Lecture 2: Berry phase
Berry phase

What is it?

Anholonomy effect in a cyclic adiabatic evolution of a closed quantum system

Time-dependent Schrödinger equation

\[ i \frac{d}{dt} |\Psi(t)\rangle = H(\vec{R}(t))|\Psi(t)\rangle \quad \vec{R}(t) = \vec{R}(t + T) \]

How to capture and exploit slowness in description of system’s dynamics?

Expand $|\Psi(t)\rangle$ in *instantaneous eigenbasis* $H(\vec{R})|\psi_m(\vec{R})\rangle = E_m(\vec{R})|\psi_m(\vec{R})\rangle$

Completeness $\hat{1} = \sum_{m}|\psi_m(\vec{R}(t))\rangle \langle \psi_m(\vec{R}(t))| \quad \text{at every } t$
\[ |\Psi(t)\rangle = \sum_{m} |\psi_m(\vec{R}(t))\rangle \langle \psi_m(\vec{R}(t))|\Psi(t)\rangle \equiv \sum_{m} |\psi_m(\vec{R}(t))\rangle \tilde{c}_m(t) \]

For convenience introduce \( \tilde{c}_m(t) = c_m(t)e^{-i \int_0^t dt' E_m(\vec{R}(t'))} \equiv c_m(t)e^{i \theta_m(t)} \)

and insert into TD-SE equations for \( c_m(t) \)

**Exercise 4:** Show that

\[ \dot{c}_n(t) = -c_n(t) \langle \psi_n| \frac{d}{dt} |\psi_n\rangle - \sum_{m \neq n} c_m(t)e^{i \theta_m(t)-i \theta_n(t)} \langle \psi_n| \frac{d}{dt} |\psi_m\rangle \]
\[ |\Psi(t)\rangle = \sum_m |\psi_m(\vec{R}(t))\rangle \langle \psi_m(\vec{R}(t)) |\Psi(t)\rangle \equiv \sum_m |\psi_m(\vec{R}(t))\rangle \tilde{c}_m(t) \]

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Solution:

\[ \sum_m \left( i|\psi_m\rangle c_m e^{i\theta_m} + i|\psi_m\rangle \dot{c}_m e^{i\theta_m} - |\psi_m\rangle c_m e^{i\theta_m} \dot{\theta}_m \right) = \sum_m E_m |\psi_m\rangle c_m e^{i\theta_m} \]

Use \( \dot{\theta}_m = -E_m \) and project on \( \langle \psi_n| \)
Exercise 5: Show that for $m \neq n$ it holds

$$
\langle \psi_n | \frac{d}{dt} | \psi_m \rangle = -\frac{\langle \psi_n | \dot{H} | \psi_m \rangle}{E_n - E_m}
$$
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$$\langle \psi_n | \frac{d}{dt} | \psi_m \rangle = -\frac{\langle \psi_n | \dot{H} | \psi_m \rangle}{E_n - E_m}$$

Solution: Differentiate instantaneous eigenvalue problem

$$\dot{H} | \psi_m \rangle + H | \dot{\psi}_m \rangle = \dot{E}_m | \psi_m \rangle + E_m | \dot{\psi}_m \rangle$$

and project on $\langle \psi_n |$
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Solution: Differentiate instantaneous eigenvalue problem

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\dot{H} | \psi_m \rangle + H | \dot{\psi}_m \rangle = \dot{E}_m | \psi_m \rangle + E_m | \dot{\psi}_m \rangle
\]

and project on \( \langle \psi_n | \) 

Conclusion:

\[
\dot{c}_n(t) = -c_n(t) \langle \psi_n | \frac{d}{dt} | \psi_n \rangle + \sum_{m \neq n} c_m(t) e^{i\theta_m(t) - i\theta_n(t)} \frac{\langle \psi_n | \dot{H} | \psi_m \rangle}{E_n - E_m}
\]
**Adiabatic approximation**

\[
\dot{H} = \frac{\partial H}{\partial \vec{R}} \cdot \frac{d\vec{R}}{dt}, \quad \frac{d\vec{R}}{dt} \propto \Omega \equiv \frac{2\pi}{T}
\]

If at every \( t \)

\[
\frac{\Omega}{|E_n(t) - E_m(t)|} \ll 1 \quad \text{(slow driving does not excite transitions between levels)}
\]

approximate

\[
\dot{c}_n(t) \approx -c_n(t)\langle \psi_n | \frac{d}{dt} | \psi_n \rangle
\]
**Adiabatic approximation**

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(slow driving does not excite transitions between levels)

approximate

\[ \dot{c}_n(t) \approx -c_n(t)\langle \psi_n | \frac{d}{dt} | \psi_n \rangle \]

**Initial conditions:**

\[ c_1(0) = 1, \quad c_{n \neq 1}(0) = 0 \]

Solution of dynamical problem

\[ |\Psi(t)\rangle \approx |\psi_1(t)\rangle e^{i\theta_1(t)} e^{i\gamma_1(t)} \]

\[ \gamma_1(t) = i \int_0^t dt' \langle \psi_1(t') | \dot{\psi}_1(t') \rangle \]

**geometric phase**
Geometric properties

After one cycle

$$\langle \Psi(0)|\Psi(T)\rangle = e^{i\theta_1(T)}e^{i\gamma_1(T)}$$

Accumulated geometric phase can not be gauged away!

Moreover, it can be observed (interferometry!) as it is a *relative* phase.
Geometric properties

After one cycle

\[ \langle \Psi(0) | \Psi(T) \rangle = e^{i\theta_1(T)} e^{i\gamma_1(T)} \]

Accumulated geometric phase can not be gauged away!

Moreover, it can be observed (interferometry!) as it is a relative phase.

How to distinguish between dynamical and geometric phases?

They have different properties. In particular,

\[ \gamma_n(T) = i \int_0^T dt \langle \psi_n | \frac{d}{dt} | \psi_n \rangle = i \oint_c d\vec{R} \cdot \langle \psi_n | \frac{\partial}{\partial \vec{R}} | \psi_n \rangle \]

does not depend on velocity of parameter change
**Geometric properties**

*Berry connection*

\[ \tilde{A}_n(\bar{R}) = i \langle \psi_n | \frac{\partial}{\partial \bar{R}} | \psi_n \rangle \]

\[ \gamma_n(C) = \oint_C d\bar{R} \cdot \tilde{A}_n(\bar{R}) \quad \text{circulation of Berry connection} \]

Geometric meaning of \( e^{i \gamma_n(C)} \): anholonomy in parallel transport

Vector \( |\psi_n(\bar{R})\rangle \) is transported along the loop on parameter manifold and does not return to itself
Geometric properties

Gauge freedom: re-define

\[ |\psi_n(\vec{R})\rangle \rightarrow e^{i\varphi_n(\vec{R})} |\psi_n(\vec{R})\rangle = |\tilde{\psi}_n(\vec{R})\rangle \]

\[ \varphi_n(\vec{R}) - \text{arbitrary differentiable function} \]

This implies

\[ \tilde{\mathcal{A}}_n(\vec{R}) = \mathcal{A}_n(\vec{R}) - \frac{\partial \varphi_n(\vec{R})}{\partial \vec{R}} \]

transformation law of a vector potential

Parallel transport gauge

\[ \varphi_n(\vec{R}(t)) = -\gamma_n(t), \quad \text{or} \quad \tilde{\mathcal{A}}_n(\vec{R}) = 0 \]

Can we choose continuous \( \varphi_n(\vec{R}) \) globally? NO! (otherwise \( e^{i\gamma_n(\vec{C})} = 1 \))
Geometric properties

What is an obstacle? *Berry curvature* and its flux (both gauge-invariant)

Stokes theorem ($d = 3$)

$$\oint_{c=\partial S} d\vec{R} \cdot \vec{A}_n(\vec{R}) = \int_S d\vec{S} \cdot \vec{\Omega}_n(\vec{R})$$  

$$\vec{\Omega}_n(\vec{R}) = \nabla \times \vec{A}_n(\vec{R})$$

In $d > 3$

$$\int_{\partial S} dR^\mu A_{n,\mu}(\vec{R}) = \int_S \Omega_n(\vec{R})$$

$$\Omega_n = dA_n = \Omega_{n,\mu\nu} dR^\mu \wedge dR^\nu$$

$$\Omega_{n,\mu\nu} = \frac{\partial}{\partial R^\mu} A_{n,\nu} - \frac{\partial}{\partial R^\nu} A_{n,\mu}$$

Explicitly: $A_{n,\mu} = i \langle \psi_n | \frac{\partial}{\partial R^\mu} | \psi_n \rangle$,  

$$\Omega_{n,\mu\nu} = -2 \text{Im} \left( \frac{\partial \psi_n}{\partial R^\mu} \frac{\partial \psi_n}{\partial R^\nu} \right)$$
Important conclusions:

- Geometric description of a (quantum closed) system in adiabatic regime: System follows instantaneous eigenstate (well-separated from other states). Effect of other states is condensed to a single number – geometric phase

- Geometric description is associated with some gauge freedom: It is necessary to identify it to pursue such a description

- Despite gauge freedom, anholonomy effect (geometric phase) is independent of a chosen gauge. Moreover, geometric phase is observable
1) Spin $\frac{1}{2}$ in slowly rotating magnetic field

$$H = \frac{1}{2} \vec{\sigma} \cdot \vec{B}(t), \quad \vec{B}(t) = B \begin{pmatrix} \cos \phi(t) \sin \theta(t) \\ \sin \phi(t) \sin \theta(t) \\ \cos \theta(t) \end{pmatrix} = B \vec{n}(t)$$

Instantaneous EV problem:

$$H|\psi_{\pm}\rangle = E_{\pm}|\psi_{\pm}\rangle, \quad E_{\pm} = \pm \frac{1}{2} B$$

Solution:

Northern gauge

$$|\psi^N_+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi} \\ \sin \frac{\theta}{2} \end{pmatrix}, \quad |\psi^N_-\rangle = \begin{pmatrix} \sin \frac{\theta}{2} e^{-i\phi} \\ -\cos \frac{\theta}{2} \end{pmatrix}$$

Southern gauge

$$|\psi^S_+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix}, \quad |\psi^S_-\rangle = \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

In both gauges wavefunctions are single-valued
Berry connections:

\[ \mathcal{A}^N_\pm = i \langle \psi^N_\pm | \frac{\partial}{\partial \vec{R}} | \psi^N_\pm \rangle \cdot d\vec{R} \]

\[ = \frac{1}{2} (1 - \cos \theta) d\phi \]

\[ \quad \text{Northern gauge} \]

\[ \mathcal{A}^S_\pm = i \langle \psi^S_\pm | \frac{\partial}{\partial \vec{R}} | \psi^S_\pm \rangle \cdot d\vec{R} \]

\[ = -\frac{1}{2} (1 + \cos \theta) d\phi \]

\[ \quad \text{Southern gauge} \]

Dirac monopole potential with \( g = \frac{1}{2} \)

Gauge transformation:
\[ |\psi^S_-\rangle = e^{i\phi} |\psi^N_-\rangle, \quad \mathcal{A}^S_- = \mathcal{A}^N_- - d\phi \]

Berry curvature:
\[ \Omega_- = \frac{1}{2} \sin \theta d\theta \wedge d\phi \]

Berry phase:
\[ \gamma_- (C) = \int_S \Omega_- = \frac{1}{2} S = \frac{1}{2} \times \text{[area enclosed by } C\text{]} \]

Analogously for excited state \( \gamma_+ (C) = -\frac{1}{2} S \)

Note that \( \gamma_+ (C) + \gamma_- (C) = 0 \)
Examples

2) Berry-Zak phase of 1d crystal band structure

Tight-binding model of 1d crystal

\[ H = \sum_{\nu', l=1}^{M} \sum_{j=1}^{N} \sum_{\delta=-1,0,1} h_{\nu' l}(\delta) c_{\nu', j}^\dagger + \delta c_{\nu, j} \]

\( N \) sites, PBC
\( M \) orbitals on each site

Basis of Bloch waves

\[ c_{l, k} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ikj} c_{l, j}, \quad k \in \frac{2\pi}{N} \cdot \left\{ -\frac{N}{2}, \ldots, \frac{N}{2} - 1 \right\} \]  
(for even \( N \))

In TD limit \( N \to \infty \):

\[ c_{l, j} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikj} c_{l, k} \]

first Brillouin zone (1BZ)
Examples

2) Berry-Zak phase of 1d crystal band structure

Bloch Hamiltonian

\[ H = \sum_k \sum_{l,l'}^{M} \hat{h}_{l',l}(k) c_{l',k}^\dagger c_{l,k} \]  

(in second quantization)

\[ \hat{h}_{l',l}(k) = \sum_{\delta = -1,0,1} h_{l',l}(\delta) e^{-ik\delta} = h_{l',l}(-1)e^{ik} + h_{l',l}(0) + h_{l',l}(1)e^{-ik} \]  

(for NN hoppings)

Periodicity:

\[ \hat{h}(k) = \hat{h}(k + 2\pi) \]

Diagonalization gives band structure \( (m = 1, \ldots, M) \)

\[ \hat{h}(k)|u^{(m)}(k)\rangle = \varepsilon^{(m)}(k)|u^{(m)}(k)\rangle \]

For each band:

\[ A^{(m)}(k) = i\langle u^{(m)}(k)|\frac{d}{dk}|u^{(m)}(k)\rangle \quad \text{and} \quad \gamma^{(m)} = \int_{-\pi}^{\pi} dk A^{(m)}(k) \]

Berry connection

Zak phase
Discrete Berry phase

Label discrete $k$ from left to right of BZ by $1, \ldots, N$

Define trace of projector’s product:

$$\text{Tr} \left[ |u_N^{(m)}\rangle \langle u_N^{(m)}| u_{N-1}^{(m)} \rangle \langle u_{N-1}^{(m)}| \ldots \langle u_n^{(m)}| u_{n-1}^{(m)} \rangle \langle u_{n-1}^{(m)}| \ldots \langle u_2^{(m)}| u_1^{(m)} \rangle \langle u_1^{(m)}| \right]$$

$$\frac{|\langle u_N^{(m)}| u_{N-1}^{(m)} \rangle| \ldots \cdot |\langle u_n^{(m)}| u_{n-1}^{(m)} \rangle| \ldots \cdot |\langle u_2^{(m)}| u_1^{(m)} \rangle| \cdot |\langle u_1^{(m)}| u_N^{(m)} \rangle|}{\prod_{n=1}^{N} |\langle u_n^{(m)}| u_{n-1}^{(m)} \rangle|} \equiv \prod_{n=1}^{N} e^{i\Delta \varphi_{n,n-1}} \equiv e^{-i\gamma^{(m)}}$$
Discrete Berry phase

Equivalence to continuous Zak phase in TD limit

\[
\frac{\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle}{|\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle|} \approx 1 + \langle u^{(m)}(k) | \frac{d}{dk} u^{(m)}(k) \rangle \Delta k
\]

\[
\prod_{n=1}^{N} \frac{\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle}{|\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle|} = \exp \left[ -i \sum_{n=1}^{N} i \ln \frac{\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle}{|\langle u^{(m)}_n | u^{(m)}_{n-1} \rangle|} \right] \approx \exp \left[ -i \int_{-\pi}^{\pi} A^{(m)}(k) dk \right]
\]

Understanding ahholonomy in \textit{parallel transport gauge}

\[
\langle \tilde{u}^{(m)}(k) | \frac{d}{dk} \tilde{u}^{(m)}(k) \rangle = 0
\]

\[
\frac{\langle \tilde{u}^{(m)}_n | \tilde{u}^{(m)}_{n-1} \rangle}{|\langle \tilde{u}^{(m)}_n | \tilde{u}^{(m)}_{n-1} \rangle|} = 1
\]

\textit{continuous} \quad \textit{discrete}
Discrete Berry phase

Explicit construction

\[ |\tilde{u}_1\rangle = |u_1\rangle, \quad |\tilde{u}_2\rangle = \frac{\langle u_2 | \tilde{u}_1 \rangle}{\langle u_2 | \tilde{u}_1 \rangle} |u_2\rangle = e^{i\Delta \varphi_{21}} |u_2\rangle, \]

\[ |\tilde{u}_3\rangle = \frac{\langle u_3 | \tilde{u}_2 \rangle}{\langle u_3 | \tilde{u}_2 \rangle} |u_3\rangle = e^{i\Delta \varphi_{32} + i\Delta \varphi_{21}} |u_3\rangle, \quad \ldots \]

\[ |\tilde{u}_N\rangle = \frac{\langle u_N | \tilde{u}_{N-1} \rangle}{\langle u_N | \tilde{u}_{N-1} \rangle} |u_N\rangle = e^{i \sum_{j=2}^{N} \Delta \varphi_{n,n-1}} |u_N\rangle \]

\[ e^{i\Delta \varphi_{n,n-1}} = \frac{\langle u_n^{(m)} | u_{n-1}^{(m)} \rangle}{\langle u_n^{(m)} | u_{n-1}^{(m)} \rangle} \]

**definition**

\[ \frac{\langle \tilde{u}_n | \tilde{u}_{n-1} \rangle}{\langle \tilde{u}_n | \tilde{u}_{n-1} \rangle} = 1 \quad (n \geq 2) \]

**property**

\[ \prod_{n=1}^{N} \frac{\langle \tilde{u}_n | \tilde{u}_{n-1} \rangle}{\langle \tilde{u}_n | \tilde{u}_{n-1} \rangle} = \frac{\langle \tilde{u}_1 | \tilde{u}_N \rangle}{\langle \tilde{u}_1 | \tilde{u}_N \rangle} = e^{i \sum_{j=2}^{N} \Delta \varphi_{n,n-1}} \frac{\langle u_1 | u_N \rangle}{\langle u_1 | u_N \rangle} = e^{i \sum_{j=1}^{N} \Delta \varphi_{n,n-1}} = e^{-i \gamma} \]

**Parallel transport gauge:** whole phase accumulated in last jump
Summary of this lecture

- Geometric description of adiabatic unitary evolution:
  - gauge freedom as a prerequisite
  - Berry phase (anholonomy in parallel transport)
  - observable (cannot be gauged away)
- Berry-Zak phase in 1d crystal band structure:
  - gauge freedom, $k$-vector periodicity
- Discrete Berry phase: explicit check of gauge invariance