Berry phase from quadratic equation

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Why do we care about Berry phase?

- Relatively new field of studies
  Quantal phase factors accompanying adiabatic changes, M.V. Berry (1983)

- Relations to:
  – quantum Hall effect
  – topological insulators, Chern number
  – electric polarization in crystals

Adiabatic theorem

Adiabatic theorem

Instantaneous energy eigenbasis $|n(t)\rangle$ given by time-independent Schrödinger equation for each time t:

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

After projection and differentiation, for $m \neq n$:

$$\langle m|\frac{d}{dt}|n\rangle = \frac{\langle m|\dot{H}(t)|n\rangle}{E_n - E_m}$$

The diagonal element defines *Berry connection*:

$$\langle n(t)|\frac{d}{dt}|n(t)\rangle \equiv -i\mathcal{A}(t)$$

Adiabatic theorem

Full solution to time-dependent Schrödinger equation:

$$|\Psi(t)\rangle = \sum_n c_n(t)\, e^{-\frac{i}{\hbar}\int_0^t E_n(t')dt'} |n(t)\rangle$$

With initial condition $|\Psi(t=0)\rangle = |k\rangle$ and for $m \neq k$ the transition to different states:

$$|c_m(t)|^2 \approx \hbar \frac{|\langle k|\dot{H}|m\rangle|^2}{(E_m - E_k)^2}$$

For slowly varying Hamiltonian $\langle m|\dot{H}(t)|k\rangle \ll (E_k - E_m)$ we can neglect transitions to other eigenstates, $m = k$:

$$c_k(t) = e^{i\int_0^t \mathcal{A}_k(t')dt'} \quad \Rightarrow \quad |\Psi(t)\rangle = e^{i\int_0^t \mathcal{A}_k(t')dt'}\, e^{-\frac{i}{\hbar}\int_0^t E_k(t')dt'} |k(t)\rangle$$

State evolves with additional phase factor, apart from the dynamical one.

Fast and slow processes in physics

$$|c_m(t)|^2 \approx \hbar \frac{|\langle k|\dot{H}|m\rangle|^2}{(E_m - E_k)^2}$$

- **Fast processes:** What is fast?

$$\hbar|\dot{H}_{km}|^2 \gg (E_m - E_k)^2$$

'frozen system':

– measurement, deep inelastic scattering

– critical slowing down (the $\Delta E \to 0$ at critical point, KZ mechanism)

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'frozen system':

– measurement, deep inelastic scattering

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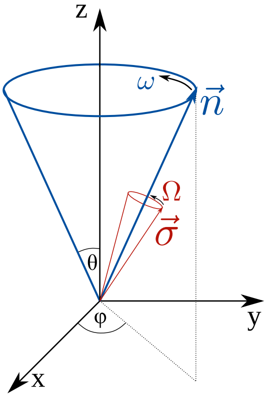
- **Slow processes:** adiabatic evolution – a state initially prepared in some eigenstate of $\hat{H}(t=0)$ remains in this eigenstate.

Berry phase
in simple setup of spin in magnetic field

Spin in varying magnetic field

$$\hat{H}(t) = \mu \vec{B}(t) \cdot \vec{\sigma}(t) = \Omega \ \vec{n}(t) \cdot \vec{\sigma}(t)$$

$$\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z), \quad \vec{n}(t) = (\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta))$$



We assume that $\theta(t) = const = \theta$ and $\varphi(t) = \omega t$, meaning that magnetic field is oscillating around the z-axis with frequency ω.

Instantenuous energy eigenstates and Berry phase

$$\mu B \begin{pmatrix} \cos(\theta) & \sin(\theta)\mathrm{e}^{-i\varphi} \\ \sin(\theta)\mathrm{e}^{i\varphi} & -\cos(\theta) \end{pmatrix} \vec{\Psi} = E\ \vec{\Psi}$$

Eigenenergies and eigenstates:

$$E_\pm = \pm\mu B, \qquad \psi_+ = \begin{pmatrix} \cos(\frac{1}{2}\theta) \\ \sin(\frac{1}{2}\theta)\mathrm{e}^{i\varphi} \end{pmatrix}, \qquad \psi_- = \begin{pmatrix} -\sin(\frac{1}{2}\theta)\mathrm{e}^{-i\varphi} \\ \cos(\frac{1}{2}\theta) \end{pmatrix}.$$

The eigenvector are not well-defined for $\theta = 0$.

New set of eigenvectors $\psi'_\pm = \mathrm{e}^{\mp i\varphi}\psi_\pm$, which are not well-defined for $\theta = \pi$.

Phases of eigenvectors are not well-defined – typical behaviour for systems with non-trivial Berry phase

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From the definition of the Berry connection:

$$\mathcal{A}_+(t) = -i\ \langle \psi_+(t) | \frac{d}{dt} | \psi_+(t) \rangle = \frac{d\varphi}{dt} \sin^2\left(\frac{\theta}{2}\right)$$

In general *Berry connection* depends on gauge transformation.
Integral over the closed path in the parameter space – gauge independent *Berry phase*

$$\gamma \equiv \oint_C \mathcal{A}(t) dt$$

Berry phase from Schrödinger equation

Time-dependent Schrödinger equation for the spinor ($\tau = t\Omega$, $\rho = \frac{\omega}{\Omega}$):

$$\begin{pmatrix} \cos(\theta) & e^{-i\rho\tau}\sin(\theta) \\ e^{i\rho\tau}\sin(\theta) & -\cos(\theta) \end{pmatrix} \begin{pmatrix} \Psi_+(\tau) \\ \Psi_-(\tau) \end{pmatrix} = i \begin{pmatrix} \dot{\Psi}_+(\tau) \\ \dot{\Psi}_-(\tau) \end{pmatrix}$$

This can be reduced to one second order differential equation for $\Psi_+(\tau)$:

$$\ddot{\Psi}_+ + i\rho\dot{\Psi}_+ + (1 - \rho\cos(\theta))\Psi_+ = 0$$

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Assuming that the state was prepared with a spin up: $\Psi_+(0) = 1, \Psi_-(0) = 0$:

$$\begin{aligned} \Psi_+(\tau) &= \mathrm{e}^{-i\frac{\rho}{2}\tau} \left(\frac{\beta + \cos(\theta) - \frac{\rho}{2}}{2\beta}\, \mathrm{e}^{-i\beta\tau} + \frac{\beta - \cos(\theta) + \frac{\rho}{2}}{2\beta}\, \mathrm{e}^{i\beta\tau} \right) \\ \Psi_-(\tau) &= \mathrm{e}^{i\frac{\rho}{2}\tau} \left(\frac{\sin(\theta)}{2\beta}\, \mathrm{e}^{-i\beta\tau} - \frac{\sin(\theta)}{2\beta}\, \mathrm{e}^{i\beta\tau} \right) \end{aligned}$$

with $\beta = \sqrt{1 - \rho\cos(\theta) + \rho^2/4}$.

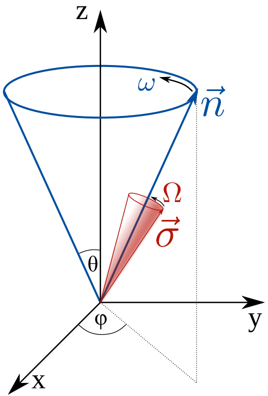
Slowly oscillating magnetic field $\rho \ll 1$, $\omega \ll \Omega$

At $t = T = \frac{2\pi}{\omega}$ expand in terms of $\rho \to 0$ limit, in the lowest order:

$$\Psi_+(T) = \cos^2\left(\frac{\theta}{2}\right) e^{-2\pi i \frac{\Omega}{\omega}} e^{-i\pi(1-\cos(\theta))} + \sin^2\left(\frac{\theta}{2}\right) e^{2\pi i \frac{\Omega}{\omega}} e^{-i\pi(1+\cos(\theta))}$$

$$\Psi_-(T) = \frac{1}{2}\sin(\theta)\left(e^{-2\pi i \frac{\Omega}{\omega}} e^{i\pi(1+\cos(\theta))} - e^{2\pi i \frac{\Omega}{\omega}} e^{i\pi(1-\cos(\theta))}\right)$$

Dynamical phase $2\pi i \frac{\Omega}{\omega} = i\Omega T$



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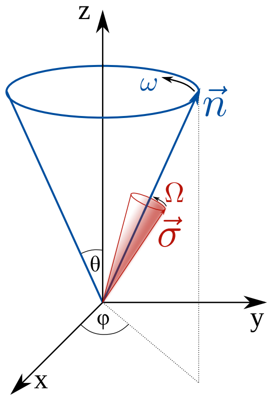

Dynamical phase $2\pi i \frac{\Omega}{\omega} = i\Omega T$

Surface area outlined by the unit vector:

$$\frac{1}{2}\int_0^{2\pi} d\varphi \int_0^{\theta} d\theta' \sin(\theta') = \frac{1}{2}\Omega_{st} = \pi\ (1-\cos(\theta))$$

but also there is a surface 'outside' of this loop:

$$\frac{1}{2}\int_0^{2\pi} d\varphi \int_{\theta}^{\pi} d\theta' \sin(\theta') = \pi\ (1+\cos(\theta)) = \frac{1}{2}(4\pi - \Omega_{st})$$

Purely geometrical feature depends only on the path in the parameter space.

Berry phase from adiabatic theorem

Time evolution of energy eigenstates: $|+\rangle, |-\rangle$ (corr. to $E = \pm\Omega = \pm\mu B$):

$$|+\rangle = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right)\, \mathrm{e}^{i\omega t} \end{pmatrix} \qquad |-\rangle = \begin{pmatrix} -\sin\left(\frac{\theta}{2}\right)\, \mathrm{e}^{-i\omega t} \\ \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

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Obtain set of 2 differential equations for c_+, c_- coefficients.

$$i \begin{pmatrix} \dot{c}_+(\tau) \\ \dot{c}_-(\tau) \end{pmatrix} = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) c_+(\tau) + \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \, \mathrm{e}^{-i\tau + 2i\frac{\tau}{\rho}} c_-(\tau) \\ -\sin\left(\frac{\theta}{2}\right) c_-(\tau) + \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \, \mathrm{e}^{i\tau - 2i\frac{\tau}{\rho}} c_+(\tau) \end{pmatrix}$$

Which leads to second order differential equation for c_+:

$$c_+'' - i(2-\rho)c_+' + 2\rho \sin^2\left(\frac{\theta}{2}\right) c_+ = 0$$

Solving by substitution $c_+(\tau) = \mathrm{e}^{i\alpha\tau}$ leads to $-\alpha^2 + (2-\rho)\alpha + 2\rho\sin^2\left(\frac{\theta}{2}\right) = 0$

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Imposing initial conditions $c_+(0) = 1$ and $c_-(0) = 0$:

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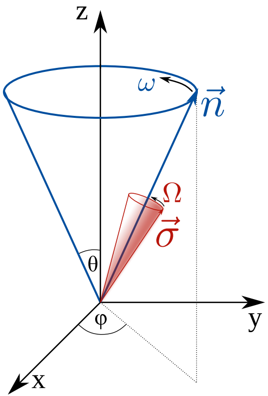
$$c_-(\tau') = -\mathrm{e}^{-i\frac{2-\rho}{2}\tau'} \left(\frac{\rho\sin(\theta)}{2\beta} \, \mathrm{e}^{i\frac{\beta}{2}\tau'} - \frac{\rho\sin(\theta)}{2\beta} \, \mathrm{e}^{-i\frac{\beta}{2}\tau'} \right)$$

Adiabatic limit $\rho = \frac{\omega}{\Omega} \ll 1$

In the lowest order approximation (0-th and 1-st in ρ):

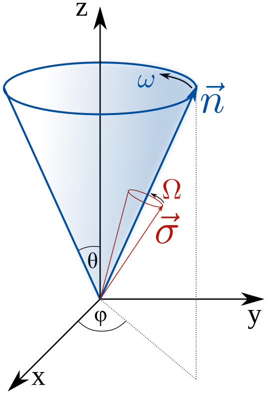
$$c_+(t) = \mathrm{e}^{-i\frac{\omega t}{2}(1-\cos(\theta))} + \mathcal{O}(\rho^2) \xrightarrow{\text{for } t=T=\frac{2\pi}{\omega}} \mathrm{e}^{-i\pi(1-\cos(\theta))}$$

$$c_-(t) = \frac{\cos(\theta)}{4}\rho\left(\mathrm{e}^{-2i\Omega t + i\omega t} - 1\right) \xrightarrow{\text{for } t=T=\frac{2\pi}{\omega}} \frac{\cos(\theta)}{4}\rho\left(\mathrm{e}^{-2i\Omega T + 2\pi i} - 1\right) \xrightarrow{\rho\to 0} 0$$



Adiabatic theorem tells us that if the evolution of the systems is slow enough, slow in comparison with the energy gap then the system initially in an eigenstate will remain in the same eigenstate and transitions to other states are supressed. Therefore the system initially in $|+\rangle$ remains in this state $|c_+(t = \frac{2\pi}{\omega})|^2 = 1$ but acquires a phase - Berry phase.

Instantaneous limit $\rho = \frac{\omega}{\Omega} \gg 1$



Very fast oscillations of magnetic field $\rho = \frac{\omega}{\Omega} \gg 1$. Expand for $\rho \to \infty$, after one full revolution of the magnetic field $\vec{B}$ around z-axis $T = \frac{2\pi}{\omega}$ (which is a very short period of time in this regime!) we see that spin remains frozen, it doesn't even have time to acquire any phase:

$$c_+\left(\frac{2\pi}{\omega}\right) \approx e^{i\pi\left(\frac{2}{\rho}-1\right)}\left(\frac{1+\cos(\theta)}{2}\, e^{i\pi\left(1-\frac{2\cos(\theta)}{\rho}\right)} + \frac{1-\cos(\theta)}{2}\, e^{i\pi\left(\frac{2\cos(\theta)}{\rho}-1\right)}\right)$$

$$\approx \frac{1+\cos(\theta)}{2} + \frac{1-\cos(\theta)}{2}\, e^{-2\pi i} = 1$$

$$c_-\left(\frac{2\pi}{\omega}\right) \approx e^{i\pi}\left(\frac{-\sin(\theta)}{2}\, e^{i\pi} + \frac{\sin(\theta)}{2}\, e^{-i\pi}\right) = 0$$

Magnetic monopole and Chern number

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Time dependance $t \rightarrow$ path in the parameter space $\vec{\lambda}(t) = (\theta(t), \varphi(t))$

Berry connection: $\vec{\mathcal{A}} = (\mathcal{A}_\theta, \mathcal{A}_\varphi)$ with $\mathcal{A}_k = -i\langle n|\frac{d}{d\lambda_k}|n\rangle$.

Berry curvature is a curl of Berry connection (gauge independent):

$$\mathcal{F}_{ij}(\lambda) = \frac{\partial \mathcal{A}_i}{\partial \lambda^j} - \frac{\partial \mathcal{A}_j}{\partial \lambda^i}$$

$$\mathcal{F}_{\theta\varphi} = \frac{1}{2}\sin(\theta) \quad \Rightarrow \quad \mathcal{F}_{ij} = \epsilon_{ijk}\frac{B^k}{2|\vec{B}|^3}$$

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for any surface S bounded by closed path C:

$$\mathrm{e}^{i\gamma} = \mathrm{e}^{-i\int_S \mathcal{F}_{ij} dS^{ij}} = \mathrm{e}^{\frac{i\Omega}{2}}$$

or its complement S', where solid angle $\Omega' = 4\pi - \Omega$:

$$\mathrm{e}^{i\gamma'} = \mathrm{e}^{-i\int_S' \mathcal{F}_{ij} dS^{ij}} = \mathrm{e}^{\frac{i(4\pi-\Omega)}{2}} = \mathrm{e}^{i\gamma}$$

Last requires that $2g \in \mathbb{Z}$.

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Chern theorem: integral of Berry curvature over any closed 2D manifold is quantized

$$\int \mathcal{F}_{ij} dS^{ij} = 2\pi C, \qquad \text{where Chern number} \quad C \in \mathbb{Z}$$

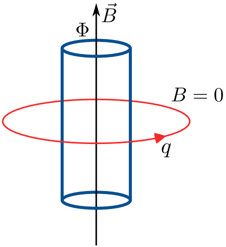
Physical examples

- **Aharonov-Bohm effect**

  Effect of gauge potential on a particle moving around the solenoid:

$$\Psi(\vec{x}) \Rightarrow \mathrm{e}^{i\gamma}\Psi(\vec{x}), \quad \mathrm{e}^{i\gamma} = \mathrm{e}^{\frac{iq}{\hbar}\oint_C \vec{A}(\vec{x})\cdot d\vec{x}} = \mathrm{e}^{iq\Phi/\hbar}$$

  Predicted in 1959.



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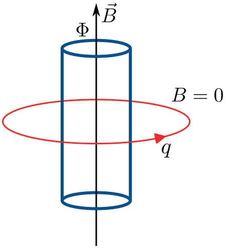
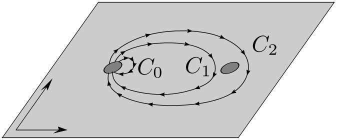


- **Anyons**

  Exchange of particles in 2D:

  - bosons $|\psi\rangle \;\rightarrow\; |\psi\rangle$
  - fermions $|\psi\rangle \;\rightarrow\; \mathrm{e}^{i\pi}|\psi\rangle \;=-|\psi\rangle$
  - anyons $|\psi\rangle \;\rightarrow\; \mathrm{e}^{i\varphi}|\psi\rangle$, φ takes any value



Physical examples

- **Quantum Hall Effect: Integer, Fractional**

  Quantized Hall conductivity

$$\sigma_{xy} = n\frac{e^2}{h}, \quad n = \frac{1}{2\pi}\int_{BZ} \mathcal{F}(k) d^2k$$

K. v Klitzing, G. Dorda, M. Pepper, Phys. Rev. Lett. **45** 494

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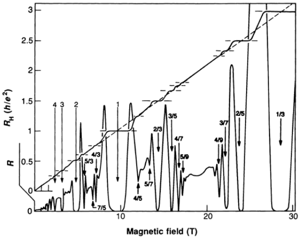

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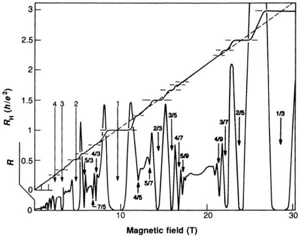

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- **Polarization in crystals**

  Definition of polarization as Berry phase in reciprocal space:

$$P = e\langle\varphi(R)|r - R|\varphi(R)\rangle = \frac{ie}{2\pi}\int_{BZ} \langle u(k)|\nabla_k|u(k)\rangle$$

where $\varphi(R)$ are localized (at R) Wannier orbitals:

$$|\varphi(R)\rangle = \int_{BZ} \frac{dk}{2\pi} \mathrm{e}^{-ik(R-r)}|u(k)\rangle$$

Conclusions

- **Adiabatic theorem**: fast and slow processes in physics:

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is gauge independent if the integral is over a closed loop in parameter space.

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  is gauge independent if the integral is over a closed loop in parameter space.

- Relations to:
  - crystals and their electric polarization
  - Aharonov-Bohm effect
  - QHE, topological order and anyons

2. General formula for phase factor

Let the Hamiltonian $\hat{H}$ be changed by varying parameters $\boldsymbol{R} = (X, Y, \ldots)$ on which it depends. Then the excursion of the system between times $t = 0$ and $t = T$ can be pictured as transport round a closed path $\boldsymbol{R}(t)$ in parameter space, with Hamiltonian $\hat{H}(\boldsymbol{R}(t))$ and such that $\boldsymbol{R}(T) = \boldsymbol{R}(0)$. The path will henceforth be called a circuit and denoted by C. For the adiabatic approximation to apply, T must be large.

The state $|\psi(t)\rangle$ of the system evolves according to Schrödinger's equation

$$\hat{H}(\boldsymbol{R}(t))\,|\psi(t)\rangle = \mathrm{i}\hbar\,|\dot{\psi}(t)\rangle. \tag{1}$$

At any instant, the natural basis consists of the eigenstates $|n(\boldsymbol{R})\rangle$ (assumed discrete) of $\hat{H}(\boldsymbol{R})$ for $\boldsymbol{R} = \boldsymbol{R}(t)$, that satisfy

$$\hat{H}(\boldsymbol{R})\,|n(\boldsymbol{R})\rangle = E_n(\boldsymbol{R})\,|n(\boldsymbol{R})\rangle, \tag{2}$$

with energies $E_n(\boldsymbol{R})$. This eigenvalue equation implies no relation between the phases of the eigenstates $|n(\boldsymbol{R})\rangle$ at different $\boldsymbol{R}$. For present purposes any (differentiable) choice of phases can be made, provided $|n(\boldsymbol{R})\rangle$ is single-valued in a parameter domain that includes the circuit C.

Adiabatically, a system prepared in one of these states $|n(\boldsymbol{R}(0))\rangle$ will evolve with $\hat{H}$ and so be in the state $|n(\boldsymbol{R}(t))\rangle$ at t.

Thus $|\psi\rangle$ can be written as

$$|\psi(t)\rangle = \exp\left\{\frac{-\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\,E_n(\boldsymbol{R}(t'))\right\}\exp\left(\mathrm{i}\gamma_n(t)\right)|n(\boldsymbol{R}(t))\rangle. \tag{3}$$

The first exponential is the familiar dynamical phase factor. In this paper the object of attention is the second exponential. The crucial point will be that its phase $\gamma_n(t)$ is *non-integrable*; γ_n cannot be written as a function of $\boldsymbol{R}$ and in particular is not single-valued under continuation around a circuit, i.e. $\gamma_n(T) \neq \gamma_n(0)$.

The function $\gamma_n(t)$ is determined by the requirement that $|\psi(t)\rangle$ satisfy Schrödinger's equation, and direct substitution of (3) into (1) leads to

$$\dot{\gamma}_n(t) = \mathrm{i}\,\langle n(\boldsymbol{R}(t))\,|\,\nabla_{\boldsymbol{R}}\, n(\boldsymbol{R}(t))\rangle\cdot\dot{\boldsymbol{R}}(t). \tag{4}$$