Berry phase, Chern number

10/11/2016
Literature:

Quantal phase factors accompanying adiabatic changes

By M. V. Berry, F.R.S.

H. H. Wills Physics Laboratory, University of Bristol,
Tyndall Avenue, Bristol BS8 1TL, U.K.

(Received 13 June 1983)
Professor Sir Micheal Victor Berry

Melville Wills Professor of Physics, University of Bristol

https://michaelberryphysics.wordpress.com/
The 2000 Ig Nobel Prize Winners

The 2000 Ig Nobel Prizes were awarded on Thursday night, October 5th, 2000 at the 10th First Annual Ig Nobel Prize Ceremony at Harvard’s Sanders Theatre. The ceremony was webcast live. You can watch the video on our YouTube Channel.

PHYSICS: Andre Geim of the University of Nijmegen (the Netherlands) and Sir Michael Berry of Bristol University (UK), for using magnets to levitate a frog. [REFERENCE: "Of Flying Frogs and Levitrons" by M.V. Berry and A.K. Geim, European Journal of Physics, v. 18, 1997, p. 307-13.]

REFERENCE: VIDEO

NOTE: Ten years later, in 2010, Andre Geim won a Nobel Prize in physics (for research on another subject).

A little frog (alive !) and a water ball levitate inside a Ø32mm vertical bore of a Bitter solenoid in a magnetic field of about 16 Tesla at the Nijmegen High Field Magnet Laboratory.

http://www.ru.nl/hfml/research/levitation/diamagnetic/
Basic definitions: Berry connection

Consider the Schrödinger equation

\[ H(R)|\psi_n(R)\rangle = E_n(R)|\psi_n(R)\rangle \]
Basic definitions: Berry connection

Consider the Schrödinger equation

\[ H(R)|\psi_n(R)\rangle = E_n(R)|\psi_n(R)\rangle \]

- \( R\): set of parameters, e.g., \( \nu \) and \( \omega \) from the SSH model
- non-degenerate state \( |\psi_n(R)\rangle \) for any value of \( R \)
Basic definitions: Berry connection

Consider the Schrödinger equation

$$H(R)|\psi_n(R)\rangle = E_n(R)|\psi_n(R)\rangle$$

- $R$: set of parameters, e.g., $v$ and $w$ from the SSH model
- non-degenerate state $|\psi_n(R)\rangle$ for any value of $R$

The phase difference between two states that are “close” in the parameter space:

$$e^{-i\Delta \gamma_n} = \frac{\langle \psi_n(R) | \psi_n(R + dR) \rangle}{|\langle \psi_n(R) | \psi_n(R + dR) \rangle|}$$
Consider the Schrödinger equation

$$H(R)|\psi_n(R)\rangle = E_n(R)|\psi_n(R)\rangle$$

- $R$: set of parameters, e.g., $v$ and $w$ from the SSH model
- non-degenerate state $|\psi_n(R)\rangle$ for any value of $R$

The phase difference between two states that are “close” in the parameter space:

$$e^{-i\Delta\gamma_n} = \frac{\langle \psi_n(R)|\psi_n(R + dR)\rangle}{|\langle \psi_n(R)|\psi_n(R + dR)\rangle|}$$

In leading order

$$-i\Delta\gamma_n \approx \langle \psi_n(R)|\nabla_R \psi_n(R)\rangle \cdot dR$$
Basic definitions: Berry connection

This equation defines the *Berry connection* (vector field):

\[ A_n = i\langle \psi_n(R) | \nabla_R \psi_n(R) \rangle = -Im[\langle \psi_n(R) | \nabla_R \psi_n(R) \rangle] \]

(here we used \( \nabla_R \langle \psi_n(R) | \psi_n(R) \rangle = 0 \)).

\[ \Delta \gamma_n = A_n \cdot dR \]  \hspace{1cm} (1)
This equation defines the *Berry connection* (vector field):

\[ A_n = i \langle \psi_n(R) | \nabla_R \psi_n(R) \rangle = -\text{Im} \left[ \langle \psi_n(R) | \nabla_R \psi_n(R) \rangle \right] \]

(here we used \( \nabla_R \langle \psi_n(R) | \psi_n(R) \rangle = 0 \)).

\[ \Delta \gamma_n = A_n \cdot dR \quad (1) \]

Note, that the Berry connection is **not gauge invariant**: 

\[ |\psi_n(R)\rangle \rightarrow e^{i\alpha(R)} |\psi_n(R)\rangle : \quad A_n(R) \rightarrow A_n(R) + \nabla_R \alpha(R). \]
Consider a **closed** directed curve $C$ in parameter space $\mathbb{R}$. The *Berry phase* along $C$ is defined in the following way:

$$\gamma_n(C) = \oint_C d\gamma_n = \oint_C A_n(R) dR$$
Consider a **closed** directed curve $C$ in parameter space $\mathbf{R}$. The *Berry phase* along $C$ is defined in the following way:

$$
\gamma_n(C) = \oint_C d\gamma_n = \oint_C A_n(\mathbf{R}) d\mathbf{R}
$$

**Important:** The Berry phase is *gauge invariant*: the integral of $\nabla_\mathbf{R} \alpha(\mathbf{R})$ depends only on the start and end points of $C \rightarrow$ for a closed curve it is zero.
Consider a **closed** directed curve $C$ in parameter space $\mathbb{R}$. The *Berry phase* along $C$ is defined in the following way:

$$\gamma_n(C) = \oint_C d\gamma_n = \oint_C A_n(R) dR$$

**Important:** The Berry phase is *gauge invariant*: the integral of $\nabla_R \alpha(R)$ depends only on the start and end points of $C \rightarrow$ for a closed curve it is zero.

Berry phase is gauge invariant $\rightarrow$ potentially observable. An observable which cannot be cast as the expectation values of any operator!
Berry curvature

In analogy to electrodynamics → express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity Berry curvature.
Berry curvature

In analogy to electrodynamics → express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity Berry curvature.

Consider a simply connected region $\mathcal{F}$ in a two-dimensional parameter space, with the oriented boundary curve of this surface denoted by $\partial \mathcal{F}$, and calculate the continuum Berry phase corresponding to the $\partial \mathcal{F}$. 
Berry curvature

In two dimensions: let $\mathbf{R} = (x, y)$. We are looking for a function $B(x, y)$ such that

$$\oint_{\partial \mathcal{F}} \mathbf{A}_n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} B_n(x, y) dx dy$$

Here $B_n(x, y)$ is the **Berry curvature**.
Berry curvature

In two dimensions: let $\mathbf{R} = (x, y)$. We are looking for a function $B(x, y)$ such that

$$\oint_{\partial \mathcal{F}} A_n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} B_n(x, y) dxdy$$

Here $B_n(x, y)$ is the *Berry curvature*.

In case $\lvert \Psi(\mathbf{R}) \rangle$ is a smooth function of $\mathbf{R}$ in $\mathcal{F}$ then we can use the *Stokes theorem*:

$$\oint_{\partial \mathcal{F}} A_n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} (\partial_x A_y^{(n)} - \partial_y A_x^{(n)}) dxdy = \int_{\mathcal{F}} B_n(x, y) dxdy$$
Berry curvature

In two dimensions: let \( \mathbf{R} = (x, y) \). We are looking for a function \( B(x, y) \) such that

\[
\oint_{\partial \mathcal{F}} \mathbf{A}_n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} B_n(x, y) dxdy
\]

Here \( B_n(x, y) \) is the Berry curvature.

In case \( |\psi(\mathbf{R})\rangle \) is a smooth function of \( \mathbf{R} \) in \( \mathcal{F} \) then we can use the Stokes theorem:

\[
\oint_{\partial \mathcal{F}} \mathbf{A}_n(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} (\partial_x A_y^{(n)} - \partial_y A_x^{(n)}) dxdy = \int_{\mathcal{F}} B_n(x, y) dxdy
\]

Generalization to higher dimensions is also possible.
Taking the explicit form of $A_n$

\[
B_{\mu\nu}^{(n)}(R) = \frac{\partial}{\partial R^\mu} A_\nu^{(n)}(R) - \frac{\partial}{\partial R^\nu} A_\mu^{(n)}(R)
= -2\text{Im} \left\langle \frac{\partial}{\partial R^\mu} \psi_n(R) \left| \frac{\partial}{\partial R^\nu} \psi_n(R) \right. \right\rangle
\]
Berry curvature

Taking the explicit form of $A_n$

$$B_{\mu\nu}^{(n)}(R) = \frac{\partial}{\partial R^\mu} A_{\nu}^{(n)}(R) - \frac{\partial}{\partial R^\nu} A_{\mu}^{(n)}(R)$$

$$= -2\text{Im} \left\langle \left. \frac{\partial}{\partial R^\mu} \psi_n(R) \right| \left. \frac{\partial}{\partial R^\nu} \psi_n(R) \right\rangle$$

- The curvature is gauge invariant; hence in principle it is physically observable.
Berry curvature

\[
B_{\mu\nu}(R) = \frac{\partial}{\partial R^\mu} A^{(n)}_\nu(R) - \frac{\partial}{\partial R^\nu} A^{(n)}_\mu(R) = -2\text{Im} \left\langle \frac{\partial}{\partial R^\mu} \psi_n(R) \left| \frac{\partial}{\partial R^\nu} \psi_n(R) \right\rangle \right.
\]

- If the wavefunction can be taken as real, the curvature \( B^{(n)} \) vanishes. Non-trivial Berry’s phase may only occur if the \( R \)-domain is not simply connected.
- If the wavefunction is unavoidably complex, then in general the curvature does not vanish. A non-trivial Berry’s phase may exist even in a simply connected domain of \( R \).
Useful formulas for the Berry curvature

Berry phase corresponding to an eigenstate $|n(R)\rangle$ of some Hamiltonian:

$$B_j^{(n)} = -\text{Im} [\varepsilon_{jkl} \partial_k \langle n | \partial_l n \rangle] = -\text{Im} [\varepsilon_{jkl} \langle \partial_k n | \partial_l n \rangle]$$

summation over repeated indeces, and $\partial_l = \partial_{R_l}$. 
Useful formulas for the Berry curvature

Berry phase corresponding to an eigenstate $|n(R)\rangle$ of some Hamiltonian:

$$B_j^{(n)} = -\text{Im}[\varepsilon_{jkl} \partial_k \langle n| \partial_l n \rangle] = -\text{Im}[\varepsilon_{jkl} \langle \partial_k n| \partial_l n \rangle]$$

summation over repeated indeces, and $\partial_l = \partial_{R_l}$.

Inserting $\mathbb{1} = \sum_{n'} |n'\rangle\langle n'|$:

$$B_n = -\text{Im} \left[ \sum_{n' \neq n} \langle \nabla_R n| n' \rangle \times \langle n'| \nabla_R n \rangle \right]$$
Useful formulas for the Berry curvature

Berry phase corresponding to an eigenstate $|n(R)\rangle$ of some Hamiltonian:

$$B_j^{(n)} = -Im[\varepsilon_{jkl} \partial_k \langle n | \partial_l n \rangle] = -Im[\varepsilon_{jkl} \langle \partial_k n | \partial_l n \rangle]$$

summation over repeated indeces, and $\partial_l = \partial_{R_l}$.

Inserting $1 = \sum_{n'} |n'\rangle\langle n'|$:

$$B_n = -Im \left[ \sum_{n' \neq n} \langle \nabla_R n | n' \rangle \times \langle n' | \nabla_R n \rangle \right]$$

Calculate $\langle n'|\nabla_R n \rangle$ (both the Hamiltonian $\hat{H}$ and the eigenstates $|n\rangle$ depend on $R$!)

$$\hat{H}|n\rangle = E_n|n\rangle$$

$$\nabla_R \hat{H}|n\rangle + \hat{H}|\nabla_R n\rangle = (\nabla_R E_n)|n\rangle + E_n|\nabla_R n\rangle$$

$$\langle n'|\nabla_R \hat{H}|n\rangle + \langle n'|\hat{H}|\nabla_R n\rangle = E_n\langle n'|\nabla_R n\rangle$$
Useful formulas for the Berry curvature

Since \( \langle n' | \hat{H} = E_{n'} \langle n' | \rangle \)

\[
\langle n' | \nabla_R \hat{H} | n \rangle + E_{n'} \langle n' | \nabla_R n \rangle = E_n \langle n' | \nabla_R n \rangle \\
\langle n' | \nabla_R \hat{H} | n \rangle = (E_n - E_{n'}) \langle n' | \nabla_R n \rangle
\]
Useful formulas for the Berry curvature

Since $\langle n'|\hat{H} = E_{n'} \langle n'|$

$$\langle n'|\nabla_R \hat{H}|n\rangle + E_{n'} \langle n'|\nabla_R n \rangle = E_n \langle n'|\nabla_R n \rangle$$

$$\langle n'|\nabla_R \hat{H}|n\rangle = (E_n - E_{n'}) \langle n'|\nabla_R n \rangle$$

Substituting this into

$$B_n = -Im \left[ \sum_{n' \neq n} \langle n'|\nabla_R n \rangle \times \langle n'|\nabla_R n \rangle \right]$$

one finds:

$$B_n = -Im \left[ \sum_{n' \neq n} \frac{\langle n|\nabla_R H|n'\rangle \times \langle n'|\nabla_R H|n\rangle}{(E_n - E_{n'})^2} \right]$$

Gauge invariant!
Berry curvature

\[ B_n = -\text{Im} \left[ \sum_{n' \neq n} \frac{\langle n | \nabla_R H | n' \rangle \times \langle n' | \nabla_R H | n \rangle}{(E_n - E_{n'})^2} \right] \]

Remarks

i) The sum of the Berry curvatures of all eigenstates of a Hamiltonian is zero

ii) Berry curvature is often the largest at near-degeneracies of the spectrum

iii) The Berry curvature is singular for such \( R_0 \) values, where \( |n(R_0)\rangle \) is degenerate with one of \( |n'(R_0)\rangle \). However, if the integration curve \( \partial F \) encircles the degeneracy point, the Berry phase can be finite.
Berry phase: the discrete version

Previously, we assumed that the phase of $|\Psi_n(R)\rangle$ varies continuously as a function of $R$.
In practical applications this is usually not the case.
Berry phase: the discrete version

Previously, we assumed that the phase of $|\Psi_n(R)\rangle$ varies continuously as a function of $R$.

In practical applications this is usually not the case.

Phase difference between two different $R$ points:

\[
e^{-i\phi_{12}^{(n)}} = \frac{\langle \Psi_n(R_1)|\Psi_n(R_2)\rangle}{|\langle \Psi_n(R_1)|\Psi_n(R_2)\rangle|}
\]

\[
\phi_{12}^{(n)} = -\text{Im} \log [\langle \Psi_n(R_1)|\Psi_n(R_2)\rangle]
\]
Berry phase: the discrete version

Previously, we assumed that the phase of $|\Psi_n(R)\rangle$ varies continuously as a function of $R$.
In practical applications this is usually not the case.

Phase difference between two different $R$ points:

$$e^{-i\phi_{12}^{(n)}} = \frac{\langle \Psi_n(R_1) | \Psi_n(R_2) \rangle}{|\langle \Psi_n(R_1) | \Psi_n(R_2) \rangle|}$$

$$\phi_{12}^{(n)} = -\text{Im} \log [\langle \Psi_n(R_1) | \Psi_n(R_2) \rangle]$$

Consider the path in parameter space:
The total phase difference along a closed path which joins the points $\mathbf{R}_i$ in a given order:

$$\gamma = \phi_{12} + \phi_{23} + \phi_{31}$$

$$= -\text{Im} \log \left[ \langle \psi_n(\mathbf{R}_1) | \psi_n(\mathbf{R}_2) \rangle \langle \psi_n(\mathbf{R}_2) | \psi_n(\mathbf{R}_3) \rangle \langle \psi_n(\mathbf{R}_3) | \psi_n(\mathbf{R}_1) \rangle \right]$$

The gauge-arbitrary phases cancel in pairs $\rightarrow$ overall phase $\gamma$ is a gauge-invariant quantity.
Berry phase: the discrete version

The total phase difference along a closed path which joins the points \( \mathbf{R}_i \) in a given order:

\[
\gamma = \phi_{12} + \phi_{23} + \phi_{31}
\]

\[
= -\text{Im} \log \left[ \langle \Psi_n(\mathbf{R}_1) | \Psi_n(\mathbf{R}_2) \rangle \langle \Psi_n(\mathbf{R}_2) | \Psi_n(\mathbf{R}_3) \rangle \langle \Psi_n(\mathbf{R}_3) | \Psi_n(\mathbf{R}_1) \rangle \right]
\]

The gauge-arbitrary phases cancel in pairs → overall phase \( \gamma \) is a gauge-invariant quantity.

In general:

\[
\gamma = \sum_{s=1}^{M} \phi_{s,s+1} = -\text{Im} \log \prod_{s=1}^{M} \langle \Psi_n(\mathbf{R}_s) | \Psi_n(\mathbf{R}_{s+1}) \rangle
\]
Example: two level system

Consider the following Hamiltonian:

\[ H_R = R_x \sigma_x + R_y \sigma_y + R_z \sigma_z = \mathbf{R} \cdot \sigma \]

where \( \mathbf{d} = (R_x, R_y, R_z) = \mathbb{R}^3 \setminus \{0\} \), to avoid degeneracy

Eigenvalues, eigenstates:

\[ H(\mathbf{R}) |\pm\rangle = \pm |\mathbf{R}| |\pm\rangle \]
Example: two level system

Consider the following Hamiltonian:

$$H_{R} = R_x \sigma_x + R_y \sigma_y + R_z \sigma_z = \mathbf{R} \cdot \sigma$$

where \( \mathbf{d} = (R_x, R_y, R_z) = \mathbb{R}^3 \setminus \{0\} \), to avoid degeneracy

Eigenvalues, eigenstates:

$$H(\mathbf{R})|\pm\rangle = \pm|\mathbf{R}|\pm\rangle$$

The \(|+\rangle\) eigenstate can be represented in the following form:

$$|+\rangle = e^{i\alpha(\theta, \phi)} \begin{pmatrix} e^{-i\phi/2} \cos(\theta/2) \\ e^{i\phi/2} \sin(\theta/2) \end{pmatrix}$$

where

$$\cos \theta = \frac{R_z}{|\mathbf{R}|}, \quad e^{i\phi} = \frac{R_x + iR_y}{\sqrt{R_x^2 + R_y^2}}$$
Example: two level system

Figure: The representation of the parameter space on a Bloch sphere
Example: two level system

The choice of phase $\alpha(\theta, \phi)$ corresponds to fixing a gauge. Several choices are possible:
The choice of phase $\alpha(\theta, \phi)$ corresponds to fixing a gauge. Several choices are possible:

1) $\alpha(\theta, \phi) = 0$ for all $\theta, \phi$.

$$|+\rangle_0 = \begin{pmatrix} e^{-i\phi/2} \cos(\theta/2) \\ e^{i\phi/2} \sin(\theta/2) \end{pmatrix}$$

We expect that $\phi = 0$ and $\phi = 2\pi$ should correspond to the same state in the Hilbert space state. However,

$$| + (\theta, \phi = 0) \rangle = -| + (\theta, \phi = 2\pi) \rangle.$$
Example: two level system

2) $\alpha(\theta, \phi) = \phi/2$. Then we have

$$|+\rangle_s = \left( \begin{array}{c} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{array} \right)$$
Example: two level system

2) \( \alpha(\theta, \phi) = \phi/2 \). Then we have

\[
|+\rangle_S = \begin{pmatrix}
\cos(\theta/2) \\
e^{i\phi}\sin(\theta/2)
\end{pmatrix}
\]

There are two interesting points: the north \( (\theta = 0) \) and the south \( (\theta = \pi) \) points.
For \( \theta = 0 \) \( |+\rangle_S = (1, 0) \) but for \( \theta = \pi \) \( |+\rangle_S = (0, e^{i\phi}) \), i.e., the value of the wave function depends on the direction one approaches the south pole.
Example: two level system

2) $\alpha(\theta, \phi) = \phi/2$. Then we have

$$|+\rangle_S = \left( \begin{array}{c} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{array} \right)$$

There are two interesting points: the north ($\theta = 0$) and the south ($\theta = \pi$) points.

For $\theta = 0$ $|+\rangle_S = (1, 0)$ but for $\theta = \pi$ $|+\rangle_S = (0, e^{i\phi})$, i.e., the value of the wave function depends on the direction one approaches the south pole.

A couple of other choices are possible. It turns out, there is no such gauge where the wavefunction is well behaved everywhere on the Bloch sphere.
Example: Berry phase for a two-level system

Let us take a closed curve $\mathcal{C}$ in the parameter space $\mathbb{R}^3 \setminus \{0\}$ and calculate the Berry phase for the state $|\pm\rangle$.

$$\gamma_{\pm} = \oint_{\mathcal{C}} A(R) dR, \quad A_{\pm}(R) = i\langle \pm | \nabla_R | \pm \rangle$$

The calculation is easier if one uses the Berry curvature.
Calculating the Berry phase for a two level system

\[ B^{\pm}(R) = -\text{Im} \frac{\langle \pm | \nabla_R \hat{H} | \mp \rangle \times \langle \mp | \nabla_R \hat{H} | \pm \rangle}{4|R|^2}, \quad \nabla_R \hat{H} = \sigma \]

This can be evaluated in any of the gauges.

\[ B^{\pm}(R) = \mp \frac{1}{2} \frac{R}{|R|^3} \]

This is the field of a pointlike monopole source in the origin.
Calculating the Berry phase for a two level system

The Berry phase of the closed loop $C$ in parameter space is the flux of the monopole field through a surface $\mathcal{F}$ whose boundary is $C$. 

\[ d_y \quad d_x \]
\[ \uparrow \quad \uparrow \]
\[ d_z \]
Calculating the Berry phase for a two level system

The Berry phase of the closed loop $C$ in parameter space is the flux of the monopole field through a surface $\mathcal{F}$ whose boundary is $C$. This is half of the solid angle subtended by the curve:

$$\gamma_- = \frac{1}{2} \Omega_C, \quad \gamma_+ = -\gamma_-$$
The Berry phase can be interpreted as a phase acquired by the wavefunction as the parameters appearing in the Hamiltonian are changing slowly in time.

\[ \hat{H}(R)|n(R)\rangle = E_n(R)|n(R)\rangle \]

where we have fixed the gauge of \( |n(R)\rangle \).
The Berry phase can be interpreted as a phase acquired by the wavefunction as the parameters appearing in the Hamiltonian are changing slowly in time.

\[ \hat{H}(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle \]

where we have fixed the gauge of \( |n(\mathbf{R})\rangle \).

Assume that the parameters of the Hamiltonian at \( t = 0 \) are \( \mathbf{R} = \mathbf{R}_0 \) and there are no degeneracies in the spectrum. The system is in an eigenstate \( |n(\mathbf{R}_0)\rangle \) for \( t = 0 \).

\[ \mathbf{R}(t = 0) = \mathbf{R}_0, \quad |\psi(t = 0)\rangle = |n(\mathbf{R}_0)\rangle \]
The Berry phase can be interpreted as a phase acquired by the wavefunction as the parameters appearing in the Hamiltonian are changing slowly in time.

\[ \hat{H}(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle \]

where we have fixed the gauge of \(|n(\mathbf{R})\rangle\).

Assume that the parameters of the Hamiltonian at \(t = 0\) are \(\mathbf{R} = \mathbf{R}_0\) and there are no degeneracies in the spectrum. The system is in an eigenstate \(|n(\mathbf{R}_0)\rangle\) for \(t = 0\).

\[ \mathbf{R}(t = 0) = \mathbf{R}_0, \quad |\psi(t = 0)\rangle = |n(\mathbf{R}_0)\rangle \]

Now consider that \(\mathbf{R}(t)\) is slowly changed in time and the values of \(\mathbf{R}(t)\) define a continuous curve \(\mathcal{C}\). Also, assume that \(|n(\mathbf{R}(t))\rangle\) is smooth along \(\mathcal{C}\).
Berry phase: physical interpretation

The wavefunction evolves according to the time-dependent Schrödinger equation:

\[
i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\mathbf{R}(t)) |\Psi(t)\rangle
\]
The wavefunction evolves according to the time-dependent Schrödinger equation:

\[ i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(R(t)) |\psi(t)\rangle \]

**Assumption:** starting from the initial state \( |n(R_0)\rangle \) the state \( |n(R(t))\rangle \) remains non-degenerate for all times.
Berry phase: physical interpretation

The wavefunction evolves according to the time-dependent Schrödinger equation:

\[ i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(R(t)) |\Psi(t)\rangle \]

**Assumption:** starting from the initial state \(|n(R_0)\rangle\) the state \(|n(R(t))\rangle\) remains non-degenerate for all times.
If the rate of change of \(R(t)\) along \(C\) slow enough, i.e.,
\[ \ll \frac{(E_n(R) - E_{n\pm 1}(R))}{\hbar} \to \text{the system remains in the eigenstate} \]
\(|n(R(t))\rangle\) (adiabatic approximation).
The wavefunction evolves according to the time-dependent Schrödinger equation:

\[ i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(R(t)) |\Psi(t)\rangle \]

**Assumption:** starting from the initial state \( |n(R_0)\rangle \) the state \( |n(R(t))\rangle \) remains non-degenerate for all times.

If the rate of change of \( R(t) \) along \( C \) slow enough, i.e.,

\[ \ll (E_n(R) - E_{n\pm1}(R))/\hbar \rightarrow \text{the system remains in the eigenstate} \]

\( |n(R(t))\rangle \) (adiabatic approximation).

The parameter vector \( R(t) \) traces out a curve \( C \) in the parameter space.
Berry phase: physical interpretation

Ansatz:

\[ |\Psi(t)\rangle = e^{i\gamma(t)} e^{-i/\hbar} \int_0^t E_n(R(t')) dt' |n(R(t))\rangle \]

Substituting the above Ansatz into the Schrödinger equation, one can show that

\[ \gamma_n(C) = i \int_C \langle n(R) | \nabla_R n(R) \rangle dR \]
Berry phase: physical interpretation

Ansatz:
\[ |\Psi(t)\rangle = e^{i\gamma(t)} e^{-i/\hbar \int_0^t E_n(R(t')) dt'} |n(R(t))\rangle \]

Substituting the above Ansatz into the Schrödinger equation, one can show that
\[ \gamma_n(C) = i \int_C \langle n(R)|\nabla_R n(R)\rangle dR \]

Consider now an *adiabatic and cyclic* change of the Hamiltonian, such that \( R(t = 0) = R(t = T) \). In this case the adiabatic phase reads
\[ \gamma_n(C) = i \oint_C \langle n(R)|\nabla_R n(R)\rangle dR \]

The phase that a state acquires during a cyclic and adiabatic change of the Hamiltonian is equivalent to the Berry phase corresponding to the closed curve representing the Hamiltonian’s path in the parameter space.
Berry phase: physical interpretation

Ansatz:

\[
|\Psi(t)\rangle = e^{i\gamma(t)} e^{-i/\hbar \int_0^t E_n(R(t'))dt'} |n(R(t))\rangle
\]

Substituting the above Ansatz into the Schrödinger equation, one can show that

\[
\gamma_n(C) = i \int_C \langle n(R)|\nabla_R n(R)\rangle dR
\]

Consider now an adiabatic and cyclic change of the Hamiltonian, such that \( R(t = 0) = R(t = T) \). In this case the adiabatic phase reads

\[
\gamma_n(C) = i \oint_C \langle n(R)|\nabla_R n(R)\rangle dR
\]

The phase that a state acquires during a cyclic and adiabatic change of the Hamiltonian is equivalent to the Berry phase corresponding to the closed curve representing the Hamiltonian’s path in the parameter space.
Considering the Berry curvature:

\[
B_n = -\text{Im} \left[ \sum_{n' \neq n} \frac{\langle n | \nabla_R H | n' \rangle \times \langle n' | \nabla_R H | n \rangle}{(E_n - E_{n'})^2} \right]
\]
Considering the Berry curvature:

\[ B_n = -\text{Im} \left[ \sum_{n' \neq n} \frac{\langle n | \nabla_R H | n' \rangle \times \langle n' | \nabla_R H | n \rangle}{(E_n - E_{n'})^2} \right] \]

- Although the system remains in the same state \(|n(R)\rangle\) during the adiabatic evolution, other states of the system \(|n'(R)\rangle\), \(n \neq n'\) nevertheless affect the state \(|n(R)\rangle\).
- This influence is manifested in the Berry curvature, which, in turn, determines the Berry phase picked up by \(|n(R)\rangle\).
Let us now consider Berry phase effects in **crystalline solids**.
Let us now consider Berry phase effects in \textit{crystalline solids}. In the non-interacting limit the Hamiltonian:

\[
\hat{H} = \frac{\hat{p}^2}{2m_e} + V(r)
\]

where \( V(r) = V(r + R_n) \) is periodic, \( R_n \) is a lattice vector.
Let us now consider Berry phase effects in **crystalline solids**. In the non-interacting limit the Hamiltonian:

\[
\hat{H} = \frac{\hat{p}^2}{2m_e} + V(r)
\]

where \( V(r) = V(r + R_n) \) is periodic, \( R_n \) is a lattice vector. Generally, the solutions of the Schrödinger equations are Bloch wavefunctions. They satisfy the following boundary condition (Bloch’s theorem):

\[
\Psi_{mk}(r + R_n) = e^{i\mathbf{k} \cdot \mathbf{R}_n} \Psi_{mk}(r)
\]

Here \( \Psi_{mk} \) is the eigenstate corresponding to the \( m \)th band and \( \mathbf{k} \) is the wave number which is defined in the Brillouin zone.
Let us now consider Berry phase effects in crystalline solids. In the non-interacting limit the Hamiltonian:

\[ \hat{H} = \frac{\hat{p}^2}{2m_e} + V(r) \]

where \( V(r) = V(r + R_n) \) is periodic, \( R_n \) is a lattice vector. Generally, the solutions of the Schrödinger equations are Bloch wavefunctions. They satisfy the following boundary condition (Bloch’s theorem):

\[ \Psi_{mk}(r + R_n) = e^{i k R_n} \Psi_{mk}(r) \]

Here \( \Psi_{mk} \) is the eigenstate corresponding to the \( m \)th band and \( k \) is the wave number which is defined in the Brillouin zone. The Brillouin zone has a topology of a torus: wave numbers \( k \) which differ by a reciprocal wave vector \( G \) describe the same state.
The Bloch wavefunctions can be written in the following form:
\[ \Psi_{mk} = e^{ikr} u_{mk}(r), \] where \( u_{mk}(r) \) is lattice periodic: \( u_{mk}(r) = u_{mk}(r + R_n) \).
The Bloch wavefunctions can be written in the following form:
\[ \Psi_{mk} = e^{ikr}u_{mk}(r), \text{ where } u_{mk}(r) \text{ is lattice periodic: } u_{mk}(r) = u_{mk}(r + R_n). \]

The functions \( u_{mk}(r) \) satisfy the following Schrödinger equation:
\[
\left[ \frac{(\hat{p} + \hbar \mathbf{k})^2}{2m_e} + V(r) \right] u_{mk}(r) = E_{mk} u_{mk}(r)
\]
The Bloch wavefunctions can be written in the following form:
\[ \Psi_{mk} = e^{ikr}u_{mk}(r), \text{ where } u_{mk}(r) \text{ is lattice periodic: } u_{mk}(r) = u_{mk}(r + R_n). \]

The functions \( u_{mk}(r) \) satisfy the following Schrödinger equation:
\[
\left[ \left( \hat{\rho} + \hbar \mathbf{k} \right)^2 + V(r) \right] u_{mk}(r) = E_{mk} u_{mk}(r)
\]

This can be written as
\[
\hat{H}(\mathbf{k})|u_m(\mathbf{k})\rangle = E_m(\mathbf{k})|u_m(\mathbf{k})\rangle
\]

\( \rightarrow \) the Brillouin zone is the parameter space for the \( \hat{H}(\mathbf{k}) \) and \( |u_m(\mathbf{k})\rangle \)
The Bloch wavefunctions can be written in the following form: 

$$\Psi_{mk} = e^{i kr} u_{mk}(r),$$

where $u_{mk}(r)$ is lattice periodic: $u_{mk}(r) = u_{mk}(r + R_n)$.

The functions $u_{mk}(r)$ satisfy the following Schrödinger equation:

$$\left[ \left( \hat{p} + \hbar k \right)^2 \frac{1}{2 m_e} + V(r) \right] u_{mk}(r) = E_{mk} u_{mk}(r)$$

This can be written as

$$\hat{H}(k) |u_m(k)\rangle = E_m(k) |u_m(k)\rangle$$

⇒ the Brillouin zone is the parameter space for the $\hat{H}(k)$ and $|u_m(k)\rangle$

Various Berry phase effects can be expected, if $k$ is varied in the wavenumber space.
Consider a two-dimensional crystalline system. Then the Berry connection of the $m$th band:

$$A^{(m)}(k) = i\langle u_m(k) | \nabla_k u_m(k) \rangle \quad k = (k_x, k_y).$$
Chern number

Consider a two-dimensional crystalline system. Then the Berry connection of the $m$th band:

$$A^{(m)}(k) = i \langle u_m(k) | \nabla_k u_m(k) \rangle \quad k = (k_x, k_y).$$

and the Berry curvature

$$\Omega^{(m)}(k) = \nabla_k \times i \langle u_m(k) | \nabla_k u_m(k) \rangle$$
Consider a two-dimensional crystalline system. Then the Berry connection of the $m$th band:

$$A^{(m)}(k) = i \langle u_m(k) | \nabla_k u_m(k) \rangle$$

$k = (k_x, k_y)$.

and the Berry curvature

$$\Omega^{(m)}(k) = \nabla_k \times i \langle u_m(k) | \nabla_k u_m(k) \rangle$$

Finally, the **Chern number** of the $m$th band is defined as

$$Q^{(m)} = -\frac{1}{2\pi} \int_{\text{BZ}} \Omega^{(m)}(k) d\mathbf{k}$$

integration is taken over the Brillouin zone (BZ).

The Chern number is an intrinsic property of the band structure and has various effects on the transport properties of the system.
Zak’s phase

One can apply an electric field to cause a linear variation of \( \mathbf{q} \). In one-dimensional systems the Berry phase calculated as \( q \) sweeps the Brillouin zone is called the Zak’s phase (Phys Rev Lett 62, 2747):

\[
\gamma_n = \int_{BZ} i d\mathbf{q} \langle \mathbf{u}_n(q) | \nabla_q | \mathbf{u}_n(q) \rangle
\]