Adiabaticity in QM

- consider Hamiltonian w/ slowly changing parameter $\lambda(t)$

  $H = H(\lambda(t))$

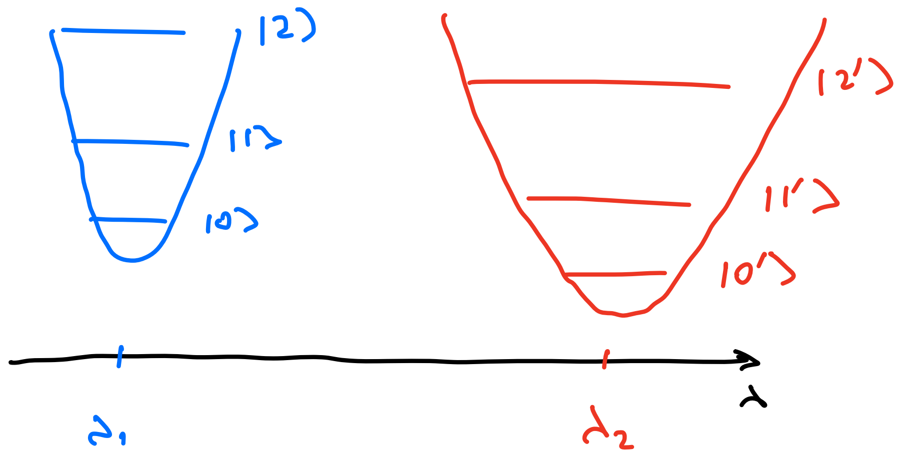
  e.g. $H(\lambda(t)) = H_0 + \lambda(t) H_1$

· instantaneous e'states: $H(\lambda)|\psi_n[\lambda]\rangle = E_n(\lambda)|\psi_n[\lambda]\rangle$

ONB: $\langle\psi_n[\lambda]|\psi_m[\lambda]\rangle = \delta_{nm}$ $\forall \lambda$ fixed ($\Rightarrow \forall t$ fixed)

· time-evolved e'states $\neq$ inst. e'states

$$|\psi_n(t)\rangle = \mathcal{T} e^{-i\int_0^t ds\, H(\lambda(s))}|\psi_n[0]\rangle \neq |\psi_n[\lambda(t)]\rangle$$



$\Rightarrow \langle\psi_n[\lambda_1]|\psi_m[\lambda_2]\rangle \neq \delta_{nm}$

<u>not</u> ONB at $\lambda_1 \neq \lambda_2$

- Adiabatic theorem

A quantum system remains in its inst. e'state upon a change of parameter $\lambda(t)$, if:

(i) the inst. e'state is gapped at all times

(ii) the rate of change in the parameter, $\dot{\lambda}$, remains small compared to the energy gap Δ to nearby levels:

$$\left|\frac{\dot{\lambda}}{\Delta(\lambda)}\right| \times |\langle\psi_m[\lambda]|\partial_\lambda H|\psi_n[\lambda]\rangle| \ll 1 \quad \forall \lambda$$

inst. gap: $\Delta(\lambda) = E_m(\lambda) - E_n(\lambda)$

intuitively: "total ramp/evolution time T should be larger than the inverse gap Δ^{-1}"

proof:

idea: apply time-dep. pert. theory on top of evolution of inst. e/states

caveat: need to take care of phase of wavefn.

starting point: $H = H(\lambda(t)) = H(t)$

$$i\partial_t |\Psi(t)\rangle = H(t)|\Psi(t)\rangle \quad (*)$$

→ if H did not depend on time:

$H|\varphi_n\rangle = E_n|\varphi_n\rangle \Rightarrow |\varphi_n(t)\rangle = e^{-itE_n}|\varphi_n(0)\rangle$

. arbitrary state: $|\Phi(t)\rangle = \sum_n c_n e^{-itE_n}|\varphi_n(0)\rangle$

→ for $H = H(t)$ time-dep.

. consider inst. e'basis $|\psi_n[\lambda(t)]\rangle = |\psi_n[t]\rangle$

$H(t)|\psi_n[t]\rangle = E_n(t)|\psi_n[t]\rangle$; $\langle\psi_n[t]|\psi_m[t]\rangle = \delta_{nm}$ ONB

↳ can expand soln. of $(*)$ at each fixed time t:

$$|\Psi(t)\rangle = \sum_n a_n(t)|\psi_n[t]\rangle$$
$$= \sum_n c_n(t)e^{i\phi_n(t)}|\psi_n[t]\rangle$$

where: $a_n(t) := c_n(t)e^{-i\int_0^t ds\, E_n(s)}$

& $\phi_n(t) = -\int_0^t ds\, E_n(s)$ dynamical phase

→ next, plug this ansatz in $(*)$:

$$i\sum_n\Big(\dot c_n|\psi_n\rangle + c_n|\dot\psi_n\rangle + c_n|\psi_n\rangle \underbrace{i\dot\phi_n}_{= E_n(t)}\Big)e^{i\phi_n} = \sum_n c_n \underbrace{H(t)|\psi_n[t]\rangle}_{= E_n(t)|\psi_n[t]\rangle} e^{i\phi_n}$$

$$\Rightarrow \cancel{i}\sum_n\big(\dot c_n|\psi_n\rangle + c_n|\dot\psi_n\rangle\big)e^{i\phi_n(t)} = 0$$

$$\sum_n \dot c_n(t)|\psi_n[t]\rangle e^{i\phi_n(t)} = -\sum_n c_n(t)|\dot\psi_n[t]\rangle e^{i\phi_n(t)} \quad / \langle\psi_m[t]|\cdot$$

$$\sum_n \dot{c}_n \underbrace{\langle \psi_m[t] | \psi_n[t] \rangle}_{=\delta_{mn}} e^{i\phi_n} = - \sum_n c_n \langle \psi_m[t] | \dot{\psi}_n[t] \rangle e^{i\phi_n}$$

$$\Rightarrow \quad \dot{c}_m(t) = - \sum_n c_n(t) \langle \psi_m[t] | \dot{\psi}_n[t] \rangle e^{i(\phi_n(t) - \phi_m(t))}$$

- fix $n \neq m$

$$\langle \psi_m[t] | \underbrace{H(t) | \psi_n[t] \rangle}_{= E_n(t) |\psi_n[t]\rangle} = E_n(t) \langle \psi_m[t] | \psi_n[t] \rangle \overset{m \neq n}{=} 0 \quad / \frac{d}{dt}$$

$$0 = \langle \dot{\psi}_m | H | \psi_n \rangle + \langle \psi_m | H | \dot{\psi}_n \rangle + \langle \psi_m | \dot{H} | \psi_n \rangle$$

$$= E_n \underbrace{\langle \dot{\psi}_m | \psi_n \rangle}_{= - \langle \psi_m | \dot{\psi}_n \rangle} + E_m \langle \psi_m | \dot{\psi}_n \rangle + \langle \psi_m | \dot{H} | \psi_n \rangle$$

$$\langle \psi_m | \psi_n \rangle = 0 \quad / d/dt$$

$$\langle \dot{\psi}_m | \psi_n \rangle + \langle \psi_m | \dot{\psi}_n \rangle = 0$$

$$= - (E_n(t) - E_m(t)) \langle \psi_m | \dot{\psi}_n \rangle + \langle \psi_m | \dot{H} | \psi_n \rangle$$

$$\Rightarrow \quad \langle \psi_m | \dot{\psi}_n \rangle = \langle \psi_m[t] | \partial_t | \psi_n[t] \rangle = -i \frac{\langle \psi_m[t] | i \partial_t H | \psi_n[t] \rangle}{E_n(t) - E_m(t)} \quad \forall n \neq m$$

Hellman - Feynman "theorem"

$$\dot{c}_m = - c_m(t) \langle \psi_m | \dot{\psi}_m \rangle - \sum_{n \neq m} c_n(t) \underbrace{\frac{\langle \psi_m[t] | \partial_t H | \psi_n[t] \rangle}{E_n(t) - E_m(t)}}_{(\square)} e^{i(\phi_n(t) - \phi_m(t))}$$

so far: exact

now: make approx. $(\square) \ll 1/t$, see condition (ii) of Ad. thm.

($\Leftrightarrow$ suppress transitions to other levels)

$$\dot{c}_m \approx i c_m \langle \psi_m[t] | i \partial_t | \psi_m[t] \rangle$$

solved by: $c_m(t) \approx c_m(0) \, e^{i \gamma_m(t)}$

where $\gamma_m(t) = \int_0^t ds \, \langle \psi_m[s] | i\partial_s | \psi_m[s] \rangle$

— geometric (Berry) phase

$\Rightarrow$ approx. soln:

initial cond. $c_m(0) = 1$; $c_n(0) = 0 \quad \forall n \neq m$

$$|\Psi(0)\rangle = c_m(0)\, |\psi_m[0]\rangle$$

$$|\Psi(t)\rangle \overset{(\square)}{\approx} c_m(0)\, e^{i\phi_m(t)}\, e^{i\gamma_m(t)}\, |\psi_m[t]\rangle$$

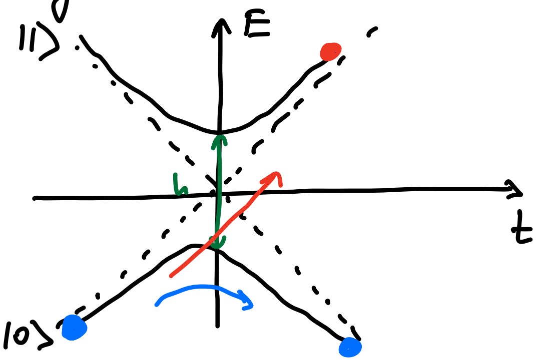
dyn. phase — geom. phase

Q: what happens $(\square)$ fails?

Landau-Zener-Problem

– two-level system (2LS) in linearly changing ext. field

$$H(t) = \frac{vt}{2}\sigma^z + \frac{h}{2}\sigma^x = \frac{1}{2}\begin{pmatrix} vt & h \\ h & -vt \end{pmatrix}$$

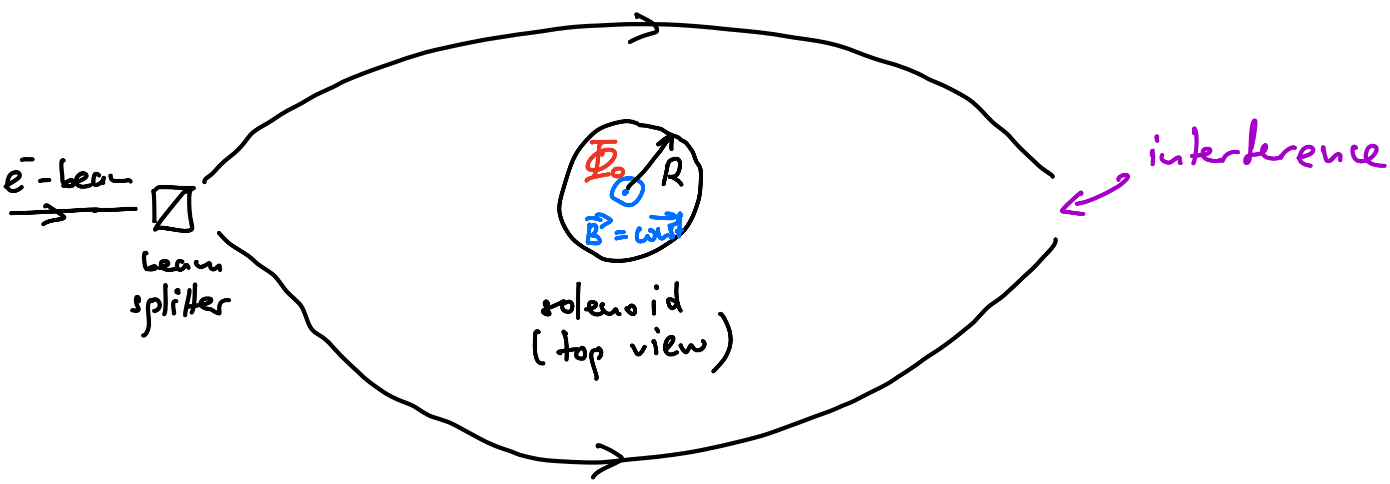


at $t \to -\infty$: $|\psi(t\to-\infty)\rangle = |0\rangle$

· interested in ratio of level occupations at $t \to +\infty$ compared to $t \to -\infty$

HW: $P_{LZ} = e^{-\frac{\pi}{2}\frac{h^2}{v}}$ exponentially suppressed in h^2/v

Aharonov-Bohm Effect



• flux thru solenoid:

$$\Phi_0 = \int \vec B\cdot d\vec a = B\pi R^2 \Rightarrow \vec B = \begin{cases} \frac{\Phi_0}{\pi R^2}\,\hat z, & \text{inside}: r\le R \\ \vec 0, & r>R \end{cases}$$

• recall $\vec B = \text{curl}\,\vec A = \vec\nabla\times\vec A$

$$\Phi_0 = \int \vec B\cdot d\vec a \underset{\substack{\uparrow\\ \text{Stokes}\\ \text{thm}}}{=} \oint_C \vec A\cdot d\vec r \Rightarrow \vec A = \begin{cases} \frac{\Phi_0}{2\pi}\frac{r}{R^2}\,\hat\varphi, & r\le R \\ \frac{\Phi_0}{2\pi r}\,\hat\varphi, & r\ge R \end{cases}$$

• Hamiltonian of charged particle

$$H = (\vec p + q\vec A)^2/2m + V(\vec r)$$

<u>want</u>: e'fns of H in terms of e'fns of $H_0 = \frac{p^2}{2m} + V(\vec r)$
w/o B-field

let $H_0\psi_0(\vec r) = E_0\psi_0(\vec r)$

<u>guess</u>: $\psi(\vec r) = e^{ig(\vec r)}\psi_0(\vec r)$

$$g(\vec r) = -q\int_{\vec r_0}^{\vec r}\vec A(\vec r')\cdot d\vec r' \qquad (*)$$
outside solenoid

<u>check</u>: $(\vec p + q\vec A)\psi(\vec r) = (-i\vec\nabla + q\vec A)\,e^{ig(\vec r)}\psi_0(\vec r)$

$$= e^{ig(\vec r)}\underbrace{(\vec\nabla g)}_{=-q\vec A}\psi_0 - ie^{ig}\nabla\psi_0 + q e^{ig}\vec A\psi_0$$

$$= e^{ig(\vec r)}\vec p\,\psi_0(\vec r)$$

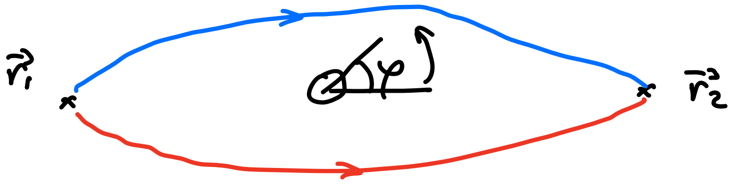
$\Rightarrow (\vec p + \vec A)^2\psi(\vec r) = e^{ig}p^2\psi_0(\vec r)$

$$\Rightarrow H\psi(\vec r) = e^{ig}\underbrace{\left(\frac{p^2}{2m} + V(\vec r)\right)\psi_0(\vec r)}_{= H_0\psi_0(\vec r) = E_0\psi_0(\vec r)} = E_0\,e^{ig}\psi_0 = E_0\psi(\vec r)$$

$\Rightarrow \psi(\vec r)$ is e'state of $H = (\vec p + q\vec A)^2/2m + V$ ✓

back to solenoid:

- consider two paths

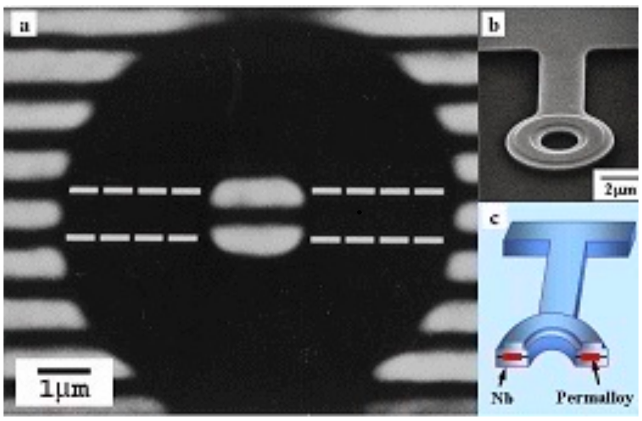


$$\varphi = -q\int_{\vec{r}_1}^{\vec{r}_2} \vec{A}\cdot d\vec{r} = \pm q \int_0^{\pi} \frac{\Phi_0}{2\pi \cancel{r}}\, \cancel{\hat{\varphi}} \cdot \cancel{r}\, d\varphi\, \cancel{\hat{\varphi}} = \pm q\, \frac{\Phi_0}{2}$$

$\Rightarrow$ phase of e^--wavefn. is different for $\frown$ & $\smile$ paths & depends on flux Φ_0 inside solenoid, although e^- never went thru region of finite B-field!

$\rightarrow$ can measure phase difference in interference experiment

$$\Delta\varphi = q\,\Phi_0 \qquad \text{Aharonov-Bohm phase}$$



Tonomura et al., PRL 1986

Q: how can we understand the AB effect using concepts from adiabaticity?

geometric phase: $\gamma_n(t) = \int_0^t ds\, \langle \psi_n[s] | i\partial_s | \psi_n[s] \rangle$

for $H = H(\lambda(t))$, s.t. $H(\lambda)|\psi_n(\lambda(t))\rangle = E_n(t)|\psi_n[\lambda(t)]\rangle$

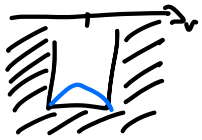
note: $i\partial_t = \dot{\lambda}\, i\partial_\lambda$

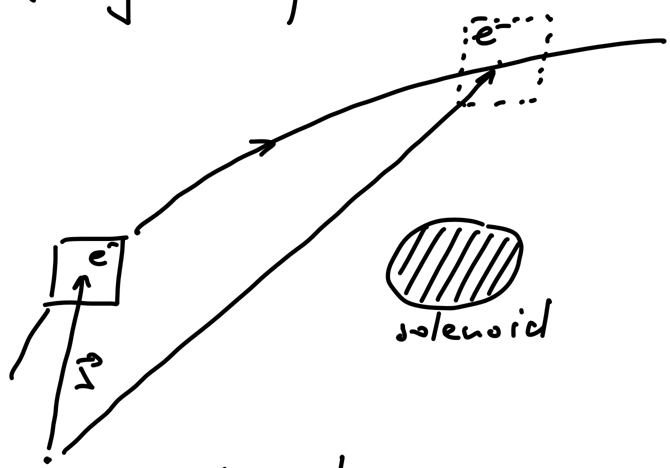
$$\Rightarrow \gamma_n = \int_{\vec{\lambda}(0)}^{\vec{\lambda}(t)} d\vec{\lambda}\, \langle \psi_n[\vec{\lambda}] | i\vec{\nabla}_\lambda | \psi_n[\vec{\lambda}] \rangle \quad \text{indep. of protocol } \vec{\lambda}(t)$$

$\rightarrow$ depends only on $\vec{\lambda}(0)$ & $\vec{\lambda}(t)$

– relation b/w AB phase & geom. phase?

• place e^- in box

$V(\vec r) =$ 



$\Rightarrow \langle \psi_0 | \vec p | \psi_0 \rangle = 0$

– wavefn of e^- in presence of solenoid

$$\psi_{\vec\lambda}(\vec r) = e^{i g_{\vec\lambda}(\vec r)} \psi_0(\vec r - \vec\lambda)$$

$$g_{\vec\lambda}(\vec r) = -q \int_{\vec\lambda}^{\vec r} \vec A(\vec r\,') \cdot d\vec r\,'$$

want.: $\gamma = \int_{\lambda_i}^{\lambda_f} d\vec\lambda \cdot \langle \psi_{\vec\lambda} | i \vec\nabla_\lambda | \psi_{\vec\lambda} \rangle$

$$i\vec\nabla_\lambda \psi_\lambda(\vec r) = q \vec A(\vec\lambda) e^{i g_\lambda(\vec r)} \psi_0(\vec r - \vec\lambda) + e^{i g_\lambda(\vec r)} \underbrace{(i\vec\nabla_\lambda)\psi_0(\vec r - \vec\lambda)}_{= -i\vec\nabla_r \psi_0(\vec r - \vec\lambda)}$$

$$\langle \psi_\lambda | i\vec\nabla_\lambda | \psi_\lambda \rangle = \int d^3 r\, e^{-i g_\lambda(\vec r)} \psi_0^*(\vec r - \vec\lambda) e^{+i g_\lambda(\vec r)} \left[q \vec A(\vec\lambda)\psi_0(\vec r - \vec\lambda) + \vec p\, \psi_0(\vec r - \vec\lambda) \right]$$

$$= q \vec A(\vec\lambda) \underbrace{\int d^3 r\, |\psi_0(\vec r - \vec\lambda)|^2}_{= \langle \psi_0 | \psi_0 \rangle = 1} + \underbrace{\int d^3 r\, \psi_0^*(\vec r - \vec\lambda)\, \vec p\, \psi_0(\vec r - \vec\lambda)}_{= \langle \psi_0 | \vec p | \psi_0 \rangle \underset{\text{box pot.}}{=} 0}$$

$$\Rightarrow \quad \langle \psi_\lambda | i\vec\nabla_\lambda | \psi_\lambda \rangle = q \vec A(\vec\lambda)$$

– geometric phase on a closed loop around solenoid:

$$\gamma = \oint q \vec A(\vec\lambda) \cdot d\vec\lambda \underset{\text{Stokes}}{=} q \int \vec\nabla_\lambda \times \vec A(\vec\lambda) \cdot d\vec a = q\, \Phi_0$$

geometric phase coincides w/ AB phase!

- analogy:

EM		QM
(i) AB phase $\varphi_{AB} = \oint \vec{A}\cdot d\vec{r}$	$\longleftrightarrow$	geom. phase $\gamma = \oint \vec{A}(\vec{\lambda})\cdot d\vec{\lambda}$
(ii) vector pot $\vec{A}(\vec{r})$	$\longleftrightarrow$	Berry connection $\vec{A}(\vec{\lambda}) = \langle \psi[\vec{\lambda}] \| i\vec{\nabla}_\lambda \| \psi[\vec{\lambda}]\rangle$
(iii) magnetic field / EM field tensor $F_{ab} = \partial_a A_b - \partial_b A_a = \varepsilon_{abc} B_c$	$\longleftrightarrow$	Berry curvature $F_{\mu\nu} = \partial_{\lambda_\mu} A_\nu - \partial_{\lambda_\nu} A_\mu$

$\hookrightarrow$ quantum geometry (later)