Asymptotic Analysis of the Quantum Dynamics in Crystals: The Bloch-Wigner Transform, Bloch Dynamics and Berry Phase

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Abstract

We study the semi-classical limit of the Schrödinger equation in a crystal in the presence of an external potential and magnetic field. We first introduce the Bloch-Wigner transform and derive the asymptotic equations governing this transform in the semi-classical setting. For the second part, we focus on the appearance of the Berry curvature terms in the asymptotic equations. These terms play a crucial role in many important physical phenomena such as the quantum Hall effect. We give a simple derivation of these terms in different settings using asymptotic analysis.

1 Introduction

This is the first of a series of papers on the asymptotic analysis of the quantum dynamics of electrons in materials. In the present paper, we introduce the Bloch-Wigner transform, which is a natural extension of the well-known Wigner transform for crystals, to study the macroscopic behavior of the electron dynamics in the presence of an external potential. We then carry out a WKB analysis of the Bloch dynamics for an electron in a bulk crystal, and focus on the derivation of the Berry phase terms and the related Bloch dynamics with Berry curvature. The asymptotic equations derived in this paper are not new. But we introduce a slightly different perspective from the existing literature and this is going to be very useful for our subsequent work.

The electronic dynamics in crystals have been studied for many years in the semiclassical 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 [13], Markowich, Mauser and Poupaud [10] derived the semiclassical 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 case when a weak random potential [3] and nonlinear interactions [7] were present.

Berry phase is an important result that appears during the adiabatic limit of quantum dynamics, as some external parameters are varied slowly [4, 14]. As B. Simon observed in [15], the adiabatic Berry phase has an elegant mathematical interpretation as the holonomy of a certain connection, the 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 [18] and related references. Panati, Spohn and Teufel later gave a rigorous derivation of such Bloch dynamics in [11, 12] by writing down the effective Hamiltonian with the help of the Weyl quantization.

The main purpose of this paper is to give a simple derivation of the effective Bloch dynamics in crystals based on asymptotic analysis. The end results that we obtain are not new, but our approach is considerably simpler than that in previous works. In particular, we give a simple derivation of the Berry curvature terms in the semi-classical limit of the Bloch dynamics. We will also introduce a natural extension of the Wigner transform for the setting of crystals. This new Wigner transform, which we call the Bloch-Wigner transform, seems to be an effective tool for analyzing the dynamics of electrons in crystals.

In subsequent papers, we will study electron dynamics in metals and insulators in the presence of external fields within the context of the time-dependent Thomas-Fermi model, Hartree-Fock model or density functional theory. Our ultimate objective is to give a unified treatment of electron dynamics in materials, with applications to nano-optics and quantum transport.

2 Preliminaries on the Bloch theory

Given a crystal lattice Γ, we consider a rescaled Schrödinger equation:

$$i\varepsilon\frac{\partial\Psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon + V_\Gamma\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\Psi^\varepsilon - \phi(\boldsymbol{x})\Psi^\varepsilon, \quad \boldsymbol{x}\in\mathbb{R}^n\,, \tag{2.1}$$

where $V_\Gamma(\cdot)$ is a potential, which is periodic with respect to Γ and $\phi(\boldsymbol{x})$ is a scalar potential. Eq. (2.1) is a standard model for describing the motion of electrons in a perfect crystal when an external macroscopic potential is applied. In physical units, the equation is given by

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V_\Gamma(\boldsymbol{x})\Psi - \phi(\boldsymbol{x})\Psi, \tag{2.2}$$

where m is the atomic mass and $\hbar$ is the reduced Planck constant. As in [2], we introduce ℓ as the lattice constant and $\tau = m\ell^2/\hbar$ as the small (quantum) time scale, and denote L and T as the large (macroscopic) length and time scales, then

$$V_\Gamma(\boldsymbol{x}) = \frac{m\ell^2}{\tau^2}\tilde{V}(\frac{\boldsymbol{x}}{\ell}), \quad \phi(\boldsymbol{x}) = \frac{mL^2}{T^2}\tilde{\phi}(\frac{\boldsymbol{x}}{L}).$$

By defining

$$\tilde{\boldsymbol{x}} = \frac{\boldsymbol{x}}{L}, \quad \tilde{t} = \frac{t}{T}, \quad \varepsilon = \frac{\ell}{L}, \quad h = \frac{\hbar T}{mL^2},$$

one obtains after dropping the tildes,

$$ih\frac{\partial\Psi}{\partial t} = -\frac{h^2}{2}\Delta\Psi + \frac{h^2}{\varepsilon^2}V_\Gamma(\frac{\boldsymbol{x}}{\varepsilon})\Psi - \phi(\boldsymbol{x})\Psi.$$

This equation has two small parameters, ε and h. We will only consider the distinguished limit when $h = \varepsilon$. This is a difficult case, as was pointed out in [2].

In the case when the external potential is absent, the time evolution is determined by the Bloch-Floquet theory [13]. Denote the Hamiltonian operator

$$H_0 = -\frac{1}{2}\Delta + V_\Gamma(\boldsymbol{z}). \tag{2.3}$$

The Bloch decomposition of H_0 is given by

$$H_0 = \frac{1}{|\Gamma^*|} \int_{\Gamma^*} H_{\boldsymbol{k}} d\boldsymbol{k}, \tag{2.4}$$

where $|\Gamma^*|$ is the measure of the first Brillouin zone, and

$$H_{\boldsymbol{k}} = -\frac{1}{2}\Delta_{\boldsymbol{k}} + V_\Gamma(\boldsymbol{z}) \tag{2.5}$$

is the Laplacian operator acting on $f \in L^2(\Gamma)$ with the Bloch boundary condition:

$$e^{-i\boldsymbol{k}\cdot\boldsymbol{z}} f \text{ is periodic on } [0, 2\pi]^n. \tag{2.6}$$

The eigenvalues and corresponding eigenfunctions of H_k are obtained from solving

$$\left[\frac{1}{2}(-i\nabla_{\boldsymbol{z}} + \boldsymbol{k})^2 + V_\Gamma(\boldsymbol{z})\right] \chi_m(\boldsymbol{k}, \boldsymbol{z}) = E_m(\boldsymbol{k})\chi_m(\boldsymbol{k}, \boldsymbol{z}). \tag{2.7}$$

with $\chi(\boldsymbol{k}, \cdot)$ periodic on Γ. It is also convenient to extend the domain of χ so that the functions involved are periodically extended.

Let us also denote the eigenvalues of (2.7) as $E_m(\boldsymbol{k})$ with the ordering that $E_1(\boldsymbol{k}) \le E_2(\boldsymbol{k}) \le \cdots$. We have

$$\sigma(H_0) = \bigcup_m E_m(\Gamma^*). \tag{2.8}$$

For each m, $E_m(\Gamma^*)$ gives a band (as a map from Γ^* to $\mathbb{R}$), and

$$\varphi_m(\boldsymbol{z}, \boldsymbol{k}) = e^{i\boldsymbol{k}\cdot\boldsymbol{z}} \chi_m(\boldsymbol{k}, \boldsymbol{z})$$

satisfies $H_0\varphi_m = E_m\varphi_m$.

3 The Bloch-Wigner transform

When $V_\Gamma = 0$,

$$i\varepsilon \frac{\partial \Psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon - \phi(\boldsymbol{x})\Psi^\varepsilon, \quad \boldsymbol{x} \in \mathbb{R}^n\,, \tag{3.9}$$

the (asymmetric) Wigner transform defined as

$$W(t, \boldsymbol{x}, \boldsymbol{k}) = \int_{\mathbb{R}^n} \frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n} \Psi^\varepsilon(t, \boldsymbol{x} - \varepsilon\boldsymbol{y})\overline{\Psi^\varepsilon}(t, \boldsymbol{x}) e^{-iky}, \tag{3.10}$$

is a useful tool for studying the Schrödinger equation in the semi-classical regime [9, 7].

In the presence of a periodic background potential V_Γ, for each n and m, we introduce the (asymmetric) Bloch-Wigner transform:

$$\sigma^\varepsilon_{mn}(t,\boldsymbol{x},\boldsymbol{k}) = \int_{\mathbb{R}^n} \frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n} \Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k}), \tag{3.11}$$

where $\boldsymbol{k}$ is in the first Brillouin zone, and $\overline{f}$ means the complex conjugate of f. The motivation of the Bloch-Wigner transform is the following. In the Wigner transform (3.10), the phase factor $\exp(-iky)$ can be understood as

$$e^{-iky} = e^{ik(x/\varepsilon - y)}e^{-ikx/\varepsilon},$$

where the Fourier term $e^{-ikx/\varepsilon}$ is the generalized eigenfunction for the operator $-\frac{1}{2}\varepsilon^2\Delta$. Now, due to the presence of the periodic background potential V_Γ, the generalized eigenfunction for the time-independent operator without external potential $-\frac{1}{2}\varepsilon^2\Delta + V_\Gamma(\boldsymbol{x}/\varepsilon)$ is no longer the Fourier wave, but the Bloch wave as we have seen in the last section. Thus, it is natural to replace the Fourier waves used in the original Wigner transform by the Bloch waves. This gives rise to the Bloch-Wigner transform defined in (3.11).

We notice that the Bloch-Wigner transform is related but different from the discrete Wigner transform introduced in [10]. In a sense, it is closer to the approach taken in [3]. Instead of decomposition of the equation into separate energy bands, the current approach treats the solution as a whole, but use a different (but natural) approach to analyze the phase space density.

Taking the time derivative of (3.11) yields

$$\begin{aligned}
\partial_t\sigma^\varepsilon_{mn} = & \frac{1}{i\varepsilon}\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\Big(-\frac{\varepsilon^2}{2}\Delta_{\boldsymbol{x}}\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y}) + V(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y})\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y}) \\
& - \phi(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\Big)\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k}) \\
& - \frac{1}{i\varepsilon}\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})\Big(-\frac{\varepsilon^2}{2}\Delta_{\boldsymbol{x}}\overline{\Psi^\varepsilon}(t,\boldsymbol{x}) \\
& + V(\frac{\boldsymbol{x}}{\varepsilon})\overline{\Psi^\varepsilon}(t,\boldsymbol{x}) - \phi(t,\boldsymbol{x})\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\Big) \\
= & I_1 + I_2 + I_3,
\end{aligned}$$

where $I_j,\ j=1,2,3$ are given by

$$\begin{aligned}
I_1 &= \frac{1}{i\varepsilon}\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\Big(-\frac{\varepsilon^2}{2}\Delta_{\boldsymbol{x}}\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})+V(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y})\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\Big)\\
&\qquad\times\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k}),\\
I_2 &= -\frac{1}{i\varepsilon}\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})\\
&\qquad\times\Big(-\frac{\varepsilon^2}{2}\Delta_{\boldsymbol{x}}\overline{\Psi^\varepsilon}(t,\boldsymbol{x})+V(\frac{\boldsymbol{x}}{\varepsilon})\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\Big),\\
I_3 &= \frac{1}{i\varepsilon}\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\big(\phi(t,\boldsymbol{x})-\phi(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\big)\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\\
&\qquad\times\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k}).
\end{aligned}$$

Using integration by parts, one obtains

$$\begin{aligned}
I_1 &= \frac{1}{i\varepsilon}E_m(\boldsymbol{k})\sigma^\varepsilon_{mn},\\
I_2 &= -\frac{1}{i\varepsilon}E_n(\boldsymbol{k})\sigma^\varepsilon_{mn}+\frac{\varepsilon}{2i}\Delta_{\boldsymbol{x}}\sigma^\varepsilon_{mn}-\frac{1}{i}\nabla_{\boldsymbol{x}}\cdot\int_{\mathbb{R}^n}\frac{\mathrm{d}\boldsymbol{y}}{(2\pi)^n}\Psi^\varepsilon(t,\boldsymbol{x}-\varepsilon\boldsymbol{y})\\
&\qquad\times\overline{\Psi^\varepsilon}(t,\boldsymbol{x})\overline{\varphi_m}(\frac{\boldsymbol{x}}{\varepsilon}-\boldsymbol{y},\boldsymbol{k})(\varepsilon\nabla_{\boldsymbol{x}})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})\\
&= -\frac{1}{i\varepsilon}E_n(\boldsymbol{k})\sigma^\varepsilon_{mn}+\frac{\varepsilon}{2i}\Delta_{\boldsymbol{x}}\sigma^\varepsilon_{mn}-\frac{1}{i}\nabla_{\boldsymbol{x}}\cdot\left(\frac{(\varepsilon\nabla_{\boldsymbol{x}})\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}{\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}\sigma^\varepsilon_{mn}\right).
\end{aligned}$$

Therefore we obtain the Bloch-Wigner equation

$$\begin{aligned}
\partial_t\sigma^\varepsilon_{mn}+\nabla_{\boldsymbol{x}}\cdot\left(\frac{\varepsilon\nabla_{\boldsymbol{x}}\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}{i\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}\sigma^\varepsilon_{mn}\right)+\frac{i\varepsilon}{2}\Delta_{\boldsymbol{x}}\sigma^\varepsilon_{mn}&\\
=\frac{1}{i\varepsilon}(E_m(\boldsymbol{k})-E_n(\boldsymbol{k}))\sigma^\varepsilon_{mn}+I_3.&\qquad(3.12)
\end{aligned}$$

We now derive the asymptotic limit of the above equation as $\varepsilon\to 0$. For this, multiplying both sides (3.12) by a smooth, compactly supported test function $f(t,\boldsymbol{x})$ and integrating in time and space, we get

$$\begin{aligned}
\iint f(t,\boldsymbol{x})\left(\partial_t\sigma^\varepsilon_{mn}+\nabla_{\boldsymbol{x}}\cdot\left(\frac{\varepsilon\nabla_{\boldsymbol{x}}\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}{i\varphi_n(\frac{\boldsymbol{x}}{\varepsilon},\boldsymbol{k})}\sigma^\varepsilon_{mn}\right)+\frac{i\varepsilon}{2}\Delta_{\boldsymbol{x}}\sigma^\varepsilon_{mn}\right)&\\
=\iint f(t,\boldsymbol{x})\left(\frac{1}{i\varepsilon}(E_m(\boldsymbol{k})-E_n(\boldsymbol{k}))\sigma^\varepsilon_{mn}+I_3\right).&\qquad(3.13)
\end{aligned}$$

Substituting into the ansatz for $\sigma^\varepsilon_{mn} = \sigma^0_{mn} + \varepsilon\sigma^1_{mn} + \cdots$, to the $\mathcal{O}(\varepsilon^{-1})$ order, we have

$$\iint f(t,\boldsymbol{x})(E_m(\boldsymbol{k}) - E_n(\boldsymbol{k}))\sigma^0_{mn} = 0. \tag{3.14}$$

For simplicity, we will assume that for $m \neq n$, $E_m(\boldsymbol{k}) \neq E_n(\boldsymbol{k})$. Hence, $\sigma^0_{mn} = 0$ for $m \neq n$.

To the $\mathcal{O}(1)$ order, we have

$$\iint \sigma^0_{mm}\partial_t f \;-\; \sigma^0_{mm}\nabla_{\boldsymbol{k}}E_m \;\cdot\; \nabla_{\boldsymbol{x}} f \;+\; \nabla_{\boldsymbol{x}}\phi \;\cdot\; \nabla_{\boldsymbol{k}}\sigma^0_{mm} f \;=\; 0, \tag{3.15}$$

where we have used the fact that

$$I_3 = -\nabla_{\boldsymbol{x}}\phi(t,\boldsymbol{x}) \cdot \nabla_{\boldsymbol{k}}\sigma^0_{mn} + \mathcal{O}(\varepsilon) \tag{3.16}$$

$$\nabla_{\boldsymbol{z}}\varphi_n(\boldsymbol{z},\boldsymbol{k}) = \nabla_{\boldsymbol{k}}E_n(\boldsymbol{k})\varphi_n(\boldsymbol{z},\boldsymbol{k}) + \sum_{m\neq n} c_m\varphi_m(\boldsymbol{z},\boldsymbol{k}). \tag{3.17}$$

Note that the terms involving $\varphi_m(\boldsymbol{z},\boldsymbol{k})$ do not contribute because $\sigma^0_{mn} = 0$ for $m \neq n$.

Summarizing, we arrive at the equation for σ^0_{mm}

$$\partial_t\sigma^0_{mm}(t,\boldsymbol{x},\boldsymbol{k}) + \nabla_{\boldsymbol{k}}E_m \cdot \nabla_{\boldsymbol{x}}\sigma^0_{mm}(t,\boldsymbol{x},\boldsymbol{k}) + \nabla_{\boldsymbol{x}}\phi \cdot \nabla_{\boldsymbol{k}}\sigma^0_{mm}(t,\boldsymbol{x},\boldsymbol{k}) = 0. \tag{3.18}$$

This gives the leading order behavior of σ^ε_{mm}.

The Bloch-Wigner transform is an elegant way for obtaining the leading order asymptotics in fairly general situations. In principle, it can also be used to study the next order behavior. However, the procedure becomes quite involved. In the following, we will turn to more traditional WKB methods. Our interest is the Berry curvature terms, which arise in the next order asymptotic equations.

4 Derivation of the Berry curvature using the WKB method

We will assume that the initial condition of (2.1) is well prepared in the sense that it is concentrated on a single isolated energy band:

$$\Psi^\varepsilon(0,\boldsymbol{x}) = a_0(\boldsymbol{x})\chi_m(\nabla_{\boldsymbol{x}}S_0, \frac{\boldsymbol{x}}{\varepsilon})\exp(\frac{iS_0(0,\boldsymbol{x})}{\varepsilon}). \tag{4.1}$$

The band index will be omitted from now on. Note that for this WKB type of initial condition, our asymptotic method is only valid before caustics. To overcome this difficulty one needs to consider for example the Gaussian beam methods [6, 8] or the Wigner functions [9, 16].

We will take the following ansatz for (2.1):

$$\Psi^{\varepsilon}_{asym}(t,\boldsymbol{x}) = a(t,\boldsymbol{x})\chi(\nabla_{\boldsymbol{x}} S_0, \frac{\boldsymbol{x}}{\varepsilon}) \exp(\frac{iS_0(t,\boldsymbol{x})}{\varepsilon}). \tag{4.2}$$

Substituting (4.2) into (2.1), we obtain the eikonal-transport equations for $a(t,\boldsymbol{x})$ and $S(t,\boldsymbol{x})$:

$$\partial_t S_0 + E(\nabla_{\boldsymbol{x}} S_0) - \phi = 0, \tag{4.3}$$

$$\begin{aligned}&\partial_t a + \nabla_{\boldsymbol{k}} E(\nabla_{\boldsymbol{x}} S_0)\cdot\nabla_{\boldsymbol{x}} a + \frac{1}{2} a \nabla_{\boldsymbol{x}}(\nabla_{\boldsymbol{k}} E(\nabla_{\boldsymbol{x}} S_0)) \\ &\quad - ia\mathcal{A}(\nabla_{\boldsymbol{x}} S_0)\cdot\nabla_{\boldsymbol{x}}\phi = 0,\end{aligned} \tag{4.4}$$

where $\mathcal{A}(\boldsymbol{k}) = \langle \chi(\boldsymbol{k},\cdot)|i\nabla_{\boldsymbol{k}}|\chi(\boldsymbol{k},\cdot)\rangle \in \mathbb{R}^n$ is the Berry connection. Here Dirac's notation of bra $\langle\cdot|$ and ket $|\cdot\rangle$ are used:

$$\langle f|g\rangle = \int \bar{f} g \mathrm{d}\boldsymbol{z},$$

$$\langle f|A|g\rangle = \int \bar{f} A g \mathrm{d}\boldsymbol{z},$$

where $\bar{f}$ is the complex conjugate of f and A is an operator. We omit the derivation of these equations here, since we will provide the derivation in appendix for more general cases.

Up to this point, the result is standard. What we have done is just a higher order expansion of WKB methods. Same equations have been obtained in a similar way, for example, in [5]. We have the following theorem which states that the WKB method works up to the formation of caustics.

Theorem 4.1 *Define Ψ^{ε} to be the solution to* (2.1) *with the single band initial condition* (4.1)*. Assume for the initial condition, $a_0(\boldsymbol{x}) \in \mathcal{S}(\mathbb{R}^n)$ and $S_0(0,\boldsymbol{x}) \in C^{\infty}(\mathbb{R}^n)$. Assume there is no caustic formed before time t_0, then the asymptotic solution given by* (4.2) *is valid up to any $t < t_0$, and there exists a constant C such that*

$$\sup_{0\le\tau\le t} \left\| \Psi^{\varepsilon}(\tau,\boldsymbol{x}) - \Psi^{\varepsilon}_{asym}(\tau,\boldsymbol{x})\right\|_{L^2(\mathbb{R}^n)} \le C\varepsilon.$$

The proof of this theorem is standard and essentially contained in the paper [5], and therefore we will omit the proof here.

Now we are going to link (4.3)-(4.4) to the Bloch dynamics with Berry curvature. As the Bloch dynamics is quite useful in physics (see for example a recent review article [18]), a better physical interpretation of the asymptotic analysis is provided.

The key observation is that the equation (4.4) is a complex equation, we can rewrite $a(t,\boldsymbol{x}) = A(t,\boldsymbol{x})\exp(iS_1(t,\boldsymbol{x}))$ and separate (4.4) into its real and imaginary parts:

$$\partial_t A + \nabla_{\boldsymbol{k}} E(\nabla_{\boldsymbol{x}} S_0)\cdot\nabla_{\boldsymbol{x}} A + \frac{1}{2}\nabla_{\boldsymbol{x}}\big(\nabla_{\boldsymbol{k}} E(\nabla_{\boldsymbol{x}} S_0)\big)A = 0, \tag{4.5}$$

$$\partial_t S_1 + \nabla_{\boldsymbol{k}} E(\nabla_{\boldsymbol{x}} S_0)\cdot\nabla_{\boldsymbol{x}} S_1 - \mathcal{A}(\nabla_{\boldsymbol{x}} S_0)\cdot\nabla_{\boldsymbol{x}}\phi = 0. \tag{4.6}$$

We now define a new phase function $S = S_0 + \varepsilon S_1$ and write an equation for S according to (4.3) and (4.6):

$$\partial_t S + E(\nabla_{\boldsymbol{x}} S) - \phi - \varepsilon\mathcal{A}(\nabla_{\boldsymbol{x}} S)\cdot\nabla_{\boldsymbol{x}}\phi = 0. \tag{4.7}$$

Taking the gradient of (4.7) with respect to $\boldsymbol{x}$ yields

$$\partial_t(\nabla_{\boldsymbol{x}} S) + \big[\nabla_{\boldsymbol{k}} E - \varepsilon\nabla_{\boldsymbol{k}}\mathcal{A}\cdot\nabla_{\boldsymbol{x}}\phi\big]\cdot\nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S - \nabla_{\boldsymbol{x}}\phi - \varepsilon\mathcal{A}\cdot\nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}}\phi = 0. \tag{4.8}$$

The equation for the characteristics of (4.8) is given by

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \nabla_{\boldsymbol{k}} E(\boldsymbol{k}) - \varepsilon\nabla_{\boldsymbol{k}}\mathcal{A}(\boldsymbol{k})\cdot\nabla_{\boldsymbol{x}}\phi(\boldsymbol{x}), \tag{4.9}$$

then (4.8) becomes, by letting $\boldsymbol{k} = \nabla_{\boldsymbol{x}} S$,

$$\frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} = \nabla_{\boldsymbol{x}}\phi(\boldsymbol{x}) + \varepsilon\mathcal{A}(\boldsymbol{k})\cdot\nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}}\phi(\boldsymbol{x}). \tag{4.10}$$

If we use the change of variables

$$\boldsymbol{x} = \tilde{\boldsymbol{x}} - \varepsilon\mathcal{A}(\tilde{\boldsymbol{k}}), \qquad \boldsymbol{k} = \tilde{\boldsymbol{k}},$$

we obtain, after dropping the tilde,

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \nabla_{\boldsymbol{k}} E(\boldsymbol{k}) - \varepsilon\frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t}\times\nabla_{\boldsymbol{k}}\times\mathcal{A}(\boldsymbol{k}), \tag{4.11}$$

$$\frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} = \nabla_{\boldsymbol{x}}\phi(\boldsymbol{x}). \tag{4.12}$$

Here $\nabla_{\boldsymbol{k}} \times \mathcal{A}(\boldsymbol{k})$ is the Berry curvature. We remark that compared with the traditional Bloch dynamics [1], the new terms depending on the Berry curvature are of higher order in ε.

The equations (4.11)-(4.12) are not new, they have been obtained from a physical argument by Sundaram and Niu [17]. In the mathematics literature, the equations have been rigorously derived by Panati, Spohn and Teufel [11]. However, the derivation here is considerably simpler than that in [11] and provides an easier way to understand the results.

It is straightforward to extend this procedure to more general cases. We will see that the above strategy can be used to derive Bloch dynamics in various situations.

5 Bloch dynamics in inhomogeneous crystals

Now we turn to a rescaled Schrödinger equation with the time dependent two scale potential:

$$i\varepsilon \frac{\partial \Psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2}\Delta \Psi^\varepsilon + V\left(t, \boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}\right)\Psi^\varepsilon, \qquad \boldsymbol{x} \in \mathbb{R}^n\,, \tag{5.1}$$

where $V(t, \boldsymbol{x}, \boldsymbol{z} = \frac{\boldsymbol{x}}{\varepsilon})$ is periodic in $\boldsymbol{z}$ on the lattice Γ.

Again we only consider initial conditions that are concentrated on one single band and drop the band index. We will use time dependent two scale WKB ansatz as:

$$\Psi^\varepsilon_{asym} = a(t, \boldsymbol{x})\chi(t, \nabla_{\boldsymbol{x}} S_0, \boldsymbol{x}, \frac{\boldsymbol{x}}{\varepsilon}) \exp(\frac{iS_0(t, \boldsymbol{x})}{\varepsilon}). \tag{5.2}$$

Here the time dependent two scale Bloch function $\chi(t, \boldsymbol{k}, \boldsymbol{x}, \boldsymbol{z})$ is the eigenfunction of the following equation

$$\left[\frac{1}{2}(-i\nabla_{\boldsymbol{z}} + \boldsymbol{k})^2 + V(t, \boldsymbol{x}, \boldsymbol{z})\right]\chi(t, \boldsymbol{k}, \boldsymbol{x}, \boldsymbol{z}) = E(t, \boldsymbol{k}, \boldsymbol{x})\chi(t, \boldsymbol{k}, \boldsymbol{x}, \boldsymbol{z}). \tag{5.3}$$

Note that in (5.3), t, $\boldsymbol{k}$ and $\boldsymbol{x}$ are parameters. In other words, we consider a cell problem in $\boldsymbol{z}$ while freezing the macroscopic position in space and time.

Substituting in the ansatz, we get the eikonal-transport equations in this case (the derivation is provided in Appendix I)

$$\partial_t S_0 + E(t, \nabla_{\boldsymbol{x}} S_0, x) = 0, \tag{5.4}$$

$$\begin{aligned} &\partial_t a + \nabla_{\boldsymbol{k}} E \cdot \nabla_{\boldsymbol{x}} a + \frac{1}{2} a \nabla_{\boldsymbol{x}} \cdot (\nabla_{\boldsymbol{k}} E|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S}) - ia\langle\chi|i\partial_t|\chi\rangle \\ &\quad + ia\nabla_{\boldsymbol{x}} E \cdot \langle\chi|i\nabla_{\boldsymbol{k}}|\chi\rangle - ia\nabla_{\boldsymbol{k}} E \cdot \langle\chi|i\nabla_{\boldsymbol{x}}|\chi\rangle = 0, \end{aligned} \tag{5.5}$$

To give a better interpretation for the equations we just obtained, we follow the same trick that we used in the last section. Define $a(t,x) = A(t,x)\exp(iS_1(t,x))$, then the first order corrected phase $S = S_0 + \varepsilon S_1$ satisfies

$$\partial_t S + E(t, \nabla_{\boldsymbol{x}} S, \boldsymbol{x}) + \varepsilon \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} E - \varepsilon \mathcal{A}_t - \varepsilon \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E = 0, \tag{5.6}$$

where the Berry connections $\mathcal{A}_{\boldsymbol{k}}$, $\mathcal{A}_t$, $\mathcal{A}_{\boldsymbol{x}}$ are given by

$$\mathcal{A}_{\boldsymbol{k}} = \langle\chi|i\nabla_{\boldsymbol{k}}|\chi\rangle, \qquad \mathcal{A}_t = \langle\chi|i\partial_t|\chi\rangle, \qquad \mathcal{A}_{\boldsymbol{x}} = \langle\chi|i\nabla_{\boldsymbol{x}}|\chi\rangle, \tag{5.7}$$

where $\chi = \chi(t, \boldsymbol{x}, \boldsymbol{k})$. Note that we now have three type of Berry connections, as the Bloch Hamiltonian depends on t, $\boldsymbol{x}$ and $\boldsymbol{k}$ as parameters.

The equation (5.6) implies the following ray (characteristics) equations:

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} &= \nabla_{\boldsymbol{k}} E + \varepsilon \nabla_{\boldsymbol{k}} \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} E + \varepsilon \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{k}} E - \varepsilon \nabla_{\boldsymbol{k}} \mathcal{A}_t \\ &\quad - \varepsilon \nabla_{\boldsymbol{k}} \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E - \varepsilon \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} \nabla_{\boldsymbol{k}} E, \\ \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} &= -\nabla_{\boldsymbol{x}} E - \varepsilon \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{x}} E - \varepsilon \nabla_{\boldsymbol{x}} \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} E + \varepsilon \nabla_{\boldsymbol{x}} \mathcal{A}_t \\ &\quad + \varepsilon \nabla_{\boldsymbol{x}} \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E + \varepsilon \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{k}} E. \end{aligned}$$

Using the change of variables,

$$\boldsymbol{x} = \tilde{\boldsymbol{x}} - \varepsilon \mathcal{A}_{\boldsymbol{k}}(\tilde{\boldsymbol{k}}, \tilde{\boldsymbol{x}}), \qquad \boldsymbol{k} = \tilde{\boldsymbol{k}} + \varepsilon \mathcal{A}_{\boldsymbol{x}}(\tilde{\boldsymbol{k}}, \tilde{\boldsymbol{x}}), \tag{5.8}$$

one recovers the Bloch dynamics in inhomogeneous crystals shown in [12, 19], after dropping the tilde, we obtain

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} &= \nabla_{\boldsymbol{k}} E - \varepsilon \Omega_{\boldsymbol{k}\boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} - \varepsilon \Omega_{\boldsymbol{k}\boldsymbol{k}} \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} - \varepsilon \Omega_{\boldsymbol{k}t}, \\ \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} &= -\nabla_{\boldsymbol{x}} E + \varepsilon \Omega_{\boldsymbol{x}\boldsymbol{x}} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} + \varepsilon \Omega_{\boldsymbol{x}\boldsymbol{k}} \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} + \varepsilon \Omega_{\boldsymbol{x}t}. \end{aligned}$$

The curvatures $\Omega_{\boldsymbol{kx}}$, $\Omega_{\boldsymbol{kk}}$, $\Omega_{\boldsymbol{xk}}$, $\Omega_{\boldsymbol{xx}}$, $\Omega_{\boldsymbol{k}t}$, $\Omega_{\boldsymbol{x}t}$ are defined as

$$\begin{aligned}
\Omega_{\boldsymbol{kx}} &= \nabla_{\boldsymbol{k}}\mathcal{A}_{\boldsymbol{x}} - (\nabla_{\boldsymbol{x}}\mathcal{A}_{\boldsymbol{k}})^T, &\qquad \Omega_{\boldsymbol{kk}} &= \nabla_{\boldsymbol{k}}\mathcal{A}_{\boldsymbol{k}} - (\nabla_{\boldsymbol{k}}\mathcal{A}_{\boldsymbol{k}})^T,\\
\Omega_{\boldsymbol{xk}} &= \nabla_{\boldsymbol{x}}\mathcal{A}_{\boldsymbol{k}} - (\nabla_{\boldsymbol{k}}\mathcal{A}_{\boldsymbol{x}})^T, &\qquad \Omega_{\boldsymbol{xx}} &= \nabla_{\boldsymbol{x}}\mathcal{A}_{\boldsymbol{x}} - (\nabla_{\boldsymbol{x}}\mathcal{A}_{\boldsymbol{x}})^T,\\
\Omega_{\boldsymbol{k}t} &= \nabla_{\boldsymbol{k}}\mathcal{A}_t - (\partial_t\mathcal{A}_{\boldsymbol{k}})^T, &\qquad \Omega_{\boldsymbol{x}t} &= \nabla_{\boldsymbol{x}}\mathcal{A}_t - (\partial_t\mathcal{A}_{\boldsymbol{x}})^T,
\end{aligned}$$

where M^T means the transpose matrix of M.

6 Magnetic Bloch dynamics in inhomogeneous crystals

In this section, we consider a more general case with the presence of magnetic field. The rescaled Schrödinger equation becomes

$$i\varepsilon\frac{\partial\Psi^\varepsilon}{\partial t} = \frac{1}{2}\left(-i\varepsilon\nabla_{\boldsymbol{x}} + \boldsymbol{b}(t,\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon})\right)^2\Psi^\varepsilon + V\left(t,\boldsymbol{x},\frac{\boldsymbol{x}}{\varepsilon}\right)\Psi^\varepsilon, \quad \boldsymbol{x}\in\mathbb{R}^n\,, \tag{6.1}$$

where $\boldsymbol{b}(\boldsymbol{x})$ is the vector potential and the magnetic field is given by $\boldsymbol{B} = \nabla\times\boldsymbol{b}$. The positive sign before $\boldsymbol{b}(\boldsymbol{x})$ comes from the negative charge of electrons.

We take an ansatz of the form (5.2), after some lengthy calculation (cf. Appendix II), we obtain the corresponding eikonal-transport equations:

$$\partial_t S_0 + E(t,\nabla_{\boldsymbol{x}}S_0,x) = 0, \tag{6.2}$$

$$\begin{aligned}
&\partial_t a + \nabla_{\boldsymbol{k}}E\cdot\nabla_{\boldsymbol{x}}a + \frac{1}{2}a\nabla_{\boldsymbol{x}}\cdot(\nabla_{\boldsymbol{k}}E|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}}S}) - ia\langle\chi|i\partial_t|\chi\rangle\\
&\quad -ia\nabla_{\boldsymbol{k}}E\cdot\langle\chi|i\nabla_{\boldsymbol{x}}|\chi\rangle - \frac{1}{2}\langle\nabla_{\boldsymbol{k}}\chi|\big[\nabla_{\boldsymbol{x}}\boldsymbol{b} - (\nabla_{\boldsymbol{x}}\boldsymbol{b})^T\big](H-E)|\nabla_{\boldsymbol{k}}\chi\rangle\\
&\quad +ia\langle\nabla_{\boldsymbol{x}}V\chi|\cdot i\nabla_{\boldsymbol{k}}|\chi\rangle + \frac{1}{2}\langle\nabla_{\boldsymbol{k}}\chi|\big[\nabla_{\boldsymbol{x}}\boldsymbol{b} - (\nabla_{\boldsymbol{x}}\boldsymbol{b})^T\big]\nabla_{\boldsymbol{k}}E|\chi\rangle = 0
\end{aligned}\tag{6.3}$$

where $\chi(t,\boldsymbol{k},\boldsymbol{x},\boldsymbol{z})$ is the eigenfunction for magnetic Bloch Schrödinger operator H,

$$\begin{aligned}
H\chi &= \left[\frac{1}{2}\big(-i\nabla_{\boldsymbol{z}} + \boldsymbol{k} + \boldsymbol{b}(t,\boldsymbol{x},\boldsymbol{z})\big)^2 + V(t,\boldsymbol{x},\boldsymbol{z})\right]\chi(t,\boldsymbol{k},\boldsymbol{x},\boldsymbol{z})\\
&= E(t,\boldsymbol{k},\boldsymbol{x})\chi(t,\boldsymbol{k},\boldsymbol{x},\boldsymbol{z}).
\end{aligned}\tag{6.4}$$

In the equation, t, $\boldsymbol{k}$ and $\boldsymbol{x}$ are parameters, therefore, similarly as in the last section, we will obtain three type of Berry connections.

To derive the magnetic Bloch dynamics, we rewrite (6.3) in terms of the Berry connections defined in (5.7) with the help of (A.11),

$$\partial_t a + \nabla_{\boldsymbol{k}} E \cdot \nabla_{\boldsymbol{x}} a + \frac{1}{2} a \nabla_{\boldsymbol{x}} \cdot (\nabla_{\boldsymbol{k}} E|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S}) - ia\mathcal{A}_t$$
$$+ia\nabla_{\boldsymbol{x}} E \cdot \mathcal{A}_{\boldsymbol{k}} - ia\nabla_{\boldsymbol{k}} E \cdot \mathcal{A}_{\boldsymbol{x}} - iaM_B = 0,$$

where M_B is given by

$$M_B = \mathrm{Im}\langle \nabla_{\boldsymbol{k}} \chi | (H-E) | \nabla_{\boldsymbol{x}} \chi \rangle.$$

Note that if $\boldsymbol{b}(t, \boldsymbol{x}, \boldsymbol{z})$ is independent of $\boldsymbol{z}$, then

$$\begin{aligned} M_B &= \frac{1}{2i} \langle \nabla_{\boldsymbol{k}} \chi | \big(\nabla_{\boldsymbol{x}} \boldsymbol{b} - (\nabla_{\boldsymbol{x}} \boldsymbol{b})^T \big) (H-E) | \nabla_{\boldsymbol{k}} \chi \rangle \\ &= \frac{1}{2i} \langle \nabla_{\boldsymbol{k}} \chi | \times (H-E) | \nabla_{\boldsymbol{k}} \chi \rangle \cdot \boldsymbol{B}. \end{aligned}$$

Similarly as before, we write $a(t, \boldsymbol{x}) = A(t, \boldsymbol{x}) \exp(S_1(t, \boldsymbol{x}))$, then the equation for the new phase function $S = S_0 + \varepsilon S_1$ is

$$\partial_t S + E(t, \nabla_{\boldsymbol{x}} S, \boldsymbol{x}) + \varepsilon \mathcal{A}_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{x}} E - \varepsilon \mathcal{A}_t - \varepsilon \mathcal{A}_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E - \varepsilon M_B = 0,$$

which implies the following dynamic equations after performing the change of variables (5.8),

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \nabla_{\boldsymbol{k}} (E - \varepsilon M_B) - \varepsilon \Omega_{\boldsymbol{kx}} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} - \varepsilon \Omega_{\boldsymbol{kk}} \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} - \varepsilon \Omega_{\boldsymbol{k}t}, \tag{6.5}$$

$$\frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} = -\nabla_{\boldsymbol{x}} (E - \varepsilon M_B) + \varepsilon \Omega_{\boldsymbol{xx}} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} + \varepsilon \Omega_{\boldsymbol{xk}} \frac{\mathrm{d}\boldsymbol{k}}{\mathrm{d}t} + \varepsilon \Omega_{\boldsymbol{x}t}. \tag{6.6}$$

We obtain the above equations for the general situation, as have been seen, the derivation using WKB method is straightforward.

We remark that, in [6], a simplified situation is considered in which the vector potential $\boldsymbol{b}(t, \boldsymbol{x}, \boldsymbol{z})$ does not depend on $\boldsymbol{z}$ and $V(t, \boldsymbol{x}, \boldsymbol{z}) = V_\Gamma(\boldsymbol{z}) - \phi(\boldsymbol{x})$. Therefore, the sum of the last four terms of (6.3) can be simplified as

$$-i\langle \chi | i\nabla_{\boldsymbol{k}} | \chi \rangle \cdot (\nabla_{\boldsymbol{x}} \phi - \nabla_{\boldsymbol{k}} E \times \boldsymbol{B}) - \frac{1}{2} \langle \nabla_{\boldsymbol{k}} \chi | \times (H-E) | \nabla_{\boldsymbol{k}} \chi \rangle \cdot \boldsymbol{B},$$

which is consistent with the equation (29) in [6].

In addition, using Peierls substitution $\boldsymbol{p} = \boldsymbol{k} + \boldsymbol{b}$, we see that (6.5)-(6.6) can be rewritten for the simplified case as

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \nabla_{\boldsymbol{p}}(E - \varepsilon M_B) - \varepsilon \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} \times \tilde{\Omega},$$

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \nabla_{\boldsymbol{x}}\phi - \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} \times \boldsymbol{B} - \varepsilon \nabla_{\boldsymbol{x}} M_B,$$

where

$$M_B = \frac{1}{2i} \langle \nabla_{\boldsymbol{k}}\chi| \times (H - E) |\nabla_{\boldsymbol{k}}\chi\rangle \cdot \boldsymbol{B}\big|_{\boldsymbol{k}=\boldsymbol{p}-\boldsymbol{b}},$$

and

$$\tilde{\Omega} = \nabla_{\boldsymbol{k}} \times \mathcal{A}_{\boldsymbol{k}}\big|_{\boldsymbol{k}=\boldsymbol{p}-\boldsymbol{b}}.$$

These are consistent with the equation (59) in [11]. Therefore one recovers the usual magnetic Bloch dynmaics in this specific case.

7 Conclusions and discussions

We have introduced a natural generalization of Wigner transform to the crystal case. We have also given a simple and unified treatment of the the Berry curvature terms in the context of Bloch dynamics, which is the semi-classical limit of one-particle Schrödinger equation in crystal. This offers an alternative approach to the work of Panati, Spohn and Teufel [11, 12]. So far we have been only focused on the case when the waves are all in a single isolated energy band. In some materials the effects from the many-body electron interaction is important. This has inspired the efforts to include the Berry phase in the density functional theory with spin degree of freedom which is going to the subject of our subsequent papers.

Appendix: Derivation of the transport equations

I. The case of the vector potential $\boldsymbol{b} = 0$

Substituting the WKB ansatz (5.2) into (5.1) yields, after taking the inner product with χ,

$$\begin{aligned}
&\partial_t a + a\langle \chi | d_t \chi\rangle + \nabla_{\boldsymbol{x}} a \cdot (\langle \chi | -i\nabla_{\boldsymbol{z}}\chi\rangle + \nabla_{\boldsymbol{x}} S) + \frac{1}{2} a \Delta_{\boldsymbol{x}} S \\
&\quad + a\langle \chi | \nabla_{\boldsymbol{k}}\chi\rangle \nabla_{\boldsymbol{x}} S : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S - a\langle \chi | i\nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{z}}\chi\rangle : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S \\
&\quad + a\langle \chi | \nabla_{\boldsymbol{x}}\chi\rangle \cdot \nabla_{\boldsymbol{x}} S - a\langle \chi | i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}}\chi\rangle = 0, \qquad \text{(A.1)}
\end{aligned}$$

where we have used the notation

$$d_t\chi = \partial_t \chi - \nabla_{\boldsymbol{k}}\chi \nabla_{\boldsymbol{k}} E : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S - \nabla_{\boldsymbol{k}}\chi \cdot \nabla_{\boldsymbol{x}} E.$$

Differentiating (5.3) with respect to $\boldsymbol{k}$ and taking the inner produce with χ, we have

$$\nabla_{\boldsymbol{k}} E = \langle \chi | -i\nabla_{\boldsymbol{z}}\chi\rangle + k. \qquad \text{(A.2)}$$

Differentiating (5.3) with respect to $\boldsymbol{k}$ twice and then taking the inner product with χ gives

$$(-\nabla_{\boldsymbol{k}} E + k)\langle \chi | \nabla_{\boldsymbol{k}}\chi\rangle - \langle \chi | i\nabla_{\boldsymbol{z}}\nabla_{\boldsymbol{k}}\chi\rangle = \frac{1}{2}\left(-I + \nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}} E\right),$$

where I is the identity tensor. Taking $\nabla_{\boldsymbol{x}}\cdot$ of (A.2) yields

$$\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E = \langle \chi | -i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}}\chi\rangle + \langle -i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}}\chi | \chi\rangle.$$

Note that

$$\frac{1}{2}\nabla_{\boldsymbol{x}} \cdot \big(\nabla_{\boldsymbol{k}} E|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S}\big) = \frac{1}{2}\big(\nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}} E : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S + \nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E\big)|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S}, \qquad \text{(A.3)}$$

and

$$\langle \chi | \nabla_{\boldsymbol{x}}\chi\rangle \cdot \nabla_{\boldsymbol{x}} S = \frac{1}{2}\big(\langle \chi | \nabla_{\boldsymbol{x}}\chi\rangle \cdot \nabla_{\boldsymbol{x}} S - \langle \nabla_{\boldsymbol{x}}\chi | \chi\rangle \cdot \nabla_{\boldsymbol{x}} S\big).$$

Putting these identities together, (A.1) is simplified to be (5.5).

II. The case of the vector potential $\boldsymbol{b} \neq 0$

The equations become more complicated when the magnetic field is nonzero. Substituting (5.2) in (6.1) produces

$$\begin{aligned}\partial_t a + a\langle\chi|d_t\chi\rangle + \nabla_{\boldsymbol{x}} a \cdot (\langle\chi| - i\nabla_{\boldsymbol{z}}\chi\rangle + \nabla_{\boldsymbol{x}} S + \langle\chi|\boldsymbol{b}\chi\rangle) + \frac{1}{2} a\Delta_{\boldsymbol{x}} S \\ + a\langle\chi|\nabla_{\boldsymbol{k}}\chi\rangle\nabla_{\boldsymbol{x}} S : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S - a\langle\chi|i\nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{z}}\chi\rangle : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S \\ + a\langle\chi|\nabla_{\boldsymbol{x}}\chi\rangle \cdot \nabla_{\boldsymbol{x}} S - a\langle\chi|i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}}\chi\rangle + a\langle\chi|\boldsymbol{b} \cdot \nabla_{\boldsymbol{x}}\chi\rangle \\ + a\langle\chi|\boldsymbol{b}\nabla_{\boldsymbol{k}}\chi\rangle : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S = 0, \qquad \text{(A.4)}\end{aligned}$$

where

$$d_t\chi = \partial_t\chi - \nabla_{\boldsymbol{k}}\chi\nabla_{\boldsymbol{k}} E : \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}} S - \nabla_{\boldsymbol{k}}\chi \cdot \nabla_{\boldsymbol{x}} E.$$

Note that $H = \frac{1}{2}\big(- i\nabla_{\boldsymbol{z}} + \boldsymbol{k} + \boldsymbol{b}(t, \boldsymbol{x}, \boldsymbol{z})\big)^2 + V(t, \boldsymbol{x}, \boldsymbol{z})$. Differentiating (6.4) with respect to $\boldsymbol{k}$ twice gives

$$(H - E)\nabla_{\boldsymbol{k}}\chi + \nabla_{\boldsymbol{k}} H\chi - \nabla_{\boldsymbol{k}} E\chi = 0, \qquad \text{(A.5)}$$

$$(H - E)\nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}}\chi + 2(\nabla_{\boldsymbol{k}} H - \nabla_{\boldsymbol{k}} E)\nabla_{\boldsymbol{k}}\chi + (\nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}} H - \nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}} E)\chi = 0.$$

Taking the inner product of the last two equations with χ yields

$$\nabla_{\boldsymbol{k}} E = \langle\chi| - i\nabla_{\boldsymbol{z}}\chi\rangle + \boldsymbol{k} + \langle\chi|\boldsymbol{b}\chi\rangle, \qquad \text{(A.6)}$$

$$\begin{aligned}(-\nabla_{\boldsymbol{k}} E + k)\langle\chi|\nabla_{\boldsymbol{k}}\chi\rangle - \langle\chi|i\nabla_{\boldsymbol{z}}\nabla_{\boldsymbol{k}}\chi\rangle + \langle\chi|\boldsymbol{b}\nabla_{\boldsymbol{k}}\chi\rangle \\ = \frac{1}{2}\left(-I + \nabla_{\boldsymbol{k}}\nabla_{\boldsymbol{k}} E\right). \qquad \text{(A.7)}\end{aligned}$$

(A.6) and (A.7) simplify (A.4) to give

$$\begin{aligned}\partial_t a + \nabla_{\boldsymbol{k}} E \cdot \nabla_{\boldsymbol{x}} a + \frac{1}{2} a\nabla_{\boldsymbol{x}} \cdot (\nabla_{\boldsymbol{k}} E|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S}) - \frac{1}{2} a\big(\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E\big)|_{\boldsymbol{k}=\nabla_{\boldsymbol{x}} S} \\ - a\nabla_{\boldsymbol{x}} E \cdot \langle\chi|\nabla_{\boldsymbol{k}}\chi\rangle + a\nabla_{\boldsymbol{x}} S \cdot \langle\chi|\nabla_{\boldsymbol{x}}\chi\rangle + a\langle\chi|\boldsymbol{b} \cdot \nabla_{\boldsymbol{x}}\chi\rangle \\ + a\langle\chi| - i\nabla_{\boldsymbol{z}}\nabla_{\boldsymbol{x}}\chi\rangle = 0, \qquad \text{(A.8)}\end{aligned}$$

in which we have also used the identity (A.3).

Since $\nabla_{\boldsymbol{x}} \cdot \boldsymbol{b} = 0$, by taking $\nabla_{\boldsymbol{x}} \cdot$ of (A.6), one has

$$\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{k}} E = \langle \chi | -i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}} \chi \rangle + \langle -i\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{z}} \chi | \chi \rangle \\ + \langle \chi | \boldsymbol{b} \cdot \nabla_{\boldsymbol{x}} \chi \rangle + \langle \boldsymbol{b} \cdot \nabla_{\boldsymbol{x}} \chi | \chi \rangle.$$

The last five terms of (A.8) simplify to give

$$\frac{1}{2}\big(- \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle + \langle \chi | \nabla_{\boldsymbol{k}} H \cdot \nabla_{\boldsymbol{x}} \chi \rangle \big) - \text{c.c.} \\ = \frac{1}{2}\big(- \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle + \langle \nabla_{\boldsymbol{k}} H \chi | \nabla_{\boldsymbol{x}} \chi \rangle \big) - \text{c.c.} \quad \text{(A.9)}$$

Differentiating (6.4) with respect to $\boldsymbol{x}$ yields

$$(H - E)\nabla_{\boldsymbol{x}} \chi + \nabla_{\boldsymbol{x}} H \chi - \nabla_{\boldsymbol{x}} E \chi = 0. \quad \text{(A.10)}$$

Therefore

$$\begin{aligned} & - \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle + \langle \nabla_{\boldsymbol{k}} H \chi | \nabla_{\boldsymbol{x}} \chi \rangle \\ = & - \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle - \langle (H - E) \nabla_{\boldsymbol{k}} \chi | \nabla_{\boldsymbol{x}} \chi \rangle + \nabla_{\boldsymbol{k}} E \cdot \langle \chi | \nabla_{\boldsymbol{x}} \chi \rangle \\ = & - \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle - \langle \nabla_{\boldsymbol{k}} \chi | (H - E) \nabla_{\boldsymbol{x}} \chi \rangle + \nabla_{\boldsymbol{k}} E \cdot \langle \chi | \nabla_{\boldsymbol{x}} \chi \rangle \qquad \text{(A.11)} \\ = & - \nabla_{\boldsymbol{x}} E \cdot \langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle - \big(\nabla_{\boldsymbol{x}} E \cdot \langle \nabla_{\boldsymbol{k}} \chi | \chi \rangle - \langle \nabla_{\boldsymbol{k}} \chi | \nabla_{\boldsymbol{x}} H \chi \rangle \big) + \nabla_{\boldsymbol{k}} E \cdot \langle \chi | \nabla_{\boldsymbol{x}} \chi \rangle \\ = & \langle \nabla_{\boldsymbol{k}} \chi | \nabla_{\boldsymbol{x}} H \chi \rangle + \nabla_{\boldsymbol{k}} E \cdot \langle \chi | \nabla_{\boldsymbol{x}} \chi \rangle. \end{aligned}$$

Here the first and third equalities come from (A.5) and (A.10) respectively, and the fourth equality is due to $\langle \chi | \nabla_{\boldsymbol{k}} \chi \rangle \in i\mathbb{R}^n$.

Since $\nabla_{\boldsymbol{x}} H = \nabla_{\boldsymbol{x}} A \nabla_{\boldsymbol{k}} H + \nabla_{\boldsymbol{x}} V$, the last equality combined with (A.8) and (A.9) imply (6.3).

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