I. BERRY CURVATURE OF BLOCH STATES

We now combine what we have learned in chapters 1 and 2 to investigate the Berry curvature of Bloch states.

A. Basics

Recall that in a crystal, the cell-periodic part \( u_{nk}(r) \) of the Bloch state \( \psi_{nk} = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(r) \) satisfies

\[
\tilde{H}_k(r) u_{nk}(r) = \varepsilon_{nk} u_{nk}(r),
\]

where

\[
\tilde{H}_k(r) = e^{-i\mathbf{k} \cdot \mathbf{r}} H(r) e^{i\mathbf{k} \cdot \mathbf{r}} = \frac{1}{2m} (\mathbf{p} + \hbar \mathbf{k})^2 + V_L(r).
\]

The Bloch momenta play the role of the slowly varying parameters, so the Berry connection for band-\( n \) is

\[
A_n(k) = i \langle u_{nk} | \frac{\partial}{\partial \mathbf{k}} | u_{nk} \rangle.
\]

The Berry curvature is

\[
F_n(k) = \nabla_k \times A_n(k) = i \langle \frac{\partial u_{nk}}{\partial k} \times \frac{\partial u_{nk}}{\partial k} \rangle.
\]

If the crystal has space inversion symmetry, then

\[
u_{nk}(r) \to u_{n-k}(-r) = u_{nk}(r),
\]

\[
A_n(k) = i \langle u_{n-k} | \frac{\partial}{\partial \mathbf{k}} | u_{n-k} \rangle = -A_n(-k)
\]

\[
F_n(k) = \nabla_k \times [-A_n(-k)] = F_n(-k)
\]

If there is time reversal transformation, then

\[
u_{nk}(r) \to u_{nk}'(r) = u_{nk}(r)
\]

\[
A_n(k) = i \langle u_{n-k} | \frac{\partial}{\partial \mathbf{k}} | u_{n-k} \rangle
\]

\[
= -i \langle u_{n-k} | \frac{\partial}{\partial \mathbf{k}} | u_{n-k} \rangle = A_n(-k)
\]

\[
F_n(k) = \nabla_k \times A_n(-k) = -F_n(-k)
\]

Therefore, if a crystal has both symmetries (and if the energy band is non-degenerate), then \( F_n(k) = 0 \) for all \( k \), and one does not need to worry about the Berry curvature. (Note: 1D is an exception. There is Berry phase, but no Berry curvature. See Eq. (??))

If the Berry curvature does exist, then it could influence the electron transport. For example, under an electric field \( \mathbf{E} \), the velocity of an electron in Bloch state \( \psi_{nk} \) is

\[
v_n(k) = \frac{1}{\hbar} \frac{\partial \varepsilon_{nk}}{\partial \mathbf{k}} + \frac{e}{\hbar} \mathbf{E} \times \mathbf{F}_n(k).
\]

\[
Pf: \text{Choose a time-dependent gauge for the electric field, } \mathbf{E} = -\partial \mathbf{A}/\partial t, \mathbf{A} = -\mathbf{E} t, \text{ then the Hamiltonian becomes,}
\]

\[
\tilde{H}_k = \frac{(\mathbf{p} + \hbar \mathbf{k})^2 + e \mathbf{E} t}{2m} + V_L(r) = \tilde{H}_k(t),
\]

where \( \mathbf{k}(t) = \mathbf{k}_0 - e \mathbf{E} t / \hbar \). To the zeroth order of approximation, one only needs to replace \( \varepsilon_{nk} \) with \( \varepsilon_{n'k} \). To the first-order, one has (see Prob. 1)

\[
|u_{nk}^{(1)}| = |u_{nk}| - i \hbar \sum_{n' \neq n} \frac{\langle u_{n'k} | \partial \mathbf{E} / \partial \mathbf{k} | u_{nk} \rangle}{\varepsilon_{nk} - \varepsilon_{n'k}},
\]

in which all of the \( k \)'s are \( k(t) \)'s.

The velocity is calculated as

\[
v_n(k) = \langle \psi^{(1)}_{nk} | \frac{\mathbf{P}}{m} | \psi^{(1)}_{nk} \rangle = \langle u^{(1)}_{nk} | \frac{\mathbf{p} + \hbar \mathbf{k}}{m} | u^{(1)}_{nk} \rangle
\]

\[
= \langle u^{(1)}_{nk} | \frac{\partial \tilde{H}_k}{\partial \mathbf{k}} | u^{(1)}_{nk} \rangle.
\]

Substitute Eqs. (1.15) into (1.18), one will get

\[
v_n(k) = \langle u_{nk} | \frac{\partial \tilde{H}_k}{\partial \mathbf{k}} | u_{nk} \rangle
\]

\[- i \sum_{n' \neq n} \left( \frac{\langle u_{nk} | \partial \tilde{H}_k | u_{n'k} \rangle \langle u_{n'k} | \partial \mathbf{E} / \partial \mathbf{k} | u_{nk} \rangle}{\varepsilon_{nk} - \varepsilon_{n'k}} \right) + c.c. \]

Before proceeding further, we need an identity: Starting from the equation,

\[
\langle u_{nk} | \tilde{H}_k | u_{n'k} \rangle = \varepsilon_{nk} \delta_{nn'},
\]

take the derivative \( \partial / \partial \mathbf{k} \) of both sides and we'll get,

\[
\langle u_{nk} | \frac{\partial \tilde{H}_k}{\partial \mathbf{k}} | u_{n'k} \rangle = (\varepsilon_{nk} - \varepsilon_{n'k}) \langle \frac{\partial u_{nk}}{\partial k} | u_{n'k} \rangle + \frac{\partial \varepsilon_{nk}}{\partial k} \delta_{nn'},
\]

\[
\langle u_{nk} | \frac{\partial \tilde{H}_k}{\partial \mathbf{k}} | u_{n'k} \rangle = (\varepsilon_{nk} - \varepsilon_{n'k}) \langle \frac{\partial u_{nk}}{\partial k} | u_{n'k} \rangle + \frac{\partial \varepsilon_{nk}}{\partial k} \delta_{nn'},
\]
With the help of this identity, the velocity can be written as,

\[ \mathbf{v}_n(k) = \frac{\partial \varepsilon_{nk}}{\hbar \partial k} - i \left( \frac{\partial u_{nk}}{\partial k} \frac{\partial u_{nk}}{\partial t} \right) = \frac{\partial \varepsilon_{nk}}{\hbar \partial k} - \mathbf{k} \times \mathbf{F}_n. \] (1.22)

Since \( \mathbf{k} = -i(e/\hbar) \mathbf{E} \), the second term is \((e/\hbar) \mathbf{E} \times \mathbf{F}_n \). End of proof.

The velocity that depends on the Berry curvature is \textit{perpendicular} to the direction of the applied \( \mathbf{E} \) field. It is called the \textit{anomalous velocity}, which first appeared in the study of \textit{anomalous Hall effect} in Karplus and Luttinger, 1954, although not in the language of Berry curvature.

The anomalous velocity plays an essential role in the theory of \textit{Quantum Hall effect} (QHE). Consider a 2D electron gas (2DEG) lying on the \( x-y \) plane subjected to a magnetic field \( \mathbf{B} \). If there is a non-zero Berry curvature \( F_z \), then the Hall current density along \( z \)-direction is given by,

\[
\mathbf{j}_z = -\frac{e}{L^2} \sum_{n,k} f(\varepsilon_{nk}) \mathbf{v}_{nz}(k)
\]

\( = -\frac{e}{L^2} \sum_{n,k} f(\varepsilon_{nk}) \partial \varepsilon_{nk} / \hbar \partial k_x \) (1.25)

\[
- \frac{e^2}{\hbar} \sum_{n,k} \frac{1}{L^2} \sum_{k} f(\varepsilon_{nk}) F_{n} z(k) E_y, \]

where \( L^2 \) is the area of the 2DEG, and \( f(\varepsilon_{nk}) \) is the Fermi-Dirac distribution function. The first term is the current density in equilibrium, which is obviously zero. The second term contributes to the Hall current.

At temperature \( T = 0 \), if \( N \) energy bands (Landau sub-bands, to be precise) are filled, then the Hall conductivity is,

\[
\sigma_{xy} = -\frac{e^2}{\hbar L^2} \sum_{n,k} F_{n} z(k) \]

\( = -\frac{e^2}{\hbar} \sum_{n=1}^{N} \left( \frac{1}{2\pi} \int_{BZ} d^2 k F_{n} z(k) \right). \) (1.28)

The integral over the Brillouin zone inside the parenthesis is a topological quantity (Thouless et al., 1982) called the \textit{first Chern number},

\[
C_1^{(n)} = \frac{1}{2\pi} \int_{BZ} d^2 k F_{n} z(k) \in \mathbb{Z}. \] (1.29)

Therefore, an insulator with \( N \) filled bands would have a quantized quantum Hall conductance \( \left( \sum_{n=1}^{N} C_1^{(n)} \right) e^2/\hbar \) (see Xiao et al., 2010).

FIG. 1 (a) Gauge-N has a string of singularity along \( -z \)-axis. (b) An atlas with two patches of gauge is singularity-free.

Some remarks are in order: 1. The discussion above applies only to integer quantum Hall effect, but does not apply to fractional quantum Hall effect.

2. In a quantum Hall system, the strong magnetic field would break the lattice translation symmetry of the Hamiltonian. Nonetheless, if the magnetic flux per unit cell is a rational fraction of the flux quantum, \( \Phi = (p/q) \Phi_0 \), then it is possible to define a \textit{magnetic translation symmetry}, such that the Bloch theory can still be applied. However, the quantities above need be interpreted as magnetic Bloch momentum \( \mathbf{k} \), magnetic Bloch band \( \varepsilon_{nk} \), and magnetic Brillouin zone (Chang and Niu, 1996).

3. The Hall conductance in Eq. (1.28) can also be obtained from linear response theory, which can be generalized to include electron interaction and disorder. It can be shown that, despite these complications, the Hall conductance remains quantized, as long as the energy gap remains open (Niu et al., 1985).

4. In experiments, disorders in a sample result in \textit{localized states} that do not conduct electric current. That is why one can observe the plateaus of the Hall conductance. In a clean system, the width of the Hall plateau would shrink to zero, and precise determination of \( e^2/\hbar \) would not be possible. So the topology is not easily revealed without the presence of disorder.

5. It is also worth emphasizing that, in the semiclassical theory of electron dynamics, Eq. (1.23) remains valid in the presence of a magnetic field \( \mathbf{B} \), but its derivation is not as easy. The \textit{semiclassical equations of motion} for electrons in band-\( n \) are

\[
\begin{array}{l}
\mathbf{r} = \frac{\varepsilon_n^{(n)}}{\hbar} - \mathbf{k} \times \mathbf{F}_n, \\
\hbar \mathbf{k} = -e \mathbf{E} - e \mathbf{r} \times \mathbf{B}.
\end{array}
\] (1.30)

in which \( \varepsilon_n^{(n)} = \varepsilon_{nk} - m_n(k) \cdot \mathbf{B} \) is the energy shifted by magnetic moment.

B. \textbf{Gauge choice of Bloch state}

Before discussing the gauge choice of Bloch state, let us look back at a simpler example: the spin-1/2 system
living on the northern hemisphere uses gauge-types of gauges are used (Wu and Yang, 1975); people
the Stokes theorem fails if the last integral approaches 0. The inequalities arise because
the Berry curvature $F = \pm \frac{1}{2 \pi}$ is well behaved along the
\( \theta = \pi \).

On the other hand, the Berry connection for the second basis is
\[ A^S_{\pm}(B) = \pm \frac{1}{2B} \frac{1 + \cos \theta}{\sin \theta} d\phi. \]  
(1.32)

It is singular along the axis of $\theta = 0$. Both $A^N_{\pm}$ and $A^S_{\pm}$ have the same Berry curvature $F$.

In Fig. 1(a), we see a loop $C_1$ near the north pole, and a loop $C_2$ near the south pole. The area inside $C_1$
marked as $S_1$; the area outside is $S_1$. Similarly the
area inside $C_2$ is called $S_2$, outside is $S_2$. It is not difficult to see that,
\[ \oint_{C_2} d\ell \cdot A^N_{\pm} = \int_{S_2} d^2 a \cdot F_{\pm} \neq \int_{S_2} d^2 a \cdot F_{\pm}. \]  
(1.33)

The LHS approaches $2\pi$ as $C_2$ shrinks to zero; while the last integral approaches 0. The inequalities arise because
the Stokes theorem fails if $A$ is singular in the domain of surface integration. That is, to ensure the validity of the Stokes theorem, the area of integration cannot contain singular points. That is why we need to choose $S_2$ for the loop $C_2$.

It is possible to remove the string of singularity if both types of gauges are used (Wu and Yang, 1975); people living on the northern hemisphere uses gauge-$N$, while people living on the southern hemisphere uses gauge-$S$ (see Fig. 1(b)). So both tribes of people feel no singularity. However, they need to switch gauges near the equator with the gauge transformation,
\[ A^S_{\pm}(B) = A^N_{\pm}(B) \pm \frac{\partial \phi}{\partial B}. \]  
(1.34)

In this case, the Stokes theorem can be applied for an integration over the whole sphere,
\[ \int_{S^2} d^2 a \cdot F_{\pm} = \int_{S^2} d^2 a \cdot \nabla \times A^N_{\pm} + \int_{S^2} d^2 a \cdot \nabla \times A^S_{\pm} \]  
(1.35)
\[ = \int_{C_{\pm}} d\ell \cdot A^N_{\pm} + \int_{C_{\pm}} d\ell \cdot A^S_{\pm} \]  
(1.36)
\[ = \int_{C_{\pm}} d\ell \cdot (A^N_{\pm} - A^S_{\pm}) \]  
(1.37)
\[ = \pm \int_{C_{\pm}} d\ell \cdot \frac{\partial \phi}{\partial B} = \mp 2\pi. \]  
(1.38)

Assume gauge-I has a singularity on the right of the $BZ$; gauge-II has a singularity on the left of the $BZ$ (see Fig. 2(b)). Then we can adopt gauge-I on the left side, and gauge-II on the right side, so that there is no singularity through the whole $BZ$. Again when crossing the boundary of different patches, one needs to switch gauges using Eq. (1.41). The single-valuedness of $\chi$ along the boundary would guarantee that the Berry curvature integrated over the whole $BZ$ (and divided by $2\pi$) is an integer value $C_1$. If there are multiple singularities for a single gauge, then more patches need be used, but the procedure remains essentially the same.

In addition to the two gauge choices above, one can also fix the phase of the Bloch state using the parallel transport gauge (see Thouless, 1984).

\[ \langle u_{k_0} | \frac{\partial}{\partial k_x} | u_{k_0} \rangle = 0, \]  
(1.42)
\[ \langle u_{k_x k_y} | \frac{\partial}{\partial k_y} | u_{k_x k_y} \rangle = 0. \]  
(1.43)
The first equation defines the phase of the states (of a band \( n \)) on the \( k_x \)-axis; the second equation defines the phase along a line with fixed \( k_x \) (see Fig. 3). As a result, the phases of any two states in the BZ have a definite relation. Be aware that the phases defined by the parallel transport gauge are not necessarily single-valued.

The states on opposite sides of the BZ boundaries represent the same physical state. Therefore, they can only differ by a \( \mathbf{k} \)-dependent phase factor. Following Eqs. (1.42) and (1.43), we can choose

\[
\begin{align*}
  u_{k_x+g_x,k_y} &= u_{k_x,k_y}, \\
  u_{k_x,k_y+g_y} &= e^{i\delta(k_x)}u_{k_x,k_y},
\end{align*}
\]

where \( g_x \) and \( g_y \) are the basis of reciprocal lattice vectors. That is, the states on the opposite sides of the vertical boundaries have the same phase. The same cannot also be true for the horizontal boundaries, otherwise the topology will be too trivial to accommodate the quantum Hall conductivity.

Periodicity of the BZ requires that

\[
\delta(k_x + g_x) = \delta(k_x) + 2\pi \times \text{integer}. \tag{1.46}
\]

In order for the integral \((1/2\pi) \int_{BZ} dk \cdot \mathbf{A}(k)\) (which is nonzero only along the upper horizontal boundary) to be the Hall conductivity \(C_1 \hbar/e^2\), the integer in Eq. (1.46) obviously has to be equal to \(C_1\).

Following the periodicity condition in Eq. (1.46), one can choose the phase to be,

\[
\delta(k_x + g_x) = \delta(k_x) + C_1 k_x a_1, \tag{1.47}
\]

where \( \delta(k_x + g_x) = \delta(k_x) \) is periodic in \( k_x \), but otherwise remains arbitrary, \( a_1 \) is a lattice constant.

In summary, when the Bloch states have non-trivial topology, the phases of the Bloch states cannot be defined uniquely and smoothly over the whole BZ. There are either points of phase ambiguity, or lines where phases are not single-valued, so that the vorticity of the whole BZ can be non-zero (Soluyanov and Vanderbilt, 2012). This is the topological obstruction mentioned at the end of ??.

1. To derive Eq. (1.15), first write

\[
|\Psi(t)\rangle = \sum_m e^{i\gamma_m(t)} e^{-\frac{i}{\hbar} \int_0^t dt' \varepsilon_{mk}(t') a_m(t)|u_{mk}\rangle
\]

\[
= \sum_m e^{-\frac{i}{\hbar} \int_0^t dt' \varepsilon_{mk}(t') a_m(t)|\tilde{u}_{mk}\rangle, \tag{1.48}
\]

in which \( a_m(t) \) vary slowly with time. This is a multi-level generalization of Eq. (??) in Chap 2. Recall that \( |\tilde{u}_{mk}\rangle = e^{i\gamma_m(t)}|u_{mk}\rangle \) satisfies the parallel transport condition (see Prob. 2.2),

\[
\langle \tilde{u}_{mk} | \partial_t | \tilde{u}_{mk} \rangle = 0. \tag{1.49}
\]

(a) Use the Schrödinger equation \( H|\Psi(t)\rangle = i\partial_t|\Psi(t)\rangle \) and show that,

\[
\frac{da_m(t)}{dt} = \frac{-e^{-\frac{i}{\hbar} \int_0^t dt' \varepsilon_{mk}(t') \langle \tilde{u}_{mk} | \partial_t | \tilde{u}_{mk} \rangle} \tag{1.50}
\]

(b) Assume the exponential factor oscillates much faster than the bracket, so that the latter can be treated as static. Integrate the equation above to get Eq. (1.15). Note: If the non-integrable phases \( \gamma_m(t) \) are not involved in a dynamical process, then they can be ignored and \( |\tilde{u}_{mk}\rangle \) are simplified as \( |u_{mk}\rangle \). (Ref: Appendix of Xiao et al., 2010)

2. Under the one-band approximation, the effective Lagrangian of a Bloch wavepacket in an external electromagnetic field can be obtained by using the time-dependent variational principle (Chang and Niu, 1996). Here we merely take the effective Lagrangian as the starting point for subsequent derivations:

\[
L(r, k; \tilde{r}, \tilde{k}) = \hbar \mathbf{k} \cdot \mathbf{\dot{r}} + \hbar \mathbf{\dot{k}} \cdot \mathbf{A}(k) - e \mathbf{\epsilon} \cdot \mathbf{A}_e(r) + e \phi_e - e^m \mathbf{F} \cdot \mathbf{m}(k) - \mathbf{B}. \tag{1.51}
\]

where \( \mathbf{A}(k) \) is the Berry connection, \( \phi_e(r) \) and \( \mathbf{A}_e(r) \) are the electromagnetic potentials, and \( e^m = \epsilon(k) - \mathbf{m}(k) \cdot \mathbf{B} \).

Treating both \( r \) and \( k \) as generalized coordinates, using the Euler-Lagrangian equation to derive the equations of motion,

\[
\hbar \mathbf{\dot{k}} = -e \mathbf{E} - e \mathbf{\epsilon} \times \mathbf{B}, \tag{1.52}
\]

\[
\hbar \mathbf{\dot{r}} = \frac{\partial e^m}{\partial k} - \hbar \mathbf{\dot{k}} \times \mathbf{F}, \tag{1.53}
\]

where \( \mathbf{B} = \nabla \times \mathbf{A}_e(r) \) and \( \mathbf{F} = \nabla_k \times \mathbf{A}(k) \).

For simplicity, assume that the electron is moving in the \( xy \)-plane and the magnetic field is along the \( z \)-direction. It would not be difficult to see that the equations of motion remain valid in more general situations.

References