Berry phase, Chern number

November 17, 2015
Literature:

Basic definitions: Berry connection, gauge invariance

Consider a quantum state $|\Psi(R)\rangle$ where $R$ denotes some set of parameters, e.g., $v$ and $w$ from the Su-Schrieffer-Heeger model.
Basic definitions: Berry connection, gauge invariance

Consider a quantum state $|\Psi(R)\rangle$ where $R$ denotes some set of parameters, e.g., $\nu$ and $w$ from the Su-Schrieffer-Heeger model.

The relative phase between two states that are close in the parameter space:

$$e^{-i\Delta\gamma} = \frac{\langle\psi(R)|\psi(R + dR)\rangle}{|\langle\psi(R)|\psi(R + dR)\rangle|} \quad \Delta\gamma = i\langle\psi(R)|\nabla_R \psi(R)\rangle \cdot dR$$
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Consider a quantum state $|\Psi(R)\rangle$ where $R$ denotes some set of parameters, e.g., $\nu$ and $\omega$ from the Su-Schrieffer-Heeger model.

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This equation defines the **Berry connection**:

$$A = i\langle \Psi(R)|\nabla_R \Psi(R)\rangle = -\text{Im}[\langle \Psi(R)|\nabla_R \Psi(R)\rangle]$$

(here we used $\nabla_R \langle \Psi(R)|\Psi(R)\rangle = 0$).
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Note, that the Berry connection is not **gauge invariant**:

$$|\psi(R)\rangle \rightarrow e^{i\alpha(R)}|\psi(R)\rangle : \quad A(R) \rightarrow A(R) + \nabla_R \alpha(R).$$
Consider a **closed** directed curve $C$ in parameter space $\mathbb{R}$.

The *Berry phase* along $C$ is defined in the following way:

$$
\sum_i \Delta \gamma_i \rightarrow \gamma(C) = -\text{Arg} \left[ \exp \left( -i \oint_C A(R) dR \right) \right]
$$
Consider a **closed** directed curve $C$ in parameter space $\mathbf{R}$. The *Berry phase* along $C$ is defined in the following way:

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

Consider the map $\mathbf{R} \mapsto |\psi(\mathbf{R})\rangle\langle\psi(\mathbf{R})|$
We assume that this map is smooth.
However, this does not imply that $\mathbf{R} \mapsto |\psi(\mathbf{R})\rangle$ is smooth!
Berry curvature

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Nevertheless, even if the gauge $R \mapsto |\psi(R)\rangle$ is not smooth in the vicinity of a point $R_0$ in the parameter space, one can always find an alternative gauge $|\psi'(R)\rangle$ which is:

i) locally smooth

ii) which generates the same map, i.e., $|\psi'(R)\rangle\langle\psi'(R)| = |\psi(R)\rangle\langle\psi(R)|$
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We want to express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity $\rightarrow \textit{Berry curvature}$. 
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We want to express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity $\rightarrow$ 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

$$\exp \left( -i \oint_{\partial \mathcal{F}} \mathbf{A}(\mathbf{R}) d\mathbf{R} \right) = \exp \left( -i \int_{\mathcal{F}} B(x, y) dx dy \right)$$

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

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

\[
\oint_{\partial \mathcal{F}} A(\mathbf{R}) d\mathbf{R} = \int_{\mathcal{F}} (\partial_x A_y - \partial_y A_x) dx dy = \int_{\mathcal{F}} B(x, y) dx dy
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Berry curvature

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In 3 dimensional parameter space:

$$B(\mathbf{R}) = \nabla_\mathbf{R} \times A(\mathbf{R})$$

Generalization to higher dimensions is also possible.
Useful formulas for the Berry curvature

We want to calculate the 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 $\partial_l = \partial_{R_l}$. 

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Secondly, inserting $1 = \sum_{n'} |n'\rangle \langle n'|$ one can write

$$B^{(n)} = -\text{Im} \left[ \sum_{n' \neq n} \langle \nabla_R n | n' \rangle \times \langle n' | \nabla_R n \rangle \right]$$
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B^{(n)} = -Im \left[ \sum_{n' \neq n} \langle \nabla_R n| n'\rangle \times \langle n'| \nabla_R n\rangle \right]
\]

To calculate \( \langle n'| \nabla_R n\rangle \), one can do the following steps: (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 \( \langle n' | \hat{H} = E_{n'} \langle n' | \) 

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

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

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

Using this result to calculate

\[
B^{(n)} = -Im \left[ \sum_{n' \neq n} \langle \nabla_R n|n' \rangle \times \langle n'|\nabla_R n \rangle \right]
\]

we find that

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

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

This form manifestly shows that the Berry curvature is \textit{gauge invariant}!
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This form manifestly show that the Berry curvature is \textit{gauge invariant}!

Remarks

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

ii) if the eigenstates are degenerate, then the dynamics must be projected onto the degenerate subspace. In this case the \textit{non-Abelian Berry curvature} naturally arises

iii) Berry curvature is often the largest at near-degeneracies
Example: two level system

Consider the following Hamiltonian:

\[ H_d = d_x \sigma_x + d_y \sigma_y + d_z \sigma_z = \mathbf{d} \cdot \mathbf{\sigma} \]

where \( \mathbf{d} = (d_x, d_y, d_z) = \mathbb{R}^3 \setminus \{0\} \), to avoid degeneracy.

Eigenvalues, eigenstates:

\[ H(\mathbf{d}) |\pm\rangle = \pm |\mathbf{d}| |\pm\rangle \]
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Eigenvalues, eigenstates:

\[ H(d)|\pm\rangle = \pm |d||\pm\rangle \]

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

\[ \cos \theta = \frac{d_z}{|d|}, \quad e^{i\phi} = \frac{d_x + id_y}{\sqrt{d_x^2 + d_y^2}} \]
Example: two level system

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

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Several choices are possible:
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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, $| + (\theta, \phi = 0) \rangle = -| + (\theta, \phi = 2\pi) \rangle$. 
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$$|+ (\theta, \phi = 0)\rangle = -|+ (\theta, \phi = 2\pi)\rangle.$$ 

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

A couple of other choices are possible, one can try to find a gauge where the wavefunction is well behaved everywhere on the Bloch sphere. It turns out that there is no such gauge.

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

$$
\gamma_- = \oint_C A(d) \, d\mathbf{d}, \quad A^-(d) = i \langle - | \nabla_d | - \rangle
$$

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

\[ B^{\pm}(d) = -Im \left\{ \frac{\langle \pm | \nabla_d \hat{H} | \mp \rangle \times \langle \mp | \nabla_d \hat{H} | \pm \rangle}{4|d|^2} \right\}, \quad \nabla_d \hat{H} = \sigma \]

This can be evaluated in any of the gauges.

\[ B^{\pm}(d) = \pm \frac{d}{|d|} \frac{1}{2|d|^2} \]

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 $C$. 
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 $F$ whose boundary is $C$. This is half of the solid angle subtended by the curve:

$$\gamma_- = \frac{1}{2} \Omega_C, \quad \gamma_+ = -\gamma_-$$
Berry phase: physical interpretation

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 $t = 0$.

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

Now consider the situation when \( \mathbf{R} \) is slowly changed in time and the values of \( \mathbf{R}(t) \) define a continuous curve \( C \). Also, assume that \( |n(\mathbf{R})\rangle \) is smooth along \( C \).
The wavefunction evolves according to the time-dependent Schrödinger equation:

\[ i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(R(t)) |\psi(t)\rangle \]
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Further important assumption: starting from the initial state \(|n(R_0)\rangle\) for all times the state \(|n(R(t))\rangle\) remains non-degenerate.
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Ansatz:

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

The parameter vector $\mathbf{R}(t)$ traces out a curve $C$ in the parameter space. Substituting the above Ansatz into the Schrödinger equation, one can show that

$$\gamma_n(C) = i \int_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle d\mathbf{R}$$
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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

$$\gamma_n(C) = i \oint_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle d\mathbf{R}$$

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.
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Considering the Berry curvature instead of the Berry connection, one can reformulate the above findings in the following way.
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Chern number

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\hat{H} = \frac{\hat{p}^2}{2m_e} + V(r)
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where \( V(r) = V(r + R_n) \) is periodic, \( R_n \) is a lattice vector.
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where \( V(r) = V(r + \mathbf{R}_n) \) is periodic, \( \mathbf{R}_n \) is a lattice vector. Generally, the solutions of the Schrödinger equations are Bloch wavefunctions. They satisfy the following boundary condition (Bloch’s theorem):

\[ \psi_{mk}(r + \mathbf{R}_n) = e^{ik\mathbf{R}_n} \psi_{mk}(r) \]

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.
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$$\psi_{mk}(r + R_n) = e^{i \mathbf{k} \cdot \mathbf{R}_n} \psi_{mk}(r)$$

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. Note, that the Brillouin zone has a topology of a torus: wave numbers $\mathbf{k}$ which differ by a reciprocal wave vector $\mathbf{G}$ describe the same state.
Chern number

The Bloch wavefunctions can be written in the following form:
\[ \psi_{mk} = e^{ikr} u_{mk}(r) \] where \( u_{mk}(r) \) is lattice periodic: \( u_{mk}(r) = u_{mk}(r + R_n) \).
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where \( u_{mk}(\mathbf{r}) \) is lattice periodic: \( u_{mk}(\mathbf{r}) = u_{mk}(\mathbf{r} + R_n) \).

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

\[
\left[ \frac{(\hat{p} + \hbar \mathbf{k})^2}{2m_e} + V(\mathbf{r}) \right] u_{mk}(\mathbf{r}) = E_{mk} u_{mk}(\mathbf{r})
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This can be written as
\[
\hat{H}(\mathbf{k})|u_m(\mathbf{k})\rangle = E_m(\mathbf{k})|u_m(\mathbf{k})\rangle
\]

\( \Longrightarrow \) the Brillouin zone can be considered as the parameter space for the Hamiltonian \( \hat{H}(\mathbf{k}) \) and \( |u_m(\mathbf{k})\rangle \) are the basis functions.
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The functions \( u_{mk}(r) \) satisfy the following Schrödinger equation:
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\hat{H}(k)|u_m(k)\rangle = E_m(k)|u_m(k)\rangle
\]

\[ \implies \] the Brillouin zone can be considered as the parameter space for the Hamiltonian \( \hat{H}(k) \) and \( |u_m(k)\rangle \) are the basis functions.

Various Berry phase effects can be expected, if \( k \) is varied in the wavenumber space.
Chern number

For simplicity, let us consider a two-dimensional crystalline system. Then the Berry connection of the $m$th band:

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

and the Berry curvature as

$$\Omega^{(m)}(\mathbf{k}) = \nabla_{\mathbf{k}} \times i \langle u_m(\mathbf{k})|\nabla_{\mathbf{k}} u_m(\mathbf{k})\rangle$$
Chern number

For simplicity, let us consider a two-dimensional crystalline system. Then the Berry connection of the $m$th band:

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

and the Berry curvature as

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

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

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

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.