Berry phase, Chern number

10/11/2016

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3. Raffaele Resta, J. Phys.: Condens. Matter **12**, (2000) R107–R143

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Quantal phase factors accompanying adiabatic changes

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(*Received* 13 *June* 1983)

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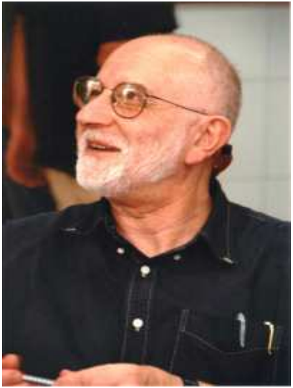

https://michaelberryphysics.wordpress.com/

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

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

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

$$e^{-i\Delta\gamma_n} = \frac{\langle\Psi_n(\mathbf{R})|\Psi_n(\mathbf{R}+d\mathbf{R})\rangle}{|\langle\Psi_n(\mathbf{R})|\Psi_n(\mathbf{R}+d\mathbf{R})\rangle|}$$

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In leading order

$$-i\Delta\gamma_n \simeq \langle\Psi_n(\mathbf{R})|\nabla_{\mathbf{R}}\Psi_n(\mathbf{R})\rangle \cdot d\mathbf{R}$$

Basic definitions: Berry connection

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

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

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

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$$\Delta\gamma_n = \mathbf{A}_n \cdot d\mathbf{R} \tag{1}$$

Note, that the Berry connection is not gauge invariant:

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

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:

$$\gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} d\gamma_n = \oint_{\mathcal{C}} \mathbf{A}_n(\mathbf{R}) d\mathbf{R}$$

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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 $\rightarrow$ express the gauge invariant Berry phase in terms of a surface integral of a gauge invariant quantity *Berry curvature*.

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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

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

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

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

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

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Generalization to higher dimensions is also possible.

Berry curvature

Taking the explicit form of $\mathbf{A}_n$

$$\begin{aligned}\mathbf{B}^{(n)}_{\mu\nu}(\mathbf{R}) &= \frac{\partial}{\partial R^\mu}A^{(n)}_\nu(\mathbf{R}) - \frac{\partial}{\partial R^\nu}A^{(n)}_\mu(\mathbf{R}) \\ &= -2\mathrm{Im}\left\langle \frac{\partial}{\partial R^\mu}\Psi_n(\mathbf{R})\right| \left.\frac{\partial}{\partial R^\nu}\Psi_n(\mathbf{R})\right\rangle\end{aligned}$$

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\end{aligned}$$

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

Berry curvature

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- If the wavefunction can be taken as real, the curvature $\mathbf{B}^{(n)}$ 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 $|n(\mathbf{R})\rangle$ 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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Inserting $\mathbb{1} = \sum_{n'} |n'\rangle\langle n'|$:

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

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

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

Useful formulas for the Berry curvature

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

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

Useful formulas for the Berry curvature

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Substituting this into

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

one finds:

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

Gauge invariant!

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

Remarks

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

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

iii) The Berry curvature is singular for such $\mathbf{R}_0$ values, where $|n(\mathbf{R}_0)\rangle$ is degenerate with one of $|n'(\mathbf{R}_0)\rangle$. However, if the integration curve $\partial\mathcal{F}$ encircles the degeneracy point, the Berry phase can be finite.

Berry phase: the discrete version

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

In practical applications this is usually not the case.

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Phase difference between two different $\mathbf{R}$ points:

$$e^{-i\phi_{12}^{(n)}} = \frac{\langle \Psi_n(\mathbf{R}_1)|\Psi_n(\mathbf{R}_2)\rangle}{|\langle \Psi_n(\mathbf{R}_1)|\Psi_n(\mathbf{R}_2)\rangle|}$$

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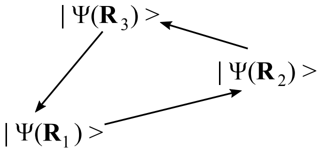
Consider the path in parameter space:



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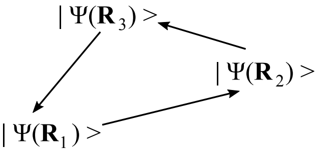

The total phase difference along a closed path which joins the points $\mathbf{R}_i$ in a given order:

$$
\begin{aligned}
\gamma &= \phi_{12} + \phi_{23} + \phi_{31} \\
&= -\mathrm{Im}\log\left[\langle\Psi_n(\mathbf{R}_1)|\Psi_n(\mathbf{R}_2)\rangle\langle\Psi_n(\mathbf{R}_2)|\Psi_n(\mathbf{R}_3)\rangle\langle\Psi_n(\mathbf{R}_3)|\Psi_n(\mathbf{R}_1)\rangle\right]
\end{aligned}
$$

The gauge-arbitrary phases cancel in pairs $\rightarrow$ overall phase γ is a gauge-invariant quantity.

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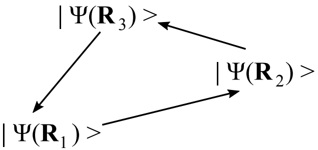

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The gauge-arbitrary phases cancel in pairs $\rightarrow$ overall phase γ is a gauge-invariant quantity.
In general:

$$\gamma = \sum_{s=1}^{M} \phi_{s,s+1} = -\mathrm{Im}\log\prod_{s=1}^{M}\langle\Psi_n(\mathbf{R}_s)|\Psi_n(\mathbf{R}_{s+1})\rangle$$

Example: two level system

Consider the following Hamiltonian:

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

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

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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

$$\cos\theta = \frac{R_z}{|\mathbf{R}|}, \qquad e^{i\phi} = \frac{R_x + iR_y}{\sqrt{R_x^2 + R_y^2}}$$

Example: two level system

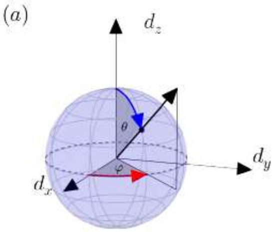

Figure: The reprentation of the parameter space on a Bloch sphere

Example: two level system

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

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Several choices are possible:

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

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

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

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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.

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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.

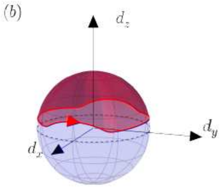
Example: Berry phase for a two-level system

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 $|-\rangle$ or $|+\rangle$.

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

The calculation is easier if one uses the Berry curvature.

Calculating the Berry phase for a two level system



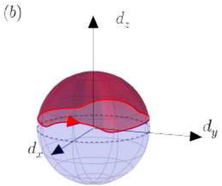
$$\mathbf{B}^{\pm}(\mathbf{R}) = -\mathrm{Im}\frac{\langle \pm|\nabla_{\mathbf{R}}\hat{H}|\mp\rangle \times \langle \mp|\nabla_{\mathbf{R}}\hat{H}|\pm\rangle}{4|\mathbf{R}|^2}, \qquad \nabla_{\mathbf{R}}\hat{H} = \sigma$$

This can be evaluated in any of the gauges.

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

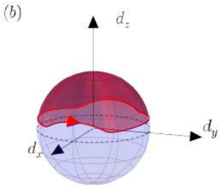
This is the field of a pointlike monopole source in the origin.

Calculating the Berry phase for a two level system



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

Calculating the Berry phase for a two level system



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: a 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 $|n(\mathbf{R})\rangle$.

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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 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:

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

Berry phase: physical interpretation

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

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

Assumption: starting from the initial state $|n(\mathbf{R}_0)\rangle$ the state $|n(\mathbf{R}(t))\rangle$ remains non-degenerate for all times.

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The parameter vector $\mathbf{R}(t)$ traces out a curve $\mathcal{C}$ in the parameter space.

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Ansatz:

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

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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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:

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

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

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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.
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.

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The Bloch wavefunctions can be written in the following form:
$\Psi_{m\mathbf{k}} = e^{i\mathbf{kr}} u_{m\mathbf{k}}(\mathbf{r})$, where $u_{m\mathbf{k}}(\mathbf{r})$ is lattice periodic: $u_{m\mathbf{k}}(\mathbf{r}) = u_{m\mathbf{k}}(\mathbf{r} + R_n)$.

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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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$\Longrightarrow$ the Brillouin zone is the parameter space for the $\hat{H}(\mathbf{k})$ and $|u_m(\mathbf{k})\rangle$
Various Berry phase effects can be expected, if $\mathbf{k}$ is varied in the wavenumber space.

Chern number

Consider a two-dimensional crystalline system.
Then the Berry connection of the mth band :

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

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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.

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):

$$\gamma_n = \int_{\mathrm{BZ}} i \mathrm{d}q \langle u_n(q) | \nabla_q | u_n(q) \rangle$$