The Berry phase in quantum mechanics

Motivation: The past decade has seen tremendous developments in various branches of physics, related to topology and (quantum) geometry.

- Nobel Prize in Physics 2016 (Thouless, Kosterlitz, Haldane)
- Breakthrough Prize 2018 (Kane, Mele) → topological insulators, quantum spin Hall effect

Key concept: quantum-mechanical wavefunctions have an intrinsic property that measures how they change when moving in some parameter space; this can lead to new forces, new phenomena, and new states of matter.

Starting point: time-dependent Schrödinger equation

\[ i \hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \]

\[ |\psi(0)\rangle = |0\rangle = \text{ground state of } \hat{H}(0) \text{ for simplicity (not necessary to define Berry phase)} \]

Assumptions:
1. Time dependence in \( \hat{H}(t) \) is slow (see below)
2. \( \hat{H}(T) = \hat{H}(0) \) periodic

Question: What is \( |\psi(T)\rangle \)? We will see that there is a non-intuitive geometric/topological contribution.

Let us assume that \( \hat{H} \) depends on time via a parameter vector \( \lambda \):
\[ i\hbar \partial_t |\psi(t)\rangle = \hat{H} \left[ \hat{\lambda}(t) \right] |\psi(t)\rangle \]
\[ \hat{\lambda}(0) = \hat{\lambda}(t) \]
e.g. magnetic field

- What does "slow" temporal variation mean?
- Define instantaneous eigenstates \( |n; t\rangle \):
  \[ \hat{H} \left[ \hat{\lambda}(t) \right] |n; t\rangle = E_n(t) |n; t\rangle \]

One can show: "slowness" (adiabaticity) \( \Leftrightarrow \)
\[ |\langle n; t | \hat{\lambda}(t) | 0; t \rangle| \ll \left[ E_n(t) - E_0(t) \right] / \tau \]
for all \( t \) and all \( n \geq 0 \).
Here \( \tau \) is a characteristic time scale for temporal variation of \( \hat{H}(t) \), e.g., \( T_{\text{wo}} \).

\[ \Rightarrow \text{for adiabatic evolution, transitions to excited states suppressed.} \]

**Geometric phase = Berry phase:**
\[
\begin{align*}
\text{Geometric} & \quad \text{Berry phase:} \\
\begin{cases} 
  i\hbar \partial_t |\psi(t)\rangle = \hat{H} \left[ \hat{\lambda}(t) \right] |\psi(t)\rangle \\
  |\psi(t)\rangle = e^{i\varphi(t)} |0; t\rangle, \quad \varphi(0) = 0
\end{cases}
\end{align*}
\]

Only phase is allowed, since norm must be conserved

\[ i\hbar \partial_t |\psi(t)\rangle = E_0(t) |\psi(t)\rangle \]
\[ \varphi(t) = -\frac{1}{\hbar} \int_0^t E_0(t') dt' + \gamma \]
\[ \gamma = \Omega_d = \text{dynamical phase} \quad \text{(always present)} \]
\[ \text{Berry phase} \]
\[ \Rightarrow \text{i} \hbar \partial_t \left[ e^{i \theta_d} e^{i \mathbf{A} \cdot \mathbf{r}} \left| 0; t \right> \right] = E_0(t) \left| 0; t \right> \]

\[ \Rightarrow \text{i} \hbar \left( \text{i} \partial_d \right) \left| \psi(t) \right> + \text{i} \hbar \left( \text{i} \partial_t \right) \left| \psi(t) \right> + \text{i} \hbar c \partial_t \left| 0; t \right> = e^{i \left( \theta_d + \mathbf{A} \cdot \mathbf{r} \right)} \left| 0; t \right> = E_0(t) \left| \psi(t) \right> \]

\[ \Rightarrow \mathbf{\dot{y}}(0; t) = \text{i} \partial_t \left| 0; t \right> \]

\[ \Rightarrow \mathbf{\gamma}(T) = \text{i} \int_0^T \left< 0; t \left| \frac{\partial}{\partial t} \left| 0; t \right> \right> dt \]

Geometric interpretation:

\[ \partial_t = \frac{\partial}{\partial t} = \frac{\partial \mathbf{A}}{\partial t} \frac{\partial}{\partial \mathbf{A}} \Rightarrow \mathbf{\gamma}_c = \text{i} \oint \left< 0; \mathbf{r} \left| \frac{\partial}{\partial \mathbf{A}} \left| 0; \mathbf{r} \right> \right> \cdot d\mathbf{A} \]

Definition:

\[ \mathbf{A}(\mathbf{r}) := \text{i} \left< 0; \mathbf{r} \left| \frac{\partial}{\partial \mathbf{A}} \right| 0; \mathbf{r} \right> \quad \text{"Berry connection"} \]

\[ = \text{vector potential} \]

\[ \Rightarrow \text{electromagnetism: magnetic field} \quad \mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) \]

Here: fictitious magnetic field

\[ \mathbf{B}(\mathbf{r}) := \nabla \times \mathbf{A}(\mathbf{r}) \]

\[ \Rightarrow \mathbf{\gamma}_c = \oint_{\mathbf{F}_c} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} = \iint \mathbf{B}(\mathbf{r}) \cdot d\mathbf{r}_c(\mathbf{r}) \]

\[ \Rightarrow \mathbf{\gamma}_c \quad \text{is the flux of a fictitious magnetic field,} \quad \mathbf{B}, \]

\[ \text{which is called Berry curvature.} \]
Question: Why is the Berry phase only well-defined on a closed loop $\gamma$?

(A) norm is not conserved on open contours
(B) adiabaticity can be violated if loop is not closed
(C) the wave function's phase can be modified at each point through a gauge transformation, hence the Berry phase is not gauge-invariant on open contours

Final remark: classical Hall effect is due to Lorentz force in $\vec{E}$ and $\vec{B}$ fields: $\vec{F} = q (\vec{E} + \vec{v} \times \vec{B})$.

The quantum (anomalous/spin) Hall effects are due to a quantum-geometric version: $\vec{F}_{\text{quantum}} = q (\vec{E} + \vec{v} \times \vec{B})$ (Berry curvature)