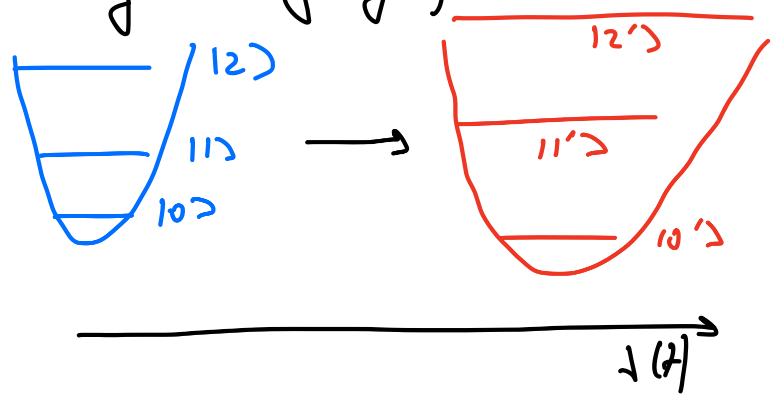
Non-adiabatic response of quantum systems

→ consider a Hamiltonian with slowly changing parameter $\lambda(t)$: $\quad H = H(\lambda(t))$



. instantaneous e'states:

$$H(\lambda)\,|\psi_n(\lambda)\rangle = E_n(\lambda)\,|\psi_n(\lambda)\rangle$$

$$\langle\psi_n(\lambda)|\psi_m(\lambda)\rangle = \delta_{nm} \qquad \forall \lambda \text{ fixed } (\forall t)$$

<u>note</u>: time-evolved states ≠ instant. e'states

$$|\psi_n(\lambda(t))\rangle \neq \mathcal{T}\exp\left(-i\int_0^t ds\; H(\lambda(s))\right)|\psi_n(\lambda(0))\rangle$$

$\Rightarrow \langle\psi_n(\lambda_1)|\psi_m(\lambda_2)\rangle$ <u>not</u> ONB at $\lambda_1 \neq \lambda_2$

Adabatic theorem

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

i) the inst. e'states are gapped at all times

ii) the change in parameter, $\dot\lambda$, remains small compared to the gap Δ to nearby levels:

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

<u>inst.</u> gap: $\quad \Delta(\lambda) = E_m(\lambda) - E_n(\lambda)$

"total ramp/evolution time T should be longer than inverse gap Δ^{-1}"

proof:

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

caveat: need to take care of dynamical phase of wavefu.

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:

$$|\Phi(t)\rangle = \sum_n c_n e^{-itE_n}|\varphi_n\rangle$$

→ $H = H(t)$ but consider inst. e'basis $|\psi_n(t)\rangle$:

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

$$\langle\psi_n(t)|\psi_m(t)\rangle = \delta_{nm} \quad \text{form ONB}$$

↳ can expand solu. of (*) for each fixed time t:

$$|\Psi(t)\rangle = \sum_n a_n(t)|\psi_n(t)\rangle$$

$$= \sum_n c_n(t) e^{i\theta_n(t)}|\psi_n(t)\rangle$$

where: $a_n(t) = c_n(t)\, e^{-i\int_0^t E_n(t')dt'}$

& $\theta_n(t) = -\int_0^t dt'\, E_n(t')$ _dynamical phase

→ plug this ansatz in (*):

$$i\sum_n \Big(\dot{c}_n|\psi_n\rangle + c_n|\dot{\psi}_n\rangle + c_n|\psi_n\rangle \underbrace{i\dot{\theta}_n}_{=E_n(t)}\Big)e^{i\theta_n} =$$

$$= \sum_n c_n(t) \underbrace{H(t)|\psi_n(t)\rangle}_{E_n(t)|\psi_n(t)\rangle} e^{i\theta_n(t)}$$

$$\Rightarrow i\sum_n \left(\dot{c}_n(t)|\psi_n(t)\rangle + c_n(t)|\dot{\psi}_n(t)\rangle\right) e^{i\theta_n(t)} = 0$$

$$\sum_n \dot{c}_n(t)|\psi_n(t)\rangle e^{i\theta_n(t)} = -\sum_n c_n(t)|\dot{\psi}_n(t)\rangle e^{i\theta_n(t)} \quad / \langle\psi_m(t)|\cdot$$

$$\sum_n \dot{c}_n \underbrace{\langle\psi_m(t)|\psi_n(t)\rangle}_{=\delta_{mn}} e^{i\theta_n} = -\sum_n c_n \langle\psi_m|\partial_t|\psi_n\rangle e^{i\theta_n}$$

$$\dot{c}_m(t) = -\sum_n c_n(t)\langle\psi_m(t)|\partial_t|\psi_n(t)\rangle e^{i(\theta_n(t)-\theta_m(t))}$$

$-$ fix $n \neq m$

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

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

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

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

$$\Rightarrow \langle\psi_m|\dot{\psi}_n\rangle = \frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m} \quad \forall n \neq m$$

$$\dot{c}_m = -c_m(t)\langle\psi_m(t)|\dot{\psi}_m(t)\rangle - \sum_{n\neq m} c_n(t)\frac{\langle\psi_m(t)|\partial_t H|\psi_n(t)\rangle}{E_n(t) - E_m(t)} e^{i(\theta_n(t)-\theta_m(t))}$$

so for : exact

make approx. $(\square) \ll 1$, see condition (ii) for ad. thm.
($\Leftrightarrow$ suppress transitions to other levels)

$$\dot{c}_m \approx i\, c_m \langle \psi_m(t) | i\partial_t | \psi_m(t) \rangle$$

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

where $\gamma_m(t) = \int_0^t dt' \langle \psi_m(t') | i\partial_{t'} | \psi_m(t') \rangle$ — Berry phase

$\Rightarrow$ approximate sln:

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

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

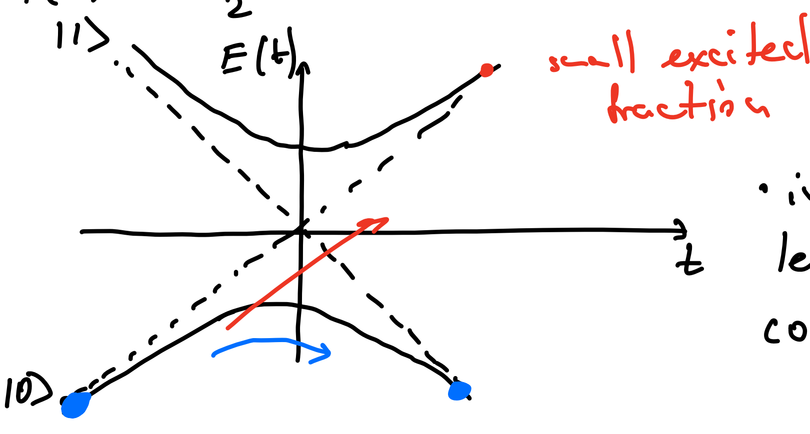
$$|\Psi(t)\rangle \overset{(\square)}{\approx} c_m(0)\, \underbrace{e^{i\theta_m(t)}}_{\text{dyn. phase}}\, \underbrace{e^{i\gamma_m(t)}}_{\text{Berry phase}}\, |\psi_m(t)\rangle$$

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

Landau - Zener Problem

- two-level system in a linearly changing field

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



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

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

ansatz: $|\psi(t)\rangle = c_1(t)\,|1\rangle + c_0(t)\,|0\rangle$

$$i\partial_t |\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$\Rightarrow \begin{cases} \dot{c}_1 = -i\frac{vt}{2}c_1 - i\frac{h}{2}c_0 \\ \dot{c}_0 = -i\frac{h}{2}c_1 + i\frac{vt}{2}c_0 \end{cases} \quad / \partial_t(\cdot)$$

$$\Rightarrow \ddot{c}_1 + \left(\frac{iv}{2} + \frac{h^2}{4} + \frac{v^2t^2}{2}\right)c_1 = 0 \qquad (*)$$

→ solved by the Weber fn

here: different approach

consider: $t \to \infty$: $H \longrightarrow \frac{vt}{2}\sigma^z$

$$c_1(t) \overset{t\to\infty}{\sim} \underbrace{|c_1|}_{=\text{const in time}} e^{-i\varphi(t)}$$

⇒ substitute in (*)

$$\Big[-i\ddot{\varphi} - \dot{\varphi}^2 + \frac{iv}{2} + \frac{h^2}{4} + \left(\frac{vt}{2}\right)^2\Big]\underbrace{c_1 = 0}_{\text{as } t\to\infty} \quad \Big/ \begin{matrix}\mathrm{Re}(\cdot)\\ \mathrm{Im}(\cdot)\end{matrix}$$

$$\begin{cases} \dot{\varphi} = \pm\frac{1}{2}\sqrt{h^2 + (vt)^2} \\ \ddot{\varphi} = \frac{v}{2} \end{cases} \quad \text{for } t \sim \infty$$

$$\dot{\varphi} = \pm\frac{v|t|}{2}\sqrt{1 + \left(\frac{h}{vt}\right)^2} \qquad \text{as } t\to\pm\infty$$

$$= \frac{vt}{2}\sqrt{1 + \left(\frac{h}{vt}\right)^2} \qquad \text{as } t\to\pm\infty$$

$$\approx \frac{vt}{2} + \frac{1}{4}\frac{h^2}{vt} + \dots \qquad \text{as } t\to\pm\infty$$

- consider : $\dfrac{c_1(\infty)}{c_1(-\infty)}$

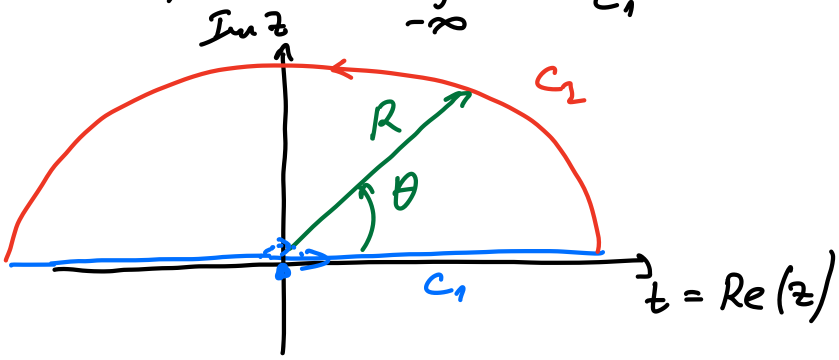
trick 1) $\log \dfrac{c_1(\infty)}{c_1(-\infty)} = \displaystyle\int_{-\infty}^{\infty} dt \, \frac{\dot{c}_1(t)}{c_1(t)}$

$$\frac{\dot{c}_1}{c_1} \overset{t\to\pm\infty}{\sim} -i\,\dot{\varphi}\Big|_{t\to\pm\infty} \approx -i\left(\frac{vt}{2} + \frac{1}{\gamma}\frac{h^2}{vt}\right)$$

trick 2) want $\displaystyle\int_{-\infty}^{\infty} dt \, \frac{\dot{c}_1}{c_1}$: use analytic continuation

$t \longrightarrow z \in \mathbb{C}$

$z = Re^{i\theta}$



$$\int_{C_1} \frac{c_1'(z)}{c_1(z)} dz + \int_{C_2} \frac{c_1'(z)}{c_1(z)} dz = 0$$

↳ c_1'/c_1 is analytic

$$\Rightarrow \int_{-\infty}^{\infty} dt \, \frac{\dot{c}_1(t)}{c_1(t)} = -\int_{C_2} dz \, \frac{\partial_z c_1(z)}{c_1(z)}$$

$$= -\lim_{R\to\infty} \int_0^{\pi} d\theta \, \frac{\partial z}{\partial \theta} \, \frac{\partial_\theta c_1(Re^{i\theta})}{c_1(Re^{i\theta})}$$

$$= +i \lim_{R\to\infty} \int_0^{\pi} d\theta \, iRe^{i\theta}\left(\frac{1}{2} v Re^{i\theta} + \frac{1}{\gamma}\frac{h^2}{vRe^{i\theta}}\right)$$

$$= -\lim_{R\to\infty} \int_0^{\pi} d\theta \left(\overset{0}{\cancel{\frac{1}{2} v R^2 e^{2i\theta}}} + \frac{1}{\gamma}\frac{h^2}{v}\right)$$

$$= -\pi \frac{h^2}{\gamma v} = \log \frac{c_1(+\infty)}{c_1(-\infty)}$$

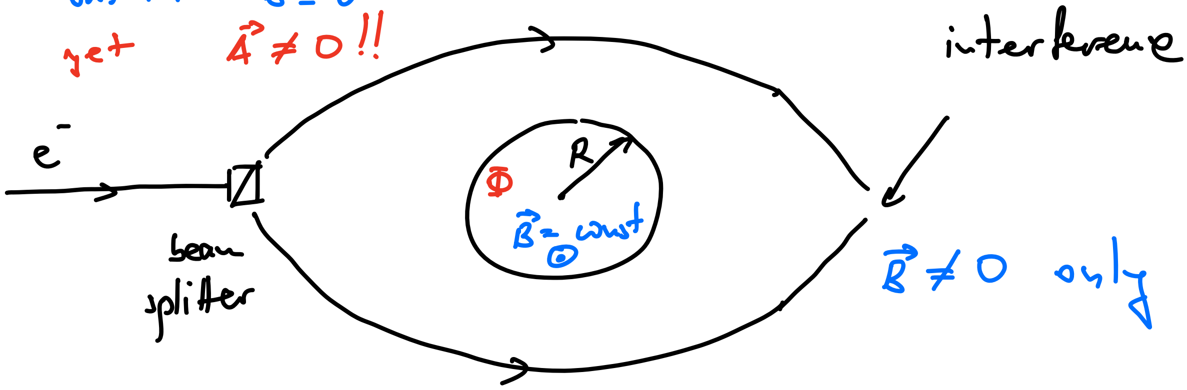
$$\frac{c_1(\infty)}{c_1(-\infty)} = e^{-\pi \frac{k^2}{4V}}$$

- for $|c(-\infty)|^2 = 1 \Rightarrow P_{LZ} = |c_1(+\infty)|^2 = e^{-\frac{\pi}{2}\frac{k^2}{V}}$

Aharonov-Bohm effect

outside: $\vec{B} \equiv \vec{0}$

yet $\vec{A} \neq 0$!!



$\vec{B} \neq 0$ only inside solenoid

- flux Φ_0 thru solenoid:

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

- recall: $\vec{B} = \operatorname{curl}\vec{A} = \vec{\nabla}\times\vec{A}$

$$\Phi_0 = \int \vec{\nabla}\times\vec{A}\cdot d\vec{a} \underset{\text{Stokes thm}}{=} \oint \vec{A}\cdot d\vec{r} \Rightarrow \vec{A} = \begin{cases} \frac{\Phi_0}{2\pi}\frac{r}{R^2}\hat{\varphi}, & r \leq R \\ \frac{\Phi_0}{2\pi r}\hat{\varphi}, & r \geq R \end{cases}$$

- Hamiltonian:

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

<u>want</u> e'fns of H in terms of e'fns of

$$H_0 = \frac{p^2}{2m} + V(\vec{r}) \quad \text{w/o magnetic field}: \vec{B} \equiv 0$$

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

def: $\psi(\vec r) = e^{ig(\vec r)}\psi_0(\vec r)$,

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

$\vec r_0$ outside solenoid

$$(\vec p + q\vec A)\psi(\vec r) = (-i\vec\nabla + q\vec A)\, e^{ig(\vec r)}\psi_0(\vec r)$$

$$= e^{ig}\underbrace{(\vec\nabla g)}_{\overset{(*)}{=}\, -q\vec A}\psi_0 - i e^{ig}\vec\nabla\psi_0 + q e^{ig}\vec A\psi_0$$

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

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

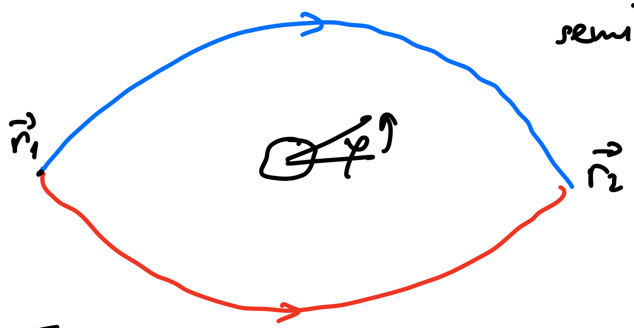
$$H\psi(\vec r) = e^{ig}\underbrace{\left(\frac{p^2}{2m}+V(\vec r)\right)\psi_0(\vec r)}_{= H_0\psi_0(\vec r) = E_0\psi_0(\vec r)} = E_0 e^{ig}\psi_0 = E_0\psi$$

$\Rightarrow \psi(\vec r) = e^{ig(\vec r)}\psi_0(\vec r)$ is an e'state of $H = \frac{(\vec p+q\vec A)^2}{2m}+V$

semi-circles

back to solenoid:

. consider two paths



$$g = -q\int_{\vec r_1}^{\vec r_2}\vec A\cdot d\vec r = \pm q\int_0^\pi \frac{\Phi_0}{2\pi\cancel{r}}\,\cancel{\hat\varphi}\cdot\cancel{r}\,d\varphi\,\cancel{\hat\varphi} = \pm q\frac{\Phi_0}{2}$$

phase of e^- is different for & paths!

$\Rightarrow$ can measure phase difference in wave function in interference experiment: $\Delta\phi = q\Phi_0$ Aharonov-Bohm phase