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BLOCH DYNAMICS WITH SECOND ORDER BERRY PHASE CORRECTION

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ABSTRACT. We derive the semiclassical Bloch dynamics with the second order Berry phase correction, based on a two-scale WKB asymptotic analysis. For uniform external electric field, the bi-characteristics system after a positional shift introduced by Berry connections agrees with the recent result in the physics literature.

1. INTRODUCTION

The understanding of dynamics of Bloch electrons and their response to external electromagnetic fields plays an important role in solid state physics (see for example [1, 2, 19, 24] and the references therein). In recent years, many physics articles such as [2, 3, 10, 24] have explored the significant role of the Berry phase in Bloch dynamics and vast related fields. There have been series of important mathematical works in this direction as well, which are devoted to rigorously justify the the validity of the physics models and provide insight for possible generalizations (see for example [4, 8, 15, 18] and the references therein).

Under the single-particle approximation, the dynamics of an electron is treated as an independent particle on the effective periodic potential generated by ions and other electrons (as a mean-field) in the crystal. After non-dimensionalization, the dynamics is given by

$$i\varepsilon\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x) = \left(-\frac{\varepsilon^2}{2}\Delta_x + V\left(\frac{x}{\varepsilon}\right) + U(x)\right)\psi(t,x), \tag{1.1}$$

where $\psi : [0,\infty)\times\mathbb{R}^d \to \mathbb{C}$ is a single particle wave function, ε is the semi-classical parameter, $V(z)$ is the lattice potential which is periodic with respect to $\mathbb{L}$, and $U(x)$ is the slowly-varying scalar potential.

It is well known that such semi-classical Schrödinger equations propagate oscillations of order $\mathcal{O}(\varepsilon)$ both in space and time. With this model, the relevant physical scale translates to the case when the typical wavelength is comparable to the period of the medium, and both of which are assumed to be small on the length-scale of the considered physical domain. This consequently leads us to a problem involving two-scales, where from now on we shall denote by $0 < \varepsilon \ll 1$ the small dimensionless parameter describing the microscopic/macroscopic scale ratio. We remark that, equation (1.1) can also be derived from the Schrödinger equation in physics units by introducing certain rescaling, which we shall omit in this paper. The readers may refer to [4, 8] for such calculations.

The electronic dynamics in crystals have been studied for many years in the semi-classical regime, where the Liouville equations replace the role of the Schrödinger equation in the limit when the rescaled Planck constant tends to zero. With the help of the Bloch-Floquet theory [19], Markowich, Mauser and Poupaud in [15] derived the semi-classical Liouville equation for describing the propagation of the phase-space density for an energy band, which controls the macroscopic dynamic behavior of the electrons. Later these results were generalized to the cases when a weak random potential in [1] and in [12] nonlinear interactions were present.

Berry phase is an important object that appears during the adiabatic limit of quantum dynamics, as some slow-changing variables enter the quantum evolution as parameters, see [2, 20]. As observed by Simon in [21], the adiabatic Berry phase has an elegant mathematical interpretation as the holonomy of a certain connection, the

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Berry connection, in the appropriate fiber bundle. This setup gives rise to the Berry curvature, which is gauge invariant and can be considered as a physical observable. It has been used in the Bloch dynamics to explain various important phenomena in crystals, see for example [10, 24] and related references. Panati, Spohn and Teufel later gave a rigorous derivation of such Bloch dynamics in [17, 18] by writing down the effective Hamiltonian with the help of the Weyl quantization. A simple derivation of the Bloch dynamics with Berry phase correction based on WKB asymptotics was also given by E, Lu and Yang in [8].

Recently in the physics literature, Gao, Yang and Niu in [10, 11] have constructed a second order semi-classical theory for Bloch electrons under uniform electromagnetic fields. The second order correction terms in Bloch dynamics are obtained, where the first order correction to the Berry curvature is derived. The second order semi-classical theory can be used to explain some important physical phenomenon, such as electric polarizability, magnetic susceptibility, and magnetoelectric polarizability, etc. This provides the motivation to our current study, which aims to extend the mathematical derivation of Bloch dynamics to include second order corrections.

The main purpose of this paper is to give a derivation of the effective Bloch dynamics in crystals based on asymptotic analysis up the second order. The final results that we obtain agree with the recent paper [10] in the situation of uniform electric field, but our approach is mathematically rigorous and is able to handle more general potentials. We also note an independent derivation of the Bloch dynamics with the second order correction [9] using Weyl quantization of operator valued symbols (see [23] for a related work).

More specifically, with a two-scaled WKB ansatz for equation (1.1), we derive the phase equation with the second order corrections, and correspondingly the perturbation in Hamiltonian and in Bloch energy. The truncated WKB solution is proved to be a valid approximation to the exact solution. The phase equation with the second order corrections is no longer a Hamilton-Jacobi equation, but it can be solved by an extended system of trajectories. Note that, since we study here WKB type solutions to the Schrödinger equation, the asymptotic solution we derive is valid only before caustics. If long time validity of the asymptotic solution is desired, one needs to consider instead for example the Gaussian beam methods [7, 13], the Wigner functions [14, 22], or the frozen Gaussian approximation for periodic media [5, 6]. The derivations of Bloch dynamics with Berry phase corrections using these approaches are interesting future directions.

The rest of the paper is organized in the following way. We present a brief review of the theory of Bloch decomposition and introduce the framework of the perturbation method to the Bloch wave function in Section 2. In Section 3, we carry out a systematic two-scaled WKB analysis to the Schrödinger equation with a lattice potential and a slow-varying external potential, where the phase equation up to second order corrections has been derived and the validity of the WKB ansatz has been justified. At last, we show in Section 4 two different ways to derive the characteristic equations of the phase equation with second order corrections, and under certain physical assumptions, the characteristic equation reduces to the bi-characteristic equations with corrected Berry curvature, which essentially agree with the recent results of the physics literature [10, 11].

Throughout this paper, we assume the following the convention in notation. If an ε dependent function f^ε admits an asymptotic expansion, we denote the $n-$th order term by f^n, and the sum of the first $n+1$ terms by $f_{(n)}$, namely,

$$f^\varepsilon = f^0 + \varepsilon f^1 + \cdots + \varepsilon^n f^n + \mathcal{O}(\varepsilon^{n+1}) = f_{(n)} + \mathcal{O}(\varepsilon^{n+1}).$$

Also we use notations as $A^{(n)}$ to stress that it is a $n-$th order tensor.

2. PRELIMINARIES AND THE STATIC PERTURBATION

2.1. **Bloch decomposition.** Recall the Schrödinger equation with a periodic lattice potential and a slow-varying scalar potential

$$i\varepsilon \frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x) = \left(-\frac{\varepsilon^2}{2}\Delta_x + V\left(\frac{x}{\varepsilon}\right) + U(x)\right)\psi(t,x). \tag{2.1}$$

In the absence of the external potential U, the Hamiltonian, after a change of variable $z = x/\varepsilon$, is given by

$$H_{\text{per}} = -\frac{1}{2}\Delta_z + V(z).$$

It is translational invariant with respect to the lattice $\mathbb{L}$. As a result, the spectrum of the Hamiltonian can be understood by the Bloch-Floquet theory, see e.g., [19]. In particular, we have the periodic Bloch wave functions $\Psi_n^0(z,p)$, given as the eigenfunctions of [1]

$$H^0(p)\Psi_n^0(z,p) := \left(\frac{1}{2}\left(-i\nabla_z + p\right)^2 + V(z)\right)\Psi_n^0(z,p) = E_n^0(p)\Psi_n^0(z,p) \tag{2.2}$$

on Γ with periodic boundary conditions. Here Γ is the *unit cell* of lattice $\mathbb{L}$ and $p \in \Gamma^*$ is the crystal momentum, where Γ^* denotes the *first Brillouin zone* (unit cell of the reciprocal lattice). For each fixed $p \in \Gamma^*$, the Bloch Hamiltonian $H^0(p)$ is a self-adjoint operator with compact resolvent, the spectrum of which is given by

$$\sigma\left(H^0(p)\right) = \left\{E_n^0(p) \mid n \in \mathbb{Z}_+\right\} \subset \mathbb{R},$$

where the eigenvalues $E_n^0(p)$ (counting multiplicity) are increasingly ordered $E_1^0(p) \leqslant \cdots \leqslant E_n^0(p) \leqslant E_{n+1}^0(p) \leqslant \cdots$. It is shown by Nenciu [16] that for any $n \in \mathbb{Z}_+$ there exists a closed set $C_n \subset \Gamma^*$ of measure zero such that

$$E_{n-1}^0(p) < E_n^0(p) < E_{n+1}^0(p), \quad p \in \Gamma^* \setminus C_n,$$

and moreover $E_n^0(p)$ and $\Psi_n^0(\cdot,p)$ are analytic on $p \in \Gamma^* \setminus C_n$. In this paper, we stick to the adiabatic regime and assume the energy band n of interest is an isolated Bloch band (*i.e.*, $C_n = \emptyset$). As a consequence, $E_n^0(p)$ and $\Psi_n^0(\cdot,p)$ are analytic with respect to p in Γ^*. Moreover, as we will focus on the particular single band, we will suppress the subscript n unless otherwise indicated.

Given $f \in L^2(\mathbb{R}^d)$, we recall the *Bloch transform*, which is an isometry from $L^2(\mathbb{R}^d)$ to $L^2(\Gamma \times \Gamma^*)$

$$\widetilde{f}(z,p) = \frac{|\Gamma|}{(2\pi)^d} \sum_{X \in \mathbb{L}} f(z+X)e^{-ip\cdot(z+X)}, \tag{2.3}$$

where $|\Gamma|$ denotes the volume of the unit cell of the lattice $\mathbb{L}$. The inverse transform is given by

$$f(z) = \int_{\Gamma^*} e^{ip\cdot z}\widetilde{f}(z,p)\,\mathrm{d}p. \tag{2.4}$$

2.2. **Perturbed Bloch wave functions.** With the external potential U, our analysis needs perturbation of the Bloch waves. For this, let us recall the perturbation theory in the context of Bloch wave functions. We assume a family of Hamiltonian $H^\varepsilon(x,p)$ on $L_z^2(\Gamma)$ parametrized by x and p admits the *static* asymptotic expansion

$$H^\varepsilon(x,p) = H^0(p) + \varepsilon H^1(x,p) + \varepsilon^2 H^2(x,p) + \mathcal{O}(\varepsilon^3).$$

This expansion is called static because it does not capture the dynamical information in the time propagation. We assume the leading order term to be just given by the Bloch Hamiltonian $H^0(p) = \frac{1}{2}(-i\nabla_z + p)^2 + V(z)$, which is independent of x. For the eigenvalue problem

$$H^\varepsilon \Psi^\varepsilon = E_s^\varepsilon \Psi^\varepsilon,$$

we assume the asymptotic expansions

$$E_s^\varepsilon(p,x) = E^0(p) + \varepsilon E_s^1(p,x) + \varepsilon^2 E_s^2(p,x) + \mathcal{O}(\varepsilon^3),$$
$$\Psi^\varepsilon(z,p,x) = \Psi^0(z,p) + \varepsilon \Psi^1(z,p,x) + \varepsilon^2 \Psi^2(z,p,x) + \mathcal{O}(\varepsilon^3).$$

[1]The superscript 0 stands for “unperturbed”, as will be clear in the sequel.

Here, we call E_s^ε the static Bloch energy, in contrast to the dynamic Bloch energy which we shall define later. But, we suppress the subcript in E^0 since E^0 is well-defined by the unperturbed Hamiltonian. The leading (zeroth) order terms in ε yields

$$H^0(p)\Psi^0(\cdot,p) = E^0(p)\Psi^0(\cdot,p), \tag{2.5}$$

which is just the unperturbed eigenvalue problem. In particular, E_s^0 and Ψ^0 are independent of the parameter x. On the other hand, the higher order terms of the Hamiltonian will depend on x explicitly, since these terms (to be specified later) will be used to capture the inhomogeneous influence by the slow-varying scalar potential $U(x)$. Thus, the higher order expansions of E^ε and Ψ^ε depend on both p and x.

Collecting the terms in the next order, one gets

$$H^0\Psi^1 + H^1\Psi^0 = E^0\Psi^1 + E_s^1\Psi^0. \tag{2.6}$$

Taking the inner product with Ψ^0 and using the leading order equation, one gets

$$E_s^1(p,x) = \left\langle \Psi^0(\cdot,p), H^1(p,x)\Psi^0(\cdot,p)\right\rangle. \tag{2.7}$$

Rewrite the first order equation as

$$(H^1 - E_s^1)\Psi^0 = (E^0 - H^0)\Psi^1.$$

Given E_s^1 and H^1, Ψ^1 is then determined up to an arbitrary constant multiple of Ψ^0. To fix the arbitrariness, we will take $\langle\Psi^1,\Psi^0\rangle = 0$, which turns out to simplify some of the calculations in our analysis.

The equation of the second order terms reads

$$H^0\Psi^2 + H^1\Psi^1 + H^2\Psi^0 = E^0\Psi^2 + E_s^1\Psi^1 + E_s^2\Psi^0. \tag{2.8}$$

To get E_s^2, it suffices to take the inner product with Ψ^0

$$\begin{aligned} E_s^2(p,x) &= \left\langle \Psi^0(\cdot,p), H^1(p,x)\Psi^1(\cdot,p,x)\right\rangle - E_s^1(p,x)\left\langle \Psi^0(\cdot,p), \Psi^1(\cdot,p,x)\right\rangle \\ &\quad + \left\langle \Psi^0(\cdot,p), H^2(p,x)\Psi^0(\cdot,p)\right\rangle \\ &= \left\langle \Psi^0(\cdot,p), H^1(p,x)\Psi^1(\cdot,p,x)\right\rangle + \left\langle \Psi^0(\cdot,p), H^2(p,x)\Psi^0(\cdot,p)\right\rangle, \end{aligned} \tag{2.9}$$

where the second equality follows from $\langle\Psi^1,\Psi^0\rangle = 0$. Moreover, Ψ^2 can be solved from (2.8) given E_s^2. This procedure can be continued to higher orders, which we will omit as only the corrections up to the second order will be considered in this paper.

To derive explicit formulas for the static expansion, we consider the Hamiltonian in (2.1). To treat the slow-varying potential $U(x)$, we assume we consider x in the neighborhood of a point x_c, with $x = x_c + \varepsilon z$ satisfied. Then, we do Taylor expansion of $U(x)$ around x_c and get

$$U(x) = U(x_c + \varepsilon z) = U(x_c) + \varepsilon z \cdot \nabla U(x_c) + \varepsilon^2 \frac{1}{2} z \cdot \nabla^2 U(x_c) z + \mathcal{O}(\varepsilon^3).$$

Clearly, $\varepsilon z \cdot \nabla U(x_c)$ corresponds to the first order correction to the unperturbed Hamiltonian, and $\varepsilon^2 \frac{1}{2} z \cdot \nabla^2 U(x_c) z$ accounts for the second order correction. We remark that, the perturbation in Hamiltonian in the form of $\varepsilon z \cdot \nabla U(x_c)$ accounts for for many physics phenomenon, such as the Wannier-Stark ladders, see e.g., [16].

To see how a perturbation like $z \cdot \nabla U(x_c)$ can be related to crystal momentum p, we note that using Bloch transformation, we have

$$z f(z) = \int_{\Gamma^*} z e^{ip\cdot z} \widetilde{f}(z,p)\,\mathrm{d}p = \int_{\Gamma^*} -i\nabla_p e^{ip\cdot z} \widetilde{f}(z,p)\,\mathrm{d}p = \int_{\Gamma^*} i e^{ip\cdot z} \nabla_p \widetilde{f}(z,p)\,\mathrm{d}p.$$

Hence, we arrived at the first order correction to the Hamiltonian

$$H^1(p,x_c) = i\nabla U(x_c) \cdot \nabla_p,$$

and according to (2.7), the first order correction to the static Bloch energy is

$$E_s^1(p, x_c) = \nabla U(x_c) \cdot i\langle \Psi^0, \nabla_p \Psi^0 \rangle. \tag{2.10}$$

Similarly, by (2.9), we obtain the second order correction to the static Bloch energy

$$E_s^2(p, x_c) = \nabla U(x_c) \cdot i\langle \Psi^0, \nabla_p \Psi^1 \rangle + \frac{1}{2}\nabla^2 U(x_c) : \langle \Psi^0, \nabla_p^2 \Psi^0 \rangle. \tag{2.11}$$

3. WKB ASYMPTOTIC ANALYSIS

3.1. **The ansatz and the zeroth order equation.** In this section, we carry out a two-scaled mono-kinetic WKB analysis to the Schrödinger equation. The starting point is the following ansatz, which is a natural extension of the ones applied in [8], to the Schrödinger equation (2.1).

$$\psi_{\mathrm{w}} = A^\varepsilon(t,x)\chi^\varepsilon\left(\frac{x}{\varepsilon}, t, \nabla_x S^\varepsilon, x\right)\exp\left(\frac{i}{\varepsilon}S^\varepsilon(t,x)\right), \tag{3.1}$$

where $\chi^\varepsilon(z,t,p,x)$ is the modified Bloch waves with the asymptotic expansion

$$\chi^\varepsilon(z,t,p,x) = \chi^0(z,p) + \varepsilon\chi^1(z,t,p,x) + \varepsilon^2\chi^2(z,t,p,x) + \mathcal{O}(\varepsilon^3).$$

We will take

$$\chi^0(z,p) = \Psi^0(z,p),$$

which does not depend on t or x, and we expect $\chi^k(z,t,p,x)$ contains $\Psi^k(z,p,x)$ and necessary modification terms to be specified. We emphasize that, even though $\Psi^k(z,p,x)$ is time-independent, $\chi^k(z,t,p,x)$ might be time-dependent due to the modification terms. We also assume the asymptotic expansions for the phase and amplitude in the ansatz (3.1)

$$S^\varepsilon(t,x) = S^0(t,x) + \varepsilon S^1(t,x) + \varepsilon^2 S^2(t,x) + \mathcal{O}(\varepsilon^3),$$

and

$$A^\varepsilon(t,x) = A^0(t,x) + \varepsilon A^1(t,x) + \varepsilon^2 A^2(t,x) + \mathcal{O}(\varepsilon^3).$$

We emphasize that here the phase function series $\{S^k\}$ and the amplitude function series $\{A^k\}$ are *real-valued*, while the functions χ^ε are complex-valued, all yet to be determined. Note that, since we will focus on a particular band throughout the analysis, we have suppressed the energy band subscript k to simplify the notation. The validity and the accuracy of this ansatz will be discussed later.

Note that, we can rewrite the ansatz in the following way

$$\psi_{\mathrm{w}} = a^\varepsilon\left(t, \frac{x}{\varepsilon}, x\right)\exp(iS^0(t,x)/\varepsilon),$$

where

$$a^\varepsilon\left(t, \frac{x}{\varepsilon}, x\right) = A^\varepsilon(t,x)\chi^\varepsilon\left(\frac{x}{\varepsilon}, t, \nabla_x S^\varepsilon, x\right)\exp\left(i(S^1 + \varepsilon S^2 + \cdots)\right),$$

is the total amplitude, which is clearly complex-valued. We remark that, the ansatz (3.1) is special in the sense that, the total amplitude a^ε depend on the χ^n in a restrictive way. To be more specific, since A^k are all real-valued, it contains no phase information at all while all the phase information is contained in the term $\exp\left(i(S^1 + \varepsilon S^2 + \cdots)\right)$. This assumption is essential to guarantee that the canonical variables have a unique trajectory. This is also why this ansatz is called mono-kinetic.

We also emphasize that, as our purpose is to derive Bloch dynamics and its corrections, we do not aim to find a general approximate solution to the Schrödinger equation up to all time, but rather a specific solution which describes the behavior of a wave packet propagating under (2.1). In particular, (3.1) poses restrictions on the initial condition, which we will discuss further below.

A straightforward calculation yields

$$e^{-iS^\varepsilon/\varepsilon}\partial_t\psi_{\rm w} = \partial_t A^\varepsilon\chi^\varepsilon + A^\varepsilon\partial_t\chi^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\chi^\varepsilon\partial_t S^\varepsilon + A^\varepsilon\nabla_p\chi^\varepsilon\cdot\nabla_x\partial_t S^\varepsilon,$$

$$e^{-iS^\varepsilon/\varepsilon}\nabla_x\psi_{\rm w} = \nabla_x A^\varepsilon\chi^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\chi^\varepsilon\nabla_x S^\varepsilon + A^\varepsilon\nabla_x\chi^\varepsilon + A^\varepsilon\nabla_x^2 S^\varepsilon\nabla_p\chi^\varepsilon + \frac{1}{\varepsilon}A^\varepsilon\nabla_z\chi^\varepsilon,$$

and

$$\begin{aligned} e^{-iS^\varepsilon/\varepsilon}\Delta_x\psi_{\rm w} = {} & \Delta_x A^\varepsilon\chi^\varepsilon + 2\frac{i}{\varepsilon}\nabla_x A^\varepsilon\cdot\nabla_x S^\varepsilon\chi^\varepsilon + 2\nabla_x A^\varepsilon\cdot\nabla_x\chi^\varepsilon + 2\nabla_x A^\varepsilon\cdot\nabla_x^2 S^\varepsilon\nabla_p\chi^\varepsilon \\ & + 2\frac{1}{\varepsilon}\nabla_x A^\varepsilon\cdot\nabla_z\chi^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\chi^\varepsilon\Delta_x S^\varepsilon - \frac{1}{\varepsilon^2}|\nabla_x S^\varepsilon|^2 A^\varepsilon\chi^\varepsilon + 2\frac{i}{\varepsilon}A^\varepsilon\nabla_x S^\varepsilon\cdot\nabla_x\chi^\varepsilon \\ & + 2\frac{i}{\varepsilon}A^\varepsilon\nabla_x S^\varepsilon\cdot\nabla_x^2 S^\varepsilon\nabla_p\chi^\varepsilon + 2\frac{i}{\varepsilon^2}A^\varepsilon\nabla_x S^\varepsilon\cdot\nabla_z\chi^\varepsilon + A^\varepsilon\Delta_x\chi^\varepsilon \\ & + 2A^\varepsilon\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_x\chi^\varepsilon + 2\frac{1}{\varepsilon}\nabla_x\cdot\nabla_z\chi^\varepsilon A^\varepsilon + \nabla_p\chi^\varepsilon\cdot\left(\nabla_x\cdot\nabla_x^2 S^\varepsilon\right)A^\varepsilon \\ & + A^\varepsilon\left(\nabla_x^2 S^\varepsilon\nabla_p\right)^2\chi^\varepsilon + 2\frac{1}{\varepsilon}A^\varepsilon\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_z\chi^\varepsilon + \frac{1}{\varepsilon^2}A^\varepsilon\Delta_z\chi^\varepsilon. \end{aligned}$$

After sorting the terms in order of ε, we obtain

$$i\varepsilon e^{-iS^\varepsilon/\varepsilon}\partial_t\psi_{\rm w} = T_0 + \varepsilon T_1, \tag{3.2}$$

$$e^{-iS^\varepsilon/\varepsilon}\left(-\frac{\varepsilon^2}{2}\Delta_x + V\left(\frac{x}{\varepsilon}\right) + U(x)\right)\psi_{\rm w} = F_0 + \varepsilon F_1 + \varepsilon^2 F_2, \tag{3.3}$$

where we have introduced the short-hand notations

$$\begin{aligned} T_0 &= -A^\varepsilon\chi^\varepsilon\partial_t S^\varepsilon, \quad T_1 = i\partial_t A^\varepsilon\chi^\varepsilon + iA^\varepsilon\partial_t\chi^\varepsilon + iA^\varepsilon\nabla_p\chi^\varepsilon\cdot\nabla_x\partial_t S^\varepsilon, \\ F_0 &= \frac{1}{2}|\nabla_x S^\varepsilon|^2 A^\varepsilon\chi^\varepsilon - iA^\varepsilon\nabla_x S^\varepsilon\cdot\nabla_z\chi^\varepsilon - \frac{1}{2}A^\varepsilon\Delta_z\chi^\varepsilon + V\left(\frac{x}{\varepsilon}\right)A^\varepsilon\chi^\varepsilon + U(x)A^\varepsilon\chi^\varepsilon \\ &= \left(H^0(p)\left(\frac{x}{\varepsilon},\nabla_x S^\varepsilon\right) + U(x)\right)\chi^\varepsilon A^\varepsilon, \\ F_1 &= -\frac{i}{2}\left(\Delta_x S^\varepsilon + 2(\nabla_x S^\varepsilon - i\nabla_z)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^\varepsilon A^\varepsilon - i(\nabla_x S^\varepsilon - i\nabla_z)\cdot\nabla_x\chi^\varepsilon A^\varepsilon \\ &\quad - i\nabla_x A^0\cdot(\nabla_x S^\varepsilon - i\nabla_z)\chi^\varepsilon. \\ F_2 &= -\frac{1}{2}\Delta_x A^\varepsilon\chi^\varepsilon - \nabla_x A^\varepsilon\cdot\nabla_x\chi^\varepsilon - \nabla_x A^\varepsilon\cdot\nabla_x^2 S^\varepsilon\nabla_p\chi^\varepsilon - \frac{1}{2}A^\varepsilon\Delta_x\chi^\varepsilon - A^\varepsilon\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_x\chi^\varepsilon \\ &\quad - \frac{1}{2}\nabla_p\chi^\varepsilon\cdot\left(\nabla_x\cdot\nabla_x^2 S^\varepsilon\right)A^\varepsilon - \frac{1}{2}A^\varepsilon\left(\nabla_x^2 S^\varepsilon\nabla_p\right)^2\chi^\varepsilon. \end{aligned}$$

Combining (3.2) and (3.3) and matching by order of ε, to the leading order, we get the following Hamilton-Jacobi equation for the leading term of the phase function

$$-\partial_t S^0 = E^0(\nabla_x S^0) + U(x), \tag{3.4}$$

where we have used the identity (2.2). Recall that, for an isolated Bloch band, $E^0(p)$ is analytic for all $p \in \Gamma^*$. Thus, the equation of S^0 can be solved by the method of characteristics, where the characteristic flow is determined by the following Hamiltonian equations:

$$\dot Q = P, \quad \dot P = -\nabla_P E^0(Q),$$

with initial conditions

$$Q(0) = x, \quad P(0) = \nabla_x S^0(0,x).$$

We remark that, the characteristic lines obtained by the above Hamiltonian flow are interpreted as the rays of geometric optics. Given the initial phase $S^0(0,x)$, the Hamiltonian system locally defines a flow map. Caustics may appear at some finite time when the characteristics initiated at different locations intersect. In the event of caustics, the Hamiltonian system no long has classical solutions and the WKB solutions to the Schrödinger equation (2.1) breaks down as well. But since we aim to derive corrections to the phase equation and to Bloch dynamics, it suffices to consider the the WKB solutions before caustics formation.

It is natural to interpret Q and P as canonical variables of the Hamilton-Jacobi equation. In Bloch dynamics, one considers a localized wave packet, in which state the expectations of the position operator and the momentum operator are called the classical variables. In the semiclassical limit, to the leading order, the classical variables agree with the canonical variables (see e.g., [18, 24]). As we will see in later sections, within the Bloch dynamical equations with corrections there is position shift introduced by Berry connections.

3.2. **The first order corrections.**

3.2.1. *Useful identities for Bloch waves.* To study the first order correction, we shall first derive some useful identities from the leading order Bloch eigenvalue problem:

$$H^0(p)\chi^0(z,p) = E^0(p)\chi^0(z,p).$$

Differentiating this equation with respect to p, we get

$$(p - i\nabla_z)\chi^0 + H^0(p)\nabla_p\chi^0 = \nabla_p E^0\chi^0 + E^0\nabla_p\chi^0. \tag{3.5}$$

The inner product with χ^0 gives (since $(H^0_p - E^0(p))\chi^0 = 0$)

$$\left\langle \chi^0, (p - i\nabla_z)\chi^0 \right\rangle = \nabla_p E^0. \tag{3.6}$$

Let us differentiate (3.5) once again with respect to p, take a product with $\nabla_x^2 S^\varepsilon$ and sum over indices (i.e., a Frobenius inner product for matrices), we arrive at

$$\begin{aligned}\Delta_x S^\varepsilon\chi^0 + 2(-i\nabla_z + p)\cdot\nabla_x^2 S^\varepsilon\nabla_p\chi^0 + H^0(p)\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_p\chi^0 = \\ \nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_p E^0\chi^0 + 2\nabla_x^2 S^\varepsilon\nabla_p E^0\cdot\nabla_p\chi^0 + E^0\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_p\chi^0,\end{aligned} \tag{3.7}$$

which implies after taking inner product with χ^0,

$$\left\langle \chi^0, \left(\Delta_x S^\varepsilon + 2(-i\nabla_z + p)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^0 \right\rangle = \nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_p E^0 + 2\nabla_x^2 S^\varepsilon\nabla_p E^0\cdot\left\langle \chi^0, \nabla_p\chi^0 \right\rangle. \tag{3.8}$$

We shall use these identities in our asymptotic derivation.

3.2.2. *Derivation of the phase equation with first order correction.* Now we collect $\mathcal{O}(1)$ and $\mathcal{O}(\varepsilon)$ terms from (3.2) and (3.3) and get

$$\begin{aligned}&-A^0\partial_t S^\varepsilon\chi^0 + \varepsilon i\partial_t A\chi^0 - \varepsilon A^1\partial_t S^\varepsilon\chi^0 - \varepsilon A^0\partial_t S^\varepsilon\chi^1 + i\varepsilon A^0\nabla_p\chi^0\cdot\nabla_x\partial_t S^\varepsilon \\ &= \left(H^0(p)\left(\frac{x}{\varepsilon},\nabla_x S^\varepsilon\right) + U(x)\right)\chi^0 A^0 \\ &+ \varepsilon\left(H^0(p)\left(\frac{x}{\varepsilon},\nabla_x S^\varepsilon\right) + U(x)\right)\chi^1 A^0 + \varepsilon\left(H^0(p)\left(\frac{x}{\varepsilon},\nabla_x S^\varepsilon\right) + U(x)\right)\chi^0 A^1 \\ &- \frac{i\varepsilon}{2}\left(\Delta_x S^\varepsilon + 2(\nabla_x S^\varepsilon - i\nabla_z)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^0 A^0 \\ &- i\varepsilon\nabla_x A^0\cdot(\nabla_x S^\varepsilon - i\nabla_z)\chi^0.\end{aligned} \tag{3.9}$$

We take inner product of both hand sides with χ^0 and simplify the result using identities (3.6) and (3.8), we obtain

$$i\varepsilon\partial_t A^0 - A^0\partial_t S^\varepsilon - i\varepsilon A^0\langle\chi^0,\nabla_q\chi^0\rangle\cdot\nabla_x U = (E^0 + U(x))A^0 - i\varepsilon\nabla_x A^0\cdot\nabla_p E^0 - \frac{i\varepsilon}{2}\nabla_x\cdot\nabla_p E^0 A^0.$$

By separating the real and imaginary parts of the above equation, we get

$$\partial_t S_{(1)} + U(x) + \left[E^0 + i\varepsilon\langle\chi^0,\nabla_p\chi^0\rangle\cdot\nabla_x U\right]\Big|_{p=\nabla_x S_{(1)}} = 0, \tag{3.10}$$

$$\partial_t A^0 = -\nabla_x A^0\cdot\nabla_p E^0 - \frac{1}{2}\nabla_x\cdot\nabla_p E^0 A^0 \tag{3.11}$$

where we denote by $S_{(1)} = S^0 + \varepsilon S^1$. Let us consider the structure of these two equations. The leading order equation (3.11) for the amplitude function is a transport equation. The phase equation (3.10) with the first order correction is still a Hamilton-Jacobi type equation. If we define

$$E^1(p,x) = i\langle \chi^0, \nabla_p \chi^0\rangle(p)\cdot\nabla_x U(x),$$

then the correction term in the phase equation is clearly $E^1(\nabla_x S_{(1)}, x)$. This correction term agrees with exactly with the first order correction to static Bloch energy, and we will identity this term with the first order correction to Bloch energy in a *dynamic* picture in Section 3.2.3. If we further differentiate (3.10) with respect to x, we get

$$\partial_t \nabla_x S_{(1)} + \nabla_x^2 S_{(1)}\cdot\nabla_p\left(E^0+\varepsilon E^1\right) + \nabla_x U + i\varepsilon\nabla_x^2 U\cdot\langle\chi^0,\nabla_p\chi^0\rangle = 0.$$

This implies the bi-characteristics in canonical variables with the notation $P = \nabla_x S_{(1)}$

$$\dot{Q} = \nabla_p\left(E^0+\varepsilon E^1\right)|_{p=P,x=Q} \tag{3.12}$$

$$\dot{P} = -\nabla_x U(Q) - i\varepsilon\nabla_x^2 U\cdot\langle\chi^0,\nabla_p\chi^0\rangle|_{p=P,x=Q}. \tag{3.13}$$

Here, $i\langle\chi^0,\nabla_p\chi^0\rangle = \mathscr{A}(p)$ is known as the Berry connection or Berry vector potential. This quantity is gauge-dependent, which means if one chooses different phase factors for χ^0, the resulting $\mathscr{A}(p)$ are actually different. Namely, for an arbitrary smooth function $\zeta(p)$, if the so-called gauge transformation

$$\chi^0 \to \exp(i\zeta(p))\chi^0,$$

is performed, the corresponding change happens for the Berry connection,

$$\mathscr{A}(p) \to \mathscr{A}(p) - \nabla_p\zeta(p).$$

By a change of variables that takes into account the position shift between classical variables and canonical variables by the Berry connection,

$$Q = \widetilde{Q} - \varepsilon\mathscr{A}(\widetilde{P}), \quad P = \widetilde{P},$$

we obtain, after dropping the tilde,

$$\dot{Q} = \nabla_P E^0(P) + \varepsilon\nabla_Q U\times\nabla_P\times\mathscr{A}(P),$$
$$\dot{P} = -\nabla_Q U(Q).$$

Here, $\nabla_p\times\mathscr{A}(p)$ is the Berry curvature, which is gauge independent. This implies, in the corrected Bloch dynamics, an anomalous velocity is introduced by the response of Bloch electrons to the external electric field. In other words, the characteristic speed has been modified due to the correction term $i\varepsilon\langle\chi^0,\nabla_p\chi^0\rangle\cdot\nabla_x U$ in the phase equation. We remark that, so far our results agree with previous works on first order corrections to the Bloch dynamics, see [8, 18, 24]. The focus of this paper is to extend this to second order corrections to the Bloch dynamics.

3.2.3. *Derivation of H^1 and E^1.* In this part, we aim to derive the specific expressions of $H^1(p,x)$ and $E^1(p,x)$, keeping in mind that they should satisfy the equation (2.1) and the solution ansatz (3.1). Also, we will establish the relation between χ^1 with Ψ^0 and Ψ^1.

We observe that, since equation (3.10) and equation (3.11) have been derived, there is a different perspective to view equation (3.9). Substitute (3.10) and (3.11) into (3.9), we obtain

$$\begin{aligned}\mathscr{A}\cdot\nabla_x U\chi^0 A^0 - i\nabla_p\chi^0\cdot\nabla_x U A^0 = \\ + i\nabla_x A^0\cdot(H^0(p)-E^0)\nabla_p\chi^0 + \frac{i}{2}(H^0(p)-E^0)\nabla_x^2 S^\varepsilon\nabla_p\cdot\nabla_p\chi^0 A^0 + (H^0(p)-E^0)\chi^1 A^0.\end{aligned} \tag{3.14}$$

The main idea here is to view this equation as the first order perturbation equation for the *dynamic* Bloch eigenvalue problem, as it has the same structure as (2.6), in particular, all the terms with time derivatives in (3.9) are canceled.

We decompose the perturbation χ^1 into $\chi^1 = w + v$, where

$$v = -\frac{i}{2}\nabla_x^2 S^0 \nabla_p \cdot \nabla_p \chi^0 - i\nabla_x \log A^0 \cdot \nabla_p \chi^0. \tag{3.15}$$

Unlike v, w contains terms that cannot be written explicitly in χ^0, which is given by

$$\mathscr{A} \cdot \nabla_x U \chi^0 - i\nabla_p \chi^0 \cdot \nabla_x U = (H^0 - E^0) w. \tag{3.16}$$

Note that this has the same structure of (2.6) (recalled here for convenience)

$$E^1 \Psi^0 - H^1 \Psi^0 = (H^0 - E^0)\Psi^1,$$

if we identify

$$\Psi^0 = \chi^0, \quad \Psi^1 = w, \quad E^1(p,x) = \mathscr{A}(p)\cdot \nabla_x U(x), \quad \text{and} \quad H^1(p,x) f = i\nabla_x U(x) \cdot \nabla_p f.$$

Note here H^1 is the first order correction to the unperturbed Hamiltonian. Clearly, the first order corrections to the Bloch energy in the static expansion is of the same form as the first order correction to the phase equation, and without confusion, hereafter, we use E^1 to denote both meanings. However, in the dynamic picture, the eigenfunction χ^1 picks up an extra time-dependent part v besides Ψ^1. This will have impact on the next order correction, as will be discussed below.

As we discussed in Section 2.2, it is natural to enforce the orthogonality condition $\langle \chi^0, w\rangle = \langle \Psi^0, \Psi^1\rangle = 0$. Moreover, this condition will simplify the results in Section 3.3.1.

We remark that χ^1 depend on x as a parameter, as clearly seen from the definition of v in (3.15) and the equation (3.16) for w. In addition, although w does not depend on t, v depends on t through S^0 and $\log A^0$, and we have

$$\partial_t v(z,t,p,x) = -\frac{i}{2}\nabla_x^2 \partial_t S^0 \nabla_p \cdot \nabla_p \chi^0 - i\nabla_x \partial_t \log A^0 \cdot \nabla_p \chi^0,$$

and hence χ^1 depends on t.

3.3. **The second order corrections.**

3.3.1. *More useful identities.* For the second order correction, we need some more identities for the Bloch waves, following similar strategies as in Section 3.2.1 applied on (3.16). We conclude with the the following identities, we omit the details for the straightforward derivations.

$$\langle \chi^0, (-i\nabla_z + p) w\rangle + \langle \chi^0, H^1(p)\nabla_p \chi^0\rangle = \nabla_p E^1 + E^1 \langle \chi^0, \nabla_p \chi^0\rangle, \tag{3.17}$$

$$\begin{aligned} &\left\langle \chi^0, \left(\Delta_x S + 2(-i\nabla_z + p)\cdot \nabla_x^2 S^\varepsilon \nabla_p\right) w\right\rangle + \left\langle \chi^0, H^1 \nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p \chi^0\right\rangle \\ &\quad = 2\nabla_x^2 S^\varepsilon \nabla_p E^0 \cdot \langle \chi^0, \nabla_p w\rangle + \nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p E^1 \\ &\qquad + 2\nabla_p E^1 \cdot \langle \chi^0, \nabla_x^2 S^\varepsilon \nabla_p \chi^0\rangle + E^1 \langle \chi^0, \nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p \chi^0\rangle, \end{aligned} \tag{3.18}$$

and

$$\langle \chi^0, (-i\nabla_z + p)\cdot \nabla_x w\rangle + \langle \chi^0, \nabla_x \cdot (H^1 \nabla_p)\chi^0\rangle = \nabla_x \cdot \nabla_p E^1 + \nabla_x E^1 \cdot \langle \chi^0, \nabla_p \chi^0\rangle. \tag{3.19}$$

Besides, from the definition of v, one gets

$$\frac{i}{2}\nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p \chi^0 = -v - i\nabla_x \log A^0 \cdot \nabla_p \chi^0.$$

Then, by direct substitution and simplification, we obtain the following two identities,

$$\frac{i}{2} A^0 E^1 \langle \chi^0, \nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p \chi^0\rangle = -A^0 E^1 \langle \chi^0, v\rangle - iE^1 \nabla_x A^0 \cdot \langle \chi^0, \nabla_p \chi^0\rangle. \tag{3.20}$$

$$-\frac{i}{2} A^0 \left\langle \chi^0, H^1 \nabla_x^2 S^\varepsilon \nabla_p \cdot \nabla_p \chi^0\right\rangle = iA^0 \langle \chi^0, \nabla_p v\rangle \cdot \nabla_x U - \nabla_x A^0 \cdot \langle \chi^0, \nabla_p^2 \chi^0\rangle \cdot \nabla_x U. \tag{3.21}$$

3.3.2. *Derivation of the corrected phase equation.* Now we collect the terms from (3.2) and (3.3) up to $\mathcal{O}(\varepsilon^2)$, this gives

$$\begin{aligned}
& i\varepsilon\partial_t A^0\chi^0 + i\varepsilon^2\partial_t A^1\chi^0 + i\varepsilon^2\partial_t A^0\chi^1 + i\varepsilon^2\partial_t v A^0 \\
&\quad - A^0\partial_t S^\varepsilon\chi^0 - \varepsilon A^1\partial_t S^\varepsilon\chi^0 - \varepsilon A^0\partial_t S^\varepsilon\chi^1 - \varepsilon^2 A^0\partial_t S^\varepsilon\chi^2 - \varepsilon^2 A^1\partial_t S^\varepsilon\chi^1 - \varepsilon^2 A^2\partial_t S^\varepsilon\chi^0 \\
&\quad + i\varepsilon A^0\nabla_p\chi^0\cdot\nabla_x\partial_t S^\varepsilon + i\varepsilon^2 A^1\nabla_p\chi^0\cdot\nabla_x\partial_t S^\varepsilon + i\varepsilon^2 A^0\nabla_p\chi^1\cdot\nabla_x\partial_t S^\varepsilon \\
&= A^0(H^0(p)+U)\chi^0 + \varepsilon A^1(H^0(p)+U)\chi^0 + \varepsilon A^0(H^0(p)+U)\chi^1 \\
&\quad + \varepsilon^2 A^2(H^0(p)+U)\chi^0 + \varepsilon^2 A^1(H^0(p)+U)\chi^1 + \varepsilon^2 A^0(H^0(p)+U)\chi^2 \\
&\quad - i\varepsilon\nabla_x A^0\cdot(\nabla_x S^\varepsilon - i\nabla_z)\chi^0 - i\varepsilon^2\nabla_x A^1\cdot(\nabla_x S^\varepsilon - i\nabla_z)\chi^0 - i\varepsilon^2\nabla_x A^0\cdot(\nabla_x S^\varepsilon - i\nabla_z)\chi^1 \\
&\quad - \frac{i\varepsilon}{2}A^0\left(\Delta_x S^\varepsilon + 2(-i\nabla_z + \nabla_x S^\varepsilon)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^0 \\
&\quad - \frac{i\varepsilon^2}{2}A^1\left(\Delta_x S^\varepsilon + 2(-i\nabla_z + \nabla_x S^\varepsilon)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^0 \\
&\quad - \frac{i\varepsilon^2}{2}A^0\left(\Delta_x S^\varepsilon + 2(-i\nabla_z + \nabla_x S^\varepsilon)\cdot\nabla_x^2 S^\varepsilon\nabla_p\right)\chi^1 \\
&\quad - i\varepsilon^2(-i\nabla_z + \nabla_x S^\varepsilon)\cdot\nabla_x\chi^1 A^0 - \frac{\varepsilon^2}{2}\Delta_x A^0\chi^0 - \varepsilon^2\nabla_x A^0\cdot\nabla_x^2 S^\varepsilon\nabla_p\chi^0 \\
&\quad - \frac{\varepsilon^2}{2}A^0(\nabla_x\cdot\nabla_x^2 S^\varepsilon)\cdot\nabla_p\chi^0 - \frac{\varepsilon^2}{2}A^0(\nabla_x^2 S^\varepsilon\nabla_p)^2\chi^0.
\end{aligned}$$

Take the inner product with χ^0 of the above equation, the real part of the resulting identity reveals[2]

$$\partial_t S_{(2)} + U(x) + \left[E^0 + \varepsilon E^1 + \varepsilon^2 E^2\right]|_{p=\nabla_x S_{(2)}} = 0, \tag{3.22}$$

where E^0 and E^1 are of the form as before but are evaluated at $\nabla_x S_{(2)}$ instead, and we denote by $S_{(2)} = S^0 + \varepsilon S^1 + \varepsilon^2 S^2$. Here E^2 is the second order correction term to the phase equation. Using the identities we derived before, we find that E^2 takes the following form

$$\begin{aligned}
E^2(p,x) &= i\langle\chi^0,\nabla_p w\rangle\cdot\nabla_x U + \langle\nabla_p\chi^0,\nabla_x^2 U\nabla_p\chi^0\rangle - \frac{\Delta_x A^0}{2A^0} + \frac{1}{2}|\nabla_x^2 S^0\nabla_p\chi^0|^2 \\
&\quad + \nabla_x\log A^0\cdot\mathrm{Im}\left(\left\langle\chi^0,\left(p - i\nabla_z - \nabla_p E^0\right)v\right\rangle\right) - \frac{1}{2}\nabla_x^2 S^0\nabla_p\cdot\nabla_p E^0\,\mathrm{Im}\left(\langle\chi^0,v\rangle\right) \\
&\quad - \nabla_x^2 S^0\nabla_p E^0\cdot\mathrm{Im}\left(\langle\chi^0,\nabla_p v\rangle\right) + \frac{1}{2}\mathrm{Im}\left(\left\langle\chi^0,(\Delta_x S^0 + 2(p - i\nabla_z)\cdot\nabla_x^2 S^0\nabla_p)v\right\rangle\right) \\
&\quad + \mathrm{Im}\left(\left\langle\chi^0,(p - i\nabla_z)\cdot\nabla_x v\right\rangle\right) + \mathrm{Im}\left(\langle\chi^0,\partial_t v\rangle\right).
\end{aligned} \tag{3.23}$$

Note that, here

$$\nabla_x v = \nabla_x v(z,t,p,x)|_{z=\frac{x}{\varepsilon},\,p=\nabla_x S_2}.$$

Since χ^0 does not depend on x, we have

$$\nabla_x v = -\frac{i}{2}\nabla_x^3 S^0 : \nabla_p^2\chi^0 - i\nabla_x^2\log A^0\cdot\nabla_p\chi^0.$$

And by using equation (3.4) and (3.11), we can directly compute that

$$\begin{aligned}
\langle\chi^0,\partial_t v\rangle &= -\frac{i}{2}\nabla_x^2\partial_t S^0 : \left\langle\chi^0,\nabla_p^2\chi^0\right\rangle - i\nabla_x\partial_t\log A^0\cdot\left\langle\chi^0,\nabla_p\chi^0\right\rangle, \\
&= \frac{i}{2}\left(\nabla_x^3 S^0\cdot\nabla_p E^0 + (\nabla_x^2 S^0\cdot\nabla_p)\otimes(\nabla_x^2 S^0\cdot\nabla)E^0 + \nabla_x^2 U\right) : \left\langle\chi^0,\nabla_p^2\chi^0\right\rangle \\
&\quad + i\left(\nabla_x^2\log A^0\cdot\nabla_p E^0 + \nabla_x\log A^0(\nabla_x^2 S^0 : \nabla_p^2 E^0)\right)\cdot\left\langle\chi^0,\nabla_p\chi^0\right\rangle
\end{aligned}$$

[2]The imaginary part leads to the equation that A_1 satisfies, which does not contribute to the second order corrections to Bloch dynamics, and will hence be neglected in this paper.

$$+ i\left(\frac{1}{2}\nabla_x^3 S^0\cdot\nabla_p\cdot\nabla_p\cdot E^0 + \frac{1}{2}(\nabla_x^2 S^0\cdot\nabla_p\cdot\nabla_p)(\nabla_x^2 S^0\cdot\nabla_p)E^0\right)\cdot\langle\chi^0,\nabla_p\chi^0\rangle.$$

Note that, the last two lines are actually real-valued, they do not enter the corrected phase equation, so we have

$$\mathrm{Im}(\langle\chi^0,\partial_t v\rangle) = \frac{1}{2}\left(\nabla_x^3 S^0\cdot\nabla_p E^0 + (\nabla_x^2 S^0\cdot\nabla_p)\otimes(\nabla_x^2 S^0\cdot\nabla)E^0 + \nabla_x^2 U\right):\mathrm{Re}\langle\chi^0,\nabla_p^2\chi^0\rangle.$$

Note, in the leading order phase equation, the unperturbed Bloch energy E^0 naturally shows up, and the first order correction term to the phase equation happens to be the first order correction of the static Bloch energy E_s^1. However, the second order correction to the phase equation E^2 does not necessarily agree with the second order correction of the static Bloch energy E_s^2. Due to the WKB ansatz (3.1) we have used, the phase equation and the amplitude equation are no longer decoupled with second order corrections, and thus some amplitude dependent terms, such as $\frac{\Delta_x A^0}{2A^0}$, enter the phase equation with second order corrections. Besides, in the first order correction analysis, we have learned that it is necessary to incorporate the term v in χ^1, v related terms also contribute to the second order correction to the phase function.

Recall that we have derived the second order correction of the Bloch energy (2.11) in the static expansion, repeated here for convenience

$$\begin{aligned} E_s^2 &= i\langle\chi^0,\nabla_p w\rangle\cdot\nabla_x U + \frac{1}{2}\langle\nabla_p\chi^0,\nabla_x^2 U\nabla_p\chi^0\rangle \\ &= i\langle\chi^0,\nabla_p w\rangle\cdot\nabla_x U - \frac{1}{4}\left(\langle\chi^0,\nabla_p^2\chi^0\rangle + \text{c.c.}\right):\nabla_x^2 U. \end{aligned} \tag{3.24}$$

As we have mentioned, this is not necessarily the same as E^2 defined in (3.23), but E^2 contains all the terms in E_s^2 (2.11).

3.3.3. *Well-posedness of initial data and accuracy of WKB approximation.* Before we turn to the characteristic equations from the phase equation (3.22), let us summarize this section by discussing the necessary assumptions such that the ansatz (3.1) is a valid approximation and the corresponding accuracy before the formation of caustics.

To this end, we reformulate (3.1) in the following form in order to apply the convergence results in [4] for two-scaled WKB analysis.

$$\begin{aligned} \psi_{\mathrm{w}} &= \sum_{j=0}^{\infty}\varepsilon^j g_j(t,\frac{x}{\varepsilon},x)\exp\left(i\sum_{m=1}^{\infty}\varepsilon^{m-1}S^m(t,x)\right)\exp\left(\frac{i}{\varepsilon}S^0(t,x)\right) \\ &:= \sum_{j=0}^{\infty}\varepsilon^j u_j(t,\frac{x}{\varepsilon},x)\exp\left(\frac{i}{\varepsilon}S^0(t,x)\right), \end{aligned} \tag{3.25}$$

where

$$u_j = g_j\exp\left(i\sum_{m=1}^{\infty}\varepsilon^{m-1}S^m(t,x)\right),$$

and g_j is determined by asymptotically matching the terms in (3.1). For example,

$$g_0 = A^0(t,x)\chi^0(t,x/\varepsilon,\nabla_x S^0(t,x)), \tag{3.26}$$

and

$$\begin{aligned} g_1 = {} & A^0(t,x)\chi^1(t,x,x/\varepsilon,\nabla_x S^0(t,x)) + A^1(t,x)\chi^0(t,x/\varepsilon,\nabla_x S^0(t,x)) \\ & + A^0(t,x)\nabla_x S^1(t,x)\cdot\nabla_p\chi^0(t,x/\varepsilon,\nabla_x S^0(t,x)). \end{aligned} \tag{3.27}$$

Taking $t=0$, the ansatz above imposes well-preparedness requirement on the initial condition to guarantee the accuracy of this approximation. For simplicity, we denote the truncated $J-$th order WKB approximation by

$$\psi_{\mathrm{w}}^J := \sum_{j=0}^{J-1}\varepsilon^j u_j\left(t,\frac{x}{\varepsilon},x\right)\exp\left(\frac{i}{\varepsilon}S^0(t,x)\right).$$

To make the leading order WKB approximation valid, we make the following assumptions, similar to those in [4].

Assumption. *The initial wave function* ψ_I^ε *is in the Schwartz space* $\mathscr{S}(\mathbb{R}^d)$*, and is of the WKB-type, i.e.*

$$\psi_I^\varepsilon(x) = u_I\left(x, \frac{x}{\varepsilon}\right) e^{i\phi_I(x)/\varepsilon} + \varepsilon\varphi_I^\varepsilon(x),$$

with $\phi_I \in C^\infty(\mathbb{R}^d, \mathbb{R})$*,* $u_I \in \mathscr{S}(\mathbb{R}^d \times \Gamma; \mathbb{C})$*. The function* φ_I^ε *is to be specified later. The amplitude* $u_I(x,y)$ *is assumed to be concentrated on a single isolated Bloch band* $E_k(p)$ *corresponding to a simple eigenvalue of* H^0*, i.e.*

$$u_I(x,y) = a_I(x)\chi_k(y, \nabla_x\phi_I(x)),$$

where $a_I \in \mathscr{S}(\mathbb{R}^d; \mathbb{C})$ *is a given amplitude.*

One can check that, with the assumptions above, relation (3.26) is always satisfied at $t = 0$, and when $t = 0$, A^0 and S^0 and S^1 are uniquely determined consequently. Moreover, from equation (3.14), χ^1 is also determined at initial time.

Next, recall that we focus on wave functions which oscillate at the scale of $\mathscr{O}(\varepsilon)$, so we define the following spaces: for $s \in \mathbb{N}$,

$$||f^\varepsilon||_{X_\varepsilon^s} = \sum_{|\alpha|+|\beta|\leq s} ||x^\alpha(\varepsilon\partial)^\beta f^\varepsilon||_{L^2},$$

and define X_ε^s as:

$$X_\varepsilon^s = \left\{ f^\varepsilon \in L^2(\mathbb{R}^d); \sup_{0<\varepsilon\leq 1} ||f^\varepsilon||_{X_\varepsilon^s} \right\}.$$

Now, we are ready to state the additional assumption for the next order WKB approximation.

Assumption. *(Well-prepared initial data.) The initial conditions* $\psi_I^\varepsilon(x)$ *satisfy the assumptions above, and the leading part of the perturbation* φ_I^ε *is of the particular form, so that there exist solutions to* $A^1 \in \mathbb{R}$ *and* $S^2 \in \mathbb{R}$ *when* $t = 0$*, whereas the residual part of* φ_I^ε *is* $\mathscr{O}(\varepsilon)$ *in* X_ε^s *for all* $s \in \mathbb{N}$*.*

This assumption also implies that, initially each term in the asymptotic expansion (3.1) is uniformly bounded in X_ε^s for all $s \in N$.

Note that, there are always initial conditions which satifiy all the assumptions above, which are WKB-type initial condition concentrated on one band with no tails. Then, by [4, Theorem 4.5], we obtain the second order approximation to the exact solution.

Theorem 3.1. *Define* $\Psi^\varepsilon(t)$ *to be the solution to equation* (2.1) *with initial conditions satisfying all the assumptions above. Assume there is no caustic formed before time* t_0*, the second order WKB approximation* ψ_W^2 *is valid up to any* $t < t_0$*, and for all* $s \in \mathbb{N}$ *there exists a constant C such that*

$$\sup_{0<\tau<t} \|\Psi^\varepsilon(\tau) - \psi_w^2(\tau)\|_{X_\varepsilon^s} \leq C\varepsilon^2.$$

4. Characteristic equations with second order corrections

In this section, we derive the bi-characteristic equations for the phase equation with second order correction in canonical variables. While we use tensor notations in this section, some expressions will be rewritten using index notation in the appendix for better clarity, since higher order derivatives are involved,

Recall that, the phase equation with first order correction (3.10) is still an Hamilton-Jacobi equation, whose characteristic equation in canonical variables Q and P are given by

$$\dot{Q} = \nabla_p\left(E^0 + \varepsilon E^1\right)|_{p=P,x=Q},$$
$$\dot{P} = -\nabla_x U(x) - i\varepsilon\nabla_x^2 U \cdot \langle\chi^0, \nabla_p\chi^0\rangle|_{p=P,x=Q}.$$

On the other hand, for phase equation with second order corrections (3.22), high order derivatives of S^0 as well as derivatives of $\log A^0$ are involved. This means, the corrected phase equation does not admit a simple bi-characteristic structure. In other words, such a characteristic system is not yet closed.

Whereas, one observes that the higher order derivatives of S^0 and $\log A^0$ are only contained in the terms of order $\mathcal{O}(\varepsilon^2)$. Therefore, we can proceed in two ways:

(1) One can solve the leading order phase equation equation and amplitude equation in the pre-processing stage, then in the phase equation with second order correction, all the higher order derivatives in the $\mathcal{O}(\varepsilon^2)$ terms are thus treated as known quantities. This is done in §4.1, the physical meaning of the resulting characteristic equations are discussed in §4.2.

(2) One can close the system of trajectories by introducing the characteristic equations of those higher order derivatives appeared in the $\mathcal{O}(\varepsilon^2)$ correction. We shall present these additional characteristic equations in §4.3.

4.1. **Bi-characteristic equations assuming S^0 and A^0.** Let us first write down the characteristics for the phase equations assuming S^0 and A^0 are known. For simplicity of notation, we introduce more notations for the auxiliary quantities

$$P^{(2)} = \nabla_x^2 S^0, \quad P^{(3)} = \nabla_x^3 S^0, \quad P^{(4)} = \nabla_x^4 S^0, \quad P^{(5)} = \nabla_x^5 S^0,$$

and

$$L^{(0)} = \log A^0, \quad L^{(1)} = \nabla_x \log A^0, \quad L^{(2)} = \nabla_x^2 \log A^0, \quad L^{(3)} = \nabla_x^3 \log A^0.$$

In the terms above, the superscripts denote the degrees of the tensors respectively. Also, one observes that all the tensors above are symmetric and only depend on S^0 and A^0. These can actually be solved also by characteristics, which will be postponed to §4.3.

Now given the auxiliary quantities above, one gets the characteristic equations of phase equation with second order corrections in canonical variables with the notation $P = \nabla_x S_{(2)}$,

$$\dot{Q} = \nabla_p \left(E^0 + \varepsilon E^1 + \varepsilon^2 E^2\right)_{p=P,x=Q},$$

and

$$\dot{P} + \left(\nabla_x U + i\varepsilon \nabla_x^2 U \cdot \langle \chi^0, \nabla_p \chi^0 \rangle + \varepsilon^2 \tilde{F}\right)_{p=P,x=Q} = 0,$$

where as before $E^1 = i\langle \chi^0, \nabla_p \chi^0 \rangle \cdot \nabla_x U$ and the second order correction is given by

$$\begin{aligned} E^2 = {} & i\langle \chi^0, \nabla_p w\rangle \cdot \nabla_x U + \langle \nabla_p \chi^0, \nabla_x^2 U \nabla_p \chi^0 \rangle - \frac{1}{2}\left((L^{(2)})_{jj} + L^{(1)} \cdot L^{(1)}\right) + \frac{1}{2}\langle P^{(2)} \cdot \nabla_p \chi^0, P^{(2)} \cdot \nabla_p \chi^0 \rangle \\ & + L^{(1)} \cdot \mathrm{Im}\left(\left\langle \chi^0, (p - i\nabla_z - \nabla_p E^0)\left(-\frac{i}{2} P^{(2)} : \nabla_p^2 \chi^0 - i\nabla_p \chi^0 \cdot L^{(1)}\right)\right\rangle\right) \\ & + \mathrm{Im}\left(\left\langle \chi^0, \left((P^{(2)})_{jj} - P^{(2)} : \nabla_p^2 E^0\right)\left(-\frac{i}{2} P^{(2)} : \nabla_p^2 \chi^0\right)\right\rangle\right) \\ & + \mathrm{Im}\left(\left\langle \chi^0, (p - i\nabla_z - \nabla_p E^0) \cdot (P^{(2)} \cdot \nabla_p)\left(-\frac{i}{2} P^{(2)} : \nabla_p^2 \chi^0 - i\nabla_p \chi^0 \cdot L^{(1)}\right)\right\rangle\right) \\ & + \mathrm{Im}\left(\left\langle \chi^0, (p - i\nabla_z - \nabla_p E^0) \cdot \left(-\frac{i}{2} P^{(3)} \cdot \nabla_p \cdot \nabla_p \chi^0 - i\nabla_p \chi^0 \cdot L^{(2)}\right)\right\rangle\right) \\ & + \frac{1}{2}\left(P^{(3)} \cdot \nabla_p E^0 + (P^{(2)} \cdot \nabla_p)(P^{(2)} \cdot \nabla) E^0 + \nabla_x^2 U\right) : \mathrm{Re}\langle \chi^0, \nabla_p^2 \chi^0 \rangle, \end{aligned}$$

and the second order "forcing" term in the equation of P is given by

$$\begin{aligned} \tilde{F} = {} & i\nabla_x^2 U \cdot \langle \chi^0, \nabla_p w \rangle + i\nabla_x U \cdot \langle \chi^0, \nabla_p \nabla_x w \rangle + \langle \nabla_p \chi^0, \nabla_x^3 U \cdot \nabla_p \chi^0 \rangle \\ & - \frac{1}{2}\left((L^{(3)})_{jjk} - 2L^{(1)} \cdot L2\right) + \mathrm{Re}\left(\langle P^{(3)} \cdot \nabla_p \chi^0, P^{(2)} \cdot \nabla_p \chi^0 \rangle\right) \\ & + L^{(2)} \cdot \mathrm{Im}\left(\left\langle \chi^0, (p - i\nabla_z - \nabla_p E^0)\left(-\frac{i}{2} P^{(2)} : \nabla_p^2 \chi^0 - i\nabla_p \chi^0 \cdot L^{(1)}\right)\right\rangle\right) \\ & + L^{(1)} \cdot \mathrm{Im}\left(\left\langle \chi^0, (p - i\nabla_z - \nabla_p E^0)\left(-\frac{i}{2} P^{(3)} \cdot \nabla_p \cdot \nabla_p \chi^0 - i\nabla_p \chi^0 \cdot L^{(2)}\right)\right\rangle\right) \end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{2}\left((P^{(3)})_{jjk}-P^{(3)}\cdot\nabla_p\cdot\nabla_p E^0\right)\mathrm{Im}\left(\left\langle\chi^0,-\frac{i}{2}P^{(2)}:\nabla_p^2\chi^0\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\cdot(P^{(3)}\cdot\nabla_p)\left(-\frac{i}{2}P^{(2)}:\nabla_p^2\chi^0-i\nabla_p\chi^0\cdot L^{(1)}\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\cdot(P^{(2)}\cdot\nabla_p)\left(-\frac{i}{2}P^{(3)}\cdot\nabla_p\cdot\nabla_p\chi^0-i\nabla_p\chi^0\cdot L^{(2)}\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\cdot\left(-\frac{i}{2}P^{(4)}\cdot\nabla_p\cdot\nabla_p\chi^0-i\nabla_p\chi^0\cdot L^{(3)}\right)\right\rangle\right)\\
&+\frac{1}{2}\left(P^{(4)}\cdot\nabla_pE^0+2(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla)E^0+\nabla_x^3U\right):\mathrm{Re}\langle\chi^0,\nabla_p^2\chi^0\rangle.
\end{aligned}
$$

For clarity, we shall also express the equations above in index form in Appendix.

4.2. **Physical interpretation of the bi-characteristic equations.** Let us understand better the bi-characteristic equations of Q and P, assuming that the auxiliary quantities ($P^{(m)}$ and $L^{(m)}$'s) are all given. Following [10, 11], we call E^2 the second order wave packet energy and define

$$E_w(Q,P)=E^2(Q,P)-E_s^2(Q,P),$$

where E_w is interpreted as the extra wave packet energy besides the static Bloch energy due to the specific profile of thel wave function. In other words, E^2 consists of two parts, the second order correction to the static Bloch energy, and extra wave packet energy which may be time-dependent due to its dependence on the phase and the amplitude. In our WKB analysis, the extra wave packet energy is given by

$$
\begin{aligned}
E_w=&\frac{1}{2}\langle\nabla_p\chi^0,\nabla_x^2U\nabla_p\chi^0\rangle-\frac{1}{2}\left((L^{(2)})_{jj}+L^{(1)}\cdot L^{(1)}\right)+\frac{1}{2}\langle P^{(2)}\cdot\nabla_p\chi^0,P^{(2)}\cdot\nabla_p\chi^0\rangle\\
&+L^{(1)}\cdot\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\left(-\frac{i}{2}P^{(2)}:\nabla_p^2\chi^0-i\nabla_p\chi^0\cdot L^{(1)}\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,\left((P^{(2)})_{jj}-P^{(2)}:\nabla_p^2E^0\right)\left(-\frac{i}{2}P^{(2)}:\nabla_p^2\chi^0\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\cdot(P^{(2)}\cdot\nabla_p)\left(-\frac{i}{2}P^{(2)}:\nabla_p^2\chi^0-i\nabla_p\chi^0\cdot L^{(1)}\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p-i\nabla_z-\nabla_pE^0)\cdot\left(-\frac{i}{2}P^{(3)}\cdot\nabla_p\cdot\nabla_p\chi^0-i\nabla_p\chi^0\cdot L^{(2)}\right)\right\rangle\right)\\
&+\frac{1}{2}\left(P^{(3)}\cdot\nabla_pE^0+(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla)E^0+\nabla_x^2U\right):\mathrm{Re}\langle\chi^0,\nabla_p^2\chi^0\rangle.
\end{aligned}
$$

We define

$$\mathscr{A}^0(p)=i\langle\chi^0,\nabla_p\chi^0\rangle,\quad \mathscr{A}^1(t,p,x)=\frac{1}{2}\left(i\langle\chi^0,\nabla_p w\rangle+c.c.\right),$$

$$\mathscr{B}=-\frac{1}{4}\left(\langle\chi^0,\nabla_p^2\chi^0\rangle+c.c.\right),$$

and

$$\mathscr{A}_{(1)}=\mathscr{A}^0+\varepsilon\mathscr{A}^1,$$

and then we can write

$$E_s^2=\mathscr{A}^1\cdot\nabla_xU+\mathscr{B}:\nabla_x^2U.$$

In the recent physics literature [10, 11], $\mathscr{A}_{(1)}$ is referred to as the Berry connection with the first order correction which responds to the first derivative of the scalar potential. While $\mathscr{B}$ is a new quantity which is yet to be explored. It responds to the second order derivative of the scalar potential and if only a uniform electric field is considered as a perturbation to periodic Hamiltonians as in [10, 11], E^2 loses the contribution from $\mathscr{B}$ because ∇_x^2U vanishes.

Then, we can rewrite the bi-characteristic equations as

$$\dot{Q}=\nabla_PE^0+\varepsilon\nabla_P(\mathscr{A}^0\cdot\nabla_QU)+\varepsilon^2\nabla_PE_s^2(Q,P)+\varepsilon^2\nabla_PE_w,$$

$$\dot{P} = -\nabla_Q U - \varepsilon \nabla_Q^2 U \cdot \mathscr{A}^0 - \varepsilon^2 \nabla_Q E_s^2(Q,P) - \varepsilon^2 \nabla_Q E_w.$$

We observe that, given that the auxiliary quantities involved in E_w are known; the canonical coordinates still satisfy a Hamiltonian flow under a modified Hamiltonian

$$\widetilde{H}_{(2)} = E^0(P) + U(Q) + \varepsilon E^1(Q,P) + \varepsilon^2 E_s^2(Q,P) + \varepsilon^2 E_w(Q,P).$$

To compare our results with those in recent work [10, 11], we consider the special case taken in these papers where the electric field is uniform, or equivalently the scaler potential is linear. Note that our results apply to more general situations. In this scenario, $\nabla_x U$ reduces to a constant vector, and all the higher order derivatives of U vanish. Moreover, H^1 and E^1 no longer depend on x, and as a result, $\mathscr{A}' = \mathscr{A}^0 + \varepsilon \mathscr{A}^1$ becomes $x-$independent.

Next, motived by [10, 11], we carry out the change of variables that incorporates into the position shift due to the Berry connection,

$$Q = Q_c - \varepsilon \mathscr{A}^0 - \varepsilon^2 \mathscr{A}^1, \quad P = P_c.$$

Dropping the subscripts c, the bi-characteristic equations reduce to

$$\dot{Q} = \nabla_P E^0 - \varepsilon \dot{P} \times \nabla_P \times \mathscr{A}' + \varepsilon^2 \nabla_P E_w,$$
$$\dot{P} = -\nabla_Q U - \varepsilon^2 \nabla_Q E_w.$$

At this stage, the characteristic equations have successfully captured the correction term the Berry curvature. However, the expression for the extra wave packet energy E_w is still complicated and may not be gauge invariant. We remark that, the physics papers [10, 11] do not give explicit expression of E_w, neither do they provide any analysis to this term. If we prepare the initial condition in some special form, the extra wave packet energy can be further simplified. For example, if the initial condition is a plane wave multiplied by a periodic Bloch wave,

$$A^0(0,x) = A_0, \quad S^0(0,x) = S_0 + K_0 x.$$

If we denote the potential function $U(x) = c_0 + c_1 x$, then, the exact solutions to equation (3.4) and equation (3.11) are

$$A^0(t,x) = A_0. \quad S^0(t,x) = b_0(t) + b_1(t)x,$$

where

$$b_1(t) = K_0 - c_1 t, \quad b_0(t) = S_0 - \int_0^t E^0(K_0 - c_1 s)\,ds - c_0 t.$$

In other words, $A^0(t,x)$ stays as an constant, and $S^0(t,x)$ remains be be a linear function in x. In this case, by direct calculations, the term v reduces to 0, and the extra wave packet energy E_w simplifies to 0. Hence the bi-characteristic equations become

$$\begin{cases} \dot{Q} &= \nabla_P E^0 - \varepsilon \dot{P} \times \nabla_P \times \mathscr{A}_{(1)}, \\ \dot{P} &= -\nabla_Q U. \end{cases} \tag{4.1}$$

This form essentially agrees with the recent results [10, 11] in the physics literature, although in the above special case, the extra wave packet energy E_w has simplified to 0. However, our derivation is open to different assumptions on the amplitude function and the phase function, and accordingly we would expect different expression of the extra wave packet energy. The work [10, 11] makes heuristic assumptions of the localization of the wave packet around the classical variables, which we do not necessarily assume in the calculation. Our results show that the second order correction to the Bloch dynamics can be derived rigorously in more general situations than that considered in [10, 11].

4.3. **Closing the system of trajectories.** Finally, let us complete the characteristic system of the phase equation with second order correction, without assuming pre-computing the auxiliary terms. That is, we aim to incorporate the Lagrangian trajectories of the auxiliary quantities with Bloch dynamics, so that a larger system of trajectories is obtained as a consequence. Since all these terms show up only in $\mathscr{O}(\varepsilon^2)$ terms, we only need to derive their characteristic equations to the zeroth order.

First, we derive that equations that $L^{(1)}$, $L^{(2)}$ and $L^{(3)}$ satisfy. Note that, if we divide the equation (3.11) by A_0, we get

$$\partial_t \log A_0 + \nabla_x \log A_0 \cdot \nabla_p E + \frac{1}{2}\nabla_x^2 S^0 \cdot \nabla_p \cdot \nabla_p E^0 = 0.$$

Then, by straight-forward differentiation, one gets the equations

$$\begin{aligned}
&\dot{L}^{(0)} + \frac{1}{2}P^{(2)} : \nabla_p^2 E^0 = 0,\\
&\dot{L}^{(1)} + (L^{(1)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0 + \frac{1}{2}P3\cdot\nabla_p\cdot\nabla_p E^0 + \frac{1}{2}(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p\cdot\nabla_p)E^0 = 0,\\
&\dot{L}^{(2)} + 2\,\mathrm{Sym}\left[(L^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + (L^{(1)}\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)E^0\\
&\quad + (L^{(1)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0 + \frac{1}{2}P^{(4)}\cdot\nabla_p\cdot\nabla_p E^0\\
&\quad + \mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + \frac{1}{2}(P^{(2)}\cdot\nabla_p\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)E^0\\
&\quad + \frac{1}{2}(P^{(2)}\cdot\nabla_p\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0 = 0,
\end{aligned}$$

and

$$\begin{aligned}
&\dot{L}^{(3)} + 3\,\mathrm{Sym}\left[(L^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + 3\,\mathrm{Sym}\left[(L^{(2)}\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)E^0\right]\\
&\quad + (L^{(1)}\cdot\nabla_p)(P^{(4)}\cdot\nabla_p)E^0 + (L^{(1)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)^3E^0 + 3\,\mathrm{Sym}\left[(L^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)^2E^0\right]\\
&\quad + 3\,\mathrm{Sym}\left[(L^{(1)}\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + \frac{1}{2}P^{(5)}\cdot\nabla_p\cdot\nabla_p E^0\\
&\quad + \frac{3}{2}\,\mathrm{Sym}\left[(P^{(4)}\cdot\nabla_p\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + \frac{3}{2}\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)E^0\right]\\
&\quad + \frac{1}{2}(P^{(2)}:\nabla_p^2)(P^{(4)}\cdot\nabla_p)E^0 + \frac{3}{2}\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)^2E^0\right]\\
&\quad + \frac{3}{2}\,\mathrm{Sym}\left[(P^{(2)}:\nabla_p^2)(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + \frac{1}{2}(P^{(2)}:\nabla_p^2)(P^{(2)}\cdot\nabla_p)^3E^0 = 0.
\end{aligned}$$

In the equations above, $\mathrm{Sym}[T]$ represents the symmetric part of tensor T, and all the expressions are evaluated at $x = Q$, $p = P$.

Next, let's switch to the derivatives of the phase function S. In the expressions of $\nabla_p E^2$ and α, the derivatives of S up to the fourth order are involved, and in the equation of $L^{(3)}$, the fifth order derivative is also included. Therefore, to close the system, we have to derive the equations for derivatives of S at least to the fifth order. By differentiating equation (3.22) with respect to x for multi-times, and keeping only $\mathscr{O}(1)$ terms, one gets

$$\begin{aligned}
&\dot{P}^{(2)} + \nabla_x^2 U + (P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0 = 0,\\
&\dot{P}^{(3)} + \nabla_x^3 U + 3\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + (P^{(2)}\cdot\nabla_p)^3E^0 = 0,\\
&\dot{P}^{(4)} + \nabla_x^4 U + 4\,\mathrm{Sym}\left[(P^{(4)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + 3(P^{(3)}\cdot\nabla_p)^2E^0\\
&\quad + 6\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + (P^{(2)}\cdot\nabla_p)^4E^0 = 0,
\end{aligned}$$

and

$$\begin{aligned}
&\dot{P}^{(5)} + \nabla_x^5 U + 5\,\mathrm{Sym}\left[(P^{(5)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + 10\,\mathrm{Sym}\left[(P^{(4)}\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)E^0\right]\\
&\quad + 10\,\mathrm{Sym}\left[(P^{(4)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right] + 15\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p)(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right]
\end{aligned}$$

$$+10\,\mathrm{Sym}\left[(P^{(3)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)(P^{(2)}\cdot\nabla_p)E^0\right]+(P^{(2)}\cdot\nabla_p)^5E^0=0.$$

In the equations above, all expressions are evaluated at $x=Q$ and $p=P$. Clearly, the the equations for $P^{(2)}$ to $P^{(5)}$ do not contain higher derivatives of S and $\log A^0$, so now the system is closed.

For clarity, we shall also express the equations in this part in index form in Appendix. To sum up, we have derived the characteristic equations (3.12)–(3.13) of Bloch dynamics with second order corrections, which are coupled with the characteristic equations of the auxiliary quantities defined above.

Appendix A. Expressions in index form

We shall express the equations in Section 4 in index form to avoid possible confusion. In the expressions below, the Einstein summation convention is used. To avoid confusion , we use i, j and k to indicate components of the variables, while we use Greek letters α, β and γ to label the components of the tensors.

In the index notation, $\nabla_p E^2$ takes the following form

$$\begin{aligned}
\partial_{p_j}E^2(p)=\partial_{p_j}\Big[&i\langle\chi^0,\partial_{p_\alpha}w\rangle\partial_{x_\alpha}U+\langle\partial_{p_\alpha}\chi^0,\partial_{x_\alpha}\partial_{x_\beta}U\partial_{p_\beta}\chi^0\rangle+\frac{1}{2}\langle(P^{(2)})_{\alpha\beta}\partial_{p_\beta}\chi^0,(P^{(2)})_{\alpha\gamma}\partial_{p_\gamma}\chi^0\rangle\\
&+(L^{(1)})_\alpha\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)\left(-\frac{i}{2}(P^{(2)})_{\beta\gamma}\partial_{p_\beta}\partial_{p_\gamma}\chi^0-i\partial_{p_\beta}\chi^0(L^{(1)})_\beta\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,\left((P^{(2)})_{\alpha\alpha}-(P^{(2)})_{\alpha\beta}\partial_{p_\alpha}\partial_{p_\beta}E^0\right)\left(-\frac{i}{2}(P^{(2)})_{\gamma\mu}\partial_{p_\gamma}\partial_{p_\mu}\chi^0\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)((P^{(2)})_{\alpha\beta}\partial_{p_\beta})\left(-\frac{i}{2}(P^{(2)})_{\gamma\mu}\partial_{p_\gamma}\partial_{p_\mu}\chi^0-i\partial_{p_\gamma}\chi^0(L^{(1)})_\gamma\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)\left(-\frac{i}{2}(P^{(3)})_{\alpha\beta\gamma}\partial_{p_\beta}\partial_{p_\gamma}\chi^0-i\partial_{p_\beta}\chi^0(L^{(2)})_{\alpha\beta}\right)\right\rangle\right)\\
&+\frac{1}{2}\left((P^{(3)})_{\alpha\beta\gamma}\nabla_{p_\gamma}E^0+((P^{(2)})_{\alpha\mu}\nabla_{p_\mu})((P^{(2)})_{\beta\nu}\nabla_{p_\nu})E^0+(\nabla_x^2U)_{\alpha\beta}\right)\mathrm{Re}(\left\langle\chi^0,\nabla_p^2\chi^0\right\rangle)_{\alpha\beta}\Big],
\end{aligned}$$

and $\tilde{F}$ takes the form

$$\begin{aligned}
\tilde{F}_j=&i\partial_{x_\alpha}\partial_{x_j}U\langle\chi^0,\partial_{x_\alpha}w\rangle+i\partial_{x_\alpha}U\langle\chi^0,\partial_{x_\alpha}\partial_{x_j}w\rangle+\langle\partial_{p_\alpha}\chi^0,\partial_{x_\alpha}\partial_{x_\beta}\partial_{x_j}U\partial_{p_\beta}\chi^0\rangle\\
&-\frac{1}{2}\left((L^{(3)})_{\alpha\alpha j}-2(L^{(1)})_\alpha(L2)_{\alpha j}\right)+\mathrm{Re}\left(\langle(P^{(3)})_{\beta\gamma j}\partial_{p_\beta}\chi^0,(P^{(2)})_{\gamma\mu}\partial_{p_\mu}\chi^0\rangle\right)\\
&+(L^{(2)})_{\alpha j}\cdot\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)\left(-\frac{i}{2}(P^{(2)})_{\beta\gamma}\partial_{p_\beta}\partial_{p_\gamma}\chi^0-i\partial_{p_\beta}\chi^0(L^{(1)})_\beta\right)\right\rangle\right)\\
&+(L^{(1)})_\alpha\cdot\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)\left(-\frac{i}{2}(P^{(3)})_{\beta\gamma j}\partial_{p_\beta}\partial_{p_\gamma}\chi^0-i\partial_{p_\beta}\chi^0(L^{(2)})_{\beta j}\right)\right\rangle\right)\\
&\frac{1}{2}\left((P^{(3)})_{\alpha\alpha j}-(P^{(3)})_{\alpha\beta\gamma}\partial_{p_\alpha}\partial_{p_\gamma}E^0\right)\mathrm{Im}\left(\left\langle\chi^0,-\frac{i}{2}(P^{(2)})_{\mu\nu}\partial_{p_\mu}\partial_{p_\nu}\chi^0\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)(P^{(3)})_{\alpha\beta j}\partial_{p_\beta}\left(-\frac{i}{2}(P^{(2)})_{\gamma\mu}\partial_{p_\gamma}\partial_{p_\mu}\chi^0-i\partial_{p_\gamma}\chi^0(L^{(1)})_\gamma\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)(P^{(2)})_{\alpha\beta}\partial_{p_\beta}\left(-\frac{i}{2}(P^{(3)})_{\gamma\mu j}\partial_{p_\gamma}\partial_{p_\mu}\chi^0-i\partial_{p_\gamma}\chi^0(L^{(2)})_{\gamma j}\right)\right\rangle\right)\\
&+\mathrm{Im}\left(\left\langle\chi^0,(p_\alpha-i\nabla_{z_\alpha}-\partial_{p_\alpha}E^0)\left(-\frac{i}{2}(P^{(4)})_{\alpha\beta\gamma j}\partial_{p_\beta}\partial_{p_\gamma}\chi^0-i\partial_{p_\beta}\chi^0(L^{(3)})_{\alpha\beta j}\right)\right\rangle\right)\\
&+\frac{1}{2}\left((P^{(4)})_{\alpha\beta\gamma j}\nabla_{p_\gamma}E^0+2((P^{(3)})_{\alpha\mu j}\nabla_{p_\mu})((P^{(2)})_{\beta\nu}\nabla_{p_\nu})E^0+(\nabla_x^2U)_{\alpha\beta j}\right)\mathrm{Re}(\left\langle\chi^0,\nabla_p^2\chi^0\right\rangle)_{\alpha\beta}.
\end{aligned}$$

The equations for the auxiliary quantities derived in Section 3.5 are given in the index notations in the following

$$(\dot{L}^{(1)})_j+(L^{(1)})_\alpha(P^{(2)})_{\beta j}\partial_{p_\alpha}\partial_{p_\beta}E^0+\frac{1}{2}(P^{(3)})_{\alpha\beta j}\partial_{p_\alpha}\partial_{p_\beta}E^0+\frac{1}{2}(P^{(2)})_{\alpha j}(P^{(2)})_{\beta\gamma}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0=0,$$

$$
\begin{aligned}
(\dot{L}^{(2)})_{jk} &+ 2\,\mathrm{Sym}\Big[(L^{(2)})_{\alpha j}(P^{(2)})_{\beta k}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] + (L^{(1)})_\alpha (P^{(3)})_{\beta jk}\partial_{p_\alpha}\partial_{p_\beta}E^0 \\
&+ (L^{(1)})_\alpha (P^{(2)})_{\beta j}(P^{(2)})_{\gamma k}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0 + \frac{1}{2}(P^{(4)})_{\alpha\beta jk}\partial_{p_\alpha}\partial_{p_\beta}E^0 \\
&+ \mathrm{Sym}\Big[(P^{(3)})_{\alpha\beta j}(P^{(2)})_{\gamma k}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] + \frac{1}{2}(P^{(2)})_{\alpha\beta}(P^{(3)})_{\gamma jk}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0 \\
&+ \frac{1}{2}(P^{(2)})_{\alpha\beta}(P^{(2)})_{\gamma j}(P^{(2)})_{\mu k}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}E^0 = 0,
\end{aligned}
$$

$$
\begin{aligned}
(\dot{L}^{(3)})_{jkl} &+ 3\,\mathrm{Sym}\Big[(L^{(3)})_{\alpha jk}(P^{(2)})_{\beta l}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] + 3\,\mathrm{Sym}\Big[(L^{(2)})_{\alpha j}(P^{(3)})_{\beta kl}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] \\
&+ (L^{(1)})_\alpha (P^{(4)})_{\beta jkl}\partial_{p_\alpha}\partial_{p_\beta}E^0 + (L^{(1)})_\alpha (P^{(2)})_{\beta j}(P^{(2)})_{\gamma k}(P^{(2)})_{\mu l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}E^0 \\
&+ 3\,\mathrm{Sym}\Big[(L^{(2)})_{j\alpha}(P^{(2)})_{\beta k}(P^{(2)})_{\gamma l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] \\
&+ 3\,\mathrm{Sym}\Big[(L^{(1)})_\alpha (P^{(3)})_{\beta jk}(P^{(2)})_{\gamma l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] \\
&+ \frac{1}{2}(P^{(5)})_{\alpha\beta jkl}\partial_{p_\alpha}\partial_{p_\beta}E^0 + \frac{3}{2}\,\mathrm{Sym}\Big[(P^{(4)})_{\alpha\beta jk}(P^{(2)})_{\gamma l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] \\
&+ \frac{3}{2}\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha\beta j}(P^{(3)})_{\gamma kl}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] + \frac{1}{2}(P^{(2)})_{\alpha\beta}(P^{(4)})_{\gamma jkl}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0 \\
&+ \frac{3}{2}\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha\beta j}(P^{(2)})_{\gamma k}(P^{(2)})_{\mu l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}E^0\Big] \\
&+ \frac{3}{2}\,\mathrm{Sym}\Big[(P^{(2)})_{\alpha\beta}(P^{(3)})_{\gamma jk}(P^{(2)})_{\mu l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}E^0\Big] \\
&+ \frac{1}{2}(P^{(2)})_{\alpha\beta}(P^{(2)})_{\gamma j}(P^{(2)})_{\mu k}(P^{(2)})_{\nu l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}\partial_{p_\nu}E^0 = 0.
\end{aligned}
$$

$$
(\dot{P}^{(2)})_{jk} + \partial_{x_j}\partial_{x_k}U + (P^{(2)})_{\alpha j}(P^{(2)})_{\beta k}\partial_{p_\alpha}\partial_{p_\beta}E^0 = 0,
$$

$$
(\dot{P}^{(3)})_{jkl} + \partial_{x_j}\partial_{x_k}\partial_{x_l}U + 3\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha jk}(P^{(2)})_{\beta l}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] + (P^{(2)})_{\alpha j}(P^{(2)})_{\beta k}(P^{(2)})_{\gamma l}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0 = 0,
$$

$$
\begin{aligned}
(\dot{P}^{(4)})_{jklm} &+ \partial_{x_j}\partial_{x_k}\partial_{x_l}\partial_{x_m}U + 4\,\mathrm{Sym}\Big[(P^{(4)})_{\alpha jkl}(P^{(2)})_{\beta m}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] \\
&+ 3(P^{(3)})_{\alpha jk}(P^{(3)})_{\beta lm}\partial_{p_\alpha}\partial_{p_\beta}E^0 + (P^{(2)}\cdot\nabla_p)^4E^0 \\
&+ 6\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha jk}(P^{(2)})_{\beta l}(P^{(2)})_{\gamma m}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] = 0,
\end{aligned}
$$

and

$$
\begin{aligned}
(\dot{P}^{(5)})_{jklmn} &+ \partial_{x_j}\partial_{x_k}\partial_{x_l}\partial_{x_m}\partial_{x_n}U + 5\,\mathrm{Sym}\Big[(P^{(5)})_{\alpha jklm}(P^{(2)})_{\beta n}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] \\
&+ 10\,\mathrm{Sym}\Big[(P^{(4)})_{\alpha jkl}(P^{(3)})_{\beta mn}\partial_{p_\alpha}\partial_{p_\beta}E^0\Big] \\
&+ 10\,\mathrm{Sym}\Big[(P^{(4)})_{\alpha jkl}(P^{(2)})_{\beta m}(P^{(2)})_{\gamma n}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] \\
&+ 15\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha jk}(P^{(3)})_{\beta lm}(P^{(2)})_{\gamma n}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}E^0\Big] \\
&+ 10\,\mathrm{Sym}\Big[(P^{(3)})_{\alpha jk}(P^{(2)})_{\beta l}(P^{(2)})_{\gamma m}(P^{(2)})_{\mu n}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}E^0\Big] \\
&+ (P^{(2)})_{\alpha j}(P^{(2)})_{\beta k}(P^{(2)})_{\gamma l}(P^{(2)})_{\mu m}(P^{(2)})_{\nu n}\partial_{p_\alpha}\partial_{p_\beta}\partial_{p_\gamma}\partial_{p_\mu}\partial_{p_\nu}E^0 = 0.
\end{aligned}
$$

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