}$ in the asymptotic expansion, for (P1) to hold it is sufficient that for $s \in (-\epsilon^{\xi'-1/2}, t^* - \epsilon^{\xi-1/2})$: $a^1_{+,inner}(y_+, s) - a^1_+(y_+, t^* + \epsilon^{1/2}s) = o_{L^2_{y_+}}(1)$ and $a^1_{-,inner}(y_-, s) = o_{L^2_{y_-}}(1)$.

We claim that we may ensure this by taking:

$$a^1_{+,inner,0}(y_+) = a^1_+(y_+, 0) = a^{1,*}(y_+), \tag{3.5.48}$$

and

$$\begin{aligned} &a^1_{-,inner,0}(y_-) = \;\; \partial_q W(q^*) \times \langle \chi_-(\cdot; p^*) | \, \partial_p \chi_+(\cdot; p^*) \rangle \\ &\times \int_{-\infty}^0 e^{i\frac{1}{2}\partial_q W(q^*)(\partial_p E_+(p^*) - \partial_p E_-(p^*))(s')^2} a_+ \left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s', t^*\right) \mathrm{d}s'. \end{aligned} \tag{3.5.49}$$

This claim follows from Taylor-expansion:

$$\begin{aligned} &\text{for all } s \in (-\epsilon^{\xi'-1/2}, t^* - \epsilon^{\xi-1/2}) : \\ &a^1_+(y_+, t^* + \epsilon^{1/2}s) - a^1_+(y_+, t^*) = O_{L^2_{y_+}}(\epsilon^{1/2}s) = O_{L^2_{y_+}}(\epsilon^{\xi'}) = o_{L^2_{y_+}}(1) \end{aligned} \tag{3.5.50}$$

since $3/8 < \xi' < 1/2$ and from integration by parts, which shows that for $s \in (-\epsilon^{\xi'-1/2}, -\epsilon^{\xi-1/2})$:

$$\begin{aligned} &a^1_{-,inner}(y_-, s) = \int_{-\infty}^s e^{i\frac{1}{2}\partial_q W(q^*)(\partial_p E_+(p^*) - \partial_p E_-(p^*))(s')^2} \\ &\times \partial_q W(q^*) a_+ \left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s', t^*\right) \langle \chi_-(\cdot; p^*) | \, \partial_p \chi_+(\cdot; p^*) \rangle \, \mathrm{d}s' \\ &= O_{L^2_{y_-}}(\epsilon^{1/2-\xi}). \end{aligned} \tag{3.5.51}$$

Since $\xi < 1/2$ by assumption, we are done.

It remains to show (P3) of Proposition 3.5.1. But by an identical argument,

$$\begin{aligned}&\text{for } s \in (\epsilon^{\xi-1/2}, \epsilon^{\xi'-1/2}):\\ &a^1_{-,inner}(y_-, s) = \partial_q W(q^*) \langle \chi_-(\cdot; p^*)| \partial_p \chi_+(\cdot; p^*)\rangle \times\\ &\int_{-\infty}^{\infty} e^{i\frac{1}{2}\partial_q W(q^*)(\partial_p E_+(p^*) - \partial_p E_-(p^*))(s')^2}\ a_+\left(y_- + [\partial_p E_-(p^*) - \partial_p E_+(p^*)]s', t^*\right) \mathrm{d}s'\\ &+ O(\epsilon^{\xi'-1/2}),\end{aligned} \tag{3.5.52}$$

so that for $\sigma = \pm$:

$$a^1_{\sigma,inner}(y_\sigma, t^* + \epsilon^{1/2} s) - a^1_\sigma(y_\sigma, t^*) = O_{L^2_{y_\sigma}}(\epsilon^{\xi'}) = o_{L^2_{y_\sigma}}(1) \tag{3.5.53}$$

for $t - t^* = \epsilon^{1/2} s \in (\epsilon^{\xi}, \epsilon^{\xi'})$. It follows that $\psi^\epsilon_{app,inner}(x,t)$ so constructed satisfies all hypotheses of Proposition 3.5.1, and so the proof of Theorem 3.3.3 is complete.

# Chapter 4

# Bound states of a periodic operator with multiple well-separated domain wall modulations

*The research described in this chapter is joint with J. Lu and M. I. Weinstein.*

## 4.1 Introduction

In this work we consider the eigenvalue problem:

$$\begin{aligned} &\mathcal{D}_{\kappa_L}\alpha = E\alpha \\ &\alpha : \mathbb{R} \to \mathcal{H} \end{aligned} \tag{4.1.1}$$

where $\mathcal{H}$ is the Hilbert space:

$$\begin{aligned} &\mathcal{H} := \left\{ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} : \text{for } j \in \{1,2\}, f_j \in L^2(\mathbb{R}) \right\} \\ &\langle f | g \rangle_{\mathcal{H}} := \sum_{j=1,2} \langle f_j | g_j \rangle_{L^2(\mathbb{R})} \end{aligned} \tag{4.1.2}$$

and $\mathcal{D}_{\kappa_L}$ is a Dirac operator with a potential $\kappa_L$ depending on a parameter $L$:

$$\mathcal{D}_{\kappa_L} := i\partial_x\sigma_3 + \kappa_L(x)\sigma_1. \tag{4.1.3}$$

Here $\sigma_1, \sigma_3$ denote the usual Pauli matrices:

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.1.4}$$

We assume $L > 1$ and let $\kappa_\infty$ denote a fixed positive constant. We define $\kappa_L$ to be the '2 domain wall' potential function (see Figure 4.1):

$$\kappa_L(x) = \begin{cases} -\kappa(x+L) & \text{for } -\infty \leq x \leq 0 \\ \kappa(x-L) & \text{for } 0 \leq x \leq \infty \end{cases} \tag{4.1.5}$$

where $\kappa$ denotes a 'domain wall' potential function which we assume to be *smooth*, *monotone increasing*, *odd*, and to satisfy:

$$\kappa(x) = \begin{cases} -\kappa_\infty & \text{if } x \leq -1 \\ \kappa_\infty & \text{if } x \geq 1 \end{cases} \tag{4.1.6}$$

where $\kappa_\infty > 0$ is a positive constant. Note that the condition that $L > 1$ ensures that $\kappa_L$ is smooth for all $x \in \mathbb{R}$. Our study of the problem (4.1.1) is motivated by recent works of Fefferman, Lee-Thorp and Weinstein [26; 25; 27] which showed that Dirac operators of the form (4.1.3) control the bifurcation of 'edge states' of periodic Schrödinger operators modulated by domain walls. It follows from their analysis that the Dirac operator (4.1.3) with the 'double' domain wall potential (4.1.5) controls the bifurcation of 'edge states' of periodic Schrödinger operators perturbed *twice* by domain wall modulations. Our analysis may be readily extended to the case of Schrödinger operators modulated $n$ times by domain walls (see Remark 4.3).

### 4.1.1 Notation

In what follows, we will make use of the following short-hand notations. For the norm induced by the $\mathcal{H}$-inner product, we will write:

$$\|f\|_{\mathcal{H}} := \langle f | f \rangle_{\mathcal{H}}^{1/2}. \tag{4.1.7}$$

For complex vectors $v, w$ in $\mathbb{C}^2$, we will write their inner product and the norm induced by this inner product as:

$$\langle v | w \rangle_{\mathbb{C}^2} := \sum_{j=1,2} \overline{v_j} w_j, \quad |v|_{\mathbb{C}^2} := \langle v | v \rangle_{\mathbb{C}^2}^{1/2}. \tag{4.1.8}$$

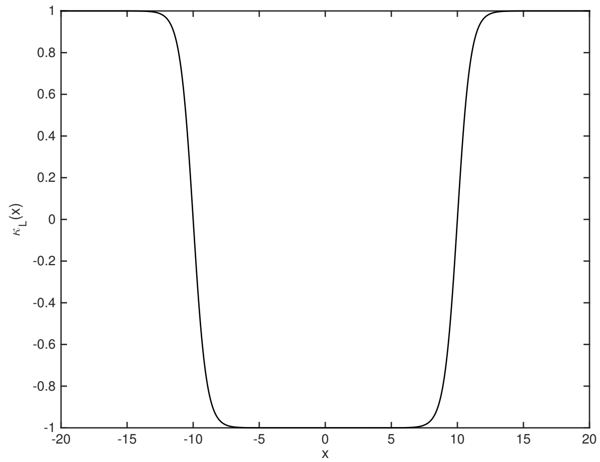



Figure 4.1: $\kappa_L(x)$ with $\kappa(x) = \tanh(x)$, $L = 10$. Note that $\tanh(x)$ doesn't strictly satisfy (4.1.6) but gives a good approximation to a function satisfying those conditions.

With this notation in hand, a short manipulation of the definition of the $\mathcal{H}$-inner product shows that:

$$\langle f | g \rangle_{\mathcal{H}} = \int_{\mathbb{R}} \langle f(x) | g(x) \rangle_{\mathbb{C}^2} \, \mathrm{d}x, \quad \|f\|_{\mathcal{H}}^2 = \int_{\mathbb{R}} |f(x)|_{\mathbb{C}^2}^2 \, \mathrm{d}x. \tag{4.1.9}$$

## 4.2 Statement of theorem

In order to state our theorem we first require some background on the case of a single domain wall potential:

### 4.2.1 The single domain wall operator

Let $\mathcal{D}_\kappa$ denote the Dirac operator with potential $\kappa(x)$ which is independent of $L$:

$$\mathcal{D}_\kappa := i\partial_x \sigma_3 + \kappa(x)\sigma_1. \tag{4.2.1}$$

The following properties are immediate:

- The operator $\mathcal{D}_\kappa$ has continuous spectrum $(-\infty, -\kappa_\infty] \cup [\kappa_\infty, \infty)$

- The operator $\mathcal{D}_\kappa$ has a zero mode: an eigenfunction $\alpha_\star$ with eigenvalue 0, given explicitly by:

$$\alpha_\star(x) := \gamma \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\int_0^x \kappa(y)\,\mathrm{d}y}, \tag{4.2.2}$$

where:

$$\gamma := \frac{1}{\sqrt{2}\|e^{-\int_0^x \kappa(y)\,\mathrm{d}y}\|_{L^2}} \tag{4.2.3}$$

ensures that $\|\alpha_\star\|_{\mathcal{H}} = 1$. It is clear from (4.1.6) that there exist constants $C > 0$ depending only on $\kappa$ such that:

$$|\alpha_\star(x)|_{\mathbb{C}^2} \leq C e^{-\kappa_\infty |x|}, \quad |\partial_x \alpha_\star(x)|_{\mathbb{C}^2} \leq C e^{-\kappa_\infty |x|}. \tag{4.2.4}$$

We will require the following 'spectral gap' assumption on the operator $\mathcal{D}_\kappa$. This assumption may be significantly weakened; see Remark 4.2.1.

**Assumption 4.2.1.** *If $\langle \alpha_\star | f \rangle_{\mathcal{H}} = 0$, then:*

$$\|\mathcal{D}_\kappa f\|_{\mathcal{H}} \geq \kappa_\infty \|f\|_{\mathcal{H}}. \tag{4.2.5}$$

**Remark 4.2.1.** *Our methods extend to the case where the operator $\mathcal{D}_\kappa$ has additional spectrum in the interval $(-\kappa_\infty, \kappa_\infty)$. Any such spectrum must be bounded a fixed distance $\delta > 0$ away from zero since the 0-eigenvalue is simple. The proof of our assertions is then identical after replacing $\kappa_\infty$ everywhere it appears with $\delta$.*

As an immediate consequence of Assumption 4.2.1 we have the following Lemma:

**Lemma 4.2.1.** *Let Assumption 4.2.1 hold. Then, for $|E| < \frac{\kappa_\infty}{2}$:*

$$\|(\mathcal{D}_\kappa - E) f\|_{\mathcal{H}} \geq \frac{\kappa_\infty}{2} \|f\|_{\mathcal{H}}. \tag{4.2.6}$$

*Furthermore, $(\mathcal{D}_\kappa - E)$ is invertible on the space $P^\perp \mathcal{H}$ where $P^\perp$ denotes the orthogonal projection operator onto $\{\alpha_\star\}^\perp$, and:*

$$\|(\mathcal{D}_\kappa - E)^{-1} P^\perp\|_{\mathcal{H} \to \mathcal{H}} \leq \frac{2}{\kappa_\infty}. \tag{4.2.7}$$

### 4.2.2 Zero modes of 'shifted' one domain wall operators

Consider the 'shifted' one domain wall operators:

$$\mathcal{D}_\kappa^+ := i\partial_x\sigma_3 + \kappa(x-L)\sigma_1, \quad \mathcal{D}_\kappa^- := i\partial_x\sigma_3 - \kappa(x+L)\sigma_1. \tag{4.2.8}$$

Then we have the following on zero modes of the operators $\mathcal{D}_\kappa^\pm$:

**Lemma 4.2.2.** *Let:*

$$\alpha_\star^+(x) := \alpha_\star(x-L), \quad \alpha_\star^-(x) := \overline{\alpha_\star(x+L)}, \tag{4.2.9}$$

*then $\alpha_\star^+$ and $\alpha_\star^-$ are zero modes of $\mathcal{D}_\kappa^+$ and $\mathcal{D}_\kappa^-$ respectively.*

*Proof.*

$$\begin{aligned} & \left(\sigma_3 i\partial_x + \kappa(x)\sigma_1\right)\alpha_\star(x) = 0 \\ \implies & \left(\sigma_3 i\partial_x + \kappa(x-L)\sigma_1\right)\alpha_\star(x-L) = 0. && \text{(changing variables, } \partial_x = \partial_{x-L}) \end{aligned}$$

$$\begin{aligned} & \left(\sigma_3 i\partial_x + \kappa(x)\sigma_1\right)\alpha_\star(x) = 0 \\ \implies & \left(\sigma_3 i\partial_x + \kappa(x+L)\sigma_1\right)\alpha_\star(x+L) = 0 && \text{(changing variables, } \partial_x = \partial_{x+L}) \\ \implies & \left(-\sigma_3 i\partial_x - \kappa(x+L)\sigma_1\right)\alpha_\star(x+L) = 0 && \text{(multiply by } -1) \\ \implies & \left(\sigma_3 i\partial_x - \kappa(x+L)\sigma_1\right)\overline{\alpha_\star(x+L)} = 0. && \text{(complex conjugate, } \kappa \text{ real)} \end{aligned}$$

□

We are now in a position to state our theorem:

**Theorem 4.2.1.** *Let Assumption 4.2.1 hold. For sufficiently large $L$, the operator $\mathcal{D}_{\kappa_L}$ has a pair of near-zero eigenvalues $E_\pm$, which satisfy:*

$$E_\pm = \pm 2\gamma^2 e^{-2\int_0^L \kappa(y)\,dy} + O(e^{-4\kappa_\infty L}). \tag{4.2.10}$$

*Their associated (normalized) eigenfunctions, which we denote $\alpha_\pm(x)$, may be written as approximate linear combinations of $\alpha_\star^+(x), \alpha_\star^-(x)$:*

$$\begin{aligned} \alpha_+(x) &= \frac{\gamma}{\sqrt{2}}\left(\alpha_\star^+(x) - i\alpha_\star^-(x)\right) + O_{\mathcal{H}}(e^{-2\kappa_\infty L}) \\ \alpha_-(x) &= \frac{\gamma}{\sqrt{2}}\left(\alpha_\star^+(x) + i\alpha_\star^-(x)\right) + O_{\mathcal{H}}(e^{-2\kappa_\infty L}) \end{aligned} \tag{4.2.11}$$

*where the functions $\alpha_\star^\pm(x)$ are the shifted zero-mode functions defined by* (4.2.9) *and the real constant $\gamma$ is as in* (4.2.3).

Our result can be seen as complementary to those obtained by Barry Simon and others for Schrödinger operators with potentials having two or more well-separated wells related by a symmetry (see [67], for example).

## 4.3 Generalization to $n$ domain walls

Our analysis may be readily extended to the case of $n$ domain walls, each separated by a distance $2L$. In this case we expect that there will be $n$ near-zero eigenvalues with exponentially small: $O(e^{-2\kappa_\infty L})$ gaps between them. When $n$ is odd, one of the $n$ non-zero eigenvalues will be an exact zero mode since in this case $\kappa_L$ is an 'odd' function of $x$ at infinity: as $|x| \to \infty$, $\kappa_L(-x) = -\kappa_L(x)$. If as $x \to \infty$, $\kappa_L(x) > 0$, the normalized zero-mode is given by:

$$\alpha_{\star,L}(x) := \gamma_L \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\int_0^x \kappa_L(y)\,\mathrm{d}y} \tag{4.3.1}$$

where:

$$\gamma_L := \frac{1}{\sqrt{2}\|e^{-\int_0^x \kappa_L(y)\,\mathrm{d}y}\|_{L^2}}. \tag{4.3.2}$$

If, as $x \to \infty$, $\kappa_L(x) < 0$, then the normalized zero-mode is given by:

$$\alpha_{\star,L}(x) := \gamma_L \begin{pmatrix} 1 \\ i \end{pmatrix} e^{\int_0^x \kappa_L(y)\,\mathrm{d}y} \tag{4.3.3}$$

## 4.4 Proof of Theorem 4.2.1 (strategy)

We now describe the strategy of the proof of Theorem 4.2.1. We seek a solution of the eigenvalue problem (4.1.1) as a linear combination of the functions $\alpha_\star^+, \alpha_\star^-$ plus a corrector function $\eta$:

$$\alpha(x) = b^+\alpha_\star^+(x) + b^-\alpha_\star^-(x) + \eta(x). \tag{4.4.1}$$

where $b^+, b^-$ are complex numbers to be determined. Let $P^{\pm,\perp}$ denote the projection operator onto $\{\alpha_\star^+, \alpha_\star^-\}^\perp$. We assume without loss of generality that $P^{\pm,\perp}\eta = \eta$. Substituting (4.4.1) into

(4.1.1) and projecting onto each of the orthogonal subspaces $\{\alpha_\star^+\}, \{\alpha_\star^-\}, \{\alpha_\star^+, \alpha_\star^-\}^\perp$ gives a coupled system of equations for $b^+, b^-$ and $\eta$:

$$i \in \pm,\ \sum_{j\in\pm} b^j \left\langle \alpha_\star^i \middle| (\mathcal{D}_{\kappa_L} - E)\alpha_\star^j \right\rangle_{\mathcal{H}} + \left\langle \alpha_\star^i \middle| (\mathcal{D}_{\kappa_L} - E)\eta \right\rangle_{\mathcal{H}} = 0 \tag{4.4.2}$$

$$\sum_{j\in\pm} b^j P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)\alpha_\star^j + P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)\eta = 0. \tag{4.4.3}$$

We claim the following key Lemma:

**Lemma 4.4.1.** *There exists an $L_0 > 1$ such that for all $L > L_0$ the following holds. If $\langle \alpha_\star^+ | f\rangle_{\mathcal{H}} = \langle \alpha_\star^- | f\rangle_{\mathcal{H}} = 0$ then:*

$$\|\mathcal{D}_{\kappa_L} f\|_{\mathcal{H}} \geq \frac{3\kappa_\infty}{4}\|f\|_{\mathcal{H}}. \tag{4.4.4}$$

*Moreover, for $|E| < \frac{\kappa_\infty}{4}$:*

$$\|(\mathcal{D}_{\kappa_L} - E)f\|_{\mathcal{H}} \geq \frac{\kappa_\infty}{2}. \tag{4.4.5}$$

*In particular, $(\mathcal{D}_{\kappa_L} - E)$ is invertible on the space $P^{\pm,\perp}\mathcal{H}$ where $P^{\pm,\perp}$ denotes the orthogonal projection operator onto $\{\alpha_\star^+, \alpha_\star^-\}^\perp$, and:*

$$\|(\mathcal{D}_{\kappa_L} - E)^{-1}P^{\pm,\perp}\|_{\mathcal{H}\to\mathcal{H}} \leq \frac{2}{\kappa_\infty}. \tag{4.4.6}$$

For the proof of Lemma 4.4.1, which follows from Lemma 4.2.1 and a partition of unity, see Section C.1.

Assuming Lemma 4.4.1, for $|E| < \frac{\kappa_\infty}{4}$ we can solve (4.4.3) in terms of $b^+, b^-$:

$$\begin{aligned}\eta &= -\sum_{j\in\pm} b^j P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)^{-1}P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)\alpha_\star^j \\ &= -\sum_{j\in\pm} b^j P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)^{-1}P^{\pm,\perp}\mathcal{D}_{\kappa_L}\alpha_\star^j.\end{aligned} \tag{4.4.7}$$

Substituting (4.4.7) back into (4.4.2), we then obtain a *closed* system for $b^+, b^-$ alone:

$$\begin{aligned}&i \in \pm,\ \sum_{j\in\pm} b^j \left\langle \alpha_\star^i \middle| (\mathcal{D}_{\kappa_L} - E)\alpha_\star^j \right\rangle_{\mathcal{H}} \\ &-\sum_{j\in\pm} \left\langle \alpha_\star^i \middle| (\mathcal{D}_{\kappa_L} - E)P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)^{-1}P^{\pm,\perp}\mathcal{D}_{\kappa_L}\alpha_\star^j \right\rangle_{\mathcal{H}} b^j = 0.\end{aligned} \tag{4.4.8}$$

Using self-adjointness of $(\mathcal{D}_{\kappa_L} - E)P^{\pm,\perp}$ (4.4.8) can be written as the following simplified matrix equation:

$$\begin{aligned} & i \in \pm, \sum_{j \in \pm} M^{ij} b^j = 0 \\ & M^{ij}(L,E) := \left\langle \alpha_\star^i \middle| \mathcal{D}_{\kappa_L} \alpha_\star^j \right\rangle_{\mathcal{H}} - E \left\langle \alpha_\star^i \middle| \alpha_\star^j \right\rangle - \left\langle P^{\pm,\perp} \mathcal{D}_{\kappa_L} \alpha_\star^i \middle| (\mathcal{D}_{\kappa_L} - E)^{-1} P^{\pm,\perp} \mathcal{D}_{\kappa_L} \alpha_\star^j \right\rangle_{\mathcal{H}} . \end{aligned} \tag{4.4.9}$$

In particular:

**Corollary 4.4.1** (of Lemma 4.4.1)**.** *For $E$ such that $|E| < \frac{\kappa_\infty}{4}$, $E$ is an eigenvalue of $\mathcal{D}_{\kappa_L}$ if and only if* $\det M^{ij}(L,E) = 0$.

Theorem 4.2.1 will follow from a detailed analysis of each component of the matrix $M^{ij}(L,E)$, assuming that $E < \frac{\kappa_\infty}{4}$ so that Lemma 4.4.1 and Corollary 4.4.1 hold. Note that the resolvent operator $(\mathcal{D}_{\kappa_L} - E)^{-1} P^{\pm,\perp}$ is actually analytic in $E$ in this case. The result of our analysis of the matrix $M(L,E)$ is the following:

**Lemma 4.4.2.** *Assume that $E < \frac{\kappa_\infty}{4}$ so that Lemma 4.4.1 holds. Then each of the entries of $M(L,E)$ varies analytically with $E$, and the matrix $M(L,E)$ may be written:*

$$M(L,E) = \begin{pmatrix} -E & 2i\gamma^2 e^{-2\int_0^L \kappa(y)\, dy} \\ -2i\gamma^2 e^{-2\int_0^L \kappa(y)\, dy} & -E \end{pmatrix} + M_1(L,E) \tag{4.4.10}$$

*where each of the entries of the matrix $M_1(L,E)$ satisfies $|M_1^{ij}(L,E)| \leq Ce^{-4\kappa_\infty L}$ for constant $C > 0$ independent of $L, E$.*

For the proof of Lemma 4.4.2, see Section C.1. We now prove Theorem 4.2.1 as follows. Note that it is clear also that $|2i\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}| \leq Ce^{-2\kappa_\infty L}$ for some constant $C > 0$ independent of $L, E$. Taking the determinant of (4.4.10) we obtain:

$$\det M^{ij}(L,E) = (E - 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y})(E + 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y})) + g(L,E) = 0 \tag{4.4.11}$$

where the function $g(L,E)$ is analytic in $E$ and satisfies the bound:

$$|g(L,E)| \leq C \left( Ee^{-4\kappa_\infty L} + e^{-6\kappa_\infty L} \right) \tag{4.4.12}$$

for some constant $C > 0$ independent of $L, E$. Let $C^* > 0$ denote a constant independent of $L, E$ such that $C^* e^{-2\kappa_\infty L} \leq |2i\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}|$, and consider the real interval $I_{R(L)}(2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y})$

centered at $E = 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}$ with radius $R(L) := C^* e^{-2\kappa_\infty L}$. We then have that for all $E \in I_{R(L)}, C^* e^{-2\kappa_\infty L} \leq E + 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}$ so that:

$$\det M^{ij}(L,E) = 0 \iff E - 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y} + \frac{g(L,E)}{E + 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}} = 0. \tag{4.4.13}$$

Now, for sufficiently large $L > 0$, we have that:

$$\begin{aligned} &\text{if } |E| = R(L), \text{ then:} \\ &\left| \frac{g(L,E)}{E + 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}} \right| \leq C_1 e^{-4\kappa_\infty L} \leq C^* e^{-2\kappa_\infty L} = |E - 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}| \end{aligned} \tag{4.4.14}$$

for some constant $C_1 > 0$ independent of $L, E$. It is now clear from the intermediate value theorem that the matrix $M(L,E)$ (4.4.10) has precisely one eigenvalue in the interval $I_{R(L)}(2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y})$. It is furthermore clear that this eigenvalue (which we denote $E_+(L)$) satisfies:

$$E_+(L) = 2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y} + O(e^{-4\kappa_\infty L}). \tag{4.4.15}$$

By an identical argument, it is clear that the matrix $M(L,E)$ (4.4.10) has precisely one eigenvalue in the interval $I_{R(L)}(-2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y})$ which satisfies:

$$E_-(L) = -2\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y} + O(e^{-4\kappa_\infty L}). \tag{4.4.16}$$

The associated eigenfunctions of these eigenvalues may be similarly expanded as:

$$\begin{aligned} \begin{pmatrix} b^+ \\ b^- \end{pmatrix}_+ &= \begin{pmatrix} 1 \\ -i \end{pmatrix} + O(e^{-2\kappa_\infty L}) \\ \begin{pmatrix} b^+ \\ b^- \end{pmatrix}_- &= \begin{pmatrix} 1 \\ i \end{pmatrix} + O(e^{-2\kappa_\infty L}), \end{aligned} \tag{4.4.17}$$

from which the statement of Theorem 4.2.1 is then clear.

# Bibliography

[1] N. I. Akhiezer. *Elements of the theory of elliptic functions.* Number 79 in Translations of Mathematical Monographs. American Mathematical Society, 1990.

[2] G. Allaire and A. Piatnitski. Homogenization of the Schrödinger equation and effective mass theorems. *Communications in Mathematical Physics*, 258(1):1–22, 2005.

[3] N.W. Ashcroft and N.D. Mermin. *Solid State Physics.* Saunders College, 1976.

[4] P. Bechouche, N. J. Mauser, and F. Poupaud. Semiclassical limit for the Schrödinger-Poisson equation in a crystal. *Communications on Pure and Applied Mathematics*, 54(7):851–890, 2001.

[5] M. V. Berry. Quantal phase factors accompanying adiabatic changes. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 392, pages 45–57. The Royal Society, 1984.

[6] M. V. Berry and M. R. Jeffrey. Conical diffraction: Hamilton's diabolical point at the heart of crystal optics. *Progress in Optics*, 50:13–50, 2007.

[7] K. Y. Bliokh, A. Niv, V. Kleiner, and E. Hasman. Geometrodynamics of spinning light. *Nature Photonics*, 2(12):748–753, 2008.

[8] I. Boaz and M. I. Weinstein. Band-edge solitons, nonlinear Schrödinger/Gross-Pitaevskii equations, and effective media. *Multiscale Modeling & Simulation*, 8(4):1055–1101, 2010.

[9] K. Cai. *Dispersive properties of Schrodinger equations.* PhD thesis, California Institute of Technology, 2005.

[10] R. Carles, C. Fermanian-Kammerer, N. J. Mauser, and H. P. Stimming. On the time evolution of Wigner measures for Schrödinger equations. *Communications on Pure and Applied Analysis*, 8(2):559–585, 2009.

[11] R. Carles, P. A. Markowich, and C. Sparber. Semiclassical asymptotics for weakly nonlinear Bloch waves. *Journal of statistical physics*, 117(1-2):343–375, 2004.

[12] L. Chai, S. Jin, and Q. Li. Semiclassical models for the Schrödinger equation with periodic potentials and band crossings. *Kinetic and related models*, 6(3):505–532, 2013.

[13] L. Chai, S. Jin, Q. Li, and O. Morandi. A multiband semiclassical model for surface hopping quantum mechanics. *Multiscale Modeling & Simulation*, 13(1):205–230, 2015.

[14] K. S. Chandrasekharan. *Elliptic functions*. Number 281 in Grundlehren der Mathematischen Wissenschaften. Springer-Verlag Berlin, 1985.

[15] M-C. Chang and Q. Niu. Berry phase, hyperorbits, and the Hofstadter spectrum: Semiclassical dynamics in magnetic Bloch bands. *Physical Review B*, 53(11):7010–7023, 1996.

[16] A. Damascelli. Probing the electronic structure of complex systems by ARPES. *Physica Scripta*, 2004(T109):61–71, 2004.

[17] Y. Colin de Verdiere, M. Lombardi, and J. Pollet. The microlocal Landau-Zener formula. *Annales de l'I.H.P. Physique théorique*, 71(1):95–127, 1999.

[18] A. Drouot. Scattering resonances for highly oscillatory potentials. https://arxiv.org/abs/1509.04198.

[19] A. Drouot. Bound states for rapidly oscillatory Schrödinger operators in dimension 2. https://arxiv.org/abs/1609.00757.

[20] V. Duchêne, I. Vukićević, and M.I. Weinstein. Scattering and localization properties of highly oscillatory potentials. *Comm. Pure Appl. Math.*, 1:83–128, 2014.

[21] V. Duchêne, I. Vukićević, and M.I. Weinstein. Homogenized description of defect modes in periodic structures with localized defects. *Commun. Math. Sci.*, 13(3):777–823, 2015.

[22] C. Duval, Z. Horváth, P.A. Horváthy, L. Martina, and P.C. Stichel. Berry phase correction to electron density in solids and 'exotic' dynamics. *Modern Physics Letters B*, 20(7):373–378, 2006.

[23] W. E, J. Lu, and X. Yang. Asymptotic analysis of quantum dynamics in crystals: the Bloch-Wigner transform, Bloch dynamics and Berry phase. *Acta Mathematicae Applicatae Sinica, English Series*, 29(3):465–476, 2013.

[24] E. Faou, V. Gradinaru, and C. Lubich. Computing semiclassical quantum dynamics with Hagedorn wavepackets. *SIAM Journal on Scientific Computing*, 31(4):3027–3041, 2009.

[25] C. Fefferman, J. Lee-Thorp, and M. Weinstein. *Topologically protected states in one-dimensional systems*, volume 247 of *Memoirs of the American Mathematical Society*. American Mathematical Society, 2017.

[26] C. L. Fefferman, J. P. Lee-Thorp, and M. I. Weinstein. Topologically protected states in one-dimensional continuous systems and Dirac points. *Proceedings of the National Academy of Sciences*, 111(24):8759–8763, 2014.

[27] C. L. Fefferman, J. P. Lee-Thorp, and M. I. Weinstein. Bifurcations of edge states—topologically protected and non-protected—in continuous 2D honeycomb structures. *2D Materials*, 3(1):014008, 2016.

[28] C. L. Fefferman and M. I. Weinstein. Honeycomb lattice potentials and Dirac points. *Journal of the American Mathematical Society*, 25(4):1169–1220, 2012.

[29] C. L. Fefferman and M. I. Weinstein. Wave packets in honeycomb structures and two-dimensional Dirac equations. *Communications in Mathematical Physics*, 326(1):251–286, 2014.

[30] C. Fermanian-Kammerer and P. Gérard. Mesures semi-classiques et croisement de modes. *Bulletin de la Société Mathématique de France*, 130(1):123–168, 2002.

[31] C. Fermanian-Kammerer and P. Gérard. A Landau-Zener formula for non-degenerated involutive codimension 3 crossings. *Annales Henri Poincaré*, 4(3):513–552, 2003.

[32] C. Fermanian-Kammerer, P. Gérard, and C. Lasser. Wigner measure propagation and conical singularity for general initial data. *Archive for Rational Mechanics and Analysis*, 209(1):209–236, 2013.

[33] C. Fermanian-Kammerer and C. Lasser. Propagation through generic level crossings: a surface hopping semigroup. *SIAM Journal on Mathematical Analysis*, 40(1):103–133, 2008.

[34] C. Fermanian-Kammerer and C. Lasser. An Egorov theorem for avoided crossings of eigenvalue surfaces. *Communications in Mathematical Physics*, 353(3):1011–1057, 2017.

[35] C. Fermanian-Kammerer and F. Mehats. A kinetic model for the transport of electrons in a graphene layer. *Journal of Computational Physics*, 327:450–483, 2016.

[36] G. A. Hagedorn. Semiclassical quantum mechanics. *Communications in Mathematical Physics*, 71(1):77–93, 1980.

[37] G. A. Hagedorn. *Molecular propagation through electron energy level crossings*, volume 536 of *Memoirs of the American Mathematical Society*. American Mathematical Society, 1994.

[38] G. A. Hagedorn. Raising and lowering operators for semiclassical wave packets. *Annals of Physics*, 269(1):77–104, 1998.

[39] G. A. Hagedorn and A. Joye. Landau-Zener transitions through small electronic eigenvalue gaps in the Born-Oppenheimer approximation. In *Annales de l'IHP Physique théorique*, volume 68, pages 85–134, 1998.

[40] E. J. Heller. Classical S-matrix limit of wave packet dynamics. *The Journal of Chemical Physics*, 65(11):4979–4989, 1976.

[41] H. Hochstadt. On the characterization of a Hill's equation from its spectrum. *Archive for Rational Mechanics and Analysis*, 19:353–611, 1965.

[42] M.A. Hoefer and M.I. Weinstein. Defect modes and homogenization of periodic Schrödinger operators. *SIAM J. Mathematical Analysis*, 43:971–996, 2011.

[43] S. G. Johnson, P. Bienstman, M. A. Skorobogatiy, M. Ibanescu, E. Lidorikis, and J. D. Joannopoulos. Adiabatic theorem and continuous coupled-mode theory for efficient taper transitions in photonic crystals. *Phys. Rev. E*, 66(6):066608, 2002.

[44] R. Karplus and J. M. Luttinger. Hall effect in ferromagnetics. *Phys. Rev.*, 95(5), 1954.

[45] H. Kitada. On a construction of the fundamental solution for Schrödinger equations. *J. Fac. Sci. Univ. Tokyo*, 27:193–226, 1980.

[46] P. Kuchment. An overview of periodic elliptic operators. *Bulletin of the American Mathematical Society*, 53(3):343–414, 2016.

[47] L. Landau. Zur theorie der energieübertragung. II. *Physics of the Soviet Union*, 2:46–51, 1932.

[48] C. Lasser, T. Swart, and S. Teufel. Construction and validation of a rigorous surface hopping algorithm for conical crossings. *Communications in Mathematical Sciences*, 5(4):789–814, 2007.

[49] C. Lasser and S. Teufel. Propagation through conical crossings: an asymptotic semigroup. *Communications on Pure and Applied Analysis*, 58(9):1188–1230, 2005.

[50] W. Magnus and S. Winkler. *Hill's Equation*. John Wiley & Sons, New York, 1966.

[51] P. A. Markowich, N. J. Mauser, and F. Poupaud. A Wigner function approach to (semi)classical limits: Electrons in a periodic potential. *Journal of Mathematical Physics*, 35(3):1066–1094, 1994.

[52] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong. Anomalous Hall effect. *Reviews of modern physics*, 82(2):1539–1592, 2010.

[53] G. De Nittis and M. Lein. Effective light dynamics in perturbed photonic crystals. *Communications in Mathematical Physics*, 332(1):221–260, 2014.

[54] G. De Nittis and M. Lein. Derivation of ray optics equations in photonic crystals via a semiclassical limit. *Annales Henri Poincaré*, 18(5):1789–1831, 2017.

[55] T. Ohsawa. The Siegel upper half space is a Marsden-Weinstein quotient: symplectic reduction and Gaussian wave packets. *Letters in Mathematical Physics*, 105(9):1301–1320, 2015.

[56] T. Ohsawa and M. Leok. Symplectic semiclassical wave packet dynamics. *Journal of Physics A: Mathematical and Theoretical*, 46(40), 2013.

[57] G. Panati, H. Spohn, and S. Teufel. Effective dynamics for Bloch electrons: Peierls substitution and beyond. *Communications in Mathematical Physics*, 242(3):547–578, 2003.

[58] G. Panati, H. Spohn, and S. Teufel. *Motion of Electrons in Adiabatically Perturbed Periodic Structures*, pages 595–617. Springer Berlin Heidelberg, Berlin, Heidelberg, 2006.

[59] J. Pöschel and E. Trubowitz. *Inverse Spectral Theory.* Number 130 in Pure and Applied Mathematics. Academic Press, 1987.

[60] F. Poupaud and C. Ringhofer. Semi-classical limits in a crystal with exterior potentials and effective mass theorems. *Communications in Partial Differential Equations*, 21(11-12):1897–1918, 1996.

[61] R. Carles and C. Sparber. Semiclassical wave packet dynamics in Schrödinger equations with periodic potentials. *Discrete Contin. Dyn. Syst. Ser. B*, 17(3):759–774, 2012.

[62] J. Ralston. Gaussian beams and the propagation of singularities. In *Studies in Partial Differential Equations*, volume 23 of *MAA Studies in Mathematics*. MAA, 1983.

[63] M. Reed and B. Simon. *Methods of modern mathematical physics, IV: analysis of operators.* Academic press, 1977.

[64] D. Robert. Propagation of coherent states in quantum mechanics and applications. In *Séminaires et Congres*, number 15, pages 181–250, 2007.

[65] O. Schnitzer. Waves in slowly-varying band-gap media. arXiv:1612.03895, 2016.

[66] R. Schubert, R. O. Vallejos, and F. Toscano. How do wave packets spread? Time evolution on Ehrenfest time scales. *Journal of Physics A: Mathematical and Theoretical*, 45(21):215–307, 2012.

[67] B. Simon. Semiclassical analysis of low lying eigenvalues, II. Tunneling. *Annals of Mathematics*, 120(1):89–118, 1984.

[68] C. Sparber. Effective mass theorems for nonlinear Schrodinger equations. *SIAM Journal on Applied Mathematics*, 66(3):820–842, 2006.

[69] C. Sparber, P. A. Markowich, and N. J. Mauser. Wigner functions versus WKB-methods in multivalued geometrical optics. *Asymptotic Analysis*, 33:153–187, 2003.

[70] H. Stiepan and S. Teufel. Semiclassical approximations for Hamiltonians with operator-valued symbols. *Communications in Mathematical Physics*, 320(3):821–849, 2013.

[71] G. Sundaram and Q. Niu. Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects. *Physical Review B*, 59(23):14915–14925, 1999.

[72] S. Teufel. *Adiabatic perturbation theory in quantum dynamics*, volume 1821 of *Lecture notes in mathematics*. Springer-Verlag Berlin Heidelberg, 2003.

[73] A. B. Watson, J. Lu, and M. I. Weinstein. Wavepackets in inhomogeneous periodic media: Effective particle-field dynamics and Berry curvature. *Journal of Mathematical Physics*, 58(2), 2017.

[74] C. E. Wayne and M. I. Weinstein. *Dynamics of partial differential equations*, volume 3 of *Frontiers in Applied Dynamical Systems: Reviews and Tutorials*. Springer International Publishing, 2015.

[75] E. T. Whittaker and G. N. Watson. *A Course of Modern Analysis*. Cambridge University Press, 1902.

[76] D. Xiao, M-C. Chang, and Q. Niu. Berry phase effects on electronic properties. *Reviews of modern physics*, 82(3):1959–2007, 2010.

[77] X. Yin, Z. Ye, J. Rho, Y. Wang, and X. Zhang. Photonic spin hall effect at metasurfaces. *Science*, 339:1404–1407, 2013.

[78] C. Zener. Non-adiabatic crossing of energy levels. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 137(833):696–702, 1932.

# Appendix A

# Chapter 2 Appendices

## A.1 Useful identities involving $E_n, \chi_n$

Let $E(p), \chi(z;p)$ satisfy the eigenvalue problem:

$$\begin{aligned} &[H(p) - E(p)]\,\chi(z;p) = 0 \\ &H(p) = \frac{1}{2}(p - i\nabla_z)^2 + V(z) \end{aligned} \tag{A.1.1}$$

and assume that $E(p), \chi(z;p)$ are smooth functions of $p$. Taking the gradient with respect to $p$ gives:

$$[(p - i\nabla_z) - \nabla_p E_n(p)]\,\chi_n(z;p) + [H(p) - E_n(p)]\,\nabla_p \chi_n(z;p) = 0 \tag{A.1.2}$$

Taking two derivatives with respect to $p$ of the equation gives:

$$\begin{aligned} &\left[\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta} E_n(p)\right] \chi_n(z;p) + [(p - i\partial_z)_\alpha - \partial_{p_\alpha} E_n(p)]\,\partial_{p_\beta}\chi_n(z;p) \\ &+ \left[(p - i\partial_z)_\beta - \partial_{p_\beta} E_n(p)\right] \partial_{p_\alpha}\chi_n(z;p) + [H(p) - E_n(p)]\,\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p) = 0 \end{aligned} \tag{A.1.3}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta. Taking the derivative with respect to $p_\gamma$ of (A.1.3) gives:

$$\begin{aligned} &[-\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma} E_n(p)]\chi_n(z;p) + [\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta} E_n(p)]\partial_{p_\gamma}\chi_n(z;p) \\ &+ [\delta_{\alpha\gamma} - \partial_{p_\alpha}\partial_{p_\gamma} E_n(p)]\partial_{p_\beta}\chi_n(z;p) + [\delta_{\beta\gamma} - \partial_{p_\beta}\partial_{p_\gamma} E_n(p)]\partial_{p_\alpha}\chi_n(z;p) \\ &+ [(p - i\partial_z)_\alpha - \partial_{p_\alpha} E_n(p)]\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p) + [(p - i\partial_z)_\beta - \partial_{p_\beta} E_n(p)]\partial_{p_\alpha}\partial_{p_\gamma}\chi_n(z;p) \\ &+ [(p - i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p)]\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p) + [H(p) - E_n(p)]\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p) = 0 \end{aligned} \tag{A.1.4}$$

## A.2 Derivation of leading-order envelope equation

Collecting terms of order $\epsilon$ in the expansion (2.3.9), using equations (2.1.21) for $\dot{S}(t)$ and (2.1.19) for $\dot{q}(t), \dot{p}(t)$, and setting equal to zero gives the following inhomogeneous self-adjoint elliptic equation in $z$ for $f^2(y,z,t)$:

$$\begin{aligned}&\left[H(p(t)) - E_n(p(t))\right] f^2(y,z,t) = \xi^2(y,z,t)\\&\text{for all } v \in \Lambda, f^2(y,z+v,t) = f^2(y,z,t);\; f^2(y,z,t) \in \Sigma_y^{R-2}(\mathbb{R}^d)\\&\xi^2 := -\left[\frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta - i\partial_t\right] f^0(y,z,t)\\&\quad - \left[\left((p(t) - i\nabla_z) - \nabla_p E_n(p(t))\right)\cdot(-i\nabla_y)\right] f^1(y,z,t).\end{aligned} \tag{A.2.1}$$

We follow the strategy outlined in Remark 2.3.1. The proof of the following Lemma will be given at the end of this section:

**Lemma A.2.1.** *$\xi^2(y,z,t)$, defined in (A.2.1) satisfies:*

$$\xi^2(y,z,t) = \tilde{\xi}^2(y,z,t) + \left[H(p(t)) - E_n(p(t))\right] u^2(y,z,t) \tag{A.2.2}$$

*where:*

$$\begin{aligned}\tilde{\xi}^2(y,z,t) = &\Bigg[i\partial_t a^0(y,t) - \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) - \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^0(y,t)\\&- \nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))\Bigg]\chi_n(z;p(t))\\&+ P_n^\perp(p(t))\left[-ia^0(y,t)\nabla_q W(q(t))\cdot\nabla_p\chi_n(z;p(t))\right]\\u^2(y,z,t) = &(-i\nabla_y)a^1(y,t)\cdot\nabla_p\chi_n(z;p(t)) + \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t)).\end{aligned} \tag{A.2.3}$$

*Here, $\mathcal{A}_n(p(t))$ is the Berry connection (2.1.26) and $P_n^\perp(p(t))$ is the orthogonal projection operator away from the subspace of $L^2_{per}$ spanned by $\chi_n(z;p(t))$ (2.3.21).*

Imposing the solvability condition of equation (A.2.1), given by (2.3.20) with $j = 2$ and $\tilde{\xi}^2(y,z,t)$ given by (A.2.3), gives the following evolution equation for $a^0(y,t)$:

$$\begin{aligned}i\partial_t a^0(y,t) = &\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^0(y,t)\\&+ \nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))a^0(y,t)\end{aligned} \tag{A.2.4}$$

Taking $a^0(y,t) = a(y,t)e^{i\phi_B(t)}$ and matching with the initial data implies equations (2.1.27) and (2.1.22). The general solution of (A.2.1) is given by (2.3.22) with $j = 2$:

$$\begin{aligned} &f^2(y,z,t) = a^2(y,t)\chi_n(z;p(t)) + (-i\nabla_y)a^1(y,t)\cdot\nabla_p\chi_n(z;p(t)) \\ &+ \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t)) \\ &[H(p(t)) - E_n(p(t))]^{-1}P_n^\perp(p(t))\left[-i\nabla_q W(q(t))a^0(y,t)\cdot\nabla_p\chi_n(z;p(t))\right] \end{aligned} \tag{A.2.5}$$

where $a^2(y,t)$ is an arbitrary function in $\Sigma_y^{R-2}(\mathbb{R}^d)$ to be fixed at higher order in the expansion.

*Proof of Lemma A.2.1.* Adding and substracting terms, using smoothness of the band $E_n(p)$ in a neighborhood of $p(t)$ (Assumption 2.1.1) we can re-write $\xi^2$ (A.2.1) as:

$$\begin{aligned} &\xi^2(y,z,t) = -\left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta - i\partial_t\right]f^0(y,z,t) \\ &-\left[\frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})\right]f^0(y,z,t) \\ &-\left[((p(t) - i\nabla_z) - \nabla_p E_n(p(t)))\cdot(-i\nabla_y)\right]f^1(y,z,t). \end{aligned} \tag{A.2.6}$$

Substituting the forms of $f^0(y,z,t)$ (2.3.14) and $f^1(y,z,t)$ (2.3.27) gives:

$$\begin{aligned} &\xi^2(y,z,t) = -\left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^0(y,t)\right. \\ &\left.- i\partial_t a^0(y,t)\right]\chi_n(z;p(t)) + ia^0(y,t)\dot{p}(t)\cdot\nabla_p\chi_n(z;p(t)) \\ &-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)\chi_n(z;p(t)) \\ &-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\left((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(p(t))\right)\partial_{p_\beta}\chi_n(z;p(t)) \\ &-(-i\nabla_y)a^1(y,t)\cdot((p(t) - i\nabla_z) - \nabla_p E_n(p(t)))\chi_n(z;p(t)). \end{aligned} \tag{A.2.7}$$

Using (A.1.2) we can simplify the term involving $a^1$:

$$\begin{aligned} &-(-i\nabla_y)a^1(y,t)\cdot((p(t) - i\nabla_z) - \nabla_p E_n(p(t)))\chi_n(z;p(t)) \\ &= (-i\nabla_y)a^1(y,t)\cdot[H(p(t)) - E_n(p(t))]\nabla_p\chi_n(z;p(t)). \end{aligned} \tag{A.2.8}$$

Using (A.1.3), and the symmetry: $(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) = (-i\partial_{y_\beta})(-i\partial_{y_\alpha})a^0(y,t)$ we can simplify the terms:

$$\begin{aligned} &-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)\chi_n(z;p(t)) \\ &-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\left((p(t) - i\partial_z)_\alpha - \partial_{p_\alpha}E_n(p(t))\right)\partial_{p_\beta}\chi_n(z;p(t)) \\ &= \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\left[H(p(t)) - E_n(p(t))\right]\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t)). \end{aligned} \tag{A.2.9}$$

Recall that $\dot{p}(t) = -\nabla_q W(q(t))$ (2.1.19). Substituting this, (A.2.8), and (A.2.9) into (A.2.1) and adding and subtracting $a^0(y,t)\nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))\chi_n(z;p(t))$ gives:

$$\xi^2(y,z,t) = \Bigg[ i\partial_t a^0(y,t) - \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t) - \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^0(y,t)$$
$$- \nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t)) \Bigg] \chi_n(z;p(t)) + P_n^\perp(p(t)) \left[ -ia^0(y,t)\nabla_q W(q(t)) \cdot \nabla_p \chi_n(z;p(t)) \right]$$
$$+ \left[ H(p(t)) - E_n(p(t)) \right] \Bigg[ \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t))$$
$$+ (-i\nabla_y)a^1(y,t) \cdot \nabla_p \chi_n(z;p(t)) \Bigg] \tag{A.2.10}$$

where $\mathcal{A}_n(p(t))$ is the Berry connection (2.1.26) and $P_n^\perp(p(t))$ is the orthogonal projection in $L^2_{per}$ away from the subspace spanned by $\chi_n(z;p(t))$. □

## A.3 Derivation of first-order envelope equation

Collecting terms of order $\epsilon^{3/2}$ in the expansion (2.3.9), using equations (2.1.21) for $\dot{S}(t)$ and (2.1.19) for $\dot{q}(t), \dot{p}(t)$, and setting equal to zero gives the following inhomogeneous self-adjoint elliptic equation in $z$ for $f^3(y,z,t)$:

$$\Big[ H(p(t)) - E_n(p(t)) \Big] f^3(y,z,t) = \xi^3(y,z,t)$$
$$\text{for all } v \in \Lambda, f^3(y,z+v,t) = f^3(y,z,t);\; f^3(y,z,t) \in \Sigma_y^{R-3}(\mathbb{R}^d)$$
$$\xi^3(y,z,t) := -\left[ \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma \right] f^0(y,z,t) \tag{A.3.1}$$
$$- \left[ \frac{1}{2}(-i\nabla_y)^2 + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta - i\partial_t \right] f^1(y,z,t)$$
$$- \Big[ \left[ (p(t) - i\nabla_z) - \nabla_p E_n(p(t)) \right] \cdot (-i\nabla_y) \Big] f^2(y,z,t)$$

We claim the following lemmas, the proofs of which will be given at the end of this section:

**Lemma A.3.1.** *$\xi^3(y,z,t)$, as defined in (A.3.1), satisfies:*

$$\xi^3(y,z,t) = \tilde{\xi}^3(y,z,t) + \left[ H(p(t)) - E_n(p(t)) \right] u^3(y,z,t) \tag{A.3.2}$$

*where* $\tilde{\xi}^3$ *is given explicitly by (A.3.24) and:*

$$\begin{aligned} u^3(y,z,t) &:= (-i\nabla_y)a^2(y,t)\cdot\nabla_p\chi_n(z;p(t)) + \frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t)) \\ &+ \frac{1}{6}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)). \end{aligned} \tag{A.3.3}$$

**Lemma A.3.2.** *The solvability condition for (A.3.1), given by (2.3.20) with* $j = 3$ *and* $\tilde{\xi}^3(y,z,t)$ *given by (A.3.24), is equivalent to the following evolution equation for* $a^1(y,t)$*:*

$$\begin{aligned} i\partial_t a^1(y,t) &= \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^1(y,t) \\ &+ \nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))a^1(y,t) \\ &+ \frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t) + \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma a^0(y,t) \\ &+ \partial_{q_\beta}W(q(t))\partial_{p_\gamma}\mathcal{A}_{n,\beta}(p(t))(-i\partial_{y_\gamma})a^0(y,t) + \partial_{q_\beta}\partial_{q_\gamma}W(q(t))\mathcal{A}_{n,\beta}(p(t))y_\gamma a^0(y,t). \end{aligned} \tag{A.3.4}$$

*Here,* $\mathcal{A}_n(p(t))$ *is the Berry connection (2.1.26).*

Taking $a^1(y,t) = b(y,t)e^{i\phi_B(t)}$ and matching with the initial data implies equation (2.1.24) for $b(y,t)$. The solution of (A.3.1) is then given by (2.3.22):

$$f^3(y,z,t) = a^3(y,t)\chi_n(z;p(t)) + u^3(y,z,t) + [H(p(t)) - E_n(p(t))]^{-1}P_n^\perp(p(t))\tilde{\xi}^3(y,z,t) \tag{A.3.5}$$

where $\tilde{\xi}^3(y,z,t)$ is given by (A.3.24) and $u^3(y,z,t)$ by (A.3.3). $a^3(y,t)$ is an arbitrary function in $\Sigma_y^{R-3}(\mathbb{R}^d)$ to be fixed at higher order in the expansion. Note that all manipulations so far are valid as long as $R \geq 3$.

*Proof of Lemma A.3.1.* Adding and subtracting terms using smoothness of the band $E_n(p)$ in a neighborhood of $p(t)$ (Assumption 2.1.1) we can re-write $\xi^3(y,z,t)$ (A.3.1) as:

$$\begin{aligned} \xi^3(y,z,t) &= -\left[\frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma}) + \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma\right]f^0(y,z,t) \\ &- \left[-\frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})\right]f^0(y,z,t) \\ &- \left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta - i\partial_t\right]f^1(y,z,t) \\ &- \left[\frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)(-i\partial_{y_\alpha})(-i\partial_{y_\beta})\right]f^1(y,z,t) \\ &- \left[((p(t) - i\nabla_z) - \nabla_p E_n(p(t)))\cdot(-i\nabla_y)\right]f^2(y,z,t) \end{aligned} \tag{A.3.6}$$

Substituting the forms of $f^0(y,z,t)$ (2.3.14), $f^1(y,z,t)$ (2.3.27), and $f^2(y,z,t)$ (A.2.5) gives a very long expression on the right-hand side. We simplify this expression by treating terms which depend on $a^2(y,t), a^1(y,t), a^0(y,t)$ in turn.

Contributions to (A.3.6) depending on $a^2(y,t)$. There is one term which depends on $a^2(y,t)$:

$$-(-i\nabla_y)a^2(y,t)\cdot((p(t)-i\nabla_z)-\nabla_p E_n(p(t)))\,\chi_n(z;p(t)) \tag{A.3.7}$$

which can be simplified using (A.1.2):

$$\begin{aligned}&-(-i\nabla_y)a^2(y,t)\cdot((p(t)-i\nabla_z)-\nabla_p E_n(p(t)))\,\chi_n(z;p(t))\\&\quad=[H(p(t))-E_n(p(t))]\left[(-i\nabla_y)a^2(y,t)\cdot\nabla_p\chi_n(z;p(t))\right].\end{aligned} \tag{A.3.8}$$

Contributions to (A.3.6) depending on $a^1(y,t)$. The terms which depend on $a^1(y,t)$ are as follows:

$$\begin{aligned}&-\left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)+\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^1(y,t)\right.\\&\left.-i\partial_t a^1(y,t)\right]\chi_n(z;p(t))+i\dot{p}(t)\cdot\nabla_p\chi_n(z;p(t))a^1(y,t)\\&-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)\frac{1}{2}\left(\delta_{\alpha\beta}-\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)\chi_n(z;p(t))\\&-(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)\left((p(t)-i\partial_z)_\alpha-\partial_p E_n(p(t))_\alpha\right)\partial_{p_\beta}\chi_n(z;p(t)).\end{aligned} \tag{A.3.9}$$

Note that these terms have an identical form to the terms depending on $a^0(y,t)$ in expression (A.2.7) for $\xi^2(y,z,t)$ which were simplified to the form (A.2.10). We may therefore manipulate these terms in an identical way (specifically, using (2.1.19), (A.1.3)) into the form:

$$\begin{aligned}&=\left[i\partial_t a^1(y,t)-\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)-\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^1(y,t)\right.\\&\left.-\nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))\right]\chi_n(z;p(t))+P_n^\perp(p(t))\left[-ia^1(y,t)\nabla_q W(q(t))\cdot\nabla_p\chi_n(z;p(t))\right]\\&+[H(p(t))-E_n(p(t))]\left[\frac{1}{2}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t)\partial_{p_\alpha}\partial_{p_\beta}\chi_n(z;p(t))\right]\end{aligned} \tag{A.3.10}$$

Contributions to (A.3.6) depending on $a^0(y,t)$. The terms which depend on $a^0(y,t)$ may be written as $T_1+T_2+T_3+T_4$ where:

$$\begin{aligned}T_1:=-&\left[\frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\right.\\&\left.+\frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma a^0(y,t)\right]\chi_n(z;p(t))\end{aligned} \tag{A.3.11}$$

$$\begin{aligned} T_2 &:= -(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\left[-\frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))\chi_n(z;p(t))\right] \\ &- (-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\left[\frac{1}{2}\left(\delta_{\alpha\beta} - \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\right)\partial_{p_\gamma}\chi_n(z;p(t))\right] \\ &- (-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\left[\frac{1}{2}\left((p(t)-i\partial_z)_\alpha - \partial_{p_\alpha}E_n(p(t))\right)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t))\right] \end{aligned} \tag{A.3.12}$$

$$\begin{aligned} &T_3 := \\ &-\left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta - i\partial_t\right](-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \end{aligned} \tag{A.3.13}$$

$$\begin{aligned} T_4 := i&\left((p(t)-i\partial_z)_\beta - \partial_{p_\beta}E_n(p(t))\right)\partial_{q_\gamma}W(q(t))(-i\partial_{y_\beta})a^0(y,t) \\ &\times [H(p(t)) - E_n(p(t))]^{-1}P_n^\perp(p(t))\partial_{p_\gamma}\chi_n(z;p(t)) \end{aligned} \tag{A.3.14}$$

Using (A.1.4) and the equality of mixed partial derivatives, we can simplify $T_2$:

$$T_2 = [H(p(t)) - E_n(p(t))]\left[\frac{1}{6}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t))\right]. \tag{A.3.15}$$

We can simplify $T_3$ using the evolution equation for $a^0(y,t)$ (A.2.4):

$$\begin{aligned} T_3 &= -\left[\frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta\right](-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &+ (-i\partial_{y_\gamma})\left[i\partial_t a^0(y,t)\right]\partial_{p_\gamma}\chi_n(z;p(t)) + (-i\partial_{y_\gamma})a^0(y,t)i\dot{p}_\beta(t)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)) \\ &= -\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &\quad + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})y_\alpha y_\beta a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &\quad + \partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &\quad - i\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)). \end{aligned} \tag{A.3.16}$$

We now write $T_3 = T_{3,1} + T_{3,2}$ where:

$$\begin{aligned} T_{3,1} := &-\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &+ \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})y_\alpha y_\beta a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \end{aligned} \tag{A.3.17}$$

$$\begin{aligned} T_{3,2} := &\,\partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\ &- i\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)). \end{aligned} \tag{A.3.18}$$

We can simplify $T_{3,1}$ as follows. We first re-arrange (A.3.17):

$$T_{3,1} = \left((-i\partial_{y_\gamma})y_\alpha y_\beta - y_\alpha y_\beta(-i\partial_{y_\gamma})\right)\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)). \tag{A.3.19}$$

Using the identity: $(-i\partial_{y_\alpha})y_\beta - y_\beta(-i\partial_{y_\alpha}) = -i\delta_{\alpha\beta}$ twice we have that:

$$(-i\partial_{y_\gamma})y_\alpha y_\beta - y_\alpha y_\beta(-i\partial_{y_\gamma}) = (-i\delta_{\alpha\gamma})y_\beta + (-i\delta_{\beta\gamma})y_\alpha. \tag{A.3.20}$$

Using the symmetry $\partial_{q_\alpha}\partial_{q_\beta}W(q(t)) = \partial_{q_\beta}\partial_{q_\alpha}W(q(t))$ we have that:

$$T_{3,1} = -i\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha a^0(y,t)\partial_{p_\beta}\chi_n(z;p(t)). \tag{A.3.21}$$

Summing $T_1 + T_2 + T_{3,1} + T_{3,2} + T_4$ (A.3.11) (A.3.15) (A.3.21) (A.3.18) (A.3.14), we have that the terms which depend on $a^0(y,t)$ in (A.3.6) are equal to:

$$\begin{aligned}
&-\left[\frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\right.\\
&\left.+\frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma a^0(y,t)\right]\chi_n(z;p(t))\\
&+[H(p(t)) - E_n(p(t))]\left[\frac{1}{6}(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t))\right]\\
&-i\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha a^0(y,t)\partial_{p_\beta}\chi_n(z;p(t))\\
&+\partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t))\\
&-i\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t))\\
&+i\left((p(t)-i\partial_z)_\beta - \partial_{p_\beta}E_n(p(t))\right)\partial_{q_\gamma}W(q(t))(-i\partial_{y_\beta})a^0(y,t)\\
&\quad\times[H(p(t)) - E_n(p(t))]^{-1}P_n^\perp(p(t))\partial_{p_\gamma}\chi_n(z;p(t)).
\end{aligned} \tag{A.3.22}$$

By adding and subtracting terms and using the definition of $\mathcal{A}_n(p(t))$ (2.1.26) we can put (A.3.22) into the form:

$$\begin{aligned}
&\Bigg[i\partial_{q_\beta} W(q(t)) \Bigg( \left\langle \chi_n(z;p(t)) \right| \partial_{p_\beta} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \left\langle \chi_n(z;p(t)) \right| \partial_{p_\gamma} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \\
&+ \Big\langle \chi_n(z;p(t)) \Big| \left( (p(t) - i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p(t)) \right) [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\beta} \chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)} \\
&- \left\langle \chi_n(z;p(t)) \right| \partial_{p_\beta} \partial_{p_\gamma} \chi_n(z;p(t)) \big\rangle_{L^2_z(\Omega)} \Bigg) (-i\partial_{y_\gamma}) a^0(y,t) - \partial_{q_\alpha} \partial_{q_\beta} W(q(t)) \mathcal{A}_{n,\beta}(p(t)) y_\alpha a^0(y,t) \\
&- \frac{1}{6} \partial_{p_\alpha} \partial_{p_\beta} \partial_{p_\gamma} E_n(p(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma}) a^0(y,t) \\
&- \frac{1}{6} \partial_{q_\alpha} \partial_{q_\beta} \partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma a^0(y,t) \Bigg] \chi_n(z;p(t)) \\
&+ P_n^\perp(p(t)) \Bigg[ - i\partial_{q_\alpha} \partial_{q_\beta} W(q(t)) y_\alpha a^0(y,t) \partial_{p_\beta} \chi_n(z;p(t)) \\
&+ \partial_{q_\beta} W(q(t)) \mathcal{A}_{n,\beta}(p(t)) (-i\partial_{y_\gamma}) a^0(y,t) \partial_{p_\gamma} \chi_n(z;p(t)) \\
&- i\partial_{q_\beta} W(q(t)) (-i\partial_{y_\gamma}) a^0(y,t) \partial_{p_\beta} \partial_{p_\gamma} \chi_n(z;p(t)) \\
&+ i \left( (p(t) - i\partial_z)_\beta - \partial_{p_\beta} E_n(p(t)) \right) \partial_{q_\gamma} W(q(t)) (-i\partial_{y_\beta}) a^0(y,t) \\
&\quad \times [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\gamma} \chi_n(z;p(t)) \Bigg] \\
&+ [H(p(t)) - E_n(p(t))] \left[ \frac{1}{6} (-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma}) a^0(y,t) \partial_{p_\alpha} \partial_{p_\beta} \partial_{p_\gamma} \chi_n(z;p(t)) \right]
\end{aligned} \tag{A.3.23}$$

Adding (A.3.8), (A.3.10) and (A.3.22) we have that $\xi^3(y,z,t)$ can be decomposed as in (A.3.2) where $u^3(y,z,t)$ is given by (A.3.3) and $\tilde{\xi}^3(y,z,t)$ is equal to:

$$
\begin{aligned}
\tilde{\xi}^3(y,z,t) = \Big[ & i\partial_t a^1(y,t) - \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t) \\
& - \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^1(y,t) - \nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t)) \\
& + i\partial_{q_\beta}W(q(t)) \Big( \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\
& + \left\langle \chi_n(z;p(t)) \middle| \left((p(t)-i\partial_z)_\gamma - \partial_{p_\gamma}E_n(p(t))\right) [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\
& - \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \Big) (-i\partial_{y_\gamma})a^0(y,t) - \partial_{q_\alpha}\partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))y_\alpha a^0(y,t) \\
& - \frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t) \\
& - \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma a^0(y,t) \Big] \chi_n(z;p(t)) \\
& + P_n^\perp(p(t)) \Big[ -ia^1(y,t)\nabla_q W(q(t)) \cdot \nabla_p \chi_n(z;p(t)) - i\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha a^0(y,t)\partial_{p_\beta}\chi_n(z;p(t)) \\
& + \partial_{q_\beta}W(q(t))\mathcal{A}_{n,\beta}(p(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\gamma}\chi_n(z;p(t)) \\
& - i\partial_{q_\beta}W(q(t))(-i\partial_{y_\gamma})a^0(y,t)\partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)) \\
& + i\left((p(t)-i\partial_z)_\beta - \partial_{p_\beta}E_n(p(t))\right)\partial_{q_\gamma}W(q(t))(-i\partial_{y_\beta})a^0(y,t) \\
& \quad \times [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\gamma}\chi_n(z;p(t)) \Big]
\end{aligned}
\tag{A.3.24}
$$

□

*Proof of Lemma A.3.2.* Imposing the orthogonality condition (2.3.20) with $j = 3$ on $\tilde{\xi}^3(y,z,t)$ given by (A.3.24) we obtain:

$$
\begin{aligned}
i\partial_t a^1(y,t) = & \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})a^1(y,t) + \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}W(q(t))y_\alpha y_\beta a^1(y,t) \\
& + \nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))a^1(y,t) \\
& + \frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a^0(y,t) + \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))y_\alpha y_\beta y_\gamma a^0(y,t) \\
& + \kappa_\gamma(t)(-i\partial_{y_\gamma})a^0(y,t) + \partial_{q_\beta}\partial_{q_\gamma}W(q(t))\mathcal{A}_{n,\beta}(p(t))y_\gamma a^0(y,t)
\end{aligned}
\tag{A.3.25}
$$

which is precisely (A.3.4) with the coefficient multiplying $(-i\partial_{y_\gamma})a^0(y,t)$ replaced by:

$$\begin{aligned}\kappa_\gamma(t) &:= i\partial_{q_\beta} W(q(t)) \Big( \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &- \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &- i \Big\langle \chi_n(z;p(t)) \Big| \big((p(t)-i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p(t))\big) \\ &\qquad \times [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\beta}\chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)} \Big).\end{aligned} \tag{A.3.26}$$

We claim that:

$$\kappa_\gamma(t) = \partial_{q_\beta} W(q(t)) \partial_{p_\gamma} \mathcal{A}_{n,\beta}(p(t)). \tag{A.3.27}$$

Adding and subtracting $i\partial_{q_\beta} W(q(t)) \left\langle \partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)}$ in (A.3.26), we have that:

$$\kappa_\gamma(t) = \partial_{q_\beta} W(q(t)) \partial_{p_\gamma} \mathcal{A}_{n,\beta}(p(t)) + \tilde{\kappa}_\gamma(t) \tag{A.3.28}$$

where:

$$\begin{aligned}\tilde{\kappa}_\gamma(t) &:= i\partial_{q_\beta} W(q(t)) \Big( - \left\langle \partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &- \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &- i \Big\langle \chi_n(z;p(t)) \Big| \big((p(t)-i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p(t))\big) \\ &\qquad \times [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \partial_{p_\beta}\chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)} \Big).\end{aligned} \tag{A.3.29}$$

Using self-adjointness of the operators:

$$(p(t)-i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p(t)), [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \tag{A.3.30}$$

on $L^2_{per}$ for each $t \geq 0$, and then identity (A.1.2) we have that the last term in (A.3.29) is equal to:

$$\begin{aligned}&- \Big\langle [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) \big((p(t)-i\partial_z)_\gamma - \partial_{p_\gamma} E_n(p(t))\big) \chi_n(z;p(t)) \Big| \partial_{p_\beta}\chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)} \\ &= \Big\langle [H(p(t)) - E_n(p(t))]^{-1} P_n^\perp(p(t)) [H(p(t)) - E_n(p(t))] \partial_{p_\gamma}\chi_n(z;p(t)) \Big| \partial_{p_\beta}\chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)}.\end{aligned} \tag{A.3.31}$$

It is clear that the operators $P_n^\perp(p(t)), [H(p(t)) - E_n(p(t))]$ commute on $L^2_{per}$ for any $t \geq 0$. We have therefore that this term:

$$= \Big\langle P_n^\perp(p(t)) \partial_{p_\gamma}\chi_n(z;p(t)) \Big| \partial_{p_\beta}\chi_n(z;p(t)) \Big\rangle_{L^2_z(\Omega)}. \tag{A.3.32}$$

Substituting (A.3.32) into (A.3.29) we obtain:

$$\begin{aligned}\tilde{\kappa}_\gamma(t) = i\partial_{q_\beta} W(q(t)) \Big[ &- \left\langle \partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &- \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &+ \left\langle P_n^\perp(p(t))\partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \Big].\end{aligned} \tag{A.3.33}$$

Recall that $\chi_n(z;p(t))$ is assumed normalized: $\langle \chi_n(z;p(t)) | \chi_n(z;p(t)) \rangle_{L^2_z(\Omega)} = 1$. Differentiating this relation with respect to $p$ and using the definition of the $L^2$-inner product we obtain:

$$\overline{\left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle}_{L^2_z(\Omega)} = - \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)}. \tag{A.3.34}$$

We now use conjugate linearity of the $L^2$-inner product in its first argument and the identity (A.3.34) to re-write the expression inside the square brackets in (A.3.33) as:

$$\begin{aligned}&- \left\langle \partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &+ \left\langle \left\langle \chi_n(z;p(t)) \middle| \partial_{p_\gamma}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)} \\ &+ \left\langle P_n^\perp(p(t))\partial_{p_\gamma}\chi_n(z;p(t)) \middle| \partial_{p_\beta}\chi_n(z;p(t)) \right\rangle_{L^2_z(\Omega)}\end{aligned} \tag{A.3.35}$$

which is clearly zero by definition of the orthogonal projection operator $P_n^\perp(p(t))$ (2.3.21). (A.3.29) is therefore zero, and the claim (A.3.27) holds. □

## A.4 Proof of $L^\infty$ bounds on $z$-dependence of residual, uniform in $p \in S_n$

In this Appendix we provide details on how to bound the $z$-dependence of terms which appear in the residual (2.3.36) in $L^\infty_z$, uniformly in $p \in S_n$, where:

$$S_n := \{p \in \mathbb{R}^d : \inf_{m \neq n} |E_m(p) - E_n(p)| \geq M\}, \text{ and } M > 0. \tag{A.4.1}$$

We consider the problem of bounding a representative term:

$$\begin{aligned}&\mathcal{J}_{\alpha\beta}(p) := \|g_{\alpha\beta}(z;p)\|_{L^\infty_z(\Omega)} \\ &g_{\alpha\beta}(z;p) := [(p_\alpha - i\partial_{z_\alpha}) - \partial_{p_\alpha}E_n(p)]\, [H(p) - E_n(p)]^{-1} P_n^\perp(p)\partial_{p_\beta}\chi_n(z;p).\end{aligned} \tag{A.4.2}$$

uniformly in $p \in S_n$. Note that although the maps $p \mapsto E_n(p)$ are periodic with respect to the lattice $\Lambda$, the map $p \mapsto g(z;p)$ is not. We claim that:

$$\sup_{p\in S_n} \mathcal{J}_{\alpha\beta}(p) = \|g_{\alpha\beta}(z;p)\|_{L^\infty_z(\Omega)} < \infty. \tag{A.4.3}$$

First, we define the 'shifted' Sobolev norms for any vector $p \in \mathbb{R}^d$ to be:

$$\|f(z)\|_{H^s_{z,p}(\Omega)} := \sum_{|j|\le s} \|(p - i\partial_z)^j f(z)\|_{L^2_z(\Omega)}. \tag{A.4.4}$$

For any fixed $p$, $H^s_{z,p}$ is equivalent to the standard norm $H^s_z$. Using Sobolev embedding we have that for any integer $s > \frac{d}{2}$:

$$\|g_{\alpha\beta}(z;p)\|_{L^\infty_z} = \|e^{ipz} g_{\alpha\beta}(z;p)\|_{L^\infty_z} \le C_{s,d}\|e^{ipz} g_{\alpha\beta}(z;p)\|_{H^s_z} = C_{s,d}\|g_{\alpha\beta}(z;p)\|_{H^s_{z,p}}. \tag{A.4.5}$$

where the constant $C_{s,d} > 0$ depends on $s$ and $d$ but is independent of $p$. We are therefore done if we can show that $\|g_{\alpha\beta}(z;p)\|_{H^s_{z,p}}$ can be bounded uniformly in $p \in S_n$ for some integer $s > d/2$.

From the definition of the $H^s_{z,p}$-norms and periodicity of $\partial_{p_\alpha} E_n(p)$ we have that for any integer $s \ge 1$, $p \in S_n$:

$$\|(p_\alpha - i\partial_{z_\alpha}) - \partial_{p_\alpha} E_n(p)\|_{H^s_{z,p} \to H^{s-1}_{z,p}} \le C', \tag{A.4.6}$$

where $C' := 1 + \sup_{p\in S_n \cap \mathcal{B}} |E_n(p)|$. By elliptic regularity, we have that for any integer $s \ge 0$, all $p \in S_n$:

$$\|[H(p) - E_n(p)]^{-1} P_n^\perp(p)\|_{H^s_{z,p} \to H^{s+2}_{z,p}} \lesssim \frac{1}{M}. \tag{A.4.7}$$

Differentiating the eigenvalue equation (2.2.6) for $\chi_n(z;p)$ with respect to $p$, we have that $P_n^\perp(p)\partial_{p_\beta}\chi_n(z;p)$ satisfies:

$$[H(p) - E_n(p)]P_n^\perp(p)\partial_{p_\beta}\chi_n(z;p) = -P_n^\perp(p)\left[(p_\beta - i\partial_{z_\beta}) - \partial_{p_\beta}E_n(p)\right]\chi_n(z;p). \tag{A.4.8}$$

Again, by elliptic regularity, for all $p \in S_n$:

$$\|P_n^\perp(p)\partial_{p_\beta}\chi_n(z;p)\|_{H^{s+2}_p} \lesssim \frac{1}{M}\|\left[(p_\beta - i\partial_{z_\beta}) - \partial_{p_\beta}E_n(p)\right]\chi_n(z;p)\|_{H^s_{z,p}}. \tag{A.4.9}$$

Using (A.4.6) we then have for all $p \in S_n$:

$$\|P_n^\perp(p)\partial_{p_\beta}\chi_n(z;p)\|_{H^{s+2}_p} \le \frac{C'}{M}\|\chi_n(z;p)\|_{H^{s+1}_{z,p}}. \tag{A.4.10}$$

Combining (A.4.6), (A.4.7), and (A.4.10) we have:

$$\begin{aligned}
\|g_{\alpha\beta}(z;p)\|_{H^s_{z,p}} &\leq C' \|[H(p) - E_n(p)]^{-1} P_n^\perp(p) \partial_{p_\beta} \chi_n(z;p)\|_{H^{s+1}_{z,p}} && \text{(using (A.4.6))} \\
&\lesssim \frac{C'}{M} \|P_n^\perp(p) \partial_{p_\beta} \chi_n(z;p)\|_{H^{s-1}_{z,p}} && \text{(using (A.4.7))} \\
&\lesssim \left(\frac{C'}{M}\right)^2 \|\chi_n(z;p)\|_{H^{s-2}_{z,p}} \quad . && \text{(using (A.4.10))} \qquad \text{(A.4.11)}
\end{aligned}$$

We now claim that for any integer $s$:

$$\sup_{p \in S_n} \|\chi_n(z;p)\|_{H^s_{z,p}} = \sup_{p \in S_n \cap \mathcal{B}} \|\chi_n(z;p)\|_{H^s_{z,p}} < \infty. \tag{A.4.12}$$

By elliptic regularity it is clear that for any fixed $p \in \mathbb{R}^d$ and fixed positive integer $s$ that:

$$\|\chi_n(z;p)\|_{H^s_{z,p}} < \infty. \tag{A.4.13}$$

Using smoothness of the map $p \mapsto \chi_n(z;p)$ in $S_n$ and compactness of the Brillouin zone $\mathcal{B}$ we have that:

$$\sup_{p \in S_n \cap \mathcal{B}} \|\chi_n(z;p)\|_{H^s_{z,p}} < \infty. \tag{A.4.14}$$

Since for any reciprocal lattice vector $b \in \Lambda^*$ we have that $\chi_n(z; p+b) = e^{-ib\cdot z}\chi_n(z;p)$, we then have that:

$$\text{for any } b \in \Lambda^*,\ \|\chi_n(z;p+b)\|_{H^s_{z,p+b}} = \|e^{-ib\cdot z}\chi_n(z;p)\|_{H^s_{z,p+b}} = \|\chi_n(z;p)\|_{H^s_{z,p}}. \tag{A.4.15}$$

The bound (A.4.12) follows.

We now turn to completing the proof of (A.4.3). Fix $\sigma$, a positive integer such that $\sigma > \max\{\frac{d}{2}, 2\}$. Then:

$$\begin{aligned}
\sup_{p \in S_n} \mathcal{J}(p) &= \sup_{p \in S_n} \|g_{\alpha\beta}(z;p)\|_{L^\infty_z} && \text{(by definition)} \\
&\leq C_{s,d} \sup_{p \in S_n} \|g_{\alpha\beta}(z;p)\|_{H^\sigma_{z,p}} && \text{(by Sobolev embedding, since } \sigma > d/2) \\
&\leq C_{s,d} \left(\frac{C'}{M}\right)^2 \sup_{p \in S_n} \|\chi_n(z;p)\|_{H^{\sigma-2}_{z,p}} && \text{(by (A.4.11), with } s = \sigma) \\
&= C_{s,d} \left(\frac{C'}{M}\right)^2 \sup_{p \in \mathcal{B} \cap S_n} \|\chi_n(z;p)\|_{H^{\sigma-2}_{z,p}} && \text{(using (A.4.12) with } s = \sigma - 2) \\
&< \infty. && \text{(by (A.4.14) with } s = \sigma - 2)
\end{aligned}$$

All other $z$-dependence in expression (2.3.36) for the residual may be bounded in $L^\infty_z$ uniformly in $p \in S_n$ by similar arguments.

## A.5 Proof of Lemma 2.4.1

First, it is clear from changing variables in the integral that:

$$\int_{\mathbb{R}^d} f(x)\, g\left(\frac{x}{\delta}+\frac{c}{\delta^2}\right)\,\mathrm{d}x = \left(\int_{\mathbb{R}^d} f(x)\,\mathrm{d}x\right)\left(\int_{\Omega} g(z)\,\mathrm{d}z\right) + O(\delta^N) \tag{A.5.1}$$

is equivalent to:

$$\int_{\mathbb{R}^d} f\left(x-\frac{c}{\delta}\right) g\left(\frac{x}{\delta}\right)\,\mathrm{d}x = \left(\int_{\mathbb{R}^d} f(x)\,\mathrm{d}x\right)\left(\int_{\Omega} g(z)\,\mathrm{d}z\right) + O(\delta^N). \tag{A.5.2}$$

Let $v_j, j \in \{1,...,d\}$ denote generators of the lattice $\Lambda$ so that if $v \in \Lambda$, there exist unique integers $n_j, j \in \{1,...,d\}$ such that:

$$v = n_1 v_1 + n_2 v_2 + ... + n_d v_d. \tag{A.5.3}$$

And let $b_j, j \in \{1,...,d\}$ denote generators of the dual lattice $\Lambda^*$ such that if $b \in \Lambda^*$, there exist unique integers $m_j, j \in \{1,...,d\}$ such that:

$$b = m_1 b_1 + m_2 b_2 + ... + m_d b_d, \tag{A.5.4}$$

and furthermore, for all $i,j \in \{1,...,d\}$, $b_i \cdot v_j = 2\pi\delta_{ij}$.

Since $g(z)$ is smooth and periodic with respect to the lattice $\Lambda$, it has a uniformly convergent Fourier series:

$$\begin{aligned} g(z) &= \sum_{(m_1,...,m_d)\in\mathbb{Z}^d} g_{m_1,...,m_d} e^{i[m_1 b_1\cdot z + m_2 b_2 \cdot z + ... m_d b_d \cdot z]} \\ g_{m_1,...,m_d} &= \int_{\mathbb{R}^d/\Lambda} e^{-i[m_1 b_1\cdot z + m_2 b_2 \cdot z + ... m_d b_d \cdot z]} g(z)\,\mathrm{d}z. \end{aligned} \tag{A.5.5}$$

We have therefore that:

$$\int_{\mathbb{R}^d} f\left(x-\frac{c}{\delta}\right) g\left(\frac{x}{\delta}\right)\,\mathrm{d}x = \sum_{(m_1,...,m_d)\in\mathbb{Z}^d} g_{m_1,...,m_d} \int_{\mathbb{R}^d} e^{i[m_1 b_1\cdot x/\delta + m_2 b_2\cdot x/\delta + ... m_d b_d \cdot x/\delta]} f(x-c/\delta)\,\mathrm{d}x \tag{A.5.6}$$

where it is valid to change the order of summation of the series with the integration by uniform convergence of the series. We now write the right-hand side of (A.5.6) as:

$$\begin{aligned} &= g_{0,...,0} \int_{\mathbb{R}^d} f(x-c/\delta)\,\mathrm{d}x \\ &+ \sum_{(m_1,...,m_d)\in\mathbb{Z}^d, (m_1,...,m_d)\neq(0,...0)} g_{m_1,...,m_d} \int_{\mathbb{R}^d} e^{i[m_1 b_1\cdot x/\delta + m_2 b_2\cdot x/\delta + ... m_d b_d \cdot x/\delta]} f(x-c/\delta)\,\mathrm{d}x \end{aligned} \tag{A.5.7}$$

By the definition of $g_{0,\ldots,0}$ (A.5.5) and by a trivial change of variables we have that:

$$g_{0,\ldots,0} \int_{\mathbb{R}^d} f(x - c/\delta)\,\mathrm{d}x = \left(\int_{\mathbb{R}^d} f(x)\,\mathrm{d}x\right)\left(\int_{\Omega} g(z)\,\mathrm{d}z\right) \tag{A.5.8}$$

To see that the second term in (A.5.7) is of $O(\delta^N)$ for arbitrary $N \in \mathbb{N}$, consider a representative term in the series where $(m_1, \ldots, m_d) = (1, 0, \ldots, 0)$:

$$\left| g_{1,0,\ldots 0} \int_{\mathbb{R}^d} e^{ib_1 \cdot x/\delta} f(x - c/\delta)\,\mathrm{d}x \right| = \left| g_{1,0,\ldots 0} \int_{\mathbb{R}^d} \left[ \left( \frac{-i\delta v_1 \cdot \nabla_x}{2\pi} \right)^N e^{ib_1 \cdot x/\delta} \right] f(x - c/\delta)\,\mathrm{d}x \right| \tag{A.5.9}$$

Integrating by parts gives:

$$\begin{aligned} &= \left| g_{1,0,\ldots 0} \int_{\mathbb{R}^d} e^{ib_1 \cdot x/\delta} \left[ \left( \frac{i\delta v_1 \cdot \nabla_x}{2\pi} \right)^N f(x - c/\delta) \right] \mathrm{d}x \right| \\ &\le \delta^N \frac{1}{(2\pi)^N} |g_{1,0,\ldots 0}| \int_{\mathbb{R}^d} \left| (v_1 \cdot \nabla_x)^N f(x - c/\delta) \right| \mathrm{d}x \end{aligned} \tag{A.5.10}$$

Using the definition of $g_{1,0,\ldots 0}$ (A.5.5) and another change of variables, we have:

$$\le \delta^N \frac{1}{(2\pi)^N} \int_{\mathbb{R}/\Lambda} |g(z)|\,\mathrm{d}z \int_{\mathbb{R}^d} \left| (v_1 \cdot \nabla_x)^N f(x) \right| \mathrm{d}x \tag{A.5.11}$$

since $f \in \mathcal{S}(\mathbb{R}^d)$, we are done:

$$\left| \int_{\mathbb{R}^d} f\left(x + \frac{c}{\delta}\right) g\left(\frac{x}{\delta}\right) \mathrm{d}x - \left(\int_{\mathbb{R}^d} f(x)\,\mathrm{d}x\right)\left(\int_{\Omega} g(z)\,\mathrm{d}z\right) \right| \le C_{N,f,g}\delta^N \tag{A.5.12}$$

where $C_N > 0$ is a positive constant which depends on $N, f, g$ but not $\delta$.

## A.6 Computation of dynamics of physical observables

In this Appendix we compute:

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\left[ \langle b(y,t) | a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \\ &\frac{\mathrm{d}}{\mathrm{d}t}\left[ \langle a(y,t) | y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right], \frac{\mathrm{d}}{\mathrm{d}t}\left[ \langle a(y,t) | (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \\ &\frac{\mathrm{d}}{\mathrm{d}t}\left[ \langle b(y,t) | y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | y b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \\ &\frac{\mathrm{d}}{\mathrm{d}t}\left[ \langle b(y,t) | (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t) | (-i\nabla_y) b(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \right] \end{aligned} \tag{A.6.1}$$

We will make use of the following simple lemmas which are each elementary to prove:

**Lemma A.6.1.** *Let $a(y,t)$ satisfy:*

$$i\partial_t a = \mathscr{H}(t)a \tag{A.6.2}$$

*where $\mathscr{H}(t)$ is self-adjoint for every $t$. Let $\mathcal{G}(t)$ denote a physical observable defined by:*

$$\mathcal{G}(t) := \int_{\mathbb{R}^d} \overline{a(y,t)} G a(y,t)\, dy \tag{A.6.3}$$

*where $G$ is self-adjoint. Then:*

$$\dot{\mathcal{G}}(t) = i \int_{\mathbb{R}^d} \overline{a(y,t)} [\mathscr{H}(t), G] a(y,t)\, dy \tag{A.6.4}$$

**Lemma A.6.2.** *Let $a(y,t)$ satisfy (A.6.2), and $b(y,t)$ satisfy:*

$$i\partial_t b = \mathscr{H}(t)b + \mathscr{I}(t)a \tag{A.6.5}$$

*where $\mathscr{I}(t)$ is self-adjoint for every $t$. Define:*

$$\mathcal{K}(t) := \int_{\mathbb{R}^d} \overline{b(y,t)} K a(y,t)\, dy + \int_{\mathbb{R}^d} \overline{a(y,t)} K b(y,t)\, dy \tag{A.6.6}$$

*where $K$ is self-adjoint. Then:*

$$\begin{aligned}\dot{\mathcal{K}}(t) &= i \int_{\mathbb{R}^d} \overline{b(y,t)} [\mathscr{H}(t), K] a(y,t)\, dy + i \int_{\mathbb{R}^d} \overline{a(y,t)} [\mathscr{H}(t), K] b(y,t)\, dy \\ &+ i \int_{\mathbb{R}^d} \overline{a(y,t)} [\mathscr{I}(t), K] a(y,t)\, dy\end{aligned} \tag{A.6.7}$$

**Lemma A.6.3.** *Let $G_1, G_2, G_3$ be operators. Then:*

$$\begin{aligned}[G_1 G_2, G_3] &= G_1 [G_2, G_3] + [G_1, G_3] G_2 \\ [G_1, G_2 G_3] &= [G_1, G_2] G_3 + G_2 [G_1, G_3]\end{aligned} \tag{A.6.8}$$

**Lemma A.6.4.**

$$[(-i\partial_{y_\alpha}), y_\beta] = -i\delta_{\alpha\beta}, [y_\alpha, (-i\partial_{y_\beta})] = i\delta_{\alpha\beta}. \tag{A.6.9}$$

We will apply the Lemmas with:

$$\mathscr{H}(t) = \frac{1}{2} \partial_{p_\alpha} \partial_{p_\beta} E_n(p(t)) (-i\partial_{y_\alpha})(-i\partial_{y_\beta}) + \frac{1}{2} \partial_{q_\alpha} \partial_{q_\beta} W(q(t)) y_\alpha y_\beta \tag{A.6.10}$$

For any operator $G$, we have:

$$\begin{aligned}i[\mathscr{H}(t), G] &= \frac{1}{2} i\partial_{p_\alpha} \partial_{p_\beta} E_n(p(t)) (-i\partial_{y_\alpha}) [(-i\partial_{y_\beta}), G] + \frac{1}{2} i\partial_{p_\alpha} \partial_{p_\beta} E_n(p(t)) [(-i\partial_{y_\alpha}), G] (-i\partial_{y_\beta}) \\ &+ \frac{1}{2} i\partial_{q_\alpha} \partial_{q_\beta} W(q(t))(t) y_\alpha [y_\beta, G] + \frac{1}{2} i\partial_{q_\alpha} \partial_{q_\beta} W(q(t))(t) [y_\alpha, G] y_\beta\end{aligned} \tag{A.6.11}$$

From (A.6.11), we have:

$$\begin{aligned} i[\mathscr{H}(t), y_\alpha] &= \partial_{p_\alpha}\partial_{p_\beta} E_n(p(t))(-i\partial_{y_\beta}) \\ i[\mathscr{H}(t), (-i\partial_{y_\alpha})] &= -\partial_{q_\alpha}\partial_{q_\beta} W(q(t)) y_\beta \end{aligned} \tag{A.6.12}$$

So that, using Lemma A.6.1:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left\langle a(y,t) \right| y_\alpha a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} &= \partial_{p_\alpha}\partial_{p_\beta} E_n(p(t)) \left\langle a(y,t) \right| (-i\partial_{y_\beta}) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} \\ \frac{\mathrm{d}}{\mathrm{d}t} \left\langle a(y,t) \right| (-i\partial_{y_\alpha}) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} &= -\partial_{q_\alpha}\partial_{q_\beta} W(q(t)) \left\langle a(y,t) \right| y_\beta a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} . \end{aligned} \tag{A.6.13}$$

Note that it follows from (A.6.13) that:

$$\begin{aligned} &\left\langle a(y,0) \right| y a(y,0) \rangle_{L^2_y(\mathbb{R}^d)} = \left\langle a(y,0) \right| (-i\nabla_y) a(y,0) \rangle_{L^2_y(\mathbb{R}^d)} = 0 \\ &\implies \text{ for all } t \geq 0, \left\langle a(y,t) \right| y a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} = \left\langle a(y,t) \right| (-i\nabla_y) a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} = 0. \end{aligned} \tag{A.6.14}$$

We will then apply Lemma A.6.2 with:

$$\begin{aligned} \mathscr{I}(t) &= \frac{1}{6}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma} E_n(p(t))(-i\partial_{y_\alpha})(-i\partial_{y_\beta})(-i\partial_{y_\gamma}) + \frac{1}{6}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\alpha y_\beta y_\gamma \\ &+ \partial_{p_\beta}\left[\nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))\right](-i\partial_{y_\beta}) + \partial_{q_\beta}\left[\nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))\right] y_\beta \end{aligned} \tag{A.6.15}$$

Calculating the commutators:

$$\begin{aligned} &i[\mathscr{I}(t), 1] = 0 \\ &i[\mathscr{I}(t), y_\alpha] = \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma} E_n(p(t))(-i\partial_{y_\beta})(-i\partial_{y_\gamma}) + \partial_{p_\alpha}\left[\nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))\right] \\ &i[\mathscr{I}(t), (-i\partial_{y_\alpha})] = -\frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma} W(q(t)) y_\beta y_\gamma - \partial_{q_\alpha}\left[\nabla_q W(q(t)) \cdot \mathcal{A}_n(p(t))\right] \end{aligned} \tag{A.6.16}$$

We have, by Lemma A.6.2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\left\langle b(y,t) \right| a(y,t) \rangle_{L^2_y(\mathbb{R}^d)} + \left\langle a(y,t) \right| b(y,t) \rangle_{L^2_y(\mathbb{R}^d)}\right] = 0 \tag{A.6.17}$$

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left[\langle b(y,t)|\, y_\alpha a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t)|\, y_\alpha b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&= \partial_{p_\alpha}\partial_{p_\beta}E_n(p(t))\left[\langle b(y,t)|\,(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t)|\,(-i\partial_{y_\alpha})b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&+ \frac{1}{2}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E_n(p(t))\left\langle a(y,t)|\,(-i\partial_{y_\beta})(-i\partial_{y_\gamma})a(y,t)\right\rangle_{L^2_y(\mathbb{R}^d)} \\
&+ \partial_{p_\alpha}\left[\nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))\right]\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)} \\
&\frac{\mathrm{d}}{\mathrm{d}t}\left[\langle b(y,t)|\,(-i\partial_{y_\alpha})a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t)|\,(-i\partial_{y_\alpha})b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&= -\partial_{q_\alpha}\partial_{q_\beta}W(q(t))\left[\langle b(y,t)|\, y_\beta a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} + \langle a(y,t)|\, y_\beta b(y,t)\rangle_{L^2_y(\mathbb{R}^d)}\right] \\
&- \frac{1}{2}\partial_{q_\alpha}\partial_{q_\beta}\partial_{q_\gamma}W(q(t))\,\langle a(y,t)|\, y_\beta y_\gamma a(y,t)\rangle_{L^2_y(\mathbb{R}^d)} \\
&- \partial_{q_\alpha}\left[\nabla_q W(q(t))\cdot\mathcal{A}_n(p(t))\right]\|a(y,t)\|^2_{L^2_y(\mathbb{R}^d)}.
\end{aligned} \tag{A.6.18}$$

## A.7 Berry phase and curvature in a two-by-two matrix example

Consider the matrix depending on parameters:

$$H(x,y,z) := \begin{pmatrix} z & x+iy \\ x-iy & -z \end{pmatrix} \tag{A.7.1}$$

where $x, y, z \in \mathbb{R}$. This matrix has eigenvalues:

$$E_\pm = \pm(x^2+y^2+z^2)^{1/2}. \tag{A.7.2}$$

so that $E_+ = E_-$ at $x = y = z = 0$. Introduce standard spherical polar co-ordinates:

$$\begin{aligned} x &= \rho\sin\theta\cos\phi \\ y &= \rho\sin\theta\sin\phi \\ z &= \rho\cos\theta \end{aligned} \tag{A.7.3}$$

where now $\rho \in \mathbb{R}, \theta \in [0,\pi), \phi \in [0,2\pi)$. Note that the Jacobian of this transformation:

$$\left|\frac{\partial(x,y,z)}{\partial(\rho,\theta,\phi)}\right| = \rho^2\sin\theta \tag{A.7.4}$$

which implies that the change of variables is not smooth anywhere on the $z-$axis (where $\rho = 0$ or $\theta = 0$). In the new variables the matrix becomes:

$$H(\rho,\theta,\phi) = \rho\begin{pmatrix} \cos\theta & \sin\theta e^{i\phi} \\ \sin\theta e^{-i\phi} & -\cos\theta \end{pmatrix}. \tag{A.7.5}$$

This matrix has eigenvalues:

$$E_{\pm} = \pm\rho \tag{A.7.6}$$

So that $E_+ = E_-$ at $\rho = 0$. The normalized eigenvectors associated with these eigenvalues are unique up to a choice of gauge. Specifically, if $\chi_\pm$ are normalized eigenvectors of the eigenvalues $E_\pm$, then so are $e^{i\delta_\pm}\chi_\pm$ where $\delta_\pm \in \mathbb{R}$. One possible choice of normalized eigenvectors is given by:

$$\chi_+ = \begin{pmatrix} \cos(\theta/2)e^{i\phi} \\ \sin(\theta/2) \end{pmatrix}, \chi_- = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{-i\phi} \end{pmatrix} \tag{A.7.7}$$

This choice is smooth away from the $z$-axis and $2\pi$-periodic in $\phi$:

$$\chi_\pm(\phi + 2\pi) = \chi_\pm(\phi) \tag{A.7.8}$$

Another choice is given by making the gauge transformation:

$$\chi'_\pm := e^{\mp i\phi/2}\chi_\pm \tag{A.7.9}$$

the new eigenvectors are:

$$\chi'_+ = \begin{pmatrix} \cos(\theta/2)e^{i\phi/2} \\ \sin(\theta/2)e^{-i\phi/2} \end{pmatrix}, \chi'_- = \begin{pmatrix} \sin(\theta/2)e^{i\phi/2} \\ -\cos(\theta/2)e^{-i\phi/2} \end{pmatrix} \tag{A.7.10}$$

This choice is smooth away from the $z-$axis and the $\phi = 0$ half-plane. Across the $\phi = 0$ half-plane the eigenfunctions change sign:

$$\chi'_\pm(\phi + 2\pi) = -\chi'_\pm(\phi) \tag{A.7.11}$$

According to the adiabatic theorem of quantum mechanics, a system prepared in an eigenstate of the Hamiltonian corresponding to an isolated eigenvalue remains proportional to the eigenstate after the parameters of the system have been varied adiabatically in a closed loop. Consider the example of the matrix Hamiltonian (A.7.5), and let $\gamma$ be a closed loop in parameter space parameterized by $\tau : \gamma(\tau) = (\rho(\tau), \theta(\tau), \phi(\tau)), \tau \in [0, 1], \gamma(1) = \gamma(0)$. Assuming that the variation is slow enough, the final state of a system prepared initially in an eigenstate of the matrix Hamiltonian:

$$\psi(0) = \chi_\pm(\gamma(0)) \tag{A.7.12}$$

is given by:

$$\psi(1) = e^{\mp i\int_0^1 \rho(\gamma(\tau))\,\mathrm{d}\tau} e^{i\phi_{B,\pm}(\gamma)}\chi_\pm(\gamma(1)) \tag{A.7.13}$$

The first factor is known as the dynamic phase and is analogous to the factor $e^{-iEt}$ which would appear in the case where the parameters remain fixed. The second factor is known as the geometric phase, and is given by integrating the Berry connection along the path:

$$\phi_{B,\pm}(\gamma) = \int_0^1 \mathcal{A}_\pm(\gamma(\tau)) \cdot \dot{\gamma}(\tau)\,\mathrm{d}\tau \tag{A.7.14}$$

where the Berry connections $\mathcal{A}_\pm$ in each eigenspace are given by:

$$\mathcal{A}_\pm := i\,\langle \chi_\pm | \,\nabla \chi_\pm \rangle \tag{A.7.15}$$

In spherical polar co-ordinates, $\dot{\gamma}(\tau)$ is:

$$\dot{\gamma}(\tau) = \dot{\rho}\hat{\rho} + \dot{\theta}\rho\hat{\theta} + \dot{\phi}\rho\sin\theta\hat{\phi}. \tag{A.7.16}$$

and $\nabla$ is given by:

$$\nabla f = \hat{\rho}\partial_\rho f + \hat{\theta}\frac{1}{\rho}\partial_\theta f + \hat{\phi}\frac{1}{\rho\sin\theta}\partial_\phi f. \tag{A.7.17}$$

Explicit computation gives:

$$\mathcal{A}_\pm = \mp\frac{1}{2}\frac{1+\cos\theta}{\rho\sin\theta}\hat{\phi} \tag{A.7.18}$$

As an example consider the path $\gamma_0(\tau) = (\rho(\tau) = 1, \theta(\tau) = \pi/2, \phi(\tau) = 2\pi\tau), \tau \in [0, 1]$. Then:

$$\phi_{B,\pm}(\gamma_0) = \mp\pi = \pi \tag{A.7.19}$$

where the final equality is understood as modulo $2\pi$. So that the final state of the system is given by:

$$\psi(1) = e^{\mp i\int_0^1 \rho(\gamma_0(\tau))\,\mathrm{d}\tau} e^{i\pi} \chi_\pm(\gamma_0(1)) \tag{A.7.20}$$

since the $\chi_\pm$ are $2\pi$-periodic in $\phi$, $\chi_\pm(\gamma_0(1)) = \chi_\pm(\gamma_0(0))$ so that:

$$\psi(1) = -e^{\mp i\int_0^1 \rho(\gamma_0(\tau))\,\mathrm{d}\tau}\psi(0) \tag{A.7.21}$$

We can study the same problem in the primed gauge. Taking initial data:

$$\psi(0) = \chi'_\pm(\gamma_0(0)) \tag{A.7.22}$$

then the final state of the system is given by:

$$\psi(1) = e^{\mp i\int_0^1 \rho(\gamma_0(\tau))\,\mathrm{d}\tau} e^{i\phi'_{B,\pm}(\gamma_0)} \chi'_\pm(\gamma_0(1)) \tag{A.7.23}$$

where:

$$\phi'_{B,\pm}(\gamma) = \int_0^1 \mathcal{A}'_\pm(\gamma(\tau)) \cdot \dot{\gamma}(\tau)\,\mathrm{d}\tau \tag{A.7.24}$$

The Berry connection in the primed gauge is:

$$\mathcal{A}'_\pm := i \left\langle \chi'_\pm \middle| \nabla \chi'_\pm \right\rangle \tag{A.7.25}$$

Explicit computation gives:

$$\mathcal{A}'_\pm = \mp \frac{1}{2} \frac{\cos\theta}{\rho \sin\theta} \hat{\phi} \tag{A.7.26}$$

which is zero for $\theta = \pi/2$. For the example loop $\gamma_0(\tau)$:

$$\psi(1) = e^{\mp i \int_0^1 \rho(\gamma_0(\tau))\,\mathrm{d}\tau} \chi'_\pm(\gamma_0(1)) \tag{A.7.27}$$

since the $\chi'_\pm$ are $2\pi$-anti-periodic, $\chi_\pm(\gamma_0(1)) = -\chi_\pm(\gamma_0(0))$ so that:

$$\psi(1) = -e^{\mp i \int_0^1 \rho(\gamma_0(\tau))\,\mathrm{d}\tau} \psi(0) \tag{A.7.28}$$

which verifies that the result of adiabatic transport of the eigenvector about a closed loop is gauge-invariant when the Berry phase is taken into account.

### A.7.1 Berry curvature

Another route to this result is as follows. Since the path $\gamma(\tau)$ is closed we can transform the line integral into a flux integral:

$$\phi_{B,\pm}(\gamma) = \int_\gamma \mathcal{A}_\pm \cdot \mathrm{d}\gamma = \int_\Omega \mathcal{F}_\pm \cdot \mathrm{d}S \tag{A.7.29}$$

where $\Omega$ is any surface whose boundary is the curve $\gamma$ and:

$$\mathcal{F}_\pm = \nabla \times \mathcal{A}_\pm \tag{A.7.30}$$

is the Berry curvature. The Berry curvature is gauge independent since under the gauge transformation:

$$\chi_\pm \to \chi'_\pm = e^{i\delta_\pm} \chi_\pm, \tag{A.7.31}$$

the Berry connection and curvature transform as:

$$\begin{aligned} \mathcal{A}_\pm &\to \mathcal{A}'_\pm = \mathcal{A}_\pm - \nabla \delta_\pm \\ \mathcal{F}_\pm &\to \mathcal{F}'_\pm \end{aligned} \tag{A.7.32}$$

For the example curve $\gamma_0$ I can take $\Omega$ to be the upper hemisphere of the sphere: $\Omega = (\rho = 1, \theta \in [0, \pi/2], \phi \in [0, 2\pi])$. Let be an arbitrary vector field, then define:

$$A_\rho := \hat{\rho} \cdot A, A_\theta := \hat{\theta} \cdot A, A_\phi := \hat{\phi} \cdot A \tag{A.7.33}$$

then the curl operator in polar co-ordinates is:

$$\begin{aligned} \nabla \times A = & \frac{1}{\rho \sin\theta} \left( \partial_\theta (A_\phi \sin\theta) - \partial_\phi A_\theta \right) \hat{\rho} \\ & + \frac{1}{\rho} \left( \frac{1}{\sin\theta} \partial_\phi A_\rho - \partial_\rho (\rho A_\phi) \right) \hat{\theta} + \frac{1}{\rho} \left( \partial_\rho (\rho A_\theta) - \partial_\theta A_\rho \right) \hat{\phi}. \end{aligned} \tag{A.7.34}$$

Applying this to $\mathcal{A}_\pm$ gives the gauge-independent Berry 'monopole' with strength 1/2 at the origin:

$$\mathcal{F}_\pm = \pm \frac{1}{2} \frac{\hat{\rho}}{\rho^2} \tag{A.7.35}$$

In spherical polars:

$$\mathrm{d}S = \rho^2 \sin\theta \mathrm{d}\theta \mathrm{d}\phi \hat{\rho} + \rho \sin\theta \mathrm{d}\rho \mathrm{d}\phi \hat{\theta} + \rho \mathrm{d}\rho \mathrm{d}\theta \hat{\phi} \tag{A.7.36}$$

Integrating the monopole over the upper hemisphere gives:

$$\phi_{B,\pm}(\gamma_0) = \pm \frac{1}{2} \int_0^{2\pi} \int_0^{\pi/2} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi = \pm\pi \tag{A.7.37}$$

as expected.

# Appendix B

# Chapter 3 Appendices

## B.1 Proof of Theorem 3.3.1 on linearity of band crossings in one spatial dimension

In this section we will prove Theorem 3.3.1 using the fact that in one spatial dimension solving the eigenvalue problem (3.2.3) is equivalent to solving a set of first-order ODEs. Throughout this section we will take $t$ as the dependent variable rather than $z$ for consistency with common presentations of ODE theory.

### B.1.1 Floquet's theorem

Consider the following general second-order ODE with periodic coefficients:

$$\begin{aligned} \ddot{f}(t) + Q(t)f(t) &= 0 \\ Q(t+1) &= Q(t). \end{aligned} \tag{B.1.1}$$

Here and throughout this section, dots will denote derivatives with respect to $t$ hence $\ddot{f}(t) := \frac{\mathrm{d}^2 f}{\mathrm{d}t^2}$. By standard ODE theory, there exist two unique linearly independent solutions $f_1(t)$ and $f_2(t)$ of (B.1.1) which satisfy:

$$\begin{aligned} f_1(0) = 1 \quad \dot{f}_1(0) = 0, \\ f_2(0) = 0 \quad \dot{f}_2(0) = 1. \end{aligned} \tag{B.1.2}$$

By periodicity of $Q$, we have that $f_1(t+1)$ and $f_2(t+1)$ are also solutions of (B.1.1). Hence, they may be written as a linear combination of $f_1(t)$ and $f_2(t)$. Using the conditions (B.1.2), we have more precisely that:

$$f_1(t+1) = f_1(1)f_1(t) + \dot{f}_1(1)f_2(t),$$
$$f_2(t+1) = f_2(1)f_1(t) + \dot{f}_2(1)f_2(t). \tag{B.1.3}$$

We now seek *quasi-periodic* solutions $f(t)$ of (B.1.1):

$$\forall t \in \mathbb{R}, f(t+1) = \rho f(t) \tag{B.1.4}$$

for any constant $\rho \in \mathbb{C}$. We will refer to $f(t)$ satisfying (B.1.4) with $\rho = 1$ as *periodic*, and to $f(t)$ satisfying (B.1.4) with $\rho = -1$ as *anti-periodic*. Any solution $f(t)$ of (B.1.1) may be expressed as $f(t) = c_1 f_1(t) + c_2 f_2(t)$ for constants $c_1, c_2 \in \mathbb{C}$. Combining (B.1.2), (B.1.3), and (B.1.4) we have that $c_1, c_2$ must satisfy:

$$M \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \rho \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \quad M := \begin{pmatrix} f_1(1) & f_2(1) \\ \dot{f}_1(1) & \dot{f}_2(1) \end{pmatrix}. \tag{B.1.5}$$

The matrix $M$ is known as the *monodromy matrix*. Since for all $t$ the Wronskian is equal to 1:

$$W(t) := f_1(t)\dot{f}_2(t) - f_2(t)\dot{f}_1(t) = 1, \tag{B.1.6}$$

the characteristic polynomial whose roots are the eigenvalues of $M$ takes the form:

$$\rho^2 - \Delta\rho + 1, \quad \Delta := f_1(1) + \dot{f}_2(1). \tag{B.1.7}$$

The constant $\Delta$ is known as the *discriminant*. Denote by $\rho_+, \rho_-$ the roots of (B.1.7):

$$\rho_\pm := \frac{\Delta \pm \sqrt{\Delta^2 - 4}}{2}. \tag{B.1.8}$$

It is easy to check that:

$$\rho_+\rho_- = 1 \text{ and } \rho_+ + \rho_- = \Delta. \tag{B.1.9}$$

There are three possibilities:

$\underline{|\Delta| < 2.}$ $\rho_+$ and $\rho_-$ have non-zero imaginary part and are complex conjugates of each other. Since $|\rho_+|^2 = \overline{\rho_+}\rho_+ = \rho_-\rho_+ = 1$ we have that there exists a unique $p \in (0, \pi)$ such that $\rho_+ = e^{ip}$ and $\rho_- = e^{-ip}$. Moreover, there exists a linearly independent set of solutions of (B.1.1) $g_+(t), g_-(t)$ satisfying:

$$g_+(t+1) = e^{ip} g_+(t), \quad g_-(t+1) = e^{-ip} g_-(t). \tag{B.1.10}$$

It follows that in this case *all* solutions of (B.1.1) remain bounded for all $t$.

$|\Delta| > 2$. $\rho_+$ and $\rho_-$ are distinct real numbers such that $\rho_-\rho_+ = 1$. In particular, $\rho_+$ and $\rho_-$ have the same sign. If $\Delta = \rho_+ + \rho_- > 2$, it follows that $\rho_+$ and $\rho_-$ are both positive and that $\rho_+ > \rho_-$. Then $\rho_+ > 1$. Define $p := \log \rho_+ > 0$. Then $\rho_+ = e^p$ and $\rho_- = e^{-p}$ and there exists a linearly independent set of solutions of (B.1.1) $g_+(t), g_-(t)$ such that:

$$g_+(t+1) = e^p g_+(t) \quad g_-(t+1) = e^{-p} g_-(t). \tag{B.1.11}$$

The case where $\Delta < 2$ is similar. It follows that in this case *no* solutions of (B.1.1) remain bounded for all $t$.

$|\Delta| = 2$. $\rho_+ = \rho_-$. It follows that $\rho_+\rho_- = \rho_+^2 = \rho_-^2 = 1$, so that $\rho_+ = \rho_- = 1$ or $\rho_+ = \rho_- = -1$. The monodromy matrix $M$ therefore has a single eigenvalue 1 or $-1$. There are then two further possibilities:

$f_2(1) = \dot{f}_1(1) = 0$. The eigenvalue $\pm 1$ has geometric multiplicity 2. If the eigenvalue is 1, then *all* solutions of (B.1.1) are periodic. If it is $-1$, then *all* solutions are anti-periodic.

Else: The eigenvalue $\pm 1$ has geometric multiplicity 1. Equation (B.1.1) has one solution which is periodic if the eigenvalue is 1 and anti-periodic if the eigenvalue is $-1$ and one solution which is unbounded as $t \to \infty$ or $t \to -\infty$.

The above result is known as *Floquet's theorem.*

### B.1.2 The Floquet-Bloch eigenvalue problem

We now consider the eigenvalue problem obtained by taking $Q(t) = E - V(t)$ in (B.1.1) where $V$ is real and 1-periodic: $V(t+1) = V(t)$ and $E \in \mathbb{R}$:

$$\begin{aligned} &-\ddot{\Phi}(t;E) + V(t)\Phi(t;E) = E\Phi(t;E), \\ &V(t+1) = V(t). \end{aligned} \tag{B.1.12}$$

Just as before we may define normalized solutions $f_1(t;E), f_2(t;E)$ of (B.1.12) and the discriminant as functions of $E$:

$$\Delta(E) := f_1(1;E) + \dot{f}_2(1;E). \tag{B.1.13}$$

We have the following theorem:

**Theorem B.1.1.** *The discriminant function $\Delta(E)$ defined by* (B.1.13) *is an entire analytic function of $E$ such that:*

(D1) *The functions $\Delta(E) - 2$ and $\Delta(E) + 2$ have infinitely many roots along the real line. The roots may have multiplicity one or two.*

(D2) *Denote by $\lambda_0 \leq \lambda_1 \leq ...$ the roots of the function $\Delta(E) - 2$ and by $\lambda'_1 \leq \lambda'_2 \leq ...$ the roots of the function $\Delta(E) + 2$, ordered with multiplicity. Then the following ordering holds:*

$$\lambda_0 < \lambda'_1 \leq \lambda'_2 < \lambda_1 \leq \lambda_2 < \lambda'_3 \leq \lambda'_4 < ... \tag{B.1.14}$$

*We will refer to the intervals $[\lambda_0, \lambda'_1], [\lambda'_2, \lambda_1], ...$ where $|\Delta(E)| \leq 2$ as* bands, *and to the intervals $(\lambda'_1, \lambda'_2), (\lambda_1, \lambda_2), ...$ where $\Delta(E) > 2$ as* gaps. *Note that gaps may be empty, or* closed*; this happens whenever $\Delta(E) - 2$ or $\Delta(E) + 2$ have a double root: $\lambda'_n = \lambda'_{n+1}$ or $\lambda_n = \lambda_{n+1}$ for some integer $n$.*

(D3) *At interior points of the bands, i.e. for $E \in (\lambda_0, \lambda'_1), (\lambda'_2, \lambda_1), ...$ the derivative of $\Delta$ with respect to $E$, $\Delta'(E)$, is never zero.*

(D4) *The double roots of $\Delta(E) - 2$ (resp. $\Delta(E) + 2$) are precisely the roots $\lambda_n$ (resp. $\lambda'_n$) where $f_2(1; E) = \dot{f}_1(1; E) = 0$ and all solutions of* (B.1.12) *are periodic (resp. anti-periodic).*

For the proof and further details, see [50]. The usual $2\pi$-periodic Bloch band dispersion functions:

$$\begin{aligned} E_n &: \mathbb{R} \to \mathbb{R} \\ &p \mapsto E_n(p), \end{aligned} \tag{B.1.15}$$

which are the eigenvalue band functions of the equivalent problems (3.2.3) and (3.2.2), may now be recovered as follows. First, we construct $E_1(p)$. For $E \in (\lambda_0, \lambda'_1)$, we have that $|\Delta(E)| < 2$. By Floquet's theorem, we may define the map:

$$\begin{aligned} (\lambda_0, \lambda'_1) &\to (0, \pi) \\ E &\mapsto p(E) \end{aligned} \tag{B.1.16}$$

where $p \in (0, \pi)$ is as in (B.1.10). To see that (B.1.16) is invertible, note that:

$$2\cos p(E) = e^{ip(E)} + e^{-ip(E)} = \Delta(E), \tag{B.1.17}$$

since $e^{ip}$ and $e^{-ip}$ are the two roots of the characteristic polynomial (B.1.7). Differentiating both sides with respect to $E$ gives:

$$-2\sin p\frac{\mathrm{d}p}{\mathrm{d}E} = \frac{\mathrm{d}\Delta}{\mathrm{d}E}. \tag{B.1.18}$$

By Theorem B.1.1 (D3) we have that for $p \in (0,\pi)$ and $E \in (\lambda_0, \lambda_1')$:

$$\frac{\mathrm{d}p}{\mathrm{d}E} = \frac{\frac{\mathrm{d}\Delta}{\mathrm{d}E}}{-2\sin p} \neq 0. \tag{B.1.19}$$

So, by the inverse function theorem the inverse map $p \mapsto E(p)$ is well-defined and smooth at each $p \in (0,\pi)$ with derivative:

$$\frac{\mathrm{d}E}{\mathrm{d}p} = \frac{-2\sin p}{\frac{\mathrm{d}\Delta}{\mathrm{d}E}(E(p))}. \tag{B.1.20}$$

We define the map $E_1$ over the interval $[0, 2\pi)$ by:

$$E_1(p) := \begin{cases} \lambda_0 & p = 0 \\ E(p) & p \in (0,\pi) \\ \lambda_1' & p = \pi \\ E(2\pi - p) & p \in (\pi, 2\pi) \end{cases} \tag{B.1.21}$$

where $E(p)$ denotes the inverse of the map (B.1.16). We then define this map for all $p \in \mathbb{R}$ by imposing $2\pi$-periodicity. By an analogous argument, all of the higher band functions $p \mapsto E_n(p)$, $n \in \{2, 3, ...\}$ may be uniquely defined.

**Remark B.1.1.** *Whenever a Bloch band $E_n(p)$ is* isolated*, i.e. for all $p_0 \in \mathbb{R}$ such that:*

$$E_{n-1}(p_0) < E_n(p_0) < E_{n+1}(p_0), \tag{B.1.22}$$

*it follows from a Lyapunov-Schmidt reduction argument that there exists a neighborhood $U_0$ of $p_0$ such that the maps $p \mapsto (E_n(p), \Phi_n(t;p))$ are both* analytic *at each $p \in U_0$.*

Now, let $E_n(p), E_{n+1}(p)$ denote spectral band functions satisfying (3.2.3) for $p \in \mathcal{B}$, and let $p^* \in \mathcal{B}$ be such that: $E_n(p^*) = E_{n+1}(p^*)$. It follows that there exist two linearly independent solutions of (B.1.12) when $E^* := E_n(p^*) = E_{n+1}(p^*)$ both satisfying:

$$\forall t \in \mathbb{R}, \quad \Phi(t+1; p^*) = e^{ip^*}\Phi(t;p^*). \tag{B.1.23}$$

By Floquet's theorem, this may only happen when $p^* = 0$ or $\pi$ (modulo $2\pi$), and implies that *all* solutions of (B.1.12) with $E = E^*$ are periodic (if $p^* = 0$) or anti-periodic (if $p^* = \pi$). We now seek quasi-periodic solutions of (B.1.12) in a neighborhood of $E = E^*$, i.e. for $E = E^* + E'$ where $|E'| \ll 1$, assuming WLOG that $p^* = 0$. Such solutions have the form $\Phi(t;E) = c_1(E) f_1(t;E) + c_2(E) f_2(t;E)$ where $c_1(E), c_2(E)$ satisfy:

$$\begin{pmatrix} f_1(1;E) & f_2(1;E) \\ \dot{f}_1(1;E) & \dot{f}_2(1;E) \end{pmatrix} \begin{pmatrix} c_1(E) \\ c_2(E) \end{pmatrix} = \rho(E) \begin{pmatrix} c_1(E) \\ c_2(E) \end{pmatrix}. \tag{B.1.24}$$

Taylor-expanding the monodromy matrix in $E'$ about $E^*$ and then using (B.1.2) and the fact that all solutions are periodic when $E = E^*$ gives:

$$\begin{pmatrix} f_1(1;E) & f_2(1;E) \\ \dot{f}_1(1;E) & \dot{f}_2(1;E) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + E' \begin{pmatrix} \partial_E f_1(1;E^*) & \partial_E f_2(1;E^*) \\ \partial_E \dot{f}_1(1;E^*) & \partial_E \dot{f}_2(1;E^*) \end{pmatrix} + O(|E'|^2) \tag{B.1.25}$$

We seek solutions of (B.1.24) where:

$$\begin{pmatrix} c_1(E) \\ c_2(E) \end{pmatrix} = \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} + E' \begin{pmatrix} \tilde{c}_1(E') \\ \tilde{c}_2(E') \end{pmatrix}, \quad \rho(E) = \rho(E^*) + E' \tilde{\rho}(E'). \tag{B.1.26}$$

Equating terms independent of $E'$ in the resulting expression gives:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} = \rho(E^*) \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} \tag{B.1.27}$$

which implies that $\rho(E^*) = 1$. The eigenvector $(c_1(E^*), c_2(E^*))^T$ is unconstrained at this order in $E'$. The remaining terms are:

$$\begin{aligned} &\left[ \begin{pmatrix} \partial_E f_1(1;E^*) & \partial_E f_2(1;E^*) \\ \partial_E \dot{f}_1(1;E^*) & \partial_E \dot{f}_2(1;E^*) \end{pmatrix} + O(|E'|) \right] \left[ \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} + E' \begin{pmatrix} \tilde{c}_1(E') \\ \tilde{c}_2(E') \end{pmatrix} \right] \\ &= \left[ \tilde{\rho}(E') \right] \left[ \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} + E' \begin{pmatrix} \tilde{c}_1(E') \\ \tilde{c}_2(E') \end{pmatrix} \right]. \end{aligned} \tag{B.1.28}$$

By constructing the Green's function (see [50] for details) we have that:

$$\begin{aligned} \partial_E f_1(1;E^*) &= \langle \Phi_2(\cdot;E^*) | \, \Phi_1(\cdot;E^*) \rangle, & \partial_E f_2(1;E^*) &= \|\Phi_2(\cdot;E^*)\|^2, \\ \partial_E \dot{f}_1(1;E^*) &= -\|\Phi_1(\cdot;E^*)\|^2, & \partial_E \dot{f}_2(1;E^*) &= -\langle \Phi_2(\cdot;E^*) | \, \Phi_1(\cdot;E^*) \rangle. \end{aligned}$$

Taking the determinant of (B.1.28) then gives:

$$\begin{aligned}
&(\langle \Phi_2(\cdot;E^*)|\,\Phi_1(\cdot;E^*)\rangle - \tilde{\rho}(E'))(\langle \Phi_2(\cdot;E^*)|\,\Phi_1(\cdot;E^*)\rangle + \tilde{\rho}(E')) \\
&-\|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 = O(E') \\
&\Longrightarrow \\
&(\tilde{\rho}(E'))^2 = \langle \Phi_2(\cdot;E^*)|\,\Phi_1(\cdot;E^*)\rangle^2 - \|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 + O(E').
\end{aligned} \tag{B.1.29}$$

Taking the square root of both sides and using the Cauchy-Schwarz inequality we have that there are two smooth solutions $\tilde{\rho}_\pm(E')$, satisfying:

$$\begin{aligned}
&\tilde{\rho}_\pm(E') = \pm i\lambda + O(|E'|) \\
&\lambda := \sqrt{\|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 - \langle \Phi_2(\cdot;E^*)|\,\Phi_1(\cdot;E^*)\rangle^2} > 0.
\end{aligned} \tag{B.1.30}$$

Substituting (B.1.30) back into (B.1.28) and setting $E' = 0$ gives:

$$\begin{pmatrix} \partial_E f_1(1;E^*) & \partial_E f_2(1;E^*) \\ \partial_E \dot{f}_1(1;E^*) & \partial_E \dot{f}_2(1;E^*) \end{pmatrix} \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} = \pm i\lambda \begin{pmatrix} c_1(E^*) \\ c_2(E^*) \end{pmatrix} \tag{B.1.31}$$

i.e. $(c_1(E^*), c_2(E^*))^T$ must be chosen to be an eigenvector of:

$$\begin{pmatrix} \partial_E f_1(1;E^*) & \partial_E f_2(1;E^*) \\ \partial_E \dot{f}_1(1;E^*) & \partial_E \dot{f}_2(1;E^*) \end{pmatrix} \tag{B.1.32}$$

with eigenvalue $\pm i\lambda$. We denote these eigenvectors by $(c_{\pm,1}(E^*), c_{\pm,2}(E^*))^T$. It now follows now from a standard Lyapunov-Schmidt reduction argument that for all $E$ sufficiently close to $E^*$ there exist two distinct eigenpair solutions $(\rho_\pm(E), (c_{1,\pm}(E), c_{2,\pm}(E))^T)$ of (B.1.24) which are *smooth in* $E$ with $\rho_\pm(E^*) = 1$, satisfying:

$$\begin{aligned}
&\rho_\pm(E) = 1 \pm i\lambda(E - E^*) + O(|E - E^*|^2), \\
&\begin{pmatrix} c_{\pm,1}(E) \\ c_{\pm,2}(E) \end{pmatrix} = \begin{pmatrix} c_{\pm,1}(E^*) \\ c_{\pm,2}(E^*) \end{pmatrix} + O(|E - E^*|).
\end{aligned} \tag{B.1.33}$$

In particular we have that:

$$\begin{aligned}
\frac{\mathrm{d}\rho_\pm}{\mathrm{d}E}(E^*) &= \pm\, i\sqrt{\|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 - \langle \Phi_2(\cdot;E^*)|\,\Phi_1(\cdot;E^*)\rangle^2} \\
&\neq 0
\end{aligned} \tag{B.1.34}$$

and that for small enough $|E - E^*|$ the $\rho_\pm(E)$ are complex. Since $\overline{\rho_+} = \rho_-$ and $\rho_+\rho_- = 1$ (B.1.9) they must be expressible as:

$$\rho_\pm(E) = e^{\pm ip(E)} \tag{B.1.35}$$

for some smooth function $p(E)$ satisfying $p(E^*) = 0$. Substituting (B.1.35) into (B.1.30) then implies that:

$$\begin{aligned}\frac{\mathrm{d}p}{\mathrm{d}E}(E^*) =& \sqrt{\|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 - \langle\, \Phi_2(\cdot;E^*)|\, \Phi_1(\cdot;E^*)\rangle^2} \\ &\neq 0\end{aligned} \tag{B.1.36}$$

which then implies, by the inverse function theorem, the existence of smooth band functions $p \mapsto E_\pm(p)$ for $p$ sufficiently close to 0 such that:

$$\frac{\mathrm{d}E_\pm}{\mathrm{d}p}(0) = \pm\frac{1}{\sqrt{\|\Phi_1(\cdot;E^*)\|^2\|\Phi_2(\cdot;E^*)\|^2 - \langle\, \Phi_2(\cdot;E^*)|\, \Phi_1(\cdot;E^*)\rangle^2}}. \tag{B.1.37}$$

By definition we have that the associated eigenfunctions $\Phi_\pm(t;E)$ are smooth in $E$ and satisfy:

$$\Phi_\pm(t+1;E) = e^{\pm ip(E)}\Phi_\pm(t;E) \tag{B.1.38}$$

for $E$ sufficiently close to $E^*$. Inverting the map $E \mapsto p$ we obtain eigenfunctions of (3.2.2) depending smoothly on $p$:

$$\Phi_\pm(t+1;p) = e^{\pm ip}\Phi_\pm(t;p) \tag{B.1.39}$$

for $p$ sufficiently close to 0. By defining $\chi_\pm(t;p) := e^{-ipt}\Phi_\pm(t;p)$ we obtain eigenfunctions of (3.2.3) depending smoothly on $p$ sufficiently close to 0. We have now proved Theorem 3.3.1 in all details.

## B.2 Proof that the "inter-band coupling coefficient" vanishes for trivial crossings

### B.2.1 Formula for $\langle\, \chi_-(\cdot;p^*)|\, \partial_p\chi_+(\cdot;p^*)\rangle$ from symmetry of Bloch band

Let $E(p)$, $\chi(z;p)$ denote an eigenpair of (3.2.3). Then:

$$\begin{aligned}&H(2\pi - p)e^{-2\pi iz}\overline{\chi(z;p)} = e^{-2\pi iz}H(-p)\overline{\chi(z;p)} \\ &= e^{-2\pi iz}\overline{H(p)\chi(z;p)} = E(p)e^{-2\pi iz}\overline{\chi(z;p)} \\ &e^{-2\pi i(z+1)}\overline{\chi(z+1;p)} = e^{-2\pi iz}\overline{\chi(z;p)}.\end{aligned} \tag{B.2.1}$$

Hence, for $p \in \mathcal{B}$ such that the eigenvalue $E(p)$ is non-degenerate, $E(p)$ and $\chi(z;p)$ obey the symmetry (after possibly multiplying $\chi(z;p)$ by a constant):

$$E(2\pi - p) = E(p) \qquad \chi(z; 2\pi - p) = e^{-2\pi i z} \overline{\chi(z;p)}. \tag{B.2.2}$$

Note further that the symmetry (B.2.2) implies that the eigenvalue $E(2\pi - p)$ is non-degenerate if and only if $E(p)$ is; if it were not, we could use (B.2.2) to generate two linearly independent eigenfunctions with eigenvalue $E(p)$ from those with eigenvalue $E(2\pi - p)$.

Now, let $E_n(p), E_{n+1}(p)$ denote eigenvalue bands of (3.2.3) which cross at $p = \pi$ (WLOG), and fix the Brillouin zone: $\mathcal{B} = [0, 2\pi]$. Let $E_+(p)$, $E_-(p)$ and $\chi_+(z;p)$, $\chi_-(z;p)$ denote the smooth eigenpairs defined in a neighborhood $U$ of $\pi$ by (3.3.3). It follows from (B.2.2) that for $p$ away from the degeneracy at $\pi$, $\chi_+(z;p)$ and $\chi_-(z;p)$ obey the symmetry:

$$\chi_-(z;p) = e^{-2\pi i z} \overline{\chi_+(z;p)}, \quad p \in U \setminus \{\pi\}. \tag{B.2.3}$$

But now recall that the maps $\chi_+(z;p), \chi_-(z;p)$ are smooth at $p = \pi$, hence:

$$\chi_-(z;\pi) = \lim_{p \uparrow \pi} \chi_-(z;p) = \lim_{p \uparrow \pi} e^{-2\pi i z} \overline{\chi_+(z;p)} = e^{-2\pi i z} \overline{\chi_+(z;\pi)}. \tag{B.2.4}$$

It follows that (B.2.3) holds for every $p \in U$:

$$\chi_-(z;p) = e^{-2\pi i z} \overline{\chi_+(z;p)}, \quad p \in U. \tag{B.2.5}$$

Substituting (B.2.5) into the formula for the "inter-band coupling coefficient" (3.3.30) gives:

$$\langle \chi_-(z;\pi) | \, \partial_p \chi_+(z;\pi) \rangle = \left\langle e^{-2\pi i z} \overline{\chi_+(z;p)} \middle| \, \partial_p \chi_+(z;\pi) \right\rangle = \int_0^1 e^{2\pi i z} \chi_+(z;\pi) \partial_p \chi_+(z;\pi) \, \mathrm{d}z. \tag{B.2.6}$$

### B.2.2 Proof that coefficient vanishes for trivial crossings

Now, suppose that $E_n(p)$ and $E_{n+1}(p)$ cross *trivially* in the sense that $V(z) = V_{1/2}(z)$, where $V_{1/2}(z)$ denotes a 1/2-periodic function, and the smooth band functions $E_+(p), E_-(p)$ and associated eigenfunctions $\chi_+(z;p)$, $\chi_-(z;p)$ defined in a neighborhood of $p = \pi$ satisfy (all equality of eigenfunctions understood as holding up to a constant phase):

$$\begin{aligned} E_+(p) &= \tilde{E}(p) & \chi_+(z;p) &= \tilde{\chi}(z;p) \\ E_-(p) &= \tilde{E}(2\pi + p) & \chi_-(z;p) &= \tilde{\chi}(z; 2\pi + p) \end{aligned} \tag{B.2.7}$$

where $\tilde{E}(p)$ is an eigenvalue band of the Bloch eigenvalue problem (3.2.3) with potential $V(z) = V_{1/2}(z)$ and 1/2 -periodic boundary conditions, considered on the Brillouin zone $[0, 4\pi]$ (see Figure 3.5).

(B.2.7) in particular implies that $\chi_+(z;p)$, $\partial_p \chi_+(z;p)$, and the function:

$$\chi_+(z;p)\partial_p \chi_+(z;p), \tag{B.2.8}$$

are all 1/2 -periodic for all $p \in U$. It follows that the function (B.2.8) has for all $p \in U$ a convergent Fourier series with only *even index* modes:

$$\chi_+(z;p)\partial_p \chi_+(z;p) = \sum_{m \in 2\mathbb{Z}} \int_0^1 e^{-2\pi i m z'} \chi_+(z';p)\partial_p \chi_+(z';p) \, \mathrm{d}z' \, e^{2\pi i m z} \tag{B.2.9}$$

and hence, by orthogonality of Fourier modes:

$$\langle \chi_-(z;\pi) | \, \partial_p \chi_+(z;\pi) \rangle = \int_0^1 e^{2\pi i z} \chi_+(z;\pi)\partial_p \chi_+(z;\pi) \, \mathrm{d}z = 0. \tag{B.2.10}$$

## B.3 Completion of proof of Theorem 3.3.2 by estimation of remaining terms

Let $t \in [t^* - \delta, t^*]$ where $\delta > 0$ is as in Proposition 3.3.1 so that:

$$\begin{aligned} &\mathrm{WP}^{1,\epsilon}[\mathfrak{S}_+(t), \mathfrak{q}_+(t), \mathfrak{p}_+(t), \mathfrak{a}^0_+(y,t), \mathfrak{a}^1_+(y,t), \mathfrak{X}_+(z;\mathfrak{p}_+(t))](x,t) \\ &= \mathrm{WP}^{1,\epsilon}[S_+(t), q_+(t), p_+(t), a^0_+(y,t), a^1_+(y,t), \chi_+(z;p(t))](x,t). \end{aligned} \tag{B.3.1}$$

Here, $q_+(t), p_+(t)$ are as in (3.3.16), $S_+(t), a^0_+(y,t), a^1_+(y,t)$ are as in Definition 3.3.1, and $\chi_+(z;p)$ is as in (3.3.3). The approximate solution $\psi^\epsilon_{app}(x,t)$ constructed in the proof of Theorem 3.2.2 [73] then takes the form:

$$\begin{aligned} &\psi^\epsilon_{app}(x,t) = \epsilon^{-1/4} e^{i\phi^\epsilon_+(y_+,t)/\epsilon} \Big\{ \\ &f^0(y_+,z,t) + \epsilon^{1/2} f^1(y_+,z,t) + \epsilon f^2(y_+,z,t) + \epsilon^{3/2} f^3(y_+,z,t) \Big\} \Big|_{y_+ = \frac{x - q_+(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} \\ &\phi^\epsilon_+(y_+,t) := S_+(t) + \epsilon^{1/2} p_+(t) y_+ \end{aligned} \tag{B.3.2}$$

where:

$$
\begin{aligned}
&f^0(z,y,t) := a_+^0(y,t)\chi_+(z;p_+(t)),\;\; f^1(z,y,t) := a_+^1(y,t)\chi_+(z;p(t)) + (-i\partial_y)a_+^0(y,t)\partial_p\chi_+(z;p_+(t)) \\
&f^2(z,y,t) := (-i\partial_y)a_+^1(y,t)\partial_p\chi_+(z;p_+(t)) + \frac{1}{2}(-i\partial_y)^2 a_+^0(y,t)\partial_p^2\chi_+(z;p_+(t)) \\
&- i\partial_q W(q_+(t))a_+^0(y,t)\mathcal{R}_+(p_+(t))P_\perp(p_+(t))\partial_p\chi_+(z;p_+(t)) \\
&f^3(y,z,t) := \frac{1}{2}(-i\partial_y)^2 a_+^1(y,t)\partial_p^2\chi_+(z;p_+(t)) + \frac{1}{6}(-i\partial_y)^3 a_+^0(y,t)\partial_p^3\chi_+(z;p_+(t)) \\
&- i\partial_q^2 W(q_+(t))y a_+^0(y,t)\mathcal{R}_+(p_+(t))P_\perp(p_+(t))\partial_p\chi_+(z;p_+(t)) \\
&+ i\partial_q W(q_+(t))\left\langle \chi_+(z;p_+(t)) \middle| \partial_p\chi_+(z;p_+(t))\right\rangle (-i\partial_y)a_+^0(y,t)\mathcal{R}_+(p_+(t))P_\perp(p_+(t))\partial_p\chi_+(z;p_+(t)) \\
&+ i\partial_q W(q_+(t))(-i\partial_y)a_+^0(y,t)\mathcal{R}_+(p_+(t))P_\perp(p_+(t))\partial_p^2\chi_+(z;p_+(t)) \\
&+ i\partial_q W(q_+(t))(-i\partial_y)a_+^0(y,t) \\
&\times \mathcal{R}_+(p_+(t))P_\perp(p_+(t))\left[(p_+(t)-i\partial_z) - \partial_p E_+(p_+(t))\right]\mathcal{R}_+(p_+(t))P_\perp(p_+(t))\partial_p\chi_+(z;p_+(t)).
\end{aligned}
\tag{B.3.3}
$$

Here, $P_+^\perp(p)$ denotes the projection operator away from the subspace of $L^2_{per}$ spanned by $\chi_+(z;p)$, while $\mathcal{R}_+(p)$ denotes the resolvent operator:

$$
\mathcal{R}_+(p) := \left(H(p) - E_+(p)\right)^{-1}. \tag{B.3.4}
$$

The residual $r^\epsilon(x,t)$ defined by (3.4.2) with $\psi^\epsilon_{app}(x,t)$ given by (B.3.2) (see [73] for details) is as follows:

$$
\begin{aligned}
r^\epsilon(x,t) = \epsilon^{-1/4}e^{i\phi_+^\epsilon(y_+,t)/\epsilon}\bigg\{&\epsilon^2\mathcal{L}^4\left(f^0 + \epsilon^{1/2}f^1 + \epsilon f^2 + \epsilon^{3/2}f^3\right) \\
+ \epsilon^2\mathcal{L}^3\left(f^1 + \epsilon^{1/2}f^2 + \epsilon f^3\right) &+ \epsilon^2\mathcal{L}^2\left(f^2 + \epsilon^{1/2}f^3\right) + \epsilon^2\mathcal{L}^1 f^3\bigg\}\bigg|_{z=\frac{x}{\epsilon},\, y=\frac{x-q_+(t)}{\epsilon^{1/2}}},
\end{aligned}
\tag{B.3.5}
$$

where:

$$
\begin{aligned}
&\mathcal{L}^1 := \left(p_+(t) - i\partial_z - \partial_p E_+(p_+(t))\right)(-i\partial_y) \qquad && \mathcal{L}^2 := -i\partial_t + \frac{1}{2}(-i\partial_y)^2 + \frac{1}{2}y^2\partial_q^2 W(q_+(t)) \\
&\mathcal{L}^3 := \frac{1}{6}y^3\partial_q^3 W(q_+(t)) && \mathcal{L}^4 := y^4\int_0^1 \frac{(\tau-1)^4}{4!}\partial_q^4 W(q_+(t) + \tau\epsilon^{1/2}y)\,\mathrm{d}\tau.
\end{aligned}
$$

Recall the discussion below (3.4.13): some terms in (B.3.5) are singular as $t \uparrow t^*$ because of the band crossing at $p^*$. We estimate $r^\epsilon(x,t)$ term by term, using identical reasoning to that given in Section 3.4.2 and using the following basic estimates which follow immediately from Taylor-expansion and the non-degeneracy conditions (3.3.4) (3.3.12):

$$\begin{aligned}
\left|(E_+(p_+(t)) - E_-(p_+(t)))^{-1}\right| &\leq \left|\frac{1}{\partial_q W(q^*)\left(\partial_p E_+(p^*) - \partial_p E_-(p^*)\right)}\right| \left(\frac{1}{|t-t^*|}\right) + O(1) \\
\left|(E_+(p_+(t)) - E_-(p_+(t)))^{-2}\right| &\leq \left|\frac{1}{\partial_q W(q^*)\left(\partial_p E_+(p^*) - \partial_p E_-(p^*)\right)}\right|^2 \left(\frac{1}{|t-t^*|^2}\right) + O\left(\frac{1}{|t-t^*|}\right) \\
\left|\partial_t\left(E_+(p_+(t)) - E_-(p_+(t))\right)^{-1}\right| &\leq \left|\frac{1}{\partial_q W(q^*)\left(\partial_p E_+(p^*) - \partial_p E_-(p^*)\right)}\right| \left(\frac{1}{|t-t^*|^2}\right) + O\left(\frac{1}{|t-t^*|}\right) \\
\left|\partial_t\left(E_+(p_+(t)) - E_-(p_+(t))\right)^{-2}\right| &\leq \left|\frac{1}{\partial_q W(q^*)\left(\partial_p E_+(p^*) - \partial_p E_-(p^*)\right)}\right|^2 \left(\frac{1}{|t-t^*|^3}\right) \\
&\quad + O\left(\frac{1}{|t-t^*|^2}\right).
\end{aligned} \tag{B.3.6}$$

Our results are that as $t \uparrow t^*$:

$$\epsilon^{-1/4}\mathcal{L}^4 f^0 = O_{L^2_x}\left(\epsilon^2\right) \qquad \epsilon^{-1/4}\mathcal{L}^4 f^1 = O_{L^2_x}\left(\epsilon^{5/2}\right) \tag{B.3.7}$$

$$\epsilon^{-1/4}\mathcal{L}^4 f^2 = O_{L^2_x}\left(\frac{\epsilon^3}{|t-t^*|}\right) \qquad \epsilon^{-1/4}\mathcal{L}^4 f^3 = O_{L^2_x}\left(\frac{\epsilon^{7/2}}{|t-t^*|^2}\right) \tag{B.3.8}$$

$$\epsilon^{-1/4}\mathcal{L}^3 f^1 = O_{L^2_x}\left(\epsilon^2\right) \qquad \epsilon^{-1/4}\mathcal{L}^3 f^2 = O_{L^2_x}\left(\frac{\epsilon^{5/2}}{|t-t^*|}\right) \tag{B.3.9}$$

$$\epsilon^{-1/4}\mathcal{L}^3 f^3 = O_{L^2_x}\left(\frac{\epsilon^3}{|t-t^*|^2}\right) \tag{B.3.10}$$

$$\epsilon^{-1/4}\mathcal{L}^2 f^2 = O_{L^2_x}\left(\frac{\epsilon^2}{|t-t^*|^2}\right) \qquad \epsilon^{-1/4}\mathcal{L}^2 f^3 = O_{L^2_x}\left(\frac{\epsilon^{5/2}}{|t-t^*|^3}\right) \tag{B.3.11}$$

$$\epsilon^{-1/4}\mathcal{L}^1 f^3 = O_{L^2_x}\left(\frac{\epsilon^2}{|t-t^*|^2}\right). \tag{B.3.12}$$

Note that the overall phase $e^{i\phi^\epsilon_+(y_+,t)/\epsilon}$ in (B.3.5) doesn't contribute. Summing up all terms in (B.3.7) we have that:

$$r^\epsilon(x,t) = O_{L^2_x}\left(\frac{\epsilon^2}{|t-t^*|^2}, \frac{\epsilon^{5/2}}{|t-t^*|^3}, \frac{\epsilon^{5/2}}{|t-t^*|}, \epsilon^2\right). \tag{B.3.13}$$

(3.3.29) then follows immediately from substituting (B.3.13) into (3.4.4).

# Appendix C

# Chapter 4 Appendices

## C.1 Proofs of key lemmas

### C.1.1 Proof of Lemma 4.4.1

We introduce the partition of unity:

$$1 = (\theta^-(x))^2 + (\theta^0(x))^2 + (\theta^+(x))^2 \tag{C.1.1}$$

where the functions $\theta^\pm, \theta^0$ satisfy:

$$\theta^-(x) = \begin{cases} 1 & \text{for } x \leq -\frac{L}{2} \\ 0 & \text{for } x \geq -\frac{L}{4} \end{cases} \tag{C.1.2}$$

$$\theta^0(x) = \begin{cases} 1 & \text{for } -\frac{L}{4} \leq x \leq \frac{L}{4} \\ 0 & \text{for } x \leq -\frac{L}{2} \text{ or } x \geq \frac{L}{2} \end{cases} \tag{C.1.3}$$

$$\theta^+(x) = \begin{cases} 1 & \text{for } x \geq \frac{L}{2} \\ 0 & \text{for } x \leq \frac{L}{4} \end{cases}. \tag{C.1.4}$$

We note two consequences of the definition. First, note that for $j \in \{+, -, 0\}$ and each positive integer $n \geq 1$:

$$\sup_{x \in \mathbb{R}} |\partial_x^n \theta^j(x)| \leq \frac{C}{L^n} \tag{C.1.5}$$

for positive constants $C > 0$ which are independent of $L$ and depend only on the particular shape of the cutoff. Second, note that if $L \geq 2$, then:

$$-L+1 \leq -\frac{L}{2} < -\frac{L}{4}. \tag{C.1.6}$$

So that for $L \geq 2$:

$$\begin{aligned} &\text{for } x \in \operatorname{supp}[\theta^+], \quad \kappa_L(x) = \kappa(x-L) \\ &\text{for } x \in \operatorname{supp}[\theta^0], \quad \kappa_L(x) = -\kappa_\infty \\ &\text{for } x \in \operatorname{supp}[\theta^-], \quad \kappa_L(x) = -\kappa(x+L). \end{aligned} \tag{C.1.7}$$

It follows that:

$$\begin{aligned} &\text{for } x \in \operatorname{supp}[\theta^+], \quad \mathcal{D}_{\kappa_L} = \mathcal{D}_{\kappa^+} \\ &\text{for } x \in \operatorname{supp}[\theta^0], \quad \mathcal{D}_{\kappa_L} = \mathcal{D}_{-\kappa_\infty} \\ &\text{for } x \in \operatorname{supp}[\theta^-], \quad \mathcal{D}_{\kappa_L} = \mathcal{D}_{\kappa^-}. \end{aligned} \tag{C.1.8}$$

where we have introduced the notation:

$$\mathcal{D}_{-\kappa_\infty} := i\partial_x\sigma_3 - \kappa_\infty\sigma_1. \tag{C.1.9}$$

We assume at this point that $L \geq 2$ so that (C.1.7) and (C.1.8) hold.

We now prove Lemma 4.4.1. Using the partition of unity, we have that:

$$\|\mathcal{D}_{\kappa_L} f\|_{\mathcal{H}}^2 = \sum_{j=0,\pm} \int (\theta^j(x))^2 |\mathcal{D}_{\kappa_L} f(x)|_{\mathbb{C}^2}^2 \,\mathrm{d}x = \sum_{j=0,\pm} \int |\theta^j(x)\mathcal{D}_{\kappa_L} f(x)|_{\mathbb{C}^2}^2 \,\mathrm{d}x. \tag{C.1.10}$$

By a trivial re-arrangement we have that:

$$j \in \{0,\pm\}, \quad \theta^j(x)\mathcal{D}_{\kappa_L} = \mathcal{D}_{\kappa_L}\theta^j(x) + [\theta^j(x), \mathcal{D}_{\kappa_L}] = \mathcal{D}_{\kappa_L}\theta^j(x) - i\partial_x\theta^j(x)\sigma_3. \tag{C.1.11}$$

Combining (C.1.10) and (C.1.11) gives:

$$\|\mathcal{D}_{\kappa_L} f\|_{\mathcal{H}}^2 = \sum_{j=0,\pm} \int |\mathcal{D}_{\kappa_L}\theta^j(x) f(x) - i\sigma_3\partial_x\theta^j(x) f(x)|_{\mathbb{C}^2}^2 \,\mathrm{d}x. \tag{C.1.12}$$

We then proceed as follows:

$$\begin{aligned} &\sum_{j=0,\pm} \int |\mathcal{D}_{\kappa_L}\theta^j(x) f(x) - i\sigma_3\partial_x\theta^j(x) f(x)|_{\mathbb{C}^2}^2 \,\mathrm{d}x \\ &= \sum_{j=0,\pm} \|\mathcal{D}_{\kappa_L}\theta^j(x) f\|_{\mathcal{H}}^2 + \|\partial_x\theta^j(x) f\|_{\mathcal{H}}^2 - 2\mathrm{Re}\left\langle i\sigma_3\partial_x\theta^j(x) f(x) \middle| \mathcal{D}_{\kappa_L}\theta^j f \right\rangle_{\mathcal{H}} \end{aligned}$$

$$\geq \sum_{j=0,\pm} \|\mathcal{D}_{\kappa_L}\theta^j(x)f\|^2_{\mathcal{H}} + \|\partial_x\theta^j(x)f\|^2_{\mathcal{H}} - 2\|\sigma_3\partial_x\theta^j f\|_{\mathcal{H}}\|\mathcal{D}_{\kappa_L}\theta^j f\|_{\mathcal{H}} \quad \text{(Cauchy-Schwarz inequality)}$$
$$\geq \sum_{j=0,\pm} (1-\epsilon^2)\|\mathcal{D}_{\kappa_L}\theta^j(x)f\|^2_{\mathcal{H}} + (1-\epsilon^{-2})\|\partial_x\theta^j f\|^2_{\mathcal{H}} \quad \text{(Young's inequality)} \tag{C.1.13}$$

for any positive $\epsilon > 0$. Fixing $\epsilon$ sufficiently small in (C.1.13) so that $(1-\epsilon^{-2}) \geq \epsilon^{-2}$ and using (C.1.5), we have that:

$$\|\mathcal{D}_{\kappa_L}f\|^2_{\mathcal{H}} \geq \sum_{j=0,\pm}(1-\epsilon^2)\|\mathcal{D}_{\kappa_L}\theta^j(x)f\|^2_{\mathcal{H}} - \epsilon^{-2}\frac{C}{L^2}\|f\|^2_{\mathcal{H}} \tag{C.1.14}$$

where the constant $C$ is independent of $L$. We now estimate the terms:

$$j \in \{0,\pm\}, \quad \|\mathcal{D}_{\kappa_L}\theta^j(x)f\|^2_{\mathcal{H}}. \tag{C.1.15}$$

First, we consider $j = +$:

$$\|\mathcal{D}_{\kappa_L}\theta^+ f\|^2_{\mathcal{H}} = \int |(i\sigma_3\partial_x + \kappa_L(x))(\theta^+(x)f(x))|^2_{\mathbb{C}^2}\,\mathrm{d}x$$
$$= \int |\mathcal{D}_{\kappa^+}(\theta^+(x)f(x))|^2_{\mathbb{C}^2}\,\mathrm{d}x = \|\mathcal{D}_{\kappa^+}\theta^+ f\|^2_{\mathcal{H}} \quad \text{(Using (C.1.8))} \tag{C.1.16}$$

We now use the fact that $\langle \alpha^+_\star | f\rangle_{\mathcal{H}} = 0$:

$$\left\langle \alpha^+_\star \middle| f\right\rangle_{\mathcal{H}} = 0$$
$$\iff \left\langle \alpha^+_\star \middle| \theta^+ f\right\rangle_{\mathcal{H}} = -\left\langle \alpha^+_\star \middle| (1-\theta^+)f\right\rangle_{\mathcal{H}}$$
$$\implies \left\langle \alpha^+_\star \middle| \theta^+ f\right\rangle_{\mathcal{H}} \leq \|\alpha^+_\star(1-\theta^+)\|_{\mathcal{H}}\|f\|_{\mathcal{H}} \quad \text{(Cauchy-Schwarz inequality)}$$

but:

$$\|(1-\theta^+)\alpha^+_\star\|^2_{\mathcal{H}} = \int |(1-\theta^+(x))\alpha_\star(x-L)|^2_{\mathbb{C}^2}\,\mathrm{d}x$$
$$\leq \int_{-\infty}^{\frac{L}{2}} |\alpha_\star(x-L)|^2_{\mathbb{C}^2}\,\mathrm{d}x \quad (\text{Supp } (1-(\theta^+)) = [-\infty, L/2])$$
$$\leq C\int_{-\infty}^{\frac{L}{2}} e^{-2\kappa_\infty|x-L|}\,\mathrm{d}x = C\int_{-\infty}^{\frac{L}{2}} e^{2\kappa_\infty(x-L)}\,\mathrm{d}x \quad (\text{Since } L/2 \geq 1, \text{ using (4.2.4)})$$
$$= Ce^{-2\kappa_\infty L}\int_{-\infty}^{L/2} e^{2\kappa_\infty x}\,\mathrm{d}x \leq Ce^{-\kappa_\infty L}$$

where $C > 0$ is a constant independent of $L > 0$. We have therefore that:

$$\left\langle \alpha_\star^+ \middle| \theta^+ f \right\rangle_{\mathcal{H}} \leq \|\alpha_\star^+(1-\theta^+)\|_{\mathcal{H}} \|f\|_{\mathcal{H}} \leq Ce^{-\kappa_\infty L/2}\|f\|_{\mathcal{H}}. \tag{C.1.17}$$

We now require the following corollary of Lemma 4.2.1:

**Corollary C.1.1.** *Let $f \in \mathcal{H}$. Then:*

$$\|\mathcal{D}_\kappa f\|_{\mathcal{H}} \geq \kappa_\infty \left| \|f\|_{\mathcal{H}} - \left| \langle \alpha_\star | f \rangle_{\mathcal{H}} \right| \right|. \tag{C.1.18}$$

*Proof.* For any $f \in \mathcal{H}$, we may write $f = P^\perp f + \langle \alpha_\star | f \rangle \alpha_\star$. Since $\alpha_\star$ is a zero mode of $\mathcal{D}_\kappa$ and using Lemma 4.2.1 we have:

$$\|\mathcal{D}_\kappa f\|_{\mathcal{H}} = \|\mathcal{D}_\kappa P^\perp f\|_{\mathcal{H}} \geq \kappa_\infty \|P^\perp f\|_{\mathcal{H}}. \tag{C.1.19}$$

Using $P^\perp f = f - \langle \alpha_\star | f \rangle \alpha_\star$, the reverse triangle inequality and normalization of $\alpha_\star : \|\alpha_\star\|_{\mathcal{H}} = 1$ we have that:

$$\|\mathcal{D}_\kappa f\|_{\mathcal{H}} \geq \kappa_\infty \|P^\perp f\|_{\mathcal{H}} = \kappa_\infty \|f - \langle \alpha_\star | f \rangle_{\mathcal{H}} \alpha_\star\|_{\mathcal{H}} \geq \kappa_\infty \left| (\|f\|_{\mathcal{H}} - \left| \langle \alpha_\star | f \rangle_{\mathcal{H}} \right|) \right|. \tag{C.1.20}$$

□

It then follows from combining (C.1.16), (C.1.17), and Corollary C.1.1 that:

$$\|\mathcal{D}_{\kappa_L} \theta^+ f\|_{\mathcal{H}}^2 = \|\mathcal{D}_{\kappa^+} \theta^+ f\|_{\mathcal{H}}^2 \geq \kappa_\infty^2 \left(1 - Ce^{-\kappa_\infty L/2}\right)^2 \|\theta^+ f\|_{\mathcal{H}}^2. \tag{C.1.21}$$

An identical argument shows that:

$$\|\mathcal{D}_L \theta^- f\|_{\mathcal{H}}^2 \geq \kappa_\infty^2 \left(1 - Ce^{-\kappa_\infty L/2}\right)^2 \|\theta^- f\|_{\mathcal{H}}^2. \tag{C.1.22}$$

where $C > 0$ again simply stands for a constant depending only on $\kappa$. Finally, we have that:

$$\begin{aligned}
\|\mathcal{D}_L \theta^0 f\|_{\mathcal{H}}^2 &= \int |(i\sigma_3 \partial_x + \kappa_L(x))(\theta^0(x) f(x))|_{\mathbb{C}^2}^2 \, \mathrm{d}x \\
&= \int |(i\sigma_3 \partial_x - \kappa_\infty \sigma_1)(\theta^0(x) f(x))|_{\mathbb{C}^2}^2 \, \mathrm{d}x \qquad \text{(Using (C.1.7))} \\
&= \left\langle \theta^0 f \middle| \mathcal{D}_{-\kappa_\infty}^2 \theta^0 f \right\rangle_{\mathcal{H}} \geq \kappa_\infty^2 \|\theta^0 f\|_{\mathcal{H}}^2.
\end{aligned} \tag{C.1.23}$$

Summing (C.1.21) (C.1.22) and (C.1.23) we see that for sufficiently large $L > 0$ (so that $1 - Ce^{-\kappa_\infty L/2} \geq 0$):

$$\sum_{j=0,\pm} \|\mathcal{D}_L \theta^j f\|_{\mathcal{H}}^2 \geq \kappa_\infty^2 \left(1 - Ce^{-\kappa_\infty L/2}\right)^2 \sum_{j=0,\pm} \|\theta^j f\|_{\mathcal{H}}^2 = \kappa_\infty^2 \left(1 - Ce^{-\kappa_\infty L/2}\right)^2 \|f\|_{\mathcal{H}}^2. \tag{C.1.24}$$

Combining this with (C.1.14) we have:

$$\begin{aligned}\|\mathcal{D}_{\kappa_L} f\|_{\mathcal{H}}^2 &\geq C\left(\left(1 - Ce^{-\kappa_\infty L/2}\right)^2 - \frac{1}{L^2}\right)\|f\|_{\mathcal{H}}^2 \\ &\geq C\left(1 - Ce^{-\kappa_\infty L/2} - \frac{1}{L^2}\right)\|f\|_{\mathcal{H}}^2\end{aligned} \tag{C.1.25}$$

from which Lemma 4.4.1 follows immediately by taking $L$ large enough.

### C.1.2 Proof of Lemma 4.4.2

#### C.1.2.1 Proof that $\left\langle \alpha_\star^i \middle| \alpha_\star^j \right\rangle_{\mathcal{H}} = \delta^{ij}$

That $\langle \alpha_\star^+ | \alpha_\star^+ \rangle_{\mathcal{H}} = \langle \alpha_\star^- | \alpha_\star^- \rangle_{\mathcal{H}} = 1$ is by definition. That $\langle \alpha_\star^- | \alpha_\star^+ \rangle_{\mathcal{H}} = \overline{\langle \alpha_\star^+ | \alpha_\star^- \rangle_{\mathcal{H}}}$ is clear from the definition of the inner product. We then have that:

$$\begin{aligned}\langle \alpha_\star^- | \alpha_\star^+ \rangle_{\mathcal{H}} &= \int_{\mathbb{R}} \langle \alpha_\star^-(x) | \alpha_\star^+(x) \rangle_{\mathbb{C}^2} \, \mathrm{d}x \\ &= \int_{\mathbb{R}} \left\langle \overline{\alpha_\star(x+L)} \middle| \alpha_\star(x-L) \right\rangle_{\mathbb{C}^2} \, \mathrm{d}x && \text{(by definition: (4.2.9))} \\ &= \int_{\mathbb{R}} \gamma^2 \left\langle \begin{pmatrix} 1 \\ -i \end{pmatrix} \middle| \begin{pmatrix} 1 \\ i \end{pmatrix} \right\rangle_{\mathbb{C}^2} e^{-\int_0^{x+L} \kappa(y)\,\mathrm{d}y} e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \, \mathrm{d}x && \text{(by definition: (4.2.2))} \\ &= 0\end{aligned}$$

#### C.1.2.2 Proof that $\langle \alpha_\star^- | \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle_{\mathbb{C}^2} = \overline{\langle \alpha_\star^+ | \mathcal{D}_{\kappa_L} \alpha_\star^- \rangle_{\mathbb{C}^2}}$ and $\langle \alpha_\star^+ | \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle_{\mathcal{H}} = \langle \alpha_\star^- | \mathcal{D}_{\kappa_L} \alpha_\star^- \rangle_{\mathcal{H}}$

That $\langle \alpha_\star^- | \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle_{\mathbb{C}^2} = \overline{\langle \alpha_\star^+ | \mathcal{D}_{\kappa_L} \alpha_\star^- \rangle_{\mathbb{C}^2}}$ is clear from self-adjointness of $\mathcal{D}_{\kappa_L}$. The other symmetry follows from:

$$\begin{aligned}
\langle \alpha_\star^+ | \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle_{\mathcal{H}} &= \int_{\mathbb{R}} \langle \alpha_\star(x-L) | \mathcal{D}_{\kappa_L} \alpha_\star(x-L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x \\
&= \int_{\mathbb{R}} \langle \alpha_\star(x-L) | (\sigma_3 i\partial_x + \kappa_L(x)\sigma_1) \alpha_\star(x-L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x \\
&= \int_{\mathbb{R}} \langle \alpha_\star(-x-L) | (\sigma_3 i\partial_{-x} + \kappa_L(-x)\sigma_1) \alpha_\star(-x-L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x && \text{(Changing variables)} \\
&= \int_{\mathbb{R}} \langle \alpha_\star(-x-L) | (-\sigma_3 i\partial_x + \kappa_L(x)\sigma_1) \alpha_\star(-x-L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x && \text{(Since } \kappa_L(-x) = \kappa_L(x)) \\
&= \int_{\mathbb{R}} \langle \alpha_\star(x+L) | (-\sigma_3 i\partial_x + \kappa_L(x)\sigma_1) \alpha_\star(x+L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x && \text{(Since } \alpha_\star(-x) = \alpha_\star(x)) \\
&= \int_{\mathbb{R}} \left\langle \overline{\alpha_\star(x+L)} \middle| \overline{(-\sigma_3 i\partial_x + \kappa_L(x)\sigma_1) \alpha_\star(x+L)} \right\rangle_{\mathbb{C}^2} \, \mathrm{d}x && \text{(Using self-adjointness)} \\
&= \int_{\mathbb{R}} \left\langle \overline{\alpha_\star(x+L)} \middle| \mathcal{D}_{\kappa_L} \overline{\alpha_\star(x+L)} \right\rangle_{\mathbb{C}^2} \, \mathrm{d}x = \langle \alpha_\star^- | \mathcal{D}_{\kappa_L} \alpha_\star^- \rangle_{\mathcal{H}} && \text{(C.1.26)}
\end{aligned}$$

#### C.1.2.3 Proof that $\langle \alpha_\star^+ | \alpha_\star^+ \rangle_{\mathcal{H}} = 0$ and $\langle \alpha_\star^- | \alpha_\star^+ \rangle_{\mathcal{H}} = 2i\gamma^2 e^{-2\int_0^L \kappa(y)\,\mathrm{d}y}$

We compute $\langle \alpha_\star^+ | \alpha_\star^+ \rangle_{\mathcal{H}}$ as follows:

$$\begin{aligned}
\langle \alpha_\star^+ | \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle_{\mathcal{H}} &= \int_{\mathbb{R}} \langle \alpha_\star(x-L) | \mathcal{D}_{\kappa_L} \alpha_\star(x-L) \rangle_{\mathbb{C}^2} \, \mathrm{d}x \\
&= \int_{\mathbb{R}} \left\langle \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \middle| (\sigma_3 i\partial_x + \sigma_1 \kappa_L(x)) \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \right\rangle_{\mathbb{C}^2} \mathrm{d}x \\
&= \int_{\mathbb{R}} \left\langle \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \middle| \begin{pmatrix} i \\ 1 \end{pmatrix} (\partial_x + \kappa_L(x)) e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \right\rangle_{\mathbb{C}^2} \mathrm{d}x \\
&= \int_{\mathbb{R}} \left\langle \begin{pmatrix} 1 \\ i \end{pmatrix} \middle| \begin{pmatrix} i \\ 1 \end{pmatrix} \right\rangle_{\mathbb{C}^2} e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} (\partial_x + \kappa_L(x)) e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \, \mathrm{d}x \\
&= 0. && \text{(C.1.27)}
\end{aligned}$$

We compute $\langle \alpha_\star^- \,|\, \mathcal{D}_{\kappa_L} \alpha_\star^+ \rangle$ as follows:

$$\begin{aligned}
\left\langle \alpha_\star^- \,\middle|\, \mathcal{D}_{\kappa_L} \alpha_\star^+ \right\rangle_{\mathcal{H}} &= \int_{\mathbb{R}} \left\langle \overline{\alpha_\star(x+L)} \,\middle|\, \mathcal{D}_{\kappa_L} \alpha_\star(x-L) \right\rangle_{\mathbb{C}^2} \mathrm{d}x \\
&= \int_{\mathbb{R}} \left\langle \overline{\alpha_\star(x+L)} \,\middle|\, (\sigma_3 i\partial_x + \sigma_1 \kappa_L(x)) \alpha_\star(x-L) \right\rangle_{\mathbb{C}^2} \mathrm{d}x \\
&= \gamma^2 \int_{\mathbb{R}} \left\langle \begin{pmatrix} 1 \\ -i \end{pmatrix} \middle| \begin{pmatrix} i \\ 1 \end{pmatrix} \right\rangle_{\mathbb{C}^2} e^{-\int_0^{x+L} \kappa(y)\,\mathrm{d}y} (\partial_x + \kappa_L(x)) e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \mathrm{d}x \\
&= 2i\gamma^2 \int_{\mathbb{R}} e^{-\int_0^{x+L} \kappa(y)\,\mathrm{d}y} (\partial_x + \kappa_L(x)) e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \mathrm{d}x
\end{aligned}$$

$$\begin{aligned}
&= 2i\gamma^2 \int_{-\infty}^0 e^{-\int_0^{x+L} \kappa(y)\,\mathrm{d}y} (\partial_x + \kappa_L(x)) e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \mathrm{d}x && \text{(Since } \kappa_L(x) = \kappa(x-L) \text{ for } x \geq 0) \\
&= -2i\gamma^2 \int_{-\infty}^0 \left[ (\partial_x - \kappa_L(x)) e^{-\int_0^{x+L} \kappa(y)\,\mathrm{d}y} \right] e^{-\int_0^{x-L} \kappa(y)\,\mathrm{d}y} \mathrm{d}x \\
&+ 2i\gamma^2 e^{-\int_0^{L} \kappa(y)\,\mathrm{d}y} e^{-\int_0^{-L} \kappa(y)\,\mathrm{d}y} && \text{(Integration by parts)} \\
&= 2i\gamma^2 e^{-\int_0^{L} \kappa(y)\,\mathrm{d}y} e^{-\int_0^{-L} \kappa(y)\,\mathrm{d}y} && \text{(Since } \kappa_L(x) = -\kappa(x+L) \text{ for } x \leq 0) \\
&= 2i\gamma^2 e^{-2\int_0^{L} \kappa(y)\,\mathrm{d}y} && \text{(Since } \kappa(-x) = -\kappa(x))
\end{aligned}$$

#### C.1.2.4 Proof of bounds on elements of $M_1(E, L)$

Very similar computations to those given above show that:

$$\|\mathcal{D}_{\kappa_L} \alpha^+\|_{\mathcal{H}} \leq C e^{-2\kappa_\infty L}, \quad \|\mathcal{D}_{\kappa_L} \alpha^-\|_{\mathcal{H}} \leq C e^{-2\kappa_\infty L}. \tag{C.1.28}$$

That all elements of the matrix $M_1(E, L)$ may be bounded by $Ce^{-4\kappa_\infty L}$ then follows from the Cauchy-Schwarz inequality using boundedness of the resolvent operator $P^{\pm,\perp}(\mathcal{D}_{\kappa_L} - E)$ in $\mathcal{H}$ for $E < \frac{\kappa_\infty}{4}$.