Berry phase, Chern number

November 17, 2015

Literature:

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2. D. Xiao, M-Ch Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959.

Basic definitions: Berry connection, gauge invariance

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

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

$$e^{-i\Delta\gamma} = \frac{\langle\Psi(\mathbf{R})|\Psi(\mathbf{R}+d\mathbf{R})\rangle}{|\langle\Psi(\mathbf{R})|\Psi(\mathbf{R}+d\mathbf{R})\rangle|} \qquad \Delta\gamma = i\langle\Psi(\mathbf{R})|\nabla_{\mathbf{R}}\Psi(\mathbf{R})\rangle \cdot d\mathbf{R}$$

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This equation defines the *Berry connection*:

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

(here we used $\nabla_{\mathbf{R}}\langle\Psi(\mathbf{R})|\Psi(\mathbf{R})\rangle = 0$).

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

$$|\Psi(\mathbf{R})\rangle \to e^{i\alpha(\mathbf{R})}|\Psi(\mathbf{R})\rangle: \qquad \mathbf{A}(\mathbf{R}) \to \mathbf{A}(\mathbf{R}) + \nabla_{\mathbf{R}}\alpha(\mathbf{R}).$$

Berry phase

Consider a **closed** directed curve $\mathcal{C}$ in parameter space $\mathbf{R}$.
The *Berry phase* along $\mathcal{C}$ is defined in the following way:

$$\sum_i \Delta\gamma_i \to \gamma(\mathcal{C}) = -Arg\left[\exp\left(-i\oint_{\mathcal{C}} \mathbf{A}(\mathbf{R})d\mathbf{R}\right)\right]$$

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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 $\mathcal{C}$, 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 asume that this map is smooth.
However, this does not imply that $\mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$ is smooth!

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Nevertheless, even if the gauge $\mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$ is not smooth in the vicinity of a point $\mathbf{R}_0$ in the parameter space, one can always find and alternative gauge $|\Psi'(\mathbf{R})\rangle$ which is :

i) locally smooth

ii) which generates the same map, i.e., $|\Psi'(\mathbf{R})\rangle\langle\Psi'(\mathbf{R})| = |\Psi(\mathbf{R})\rangle\langle\Psi(\mathbf{R})|$

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We want to express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity $\rightarrow$ *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

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

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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*:

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

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In 3 dimensional parameter space:

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

Generalization to higher dimensions is also possible.

Useful formulas for the Berry curvature

We want to calculate the Berry phase corresponding to an eigenstate $|n(\mathbf{R})\rangle$ 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 $\mathbb{1} = \sum_{n'} |n'\rangle\langle n'|$ one can write

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

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To calculate $\langle n'|\nabla_{\mathbf{R}} n\rangle$, one can do the following steps: (both the Hamiltonian $\hat{H}$ and the eigenstates $|n\rangle$ depend on $\mathbf{R}$!)

$$\begin{aligned}
\hat{H}|n\rangle &= E_n|n\rangle \\
\nabla_{\mathbf{R}}\hat{H}|n\rangle + \hat{H}|\nabla_{\mathbf{R}} n\rangle &= (\nabla_{\mathbf{R}} E_n)|n\rangle + E_n|\nabla_{\mathbf{R}} n\rangle \\
\langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle + \langle n'|\hat{H}|\nabla_{\mathbf{R}} n\rangle &= E_n\langle n'|\nabla_{\mathbf{R}} n\rangle
\end{aligned}$$

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

$$\begin{aligned} \langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle + E_{n'}\langle n'|\nabla_{\mathbf{R}} n\rangle &= E_n\langle n'|\nabla_{\mathbf{R}} n\rangle \\ \langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle &= (E_n - E_{n'})\langle n'|\nabla_{\mathbf{R}} n\rangle \end{aligned}$$

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Using this result to calculate

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

we find that

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

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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 *non-Abelian Berry curvature* naturally arises

iii) Berry curvature is often the larges at near-degeneracies

Example: two level system

Consider the following Hamiltonian:

$$H_{\mathbf{d}} = d_x\sigma_x + d_y\sigma_y + d_z\sigma_z = \mathbf{d}\cdot\sigma$$

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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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

$$\cos\theta = \frac{d_z}{|\mathbf{d}|}, \qquad e^{i\phi} = \frac{d_x + id_y}{\sqrt{d_x^2 + d_y^2}}$$

Example: two level system

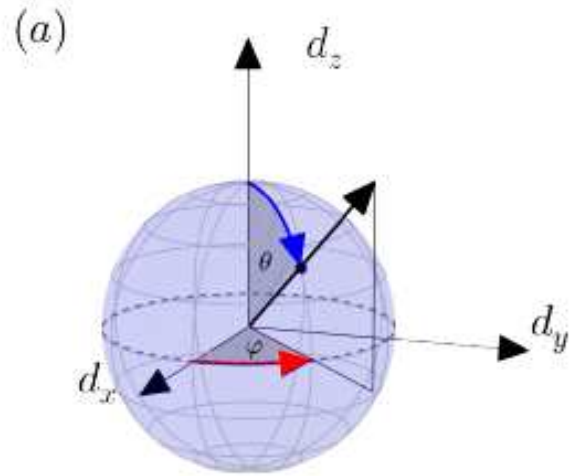

Figure : The reprentation of the parameter space on a Bloch sphere

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

We except 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.

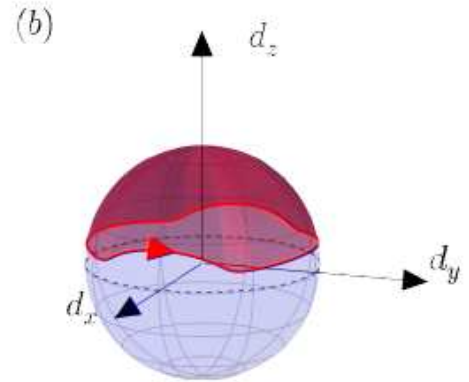
Calculating the Berry phase for a two level system

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

$$\gamma_- = \oint_{\mathcal{C}} \mathbf{A}(\mathbf{d}) d\mathbf{d}, \qquad \mathbf{A}^-(\mathbf{d}) = i\langle -|\nabla_{\mathbf{d}}|-\rangle$$

The calculation is easier if one uses the Berry curvature.

Calculating the Berry phase for a two level system



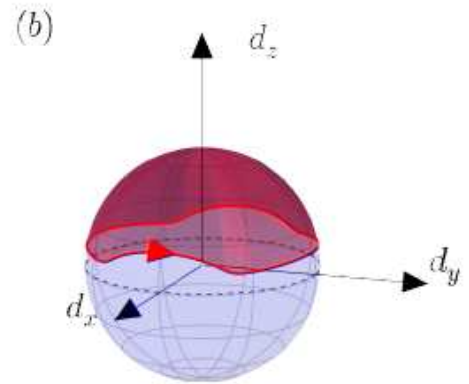
$$\mathbf{B}^{\pm}(\mathbf{d}) = -Im\frac{\langle \pm|\nabla_{\mathbf{d}}\hat{H}|\mp\rangle \times \langle \mp|\nabla_{\mathbf{d}}\hat{H}|\pm\rangle}{4|\mathbf{d}|^2}, \qquad \nabla_{\mathbf{d}}\hat{H} = \sigma$$

This can be evaluated in any of the gauges.

$$\mathbf{B}^{\pm}(\mathbf{d}) = \pm\frac{\mathbf{d}}{|\mathbf{d}|}\frac{1}{2|\mathbf{d}|^2}$$

This is the field of a pointlike monopole source in the origin.

Calculating the Berry phase for a two level system



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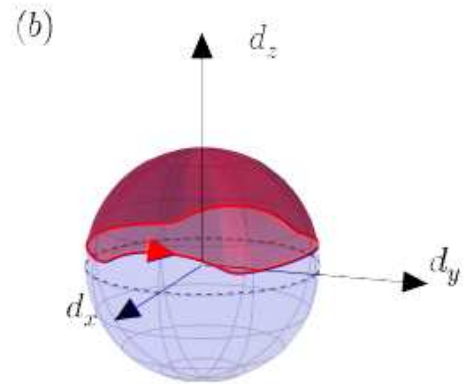

The Berry phase of the closed loop $\mathcal{C}$ in parameter space is the flux of the monopole field through a surface $\mathcal{F}$ whose boundary is $\mathcal{C}$.
This is half of the solid angle subtended by the curve:

$$\gamma_- = \frac{1}{2}\Omega_{\mathcal{C}}, \qquad \gamma_+ = -\gamma_-$$

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 $t = 0$.

$$\mathbf{R}(t = 0) = \mathbf{R}_0, \qquad |\Psi(t = 0)\rangle = |n(\mathbf{R}_0)\rangle$$

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

Berry phase: physical interpretation

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

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

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In this case one can choose the rate of change $R(t)$ along $\mathcal{C}$ slow enough such that the system remains in an eigenstate $|n(\mathbf{R}(t))\rangle$ (*adiabatic approximation*). However, $|n(\mathbf{R}(t))\rangle$ picks up a phase factor during the time evolution.

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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 $\mathcal{C}$ in the parameter space. Substituting the above Ansatz into the Schrödinger equation, one can show that

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

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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

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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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Although the system remains in the same state $|n(\mathbf{R})\rangle$ during the adiabatic evolution, other states of the system $|n'(\mathbf{R})\rangle$, $n \neq n'$ are nevertheless influencing the state $|n(\mathbf{R})\rangle$. This influence is manifested in the Berry curvature, which, in turn, determines the Berry phase picked up by $|n(\mathbf{R})\rangle$.

Chern number

Let us now consider Berry phase effects in *crystalline solids*.

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Generally, the solutions of the Schrödinger equations are Bloch wavefunctions.
They satisfy the following boundary condition (Bloch's theorem):

$$\Psi_{m\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) = e^{i\mathbf{k}\mathbf{R}_n}\Psi_{m\mathbf{k}}(\mathbf{r})$$

Here $\Psi_{m\mathbf{k}}$ is the eigenstate corresponding to the mth band and $\mathbf{k}$ is the wave number which is defined in the Brillouin zone.

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Here $\Psi_{m\mathbf{k}}$ is the eigenstate corresponding to the mth 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:
$\Psi_{m\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{m\mathbf{k}}(\mathbf{r})$ where $u_{m\mathbf{k}}(\mathbf{r})$ is lattice periodic: $u_{m\mathbf{k}}(\mathbf{r}) = u_{m\mathbf{k}}(\mathbf{r} + R_n)$.

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

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

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

$\Longrightarrow$ 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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$\Psi_{m\mathbf{k}} = e^{i\mathbf{kr}} u_{m\mathbf{k}}(\mathbf{r})$ where $u_{m\mathbf{k}}(\mathbf{r})$ is lattice periodic: $u_{m\mathbf{k}}(\mathbf{r}) = u_{m\mathbf{k}}(\mathbf{r} + R_n)$.

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

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

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Various Berry phase effects can be expected, if $\mathbf{k}$ is varied in the wavenumber space.

Chern number

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

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

and the Berry curvature as

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

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Finally, the *Chern number* of the mth 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.