Michael Sentef – Lecture Turku (20 minutes)

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.

'TKNN', quantum Hall effect
quantum anomalous Hall effect

- 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

$$i\hbar \partial_t |\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

$$|\psi(0)\rangle = |0\rangle$$ = ground state of $\hat{H}(0)$ 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

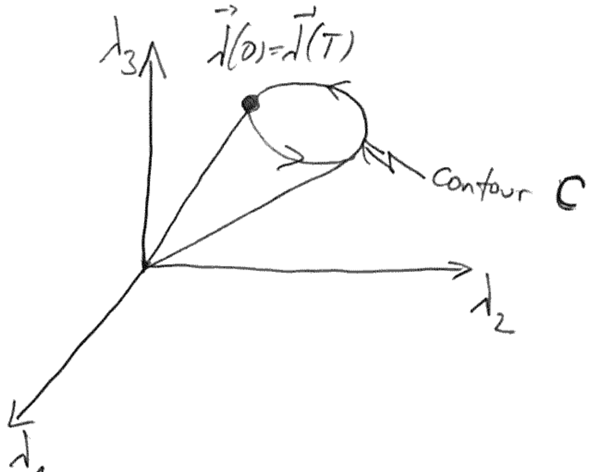
Question: What is $|\psi(T)\rangle$? We will see that there is a non-intuitive geometric/topological contribution.

Let us assume that $\hat{H}$ depends on time via a parameter, $\vec{\lambda}$:
vector

$$i\hbar\,\partial_t |\psi(t)\rangle = \hat{H}[\vec{\lambda}(t)]\,|\psi(t)\rangle$$

$$\vec{\lambda}(0) = \vec{\lambda}(t)$$

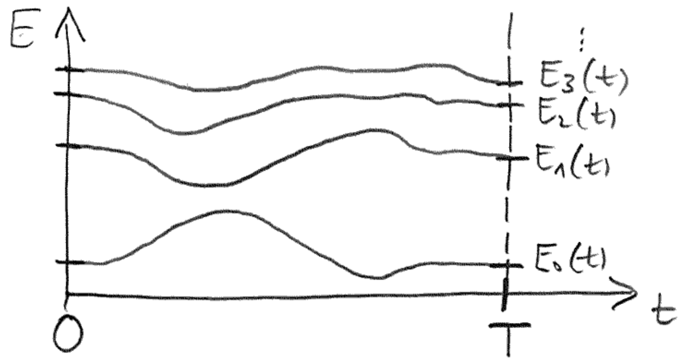
e.g. magnetic field



- what does "slow" temporal variation mean?

Define instantaneous eigenstates $|n;t\rangle$:

$$\hat{H}[\vec{\lambda}(t)]\,|n;t\rangle = E_n(t)\,|n;t\rangle$$



One can show: "slowness" (adiabaticity) $\Longleftrightarrow$

$$|\langle n;t|\,\dot{\hat{H}}(t)\,|0;t\rangle| \ll [E_n(t) - E_0(t)]/\tau$$

for all t and all $n>0$.

Here τ is a characteristic time scale for temporal variation of $\hat{H}(t)$, e.g., $\tau \sim T$.

$\Rightarrow$ for adiabatic evolution, transitions to excited states suppressed.

Geometric phase = Berry phase:

$$\begin{cases} i\hbar\,\partial_t |\psi(t)\rangle = H[\vec{\lambda}(t)]\,|\psi(t)\rangle \\ |\psi(t)\rangle = \underbrace{e^{i\varphi(t)}}_{\text{only phase is allowed, since norm must be conserved}}\,|0;t\rangle\,, \quad \varphi(0)=0 \end{cases}$$

$$\Rightarrow\ i\hbar\,\partial_t |\psi(t)\rangle = E_0(t)\,|\psi(t)\rangle$$

$$\varphi(t) = \underbrace{-\frac{1}{\hbar}\int_0^t E_0(t')\,dt'}_{=:\ \theta_d\ =\ \text{dynamical phase (always present)}} + \gamma$$

γ: Berry phase

$$\Rightarrow i\hbar\partial_t\left[e^{i\theta_d}e^{i\gamma}|0;t\rangle\right] = E_0(t)\,|\Psi(t)\rangle$$

$$\Rightarrow \underbrace{i\hbar\,(i\dot{\theta}_d)\,|\Psi(t)\rangle}_{=E_0(t)\,|\Psi(t)\rangle} + i\hbar\,(i\dot{\gamma})\underbrace{|\Psi(t)\rangle}_{=e^{i(\theta_d+\gamma)}|0;t\rangle} + i\hbar\, e^{i(\theta_d+\gamma)}\partial_t|0;t\rangle = E_0(t)\,|\Psi(t)\rangle$$

→ cancels against right-hand side

$$\Rightarrow \left.\begin{array}{l}\dot{\gamma}(0;t) = i\partial_t|0;t\rangle \\ \oplus \text{ normalization } \langle 0;t|0;t\rangle = 1\end{array}\right\} \Rightarrow \boxed{\gamma(T) = i\int_0^T \langle 0;t|\frac{\partial}{\partial t}|0;t\rangle\, dt}$$

Berry phase (Berry 1948)

<u>Geometric interpretation:</u>

$$\partial_t = \frac{\partial}{\partial t} = \frac{\partial\vec{\lambda}}{\partial t}\frac{\partial}{\partial\vec{\lambda}} \rightarrow \boxed{\gamma_C = i\oint \langle 0;\vec{\lambda}|\frac{\partial}{\partial\vec{\lambda}}|0;\vec{\lambda}\rangle \cdot d\vec{\lambda}}$$

geometric phase

<u>Def.:</u> $\vec{\mathcal{A}}(\vec{\lambda}) := i\langle 0;\vec{\lambda}|\frac{\partial}{\partial\vec{\lambda}}|0;\vec{\lambda}\rangle$ "Berry connection"

$\hat{=}$ vector potential

→ electromagnetism: magnetic field $\vec{B}(\vec{r}) = \vec{\nabla}_{\vec{r}} \times \vec{A}(\vec{r})$

Here: fictitious magnetic field

$$\vec{\mathcal{B}}(\vec{\lambda}) := \vec{\nabla}_{\vec{\lambda}} \times \vec{\mathcal{A}}(\vec{\lambda})$$

$$\Rightarrow \gamma_C = \oint \vec{\mathcal{A}}(\vec{\lambda})\cdot d\vec{\lambda} = \iint_{F_C} \vec{\mathcal{B}}(\vec{\lambda})\cdot d\vec{f}_C(\vec{\lambda})$$

⇒ γ_C is the flux of a fictitious magnetic field, $\mathcal{B}$, which is called Berry curvature.

Question: Why is the Berry phase only well-defined on a closed loop $\oint$?

(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: "$\vec{F}_{quantum} = q(\vec{E} + \vec{v} \times \vec{\mathcal{B}})$"

Berry curvature