The objective of this article is to provide a comprehensive review of the Hall effect family. Grasping the intricate physics underlying the various manifestations of the Hall effect is no straightforward feat. In this regard, we present a step-by-step analysis. The structure of the entire article is as follows:

1) We commence by delving into the conventional theory of conductivity, spanning from classical principles to the realm of quantum mechanics.

2) Upon entering the quantum realm, we proceed to derive the current operator, encompassing two distinct contributions. The initial term corresponds to the gradient of the energy eigenvalue in k-space, impacting the conductivity of most metals. The subsequent term, connected to the Berry curvature, assumes significance in situations where time-reversal symmetry is violated.

3) It is worth noting that the Berry curvature-associated second term possesses a captivating property. The integration of the Berry curvature across the Brillouin zone, summed over all bands, results in an integer value of 2π.

1 Brief Summary of Conductance Theory

To elucidate conductivity, physicists have formulated multiple models, spanning from the classical and semiclassical to the quantum approaches. These models can be summarized as follows:

1) In classical model, the electrons are treated classically, and the movement is governed by the Newton's law and the forces on the electrons are described by electromagnetism . This model is good enough to explain the Ohm's law.

2) The semiclassical model views electrons as both particles and waves. Electron movement is likened to wavepacket propagation, with the electron's velocity representing the group velocity of the wave. This model leverages particle-wave duality and effectively accounts for conduction in metals.

3) In the quantum model, velocity is represented by the expectation value of the velocity operator within a given wavefunction. This theoretical approach is essential for deriving Hall conductance and comprehending the topological intricacies of Hall conductance.

2 Classical Conductance Theory Example: Hall Effect

We consider the electrons inside conductors. When we apply both an electric field E and a magnetic filed B, the electrons have the equation of motion following the Newtons' law

$$m\frac{d\mathbf{v}}{dt} = -e\mathbf{E} - e\mathbf{v} \times \mathbf{B} - m\frac{\mathbf{v}}{\tau}$$

The first term in right hand side is the force by the electric field, and the second term is the force by the magnetic field. The third term electron collision by the ions. When collision happens, the momentum of the electron changes to zero within a certain mean free time τ. At the equilibrium states, we have $\frac{d\mathbf{v}}{dt} = 0$.

The velocity satisfies

$$\frac{e\tau}{m}\mathbf{v} \times \mathbf{B} + \mathbf{v} = -\frac{e\tau}{m}\mathbf{E} \tag{1}$$

As $\mathbf{v} = (v_x, v_y)$, so the above equation can be written as

$$v_x + \frac{e\tau}{m}v_y B = -\frac{e\tau}{m}E_x$$

The current density J is related to the velocity by

$$\mathbf{J} = -ne\mathbf{v}$$

So

$$j_x + \frac{e\tau B}{m}j_y = \frac{ne^2\tau}{m}E_x$$

We define the conductivity as

$$\mathbf{J} = \sigma\mathbf{E}$$

so $\sigma_{xx} = \frac{ne^2\tau}{m}$, $\sigma_{xy} = \frac{ne}{B}$.

3   Hall conductivity of 2D electrons

Solution to 2D electron system subject to a magnetic field
A Hamiltonian for 2D electrons in a magnetic field $A = xB\hat{y}$ is

$$H = \frac{1}{2m}(p_x^2 + (p_y + eBx)^2)$$

Because this Hamiltonian commutes with p_y, so they share the same eigenstates, therefore, we can write the solution for the Hamiltonian as

$$\psi_k(x, y) = e^{iky}f_k(x)$$

$$H\psi_k(x, y) = \frac{1}{2m}(p_x^2 + (\hbar k + eBx)^2)\psi_k(x, y) = H_k\psi_k(x, y)$$

$$H_k = \frac{1}{2m}p_x^2 + \frac{m\omega_B^2}{2}(x + \frac{\hbar k}{eB})^2$$

This H_k is the Hamiltonian for a harmonic oscillator in the x direction, with the center displaced form the origin. The solution to H_k is very similar to harmonic oscillator. The energy eigenvalues are

$$E_n = \hbar\omega_B(n + \frac{1}{2})$$

where $\omega_B = \frac{eB}{m}$. And the eigenstate wavefunctions are

$$\psi_{n,k}(x,y) \propto e^{iky} H_n(x + \frac{\hbar k}{eB}) e^{-(x+\frac{\hbar k}{eB})^2 eB/2\hbar}$$

Adding an electric filed for 2D electron system subjected to a magnetic field

$$H = \frac{1}{2m}(p_x^2 + (p_y + eBx)^2) + eEx$$

Its solution is again similar to harmonic oscillator with additional shift

$$\psi(x,y) = \psi_{n,k}(x + mE/eB^2, y)$$

and the energies are

$$E_{n,k} = \hbar\omega_B(n + \frac{1}{2}) - eE(\frac{\hbar k}{eB} + \frac{eE}{m\omega_B^2}) + \frac{m}{2}\frac{E^2}{B^2}$$

Since we get the wavefunction and eigenenergy, there are two ways to find out the current. One way is to use the semiclassical approach. We can calculate group velocity given a wavevector k

$$v_y = \frac{1}{\hbar}\frac{\partial E_{n,k}}{\partial k} = -\frac{E}{B}$$

So we surprisingly see add an electric filed in x direction generates the movement in y! To find out the total current in y direction, we have to know the degeneracy, which means how many electrons are in the state with the momentum k to k + dk. In y direction, electrons are free particle with momentum k confined in a finite size L_y. So

$$\frac{dn}{dk} = \frac{L_y}{2\pi}$$

The total current is

$$I_y = e\frac{E}{B}\int \frac{dn}{dk}dk = \frac{eEL_y}{2\pi B}\int k$$

The range of k in the above integral is tricky. From the wavefunction, we see the center of the harmonic oscillator in x direction is $x = -k\hbar/eB$, while $0 \leq x \leq L_x$, then $-L_x eB/\hbar \leq k \leq 0$.

$$I_y = \frac{eEL_y}{2\pi B}\int_{-L_x eB/\hbar}^{0} k = \frac{e^2}{h}EA$$

4   Current derivation in quantum approach

The second way is purely quantum approach. In quantum mechanics, the average position is defined as

$$< r(t) > = < \Psi(t)|\hat{r}|\Psi(t) >$$

and the average velocity is the total derivative of above.

$$< \dot{r}(t) >= \frac{d}{dt} < \Psi(t)|\hat{r}|\Psi(t) >$$

We first need to derive $\Psi(t)$.

4.1 Wavefunction subject to adiabatic approximation

Based on Bloch theorem, the wave function can be written as

$$|\Psi_n(t) >= e^{i\theta_n(t)}|u_n(R(t) >$$

and its derivative is

$$\frac{d}{dt}|\Psi_n(t) >= i\dot{\theta}_n e^{i\theta_n(t)}|u_n > +e^{i\theta_n}\frac{d}{dt}|u_n >$$

Substituting $|\Psi_n(t)$ into Schrodinger equation,

$$i\hbar\frac{d}{dt}|\Psi_n(t) >= H(R(t))|\Psi_n(t) >$$

yields

$$i\hbar[i\dot{\theta}_n|u_n > +\frac{d}{dt}|u_n >]e^{i\theta_n(t)} = H(R(t))e^{i\theta_n}|u_n >$$

Canceling $e^{i\theta_n(t)}$ on both sides:

$$-\hbar\dot{\theta}_n|u_n > +i\hbar\frac{d}{dt}|u_n >= E_n(R(t))|u_n >$$

Multiplying $|u_n >$ on the left:

$$-\hbar\dot{\theta}_n + i\hbar < u_n|\frac{d}{dt}|u_n >= E_n(R(t))$$

So

$$\dot{\theta}_n = i < u_n|\frac{d}{dt}|u_n > -\frac{1}{\hbar}E_n(R(t))$$

Integrating over time gives

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt' + i\int_0^t < u_n(t')|\frac{d}{dt'}u_n(t') > dt'$$

Define

$$\gamma_n(t) = i\int_0^t < u_n(t')|\frac{d}{dt'}u_n(t') > dt'$$

which is the Berry phase. The final result of adiabatic solution is

$$|\Psi_n(t) >= e^{i\gamma_n(t)}exp(-\frac{i}{\hbar}\int_0^t E_n(t')dt')|u_n(R(t)) >$$

The final state at time t acquires both a dynamical phase from the energy eighenvalue and a geometric Berry phase from the parametric evolution of the eigenstate.

4.2 Expectation value of velocity given the wavefunction

$$< \dot{r}(t) > = \frac{d}{dt} < \Psi(t)|\hat{r}|\Psi(t) >$$

$$=< \frac{d}{dt}\Psi(t)|\hat{r}|\Psi(t) > + < \Psi(t)|\frac{d}{dt}\hat{r}|\Psi(t) > + < \Psi(t)|\hat{r}|\frac{d}{dt}\Psi(t) >$$

Derivation of the 2nd term $< \Psi(t)|\frac{d}{dt}\hat{r}|\Psi(t) >$
1)Based on Heisenburg equation

$$\frac{d}{dt}\hat{r} = \frac{i}{\hbar}[H, r] = \frac{1}{i\hbar}[\hat{r}, \hat{H}]$$

So

$$< \Psi(t)|\frac{d}{dt}\hat{r}|\Psi(t) >= \frac{1}{i\hbar} < \Psi(t)|[\hat{r}, \hat{H}]|\Psi(t) >$$

2)Schrodinger equation with periodic Hamiltonian. Consider Bloch eigenstate

$$|\Psi_{nk} >= e^{ikr}|u_{nk} >$$

Then Schrodinger equation give the Block eigenstate becomes

$$\hat{H}(k)e^{ikr}|u_{nk} >= \epsilon_{nk}e^{ikr}|u_{nk} >$$

Multiplying e^{-ikr} on the left hand side,

$$e^{-ikr}\hat{H}(k)e^{ikr}|u_{nk} >= e^{-ikr}\epsilon_{nk}e^{ikr}|u_{nk} >= \epsilon_{nk}|u_n nk >$$

Define the cell-periodic Hamiltonian

$$\hat{H}(k) \equiv e^{-ikr}\hat{H}e^{ikr}$$

then we have

$$\hat{H}(k)|u_{nk} >= \epsilon_n(k)|u_{nk} >$$

3)link $[r, \hat{H}]$ to $\partial_k H(k)$,
Differentiating $\hat{H}(k)$:

$$\frac{d}{dk}\hat{H}(k) = \frac{d}{dk}[e^{-ik\dot{r}}\hat{H}e^{ik\dot{r}}]$$

$$= -i[e^{-ik\dot{r}}r\hat{H}e^{ik\dot{r}}] + [e^{-ik\dot{r}}\hat{H}re^{ik\dot{r}}]$$

$$= -ie^{-ikr}[r, \hat{H}]e^{ikr}$$

4)Evaluating the expectation value of $[r, \hat{H}]$,

$$< \Psi_{nk}|[\hat{r}, \hat{H}]|\Psi_{nk} >=< u_{nk}|e^{-ikr}[\hat{r}, \hat{H}]e^{ikr}|u_{nk} >$$

$$=< u_{nk}|i\nabla_k\hat{H}(k)|u_{nk} >$$

According to Hellmann–Feynman theorem

$$< u_{nk}|i\nabla_k \hat{H}(k)|u_{nk} >= i\nabla_k \epsilon(k)$$

Combining 1) through 4)

$$< \Psi(t)|\frac{d}{dt}\hat{r}|\Psi(t) >= \frac{1}{i\hbar} < \Psi(t)|[\hat{r},\hat{H}]|\Psi(t) >= \frac{1}{\hbar}\nabla_k \epsilon_n(k)$$

This shows the current contribution coming directly from band structure, and it allows us to explain the conductivity of metal, which will be explained in later sections.

Derivation of 1st and 3rd term The 3rd term is the complex conjugate of the 1st term.   (1)Derivative of wavefunction
The time-dependent wavefunction is the Bloch form with a Berry phase.

$$|\Psi >= e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >$$

$$|\partial_t \Psi >= [i\dot{\theta}(t) + (i\dot{k}(t)r)]e^{i\theta}e^{ik(t)r}|u(k(t)) > +e^{i\theta}e^{ik(t)r}\dot{k}(t)|\partial_k u(k(t)) >$$
$$< \partial_t \Psi |=< u(k(t))|e^{-ik(t)r}e^{-i\theta}[-i\dot{\theta}(t) + (-ik(t)r)]+ < \partial_k u(k(t))|e^{-ik(t)r}e^{-i\theta}\dot{k}(t)$$

So

$$\begin{aligned}
< \Psi|r|\partial_t \Psi >&=< u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}ir\dot{\theta}(t)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}irk(t)re^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|\partial_k u(k(t)) >\\
< \partial_t \Psi|r|\Psi >&=< u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}(-ir\dot{\theta}(t))e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}(-irk(t)r)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < \partial_k u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
< \Psi|r|\partial_t \Psi > + < \partial_t \Psi|r|\Psi >&=< u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}(ir\dot{\theta}(t) - ir\dot{\theta}(t))e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}(irk(t)r - irk(t)r)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&+ < u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|\partial_k u(k(t)) >\\
&+ < \partial_k u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >\\
&=< u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|\partial_k u(k(t)) >\\
&+ < \partial_k u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|u(k(t)) >
\end{aligned}$$

Define S_{geom}

$$S_{geom} =< u(k(t))|e^{-ik(t)r}e^{-i\theta(t)}r\dot{k}(t)e^{i\theta(t)}e^{ik(t)r}|\partial_k u(k(t)) > +c.c$$

Based on an identity

$$< u_k|e^{-ikr}\hat{r}e^{ikr}|u_k >= i\partial_k+ < u_k|i\partial_k u_k >$$

The component of $S_{geom,i}$ is

$$S_{geom,\alpha} = \dot{k}_\beta[\partial_{k_\beta}(i < u|\partial_{k_\alpha}u >) - \partial_k k_\alpha(i < \partial_{k_\beta}u|u >)] = \dot{k}_\beta(\partial_{k_\beta}A_\alpha - \partial_{k_\alpha}A_\beta)$$

6

Define Berry connection

$$A_\alpha(k) = i < u|\partial_{k_\alpha} u >$$

The corresponding Berry curvature is

$$\Omega_\gamma = (\nabla_k \times A)_\gamma$$

$$S_{geom} = -\dot{k} \times \Omega(k)$$

When the electric field E is present

$$\hbar\dot{k} = -eE$$

The expectation value of the velocity

$$< v >= \frac{1}{\hbar}\nabla_k \epsilon_n(k) + \frac{e}{\hbar}E \times \Omega_n(k) = v_{Bloch} + v_{anomalous}$$

So the contribution of electron velocity comes from two terms: one is Bloch velocity $v_{Bloch} = \frac{1}{\hbar}\nabla_k \epsilon_n(k)$ which can explan the conductivity of metal, the other one is anomalous velocity $\frac{e}{\hbar}E \times \Omega_n(k)$, which explains the conductivity for Hall effect, topological insulators, etc.

4.3   Current expression

$$j = -e \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} f(\mathbf{k})v_n(\mathbf{k})$$

where $f(\mathbf{k})$ is Fermi-Dirac distribution and summation over n means summation over all occupied bands. We can decompose the current into two terms,
Bloch current:

$$j_{Bloch} = -e \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} f(\mathbf{k})v_{Bloch}(\mathbf{k})$$

and anomalous current:

$$j_{anomalous} = -e \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} f(\mathbf{k})v_{Bloch}(\mathbf{k})$$

4.3.1   Bloch Current

1) Electric field is not present. We have symmetrical engery band $E_n(\mathbf{k}) = E_n(-\mathbf{k})$, so $\nabla_k E_n(\mathbf{k})$ is odd function. $\nabla_\mathbf{k} E_n(-\mathbf{k}) = -\nabla_\mathbf{k} E_n(\mathbf{k})$. Also $f(\mathbf{k})$ is symmetrical with respect to $\mathbf{k}$, $f(\mathbf{k}) = f(E(\mathbf{k})) = f(e(-\mathbf{k}))$. So $f(\mathbf{k})v_{Bloch}(\mathbf{k})$ is an odd function with respect to k. As a consequence the integral over the Brillion zone is zero

$$j_{Bloch} = -e \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} f(\mathbf{k})v_{Bloch}(\mathbf{k}) = 0$$

So the net current without eletric field.

2) Electric field is present

a) If all the bands are fully occupied, the distribution function does not change when electric field is applied because all the states are occupied. Therefore the net current is still zero.

b) When some bands are partially filled, the distribution function becomes

$$f(\mathbf{k}) = f_0(\mathbf{k}) + \delta f(\mathbf{k})$$

Where $f_0(\mathbf{k})$ is the distribution function without electric field. Based on Boltzman relaxation time approximation

$$\delta f(\mathbf{k}) = \frac{e\tau}{\hbar} \hat{E} \cdot \nabla_k f_0(k)$$

$$
\begin{aligned}
j_{Bloch} &= -e \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} \delta f(\mathbf{k}) v_{Bloch}(k) \\
&= e^2\tau \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} (E \cdot \nabla_k f_0) v_n(k) \\
&= e^2\tau \sum_n \int_{BZ} \frac{d^3k}{(2\pi)^3} (E \cdot \frac{\partial f}{\partial \epsilon} \frac{\partial \epsilon}{\partial k}) v_n(k)
\end{aligned}
$$

Define

$$\sigma_{ij} = e^2\tau \sum_n \int \frac{d^3k}{(2\pi)^3} v_i(k) v_j(k) (-\frac{df_0}{d\epsilon})$$

We have

$$\mathbf{j} = \sigma \mathbf{E}$$

4.3.2 Anomalous Current

$$v_{anomalous} = -\frac{e}{\hbar} E \times \Omega_n \mathbf{k}$$

Imagine we apply an electric field in x direction, and we would like to know the current in y

$$j_y = -e \sum_n \int \frac{d^2k}{(2\pi)^2} f_n(\mathbf{k}) [-\frac{\mathbf{e}}{\hbar} (\mathbf{E} \times \mathbf{\Omega_n}(\mathbf{k}))_\mathbf{y}]$$

For 2D system, $E = (E_x, E_y)$, and Ω is in z direction. So

$$(E \times \Omega_n)_y = E_z \Omega_n^x - E_x \Omega_n^z$$

Because $E_z = 0$, and $\Omega_n^x = 0$

$$(E \times \Omega_n)_y = -E_x \Omega_n^z(\mathbf{k})$$

Plugging this into the formula of j_y

$$j_y = [-\frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} f_n(\mathbf{k})\Omega_n(\mathbf{k})]E_x$$

The conductivity is

$$\sigma_{xy} = -\frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} f_n(\mathbf{k})\Omega_n(k_x, k_y)$$

In the insulator, all valence bands are occupied, $f_n(\mathbf{k}) = 1$.

$$\sigma_{xy} = -\frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} \Omega_n(k_x, k_y)$$

Define Chern number for the nth band

$$C_n = \frac{1}{2\pi} \int_{BZ} d^2k \, \Omega_n(\mathbf{k})$$

For all the occupied band, the total Chern number is

$$C = \sum_n C_n$$

Plugging in C into σ_{xy}

$$\sigma_{xy} = -\frac{e^2}{\hbar} \sum_n (2\pi C_n)\frac{1}{(2\pi)^2} = -\frac{e^2}{2\pi\hbar} \sum_n C_n = -\frac{e^2}{2\pi\hbar}C = -\frac{e^2}{h}C$$

4.4 The Chern number is an integer

The Brillouin zone (BZ) is a torus T^2, which has no boundary. To apply Stokes' theorem, we divide it into two overlapping regions where the Bloch wavefunctions $|u_{n\mathbf{k}}\rangle$ can be defined with smooth, single-valued gauges.

- Let R_I be the region $0 \leq k_y \leq \pi$.

- Let R_{II} be the region $\pi \leq k_y \leq 2\pi$.

These regions share the boundaries:

- C_1: the line $k_y = \pi$ (traversed from $k_x = 0$ to 2π).

- C_2: the line $k_y = 0$ and $k_y = 2\pi$, identified as the same line on the torus (traversed from $k_x = 2\pi$ to 0).

We choose smooth gauges for the wavefunctions in each region:

- In R_I: $|u_{n\mathbf{k}}^I\rangle$ with Berry connection $\mathbf{A}_n^I(\mathbf{k}) = i\langle u_{n\mathbf{k}}^I|\nabla_{\mathbf{k}} u_{n\mathbf{k}}^I\rangle$.

- In R_{II}: $|u_{n\mathbf{k}}^{II}\rangle$ with Berry connection $\mathbf{A}_n^{II}(\mathbf{k})$.

On the boundaries C_1 and C_2, the wavefunctions in different gauges are related by a $U(1)$ gauge transformation:

$$|u_{n\mathbf{k}}^{II}\rangle = e^{i\chi_1(\mathbf{k})}|u_{n\mathbf{k}}^{I}\rangle \quad \text{for } \mathbf{k} \in C_1$$

$$|u_{n\mathbf{k}}^{II}\rangle = e^{i\chi_2(\mathbf{k})}|u_{n\mathbf{k}}^{I}\rangle \quad \text{for } \mathbf{k} \in C_2$$

Under this transformation, the Berry connections are related by:

$$\mathbf{A}_n^{II}(\mathbf{k}) = \mathbf{A}_n^{I}(\mathbf{k}) - \nabla_{\mathbf{k}}\chi_{1,2}(\mathbf{k})$$

We express the Chern number as an integral of the Berry curvature $\Omega_n = (\nabla_{\mathbf{k}} \times \mathbf{A}_n)_z$. Using Stokes' theorem on each region:

$$C_n = \frac{1}{2\pi} \iint_{R_I} \Omega_n \, d^2k + \frac{1}{2\pi} \iint_{R_{II}} \Omega_n \, d^2k = \frac{1}{2\pi} \oint_{\partial R_I} \mathbf{A}_n^{I} \cdot d\mathbf{k} + \frac{1}{2\pi} \oint_{\partial R_{II}} \mathbf{A}_n^{II} \cdot d\mathbf{k}$$

The boundaries are traversed as follows:

- ∂R_I: along C_1 in the $+\hat{k}_x$ direction, then C_2 in the $-\hat{k}_x$ direction.

- ∂R_{II}: along C_1 in the $-\hat{k}_x$ direction, then C_2 in the $+\hat{k}_x$ direction.

Adding the contributions carefully, the total line integral becomes:

$$C_n = \frac{1}{2\pi} \left[\int_{C_1} (\mathbf{A}_n^{I} - \mathbf{A}_n^{II}) \cdot d\mathbf{k} + \int_{C_2} (\mathbf{A}_n^{II} - \mathbf{A}_n^{I}) \cdot d\mathbf{k} \right]$$

Using the gauge relation $\mathbf{A}_n^{II} = \mathbf{A}_n^{I} - \nabla_{\mathbf{k}}\chi$, we find:

$$\mathbf{A}_n^{I} - \mathbf{A}_n^{II} = \nabla_{\mathbf{k}}\chi_1 \quad \text{on } C_1$$

$$\mathbf{A}_n^{II} - \mathbf{A}_n^{I} = -\nabla_{\mathbf{k}}\chi_2 \quad \text{on } C_2$$

Substituting these in:

$$C_n = \frac{1}{2\pi} \left[\int_{C_1} \nabla_{\mathbf{k}}\chi_1 \cdot d\mathbf{k} - \int_{C_2} \nabla_{\mathbf{k}}\chi_2 \cdot d\mathbf{k} \right]$$

Each integral is now a total derivative along a closed path:

$$\int_{C_1} \nabla_{\mathbf{k}}\chi_1 \cdot d\mathbf{k} = \chi_1(2\pi, \pi) - \chi_1(0, \pi)$$

$$\int_{C_2} \nabla_{\mathbf{k}}\chi_2 \cdot d\mathbf{k} = \chi_2(2\pi, 0) - \chi_2(0, 0)$$

Therefore,

$$C_n = \frac{1}{2\pi} \left[(\chi_1(2\pi, \pi) - \chi_1(0, \pi)) - (\chi_2(2\pi, 0) - \chi_2(0, 0)) \right]$$

The Bloch wavefunction must be single-valued on the torus. This imposes a quantization condition on the gauge transformation functions after a closed loop:

$$\chi_1(2\pi, \pi) - \chi_2(0, 0) = 2\pi m_1, \quad \chi_2(2\pi, 0) - \chi_1(0, \pi) = 2\pi m_2$$

for some integers $m_1, m_2 \in \mathbb{Z}$.

Using these relations, the expression in the bracket simplifies to:

$$[\cdots] = (\chi_1(2\pi, \pi) - \chi_1(0, \pi)) - (\chi_2(2\pi, 0) - \chi_2(0, 0)) = 2\pi m_1 - 2\pi m_2$$

Substituting back, the factors of 2π cancel:

$$C_n = \frac{1}{2\pi}(2\pi m_1 - 2\pi m_2) = m_1 - m_2$$

Since m_1 and m_2 are integers, their difference C_n is also an integer.

$$\boxed{C_n \in \mathbb{Z}}$$

So

$$\sigma_{xy} = -\nu \frac{e^2}{h}$$

Where ν is an integer.

5   Modern Theory of Polarization

5.1   Introduction

The modern theory of polarization, developed by King-Smith, Vanderbilt, and Resta, shows that the **change** in macroscopic polarization $\Delta \mathbf{P}$ of an insulator can be expressed as a geometric phase (Berry phase) of the electronic wavefunctions. This note outlines the derivation in one dimension for clarity.

5.2   Derivation of Current Density

Step 1: General expression for the current operator The current density operator for a single electron is derived from the probability current in quantum mechanics. In one dimension:

$$\hat{j}(x) = -\frac{e}{2m}\left[\hat{p}\delta(\hat{x} - x) + \delta(\hat{x} - x)\hat{p}\right]$$

where $\hat{p} = -i\hbar\partial_x$ is the momentum operator, and e is the magnitude of the electron charge (so the electron's charge is $-e$).

We are interested in the **macroscopic current density** $j(t)$, which is the spatial average of $\hat{j}(x)$. For a state $|\Psi\rangle$, the average current is:

$$j(t) = \frac{1}{L}\int_0^L dx \, \langle\Psi|\hat{j}(x)|\Psi\rangle$$

Step 2: Current for a single Bloch state Consider first a single Bloch state $|\psi_{nk}(t)\rangle$. Its contribution to the current density is:

$$j_{nk}(t) = \frac{1}{L}\int_0^L dx \, \langle\psi_{nk}(t)|\hat{j}(x)|\psi_{nk}(t)\rangle$$

After substituting the Bloch form and carrying out the integral (details omitted), one obtains the well-known result:

$$j_{nk}(t) = -\frac{e}{\hbar}\frac{\partial E_{nk}(t)}{\partial k}$$

This is the **group velocity** contribution. However, this formula assumes the state is a strict eigenstate of the instantaneous Hamiltonian. In an adiabatic process, the actual time-evolving state is **not** exactly the instantaneous eigenstate; it acquires an additional phase and possible corrections.

Step 3: Adiabatic time evolution and first-order correction Under adiabatic evolution, the true time-dependent state $|\Psi_{nk}(t)\rangle$ that starts in $|\psi_{nk}(0)\rangle$ at $t=0$ is given, to first order in the adiabatic parameter, by:

$$|\Psi_{nk}(t)\rangle \approx e^{i\gamma_{nk}(t)}e^{-\frac{i}{\hbar}\int_0^t E_{nk}(t')dt'}\left[|\psi_{nk}(t)\rangle + i\hbar\sum_{m\neq n}\frac{|\psi_{mk}(t)\rangle\langle\psi_{mk}(t)|\partial_t\psi_{nk}(t)\rangle}{E_{nk}(t) - E_{mk}(t)}\right]$$

where $\gamma_{nk}(t)$ is the **Berry phase**:

$$\gamma_{nk}(t) = i\int_0^t dt'\,\langle\psi_{nk}(t')|\partial_{t'}\psi_{nk}(t')\rangle$$

The term proportional to $\sum_{m\neq n}$ is the **first-order adiabatic correction** due to mixing with other bands.

5.2.1 Step 4: Current to first order in adiabaticity

We now compute the current for the true adiabatically evolved state $|\Psi_{nk}(t)\rangle$, keeping terms up to first order in the time derivative.

The expectation value of the current operator is:

$$j_{nk}^{\text{true}}(t) = \frac{1}{L}\int_0^L dx\,\langle\Psi_{nk}(t)|\hat{j}(x)|\Psi_{nk}(t)\rangle$$

Substituting the expanded form of $|\Psi_{nk}(t)\rangle$ and keeping terms linear in ∂_t, we find (after substantial algebra) two contributions:

1. **Zeroth-order term**: The group velocity term $-\frac{e}{\hbar}\partial_k E_{nk}(t)$. This is the same as if the state were an exact eigenstate.

2. **First-order correction**: Comes from the interband mixing. This correction is essential for capturing the full adiabatic current.

Step 5: The final compact form Remarkably, the sum of the zeroth-order and first-order corrections can be combined into a single, elegant expression involving only the periodic part u_{nk} of the Bloch function:

$$\boxed{j_n(t) = \frac{e}{2\pi}\int_{-\pi/a}^{\pi/a}\frac{dk}{i}\,\langle u_{nk}(t)|\partial_t u_{nk}(t)\rangle}$$

Here $j_n(t)$ is the current density contribution from band n, and we have summed over all k-states in the Brillouin zone (assuming the band is fully occupied, as in an insulator). The total current density is the sum over all occupied bands:

$$j(t) = \sum_n^{\text{occupied}} j_n(t)$$

Step 6: Verification and interpretation To check this formula, consider the case where the time dependence comes solely from a uniform electric field E. Then, via the acceleration theorem $\hbar \dot{k} = -eE$, we have $\partial_t = \dot{k}\partial_k = -\frac{eE}{\hbar}\partial_k$. Substituting:

$$j_n = \frac{e}{2\pi} \int dk \left(-\frac{eE}{\hbar}\right) \frac{1}{i} \langle u_{nk}|\partial_k u_{nk}\rangle = -\frac{e^2 E}{2\pi\hbar} \int dk \, A_n(k)$$

where $A_n(k) = i\langle u_{nk}|\partial_k u_{nk}\rangle$ is the Berry connection. For a full cycle, this leads to the polarization change $\Delta P_n = \frac{e}{2\pi}\Delta\phi_n$, where $\phi_n = \oint A_n(k)dk$ is the Zak phase, consistent with the modern theory of polarization.

Key Points

- The derivation assumes **adiabatic evolution**: the Hamiltonian changes slowly compared to the band gap.

- The formula $j_n(t) = \frac{e}{2\pi} \int \frac{dk}{i} \langle u_{nk}|\partial_t u_{nk}\rangle$ captures both the **intraband** (group velocity) and **interband** (polarization) contributions to the current in a unified way.

- This current is a **transient** polarization current, not a steady-state transport current. It exists only while the Hamiltonian is changing.

- The expression is **gauge invariant** (modulo integer multiples of e) because it involves the time derivative of a Berry phase.

5.3 Derivation of Polarization

5.3.1 Setup: Adiabatic Evolution

Consider a one-dimensional insulator of length $L = Na$, with lattice constant a and N unit cells (periodic boundary conditions). The Hamiltonian depends adiabatically on a parameter $\lambda(t)$ (e.g., atomic positions, external field), with t parameterizing time or an adiabatic process.

The goal is to compute the **change in polarization** ΔP between an initial state at $t = 0$ and a final state at $t = T$:

$$\Delta P = P(T) - P(0)$$

5.3.2 Step-by-Step Derivation

Step 1: Polarization Change from Integrated Current The fundamental relation between polarization and current density is:

$$\frac{dP(t)}{dt} = j(t)$$

where $j(t)$ is the macroscopic current density. Integrating over the adiabatic process:

$$\Delta P = \int_0^T j(t)\, dt$$

Thus, the problem reduces to computing the adiabatic current $j(t)$.

Step 2: Current Density in the Independent Electron Picture Consider a one-dimensional crystal with lattice constant a and length $L = Na$ (periodic boundary conditions). The time-dependent Hamiltonian $H(t)$ depends adiabatically on a parameter $\lambda(t)$, which could represent atomic displacements or a slowly varying external field.

We work within the **independent electron approximation** and the **adiabatic approximation**: the system remains in its instantaneous eigenstates as $H(t)$ changes.

Let $|\psi_{nk}(t)\rangle$ be the Bloch eigenstate of $H(t)$ with band index n and crystal momentum k:

$$H(t)|\psi_{nk}(t)\rangle = E_{nk}(t)|\psi_{nk}(t)\rangle$$

The Bloch wavefunction has the form:

$$\psi_{nk}(x,t) = e^{ikx} u_{nk}(x,t)$$

where $u_{nk}(x,t)$ is the periodic part, satisfying $u_{nk}(x+a,t) = u_{nk}(x,t)$. For a system of independent electrons, the total current is the sum over all occupied Bloch states. For a single occupied band n (the multi-band case is a simple summation), the contribution is:

$$j_n(t) = \frac{e}{2\pi} \int_{-\pi/a}^{\pi/a} \frac{dk}{i} \langle u_{nk}(t)|\partial_t u_{nk}(t)\rangle$$

where $|u_{nk}(t)\rangle$ is the periodic part of the Bloch wavefunction for band n and crystal momentum k, evolving under the time-dependent Hamiltonian $H(\lambda(t))$. The factor e is the electron charge (with sign convention such that $-e$ is the electron's charge).

Step 3: Express Current in Terms of Berry Connection Define the **Berry connection** in parameter space. In addition to the usual k-space Berry connection $A_n^{(k)} = i\langle u_{nk}|\partial_k u_{nk}\rangle$, we have a "time" or "$\lambda$" connection:

$$A_n^{(t)}(k,t) = i\langle u_{nk}(t)|\partial_t u_{nk}(t)\rangle$$

Then the current becomes:

$$j_n(t) = \frac{e}{2\pi} \int_{-\pi/a}^{\pi/a} dk \, [-i\langle u_{nk}(t)|\partial_t u_{nk}(t)\rangle] = \frac{e}{2\pi} \int_{-\pi/a}^{\pi/a} dk \, A_n^{(t)}(k,t)$$

Step 4: Integrate Current to Get Polarization Change Integrate the current over time to get the total polarization change contributed by band n:

$$\Delta P_n = \int_0^T j_n(t)\, dt = \frac{e}{2\pi} \int_0^T dt \int_{-\pi/a}^{\pi/a} dk \, A_n^{(t)}(k,t)$$

Interchange the order of integration (Fubini's theorem):

$$\Delta P_n = \frac{e}{2\pi} \int_{-\pi/a}^{\pi/a} dk \left[\int_0^T dt \, A_n^{(t)}(k,t) \right]$$

The term in brackets, $\int_C A_n^{(t)} dt$, is a line integral of the Berry connection along the time/λ direction for a fixed k.

Step 5: Link to Berry Phase via 2D Parameter Space Consider the two-dimensional parameter space (k, t) (or (k, λ)). Define a generalized Berry connection one-form:

$$\mathcal{A}_n = A_n^{(k)} dk + A_n^{(t)} dt$$

Now consider a rectangular loop $\mathcal{C}$ in this parameter space:

- Path 1: At $t = 0$, k goes from $-\pi/a$ to π/a.

- Path 2: At $k = \pi/a$, t goes from 0 to T.

- Path 3: At $t = T$, k goes from π/a to $-\pi/a$.

- Path 4: At $k = -\pi/a$, t goes from T to 0.

The Berry phase γ_n for this loop is:

$$\gamma_n = \oint_{\mathcal{C}} \mathcal{A}_n$$

By Stokes' theorem, this equals the integral of the Berry curvature $\Omega_n^{(k,t)} = \partial_k A_n^{(t)} - \partial_t A_n^{(k)}$ over the enclosed surface.

Evaluating $\oint_{\mathcal{C}} \mathcal{A}_n$ explicitly along the four paths, one finds that:

$$\gamma_n = [\phi_n(T) - \phi_n(0)] + (\text{terms that cancel or are zero due to periodicity in } k)$$

where $\phi_n(t)$ is the **Zak phase** (the k-space Berry phase across the Brillouin zone) at a fixed time t:

$$\phi_n(t) = \int_{-\pi/a}^{\pi/a} dk\, A_n^{(k)}(k, t) = i \int_{-\pi/a}^{\pi/a} dk\, \langle u_{nk}(t) | \partial_k u_{nk}(t) \rangle$$

Crucially, the time-integral term $\int dk \int dt\, A_n^{(t)}$ appears as part of γ_n.

Step 6: Final Result: Polarization Change as Berry Phase Difference After carefully tracking the contributions from all four paths of the loop and using the periodicity of the wavefunction in k-space ($|u_{n,k+2\pi/a}\rangle = |u_{nk}\rangle$), one arrives at the central result:

$$\boxed{\Delta P_n = \frac{e}{2\pi} [\phi_n(T) - \phi_n(0)]}$$

For a multi-band insulator, we sum over all occupied bands:

$$\boxed{\Delta \mathbf{P} = \frac{e}{2\pi} \sum_n^{\text{occ}} \Delta \phi_n\, \hat{\mathbf{G}}}$$

where in higher dimensions, ϕ_n becomes a vectorial Zak phase integrated over the Brillouin zone, and $\hat{\mathbf{G}}$ is a reciprocal lattice vector direction. In 1D, it simplifies to the scalar form above.

5.3.3 Interpretation

- **Not absolute polarization**: The formula gives only the **change** ΔP, not the absolute value of P. This resolves the long-standing ambiguity in defining polarization for a periodic crystal.

- **Geometric origin**: The change is expressed as the difference in a **geometric phase** (Berry/Zak phase) of the occupied Bloch states. It is a bulk property, independent of surface details.

- **Quantization**: In a cyclic adiabatic process where the Hamiltonian returns to itself, $\Delta\phi_n$ must be an integer multiple of 2π, so ΔP is quantized in units of e (times a lattice vector). This manifests in phenomena like charge pumping.