Adiabatic Gauge Potentials

<u>setup</u>: Hamiltonian $H(\vec{\lambda})$ depends on ext. param. $\vec{\lambda}$
→ often, $\vec{\lambda}$ is a vector, but we'll consider single λ for simplicity

- inst. e'basis: $H(\lambda)|n[\lambda]\rangle = E_n(\lambda)|n(\lambda)\rangle$

<u>def</u>: <u>gauge pot</u>: $\mathcal{A}_\lambda(\cdot) := i\partial_\lambda(\cdot)$ as follows:

- diag. matrix elements:

$\langle n[\lambda]|\mathcal{A}_\lambda|n[\lambda]\rangle = \langle n[\lambda]|i\partial_\lambda|n[\lambda]\rangle =: A_n$ Berry connection of e'state $|n[\lambda]\rangle$

- off-diag. matrix el.: $n\neq m$

$$\langle n[\lambda]|\mathcal{A}_\lambda|m[\lambda]\rangle := -i\,\frac{\langle n[\lambda]|\partial_\lambda H|m[\lambda]\rangle}{E_n(\lambda)-E_m(\lambda)} \quad \forall n\neq m$$

if $U_\lambda^+ H_\lambda U_\lambda = \text{diag} \Rightarrow \mathcal{A}_\lambda = (i\partial_\lambda U_\lambda)U_\lambda^+$

– why "gauge" potential?
gauge freedom associated w/ re-phasing individual e'states:

$$|n[\lambda]\rangle \longmapsto |n'[\lambda]\rangle := e^{i\chi_n(\lambda)}|n[\lambda]\rangle$$

U(1) gauge group

physics remains unchanged (↔ gauge freedom)

<u>but</u>:

$$A_n = \langle n[\lambda]|i\partial_\lambda|n[\lambda]\rangle \longmapsto \langle n[\lambda]|e^{-i\chi_n(\lambda)}i\partial_\lambda\left(e^{+i\chi_n(\lambda)}|n[\lambda]\rangle\right)$$

$$= \langle n[\lambda]|i\partial_\lambda|n[\lambda]\rangle - \partial_\lambda\chi_n(\lambda)\underbrace{\langle n[\lambda]|n[\lambda]\rangle}_{=1}$$

$$= A_n - \partial_\lambda\chi_n$$

Berry connection not gauge invariant
→ unphysical, cannot be measured

but: $\oint A_n\cdot d\lambda = \gamma_n$ geom./Berry phase along <u>closed</u> loop is gauge-inv. (cf. magnetic flux in EM)

want: basis indep. def. of A_λ:

1) def. e'state projector $P_n(\lambda) := |n[\lambda]\rangle\langle n[\lambda]|$

$$(i\partial_\lambda P_n(\lambda))(\cdot) = i\partial_\lambda\big(P_n(\lambda)(\cdot)\big) - P_n(\lambda)\, i\partial_\lambda(\cdot)$$
$$= \big(A_\lambda P_n(\lambda) - P_n(\lambda)A_\lambda\big)(\cdot)$$
$$= [A_\lambda, P_n(\lambda)](\cdot) \qquad (*)$$

2) consider $H(\lambda) = \sum_n E_n(\lambda)|n[\lambda]\rangle\langle n[\lambda]| = \sum_n E_n(\lambda) P_n(\lambda)$

$$i\partial_\lambda H(\lambda) = -i \underbrace{\sum_n (-\partial_\lambda E_n(\lambda)) P_n(\lambda)}_{=: M_\lambda \text{ generalized force}} + \underbrace{\sum_n E_n(\lambda)\, \underbrace{i\partial_\lambda P_n(\lambda)}_{\overset{(*)}{=} [A_\lambda, P_n(\lambda)]}}_{= [A_\lambda, \sum_n E_n(\lambda) P_n(\lambda)]}$$

$$= -i M_\lambda + [A_\lambda, H(\lambda)]$$

$$\Rightarrow \quad i\partial_\lambda H(\lambda) = [A_\lambda, H(\lambda)] - i M_\lambda \qquad / [H(\lambda), \cdot\,]$$

$$[H, i\partial_\lambda H] - [H, [A_\lambda, H]] = -i[H, M_\lambda] = 0$$

$$\boxed{[H,\ i\partial_\lambda H - [A_\lambda, H]] = 0}$$ defining eq. for AGP A_λ

notice: above eq. does not fix diag. matrix el. $\langle n|A_\lambda|n\rangle$ in inst. e'basis of H

indeed, if $\mathcal{D}_\lambda := \sum_n d_n(\lambda) P_n(\lambda)$ is <u>any</u> diag. op.,

then $[\mathcal{D}_\lambda, H] = 0$, & hence

$A_\lambda + \mathcal{D}_\lambda$ is another valid gauge pot.

$\rightarrow$ manifestation of $U(1)$ gauge dependence

$$A_\lambda \longmapsto A_\lambda' = A_\lambda - \sum_n (\partial_\lambda \chi_n(\lambda)) P_n(\lambda)$$

Q: is there a gauge-inv. description of the AGP?

recall from EM coupled to cpx. scalar field ϕ

Lagrangian density: $\mathcal{L} = -\frac{1}{4g} F_{\mu\nu}F^{\mu\nu} + (D^\mu \phi)(D_\mu \phi)$

U(1) gauge transf.:

$A_\mu \mapsto A_\mu - \partial_\mu \chi$

$\phi \mapsto e^{\chi} \phi$

gauge pot.: A_μ

field tensor: $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$

$\to$ gauge-inv. (physical, contains E&M fields)

covariant derivative: $iD_\mu = i\partial_\mu - A_\mu$

but: $iD_\mu \longmapsto iD_\mu' = i\partial_\mu - A_\mu'$

$= i\partial_\mu - A_\mu + \partial_\mu \chi$ not gauge-inv.

however: $iD_\mu \phi = (i\partial_\mu - A_\mu)\phi$

$\longmapsto (i\partial_\mu - A_\mu + \partial_\mu \chi)(e^{i\chi}\phi)$

$= e^{i\chi}(-\partial_\mu \chi + i\partial_\mu - A_\mu + \partial_\mu \chi)\phi$

$= e^{i\chi} D_\mu \phi$

$\Rightarrow |D_\mu \phi|^2 \longmapsto |D_\mu \phi|^2$ is gauge inv.!

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back to QM: if $A_\lambda = i\partial_\lambda$, let's consider:

Kato AGP:

$A_\lambda^K := iD_\lambda = i\partial_\lambda - \sum_n A_n(\lambda) P_n(\lambda)$

$= A_\lambda - \underbrace{\sum_n A_n(\lambda) P_n(\lambda)}_{\text{subtracts diag. matrix el. of } A_\lambda \text{ in inst. e'basis}}$

$= \sum_{n,m} \overbrace{(1-\delta_{mn})} \langle n[\lambda]| i\partial_\lambda |m[\lambda]\rangle\, |n[\lambda]\rangle\langle m[\lambda]|$

compare w/

$A_\lambda = \sum_{n,m} \langle n[\lambda]| i\partial_\lambda |m[\lambda]\rangle\, |n[\lambda]\rangle\langle m[\lambda]|$

• Kato AGP is manifestly gauge inv.:

$$A_\lambda^K \longmapsto A_\lambda^{K\prime} = \sum_{n,m}(1-\delta_{nm}) \underbrace{\langle n'[\lambda]|\, i\partial_\lambda \,|m'[\lambda]\rangle}_{=\langle n|i\partial_\lambda|m\rangle e^{i(\chi_m-\chi_n)} - \partial_\lambda \chi_m \underbrace{\langle n|m\rangle}_{=\delta_{nm}} e^{i\chi_m-\chi_n}} \; \underbrace{|n'[\lambda]\rangle\langle m'[\lambda]|}_{=e^{i(\chi_n-\chi_m)}|n[\lambda]\rangle\langle m[\lambda]|}$$

$$= \sum_{n,m}(1-\delta_{nm})\langle n[\lambda]|\,i\partial_\lambda\,|m[\lambda]\rangle\, |n[\lambda]\rangle\langle m[\lambda]|$$

$$- \underbrace{(1-\delta_{mn})\,\delta_{mn}}_{=0}\, \partial_\lambda \chi\, |n[\lambda]\rangle\langle m[\lambda]|$$

$$= A_\lambda^K \checkmark$$

<u>can show</u>: $A_\lambda^K = \frac{1}{2}\sum_n \left[P_n(\lambda),\, i\partial_\lambda P_n(\lambda)\right]$, $\quad P_n(\lambda) = |n[\lambda]\rangle\langle n[\lambda]|$

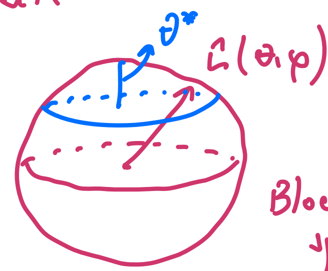
Kato AGP generates parallel transport on parameter manifold

- Example (HW): 2LS parametrized by Hamiltonian

$H(\theta,\varphi) = E\, \hat{n}(\theta,\varphi)\cdot\vec{\sigma}$, where E sets energy

$$\hat{n}(\theta,\varphi) = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} \; ; \quad \vec{\sigma} = \begin{pmatrix} \sigma^x \\ \sigma^y \\ \sigma^z \end{pmatrix} \quad \text{vector of Pauli matrices}$$

here $\vec{\lambda} = (\theta,\varphi)$ two-parameter manifold



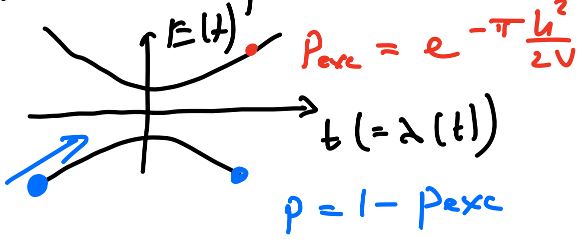
Bloch sphere

→ two gauge potentials: A_θ, A_φ
each is 2×2 matrix

→ two Kato potentials: A_θ^K, A_φ^K

Counterdiabatic Driving

- recall LZ problem: $H(t) = \frac{vt}{2}\sigma^z + \frac{h}{2}\sigma^x$



- excited fraction is exp. small but finite; depends h^2/v

<u>issues</u>: 1) p_{exc} increases if speed v increases
2) expression valid in regime $t \to \infty$; what about finite times?

Q: can we suppress excitations completely & at <u>all</u> times during the ramp

<u>Yes!</u> → transitionless driving / shortcut to adiabaticity

consider $H = H(\lambda) = H_\lambda$

. let U_λ diagonalize H_λ instantaneously, i.e.

$$U^\dagger(\lambda)\, H(\lambda)\, U(\lambda) = \begin{pmatrix} E_1(\lambda) & & 0 \\ & E_2(\lambda) & \\ 0 & & \ddots \end{pmatrix} =: \mathcal{D}(\lambda)$$

. recall that $\lambda = \lambda(t)$ changes in real time:
$U(\lambda(t))$ induces a change-of-frame transformation:
consider $|\psi(t)\rangle$ & $|\tilde\psi(t)\rangle := U^\dagger(\lambda(t))|\psi(t)\rangle$

Schr. eq. for $|\psi(t)\rangle$: $\;i\partial_t|\psi(t)\rangle = H(\lambda(t))|\psi(t)\rangle$

which Hamiltonian $\tilde H(t)$ generates time-evo. of $|\tilde\psi(t)\rangle$?

$$i\partial_t|\tilde\psi(t)\rangle = i\partial_t\left(U^\dagger(\lambda(t))\,|\psi(t)\rangle\right)$$

$$= \underbrace{(i\partial_t U^\dagger)U}_{= -U^\dagger i\partial_t U}\;\underbrace{U^\dagger|\psi(t)\rangle}_{= |\tilde\psi(t)\rangle} + U^\dagger \underbrace{i\partial_t|\psi(t)\rangle}_{= H(t)|\psi(t)\rangle = HU|\tilde\psi(t)\rangle}$$

$U^\dagger U = \mathbb{1}\;/\partial_t(\cdot)$

$(\partial_t U^\dagger)U = -U^\dagger\partial_t U$

$$= \underbrace{\left(U_\lambda^\dagger H_\lambda U_\lambda - U_\lambda^\dagger\, i\partial_t U_\lambda\right)}_{= \tilde H(t)\ \text{co-moving frame Hamiltonian}}|\tilde\psi(t)\rangle$$

$$\Rightarrow \tilde{H}(t) = U^{\dagger}(\lambda(t))\, H(\lambda(t))\, U(\lambda(t)) - U^{\dagger}(\lambda(t))\, i\partial_t\, U(\lambda(t))$$

$$= \underbrace{U_\lambda^{\dagger} H_\lambda U_\lambda}_{=\mathcal{D}_\lambda \text{ diag. matrix}} - \dot{\lambda}\, \underbrace{U_\lambda^{\dagger} i\partial_\lambda U_\lambda}_{=\tilde{\mathcal{A}} \text{ gauge pot. in co-mov. frame in e'basis } U(\lambda)}$$

<u>notice</u>: $\mathcal{D}(\lambda)$ is diagonal; therefore: any excitations during the evo. under $H(\lambda(t))$ must necessarily be caused by AGP $\tilde{\mathcal{A}}_\lambda$ in co-mov. frame

<u>idea</u>: apply extra "force" to counteract excitations

e.g. consider $H(\lambda) \longrightarrow H(\lambda) + \underbrace{\dot{\lambda} \mathcal{A}_\lambda}_{\text{cancels all excitations}} =: H_{CD}$ counterdiabatic Hamiltonian (CD driving)

w/ $\mathcal{A}_\lambda = U_\lambda \tilde{\mathcal{A}}_\lambda U_\lambda^{\dagger} = (i\partial_\lambda U)U^{\dagger}$ AGP in lab frame

<u>check</u>: $\tilde{H}_{CD} = U_\lambda^{\dagger}(H_\lambda + \dot{\lambda}\mathcal{A}_\lambda)U_\lambda - \dot{\lambda}\, U^{\dagger} i\partial_\lambda U$

$= U_\lambda^{\dagger} H_\lambda U_\lambda + \dot{\lambda}\, U_\lambda^{\dagger}\mathcal{A}_\lambda U_\lambda - \dot{\lambda}\, \tilde{\mathcal{A}}_\lambda$

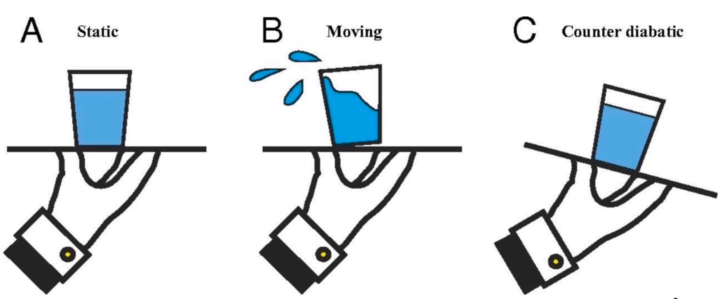
$= \mathcal{D}_\lambda$ no more excitations!

$\Rightarrow$ for time evo under $H_{CD}(\lambda(t))$, a system starting in an e'state of $H(\lambda(0))$ remains in the inst. e'state of $H(\lambda(t))$ at all times, up to an overall phase (depends on $U(1)$ gauge)

$\rightarrow$ transitionless driving

$$|n(t)\rangle = \mathcal{T} e^{-i\int_0^t H_{CD}(\lambda(s))\, ds} |n[0]\rangle = e^{i\gamma_n(t)} |n[\lambda(t)]\rangle$$

<u>note</u>: we achieve transitionless driving for <u>any</u> protocol $\lambda(t)$!



Sels & Polkovnikov, PNAS '17

<u>intuition</u>: limiting cases

a) $\dot\lambda \to \infty \Rightarrow H_{CD} \approx \dot\lambda A_\lambda$

Schr. eq. $i\partial_t |\psi(t)\rangle = H_{CD}(t)|\psi(t)\rangle$
$\approx \dot\lambda A_\lambda |\psi(t)\rangle$

change variables: $i\partial_\lambda |\psi[\lambda]\rangle = A_\lambda |\psi[\lambda]\rangle$

$\Rightarrow A_\lambda$ generates evo. in parameter space ($\hookrightarrow$ parallel transport) which becomes exact as $\dot\lambda \to \infty$

b) adiabatic limit: $\dot\lambda \to 0 \Rightarrow H_{CD} \approx H$
$\to$ time evo is generated by $H(\lambda)$ ("LZ" limit)

<u>therefore</u>: $H_{CD} = H(\lambda) + \dot\lambda A_\lambda$ interpolates b/w infinitely slow adiabatic evo. generated by H_λ & rapid evo generated by AGP $\dot\lambda A_\lambda$

<u>Example</u>: two-level system under <u>arbitrary</u> protocol:

$H(\lambda) = \Delta\sigma^z + \lambda(t)\sigma^x$

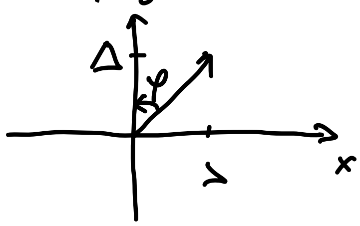
<u>step (i)</u> [cheap trick]: use $\tilde A = U^+ i\partial_\lambda U$, where $U_\lambda^+ H_\lambda U_\lambda = \mathrm{diag}_\lambda$

& note: H_λ is real-valued $\Rightarrow$ e'states real $\Leftrightarrow U$ is orthogonal

most general orth. transform. for 2LS:

$U_\lambda = e^{i f(\lambda)\sigma^y}$ $\to \sigma^y$ is imaginary-valued
$\to$ overall factor i

Bloch sphere $\longrightarrow$ zx-plane



$$U(\lambda) = e^{-i\varphi(\lambda,\Delta)\frac{\sigma^y}{2}}$$

s.t. $\tan\varphi = \frac{\lambda}{\Delta}$

(ii) need $\mathcal{A}_\lambda = U_\lambda^\dagger\, i\partial_\lambda U_\lambda = U^\dagger \partial_\lambda \varphi \frac{\sigma^y}{2} U = \frac{1}{2}\partial_\lambda\varphi\, \sigma^y$

$$\partial_\lambda \varphi = \partial_\lambda \arctan\left(\frac{\lambda}{\Delta}\right) = \frac{1}{\Delta}\frac{1}{1+[\lambda/\Delta]^2} = \frac{\Delta}{\Delta^2+\lambda^2}$$

$$\Rightarrow \mathcal{A}_\lambda = \frac{1}{2}\frac{\Delta}{\Delta^2+\lambda^2}\sigma^y \underset{[A,U]=0}{=} A_\lambda$$

(iii) construct H_{CD}:

$$H_{CD}(\lambda(t)) = \Delta\sigma^z + \lambda(t)\sigma^x + \frac{\dot\lambda(t)}{2}\frac{\Delta}{\Delta^2+\lambda^2(t)}\sigma^y$$

<u>Rmk</u>: AGP $A_\lambda = (i\partial_\lambda U_\lambda)U_\lambda^\dagger$ does not contain information about change-of-basis transformation; it only tells us how to move from one inst. e'basis to another:

$i\partial_\lambda U_\lambda = A_\lambda U_\lambda$ Schr. eq. for A_λ on param. mfd

$$\Rightarrow U(\lambda_f,\lambda_i) = \underbrace{P e^{-i\int_{\lambda_i}^{\lambda_f} d\lambda A_\lambda}}_{\text{path-ordered exp.; changes b/w e'bases}} \underbrace{U(\lambda_i,\lambda_i)}_{\text{initial condition, defines diagonalizing transformation}}$$

- CD Hamiltonian is <u>not</u> unique, since AGP can be changed using $U(1)$ gauge transformation

↪ • all valid CD Hamiltonians generate transitionless driving
• only difference is in accumulated global phase

consider Schr. eq: $i\partial_t |n(t)\rangle = \mathcal{H}(t)|n(t)\rangle$

where $\mathcal{H}(0)|n(0)\rangle = E(0)|n(0)\rangle$

drive	Hamiltonian $\mathcal{H}(t)$	acc. phase
adiabatic; $T\to\infty$	$\mathcal{H}(t) = H_{ctrl}(t)$	$\gamma_n(t) + \phi_n(t)$ proof: cf. adiabatic thm.
dynamical CD fixed gauge: $\chi_n(t) \equiv 0$	$\mathcal{H}(t) = H_{ctrl}(t) + \dot\lambda A_\lambda$; $A_\lambda = (i\partial_\lambda U_\lambda)U_\lambda^\dagger$ & $U_\lambda^\dagger H_{ctrl} U_\lambda = \text{diag}$	$\phi_n(t)$ proof: • in co-mov. frame $\tilde{\mathcal{H}}(t) = \mathcal{D}(\lambda(t))$ diag. $\Rightarrow |\tilde n(t)\rangle = \underbrace{e^{-i\int_0^t E_n(s)ds}}_{= e^{i\phi(t)} \text{ dyn. phase}}|\tilde n(0)\rangle$ $\Rightarrow |n(t)\rangle = U(\lambda(t))|\tilde n(t)\rangle$ $= e^{i\phi_n(t)}U_\lambda|\tilde n(0)\rangle$ $= e^{i\phi_n(t)}|n[\lambda(t)]\rangle$
Kato CD gauge-inv.	$\mathcal{H}(t) = H_{ctrl}(t) + \dot\lambda A_\lambda^K$; $A_\lambda^K = \frac{1}{2}\sum_n [P_n, i\partial_\lambda P_n]$ $P_n = |n[\lambda]\rangle\langle n[\lambda]|$	$\phi_n(t) + \gamma_n(t)$ same as in the adiabatic theorem, but w/o restriction on being in adiabatic limit proof: $\tilde{\mathcal{H}}(t) = \mathcal{D}(t) + \dot\lambda\underbrace{(\tilde A_\lambda^K - \tilde A_\lambda)}_{\text{differ by Berry conn.}}$ $= \sum_n (E_n(t) + \dot\lambda A_n) P_n(\lambda)$ $\Rightarrow |n(t)\rangle = e^{i\phi_n(t) + i\gamma_n(t)}|n[\lambda(t)]\rangle$ w/ $\underbrace{\gamma_n(t) = \int_0^t ds\, \dot\lambda(s) A_n(\lambda(s))}_{\text{geom. phase}}$

generic CD $x_n(t)$ arbitrary (but fixed)	$\mathcal{H}(t) = H_{ctrl}(t) + \mathcal{A}'_\lambda$; $A'_\lambda = A_\lambda - \sum_n \partial_\lambda x_n P_n$	$x_n(t) + \phi_n(t)$ proof: same as for A_λ but now w/ extra phase $\int_0^t \dot{\lambda}(s)\, \partial_\lambda x_n(\lambda(s))\, ds$ $= x_n(\lambda(t))$
Kato AGP gauge-inv.	$\mathcal{H}(t) = \dot{\lambda} A^K_\lambda$	$\gamma_n(t)$ proof: $\tilde{\mathcal{H}}(t) = \dot{\lambda}(\tilde{A}^K_\lambda - \tilde{A}_\lambda)$ $= \sum_n \dot{\lambda} A_n P_n(\lambda(t))$ & same as above
periodic AGP fixed gauge $x_n(t) = 2\pi l_n \frac{t}{T}$ $l_n \in \mathbb{Z}$	$\mathcal{H}(t) = \mathcal{A}(t)$ [here $\lambda = t$] & $\mathcal{A}(t+T) = \mathcal{A}(t)$ periodic w/ period T $\lvert n[T]\rangle = \lvert n[0]\rangle$ periodic ONB for $\mathcal{A}(t)$	$2\pi l_n$, $l_n \in \mathbb{Z}$ (at $t=T$) proof: $\lambda = t \Rightarrow \dot{\lambda} = 1$ $\tilde{\mathcal{H}}(t) = \mathcal{A}(t)$ $= \sum_n A_n(t) P_n(t) + A^K(t)$ $\Rightarrow$ $\lvert n(T)\rangle = \mathcal{T} e^{-i\oint A^K(t)dt}\, e^{i\gamma_n(T)} \lvert n[T]\rangle$ $= e^{2\pi i l_n + i\gamma_n(T) - i\gamma_n(0)} \lvert n[0]\rangle$ $= e^{2\pi i l_n} \lvert n[0]\rangle$