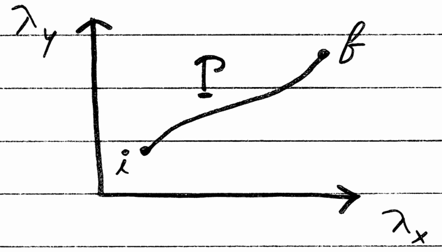
ADIABATIC PERTURBATION THEORY

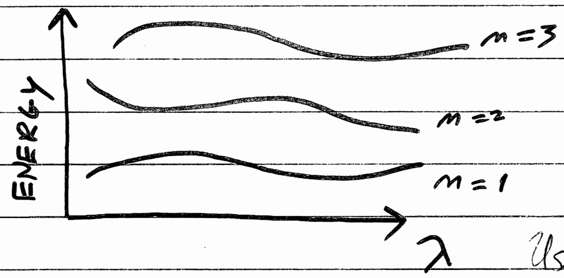
$H = H[\underline{\lambda}(t)]$

slowly-varying param.



Instantaneous eigenstates:

$$H[\underline{\lambda}(t)]\,|u_m[\underline{\lambda}(t)]\rangle = E_m[\underline{\lambda}(t)]\,|u_m[\underline{\lambda}(t)]\rangle$$



No level crossing

Ansatz:

$$|\Psi_m(t)\rangle = \underbrace{\exp\left[-\frac{i}{\hbar}\int_0^t E_m[\underline{\lambda}(t')]\,dt'\right]}_{\text{Usual Dynamical phase}} \overbrace{e^{i\phi_m(t)}}^{\text{Allow for extra phase factor}} |u_m[\underline{\lambda}(t)]\rangle$$

Plug into $i\hbar|\dot{\Psi}_m\rangle = H|\Psi_m(t)\rangle$:

$$\begin{aligned} \text{LHS} &= E_m[\underline{\lambda}]\exp[\ldots]e^{i\phi_m}|u_m(\underline{\lambda})\rangle \\ &+ i\hbar\exp[\ldots]\,i\dot{\phi}_m e^{i\phi_m}|u_m(\underline{\lambda})\rangle \\ &+ i\hbar\exp[\ldots]e^{i\phi_m}\,\dot{\underline{\lambda}}\cdot\frac{d|u_m\rangle}{d\underline{\lambda}} \end{aligned}$$

$$\text{RHS} = \exp[\ldots]e^{i\phi_m}E_m[\underline{\lambda}]\,|u_m(\underline{\lambda})\rangle$$

Cancel

$$\Rightarrow\quad i\dot{\phi}_m|u_m\rangle = -\dot{\underline{\lambda}}\cdot\frac{d|u_m\rangle}{d\underline{\lambda}}$$

$\langle u_m| \times (\ldots)$

$$\dot{\phi}_m = +i\,\dot{\underline{\lambda}}\cdot\langle u_m|\frac{d}{d\underline{\lambda}}u_m\rangle$$

$$\equiv \underline{A}_m(\underline{\lambda})\cdot\dot{\underline{\lambda}}$$

$$\boxed{\underline{A}_m(\underline{\lambda}) = i\langle u_m|\frac{d}{d\underline{\lambda}}u_m\rangle}$$

Berry connection

Integrate from t_i to t_f:

$$\phi_n(t_f) = \int_{t_i}^{t_f} \underline{A}_n(\underline{\lambda}) \cdot \frac{d\underline{\lambda}}{dt}\, dt$$

$$\boxed{\phi_n(P) = \int_{\underline{\lambda}_i}^{\underline{\lambda}_f} \underline{A}_n(\underline{\lambda}) \cdot d\underline{\lambda}}$$

Only depends on the path, not on the traversal rate: **GEOMETRIC!**

- ϕ_n is real, because $\underline{A}_n$ is real, i.e.,

$\langle u_n | \frac{d}{d\underline{\lambda}} u_n \rangle$ is purely imaginary:

$$2\,\mathrm{Re} \langle u_n | \frac{d}{d\lambda} u_n \rangle = \langle u_n | \frac{d}{d\lambda} u_n \rangle + \langle \frac{d}{d\lambda} u_n | u_n \rangle$$

$$= \frac{d}{d\lambda} \langle u_n(\lambda) | u_n(\lambda) \rangle = 0 \;//$$

- Gauge transformations: Eigenstates only defined ~~up~~ to a phase,

$$|\tilde{u}_n(\lambda)\rangle = e^{-i\beta_n(\lambda)} |u_n(\lambda)\rangle$$

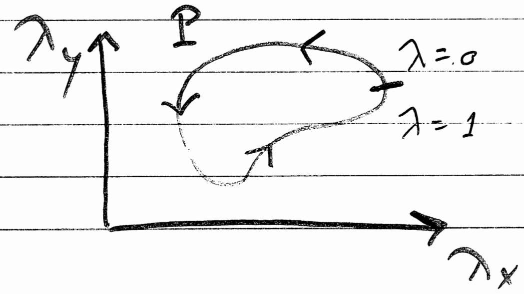
also valid eigenstate

Real, assume smooth in λ

$$\Rightarrow \begin{cases} \underline{\tilde{A}}_n(\underline{\lambda}) = \underline{A}_n(\underline{\lambda}) + \dfrac{d\beta_n}{d\underline{\lambda}} \\ \tilde{\phi}_n = \phi_n + \beta_n(\underline{\lambda}_f) - \beta_n(\underline{\lambda}_i) \end{cases}$$

$\therefore$ Can choose a gauge where the geometric phase of the path vanishes, and only the dynamical phase remains

But consider now a <u>closed path</u> (Berry 1984)



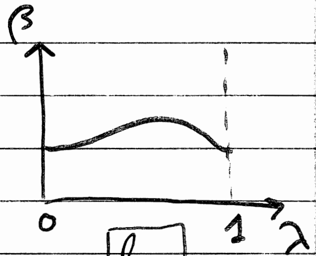
Parametrize circuit by a scalar $\lambda \in [0,1]$

Since $\lambda=0$ and $\lambda=1$ label the same state, we require

$$\begin{cases} |u_n(\lambda=1)\rangle = |u_n(\lambda=0)\rangle \\ |\tilde{u}_n(\lambda=1)\rangle = |\tilde{u}_n(\lambda=0)\rangle \end{cases}$$ "single-valued"

$$\Rightarrow \beta_n(\lambda=1) = \beta_n(\lambda=0) + 2\pi l$$

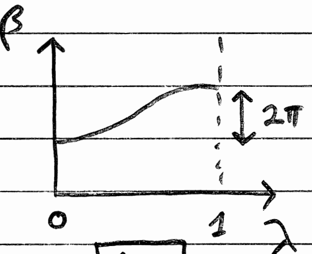
↑ "winding number" of gauge transf.



$\boxed{l=0}$

$$\therefore \quad \boxed{\tilde{\phi}_n = \phi_n + 2\pi l}$$

$$\boxed{\phi_n(P) = \oint \underline{A}_n(\underline{\lambda})\cdot d\underline{\lambda}}$$ **Berry phase**

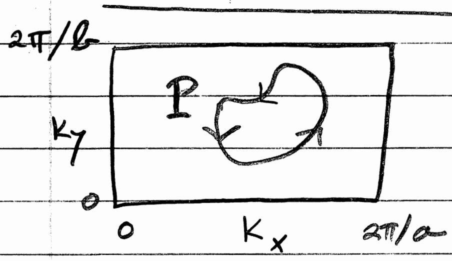


$\boxed{l=1}$

For closed path, $e^{i\phi_n}$ is gauge invariant, and so it cannot be removed by a gauge Transf.!

$\Rightarrow$ $\boxed{\text{potentially a physical observable}}$

• Example: Berry phase in a 2D Brillouin zone



$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r}) \qquad \underline{r}=(x,y)$$

$$V(\underline{r}+\underline{R}) = V(\underline{r}), \quad \underline{R} = i\underline{a} + j\underline{b}$$

Eigenstates labelled by $\underline{k} = (k_x, k_y) \in 1^{ST}$ BZ

$$\begin{cases} H|\psi_{n\underline{k}}\rangle = E_{n\underline{k}}|\psi_{n\underline{k}}\rangle \\ |\psi_{n,\underline{k}+\underline{G}}\rangle = |\psi_{n\underline{k}}\rangle \end{cases}$$

Bloch's theorem: $$\begin{cases} \psi_{n\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}\, u_{n\underline{k}}(\underline{r}) \\ u_{n\underline{k}}(\underline{r}+\underline{R}) = u_{n\underline{k}}(\underline{r}) \end{cases}$$

④

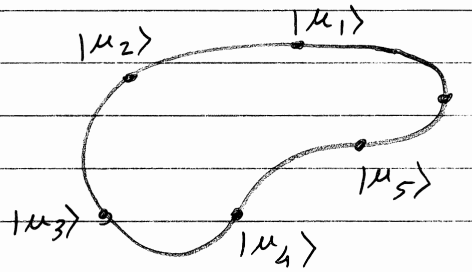
$$\Rightarrow \begin{cases} H(\underline{k})\,|u_{n\underline{k}}\rangle = E_{n\underline{k}}\,|u_{n\underline{k}}\rangle \\ H(\underline{k}) = e^{-i\underline{k}\cdot\underline{r}}\, H\, e^{+i\underline{k}\cdot\underline{r}} \end{cases}$$ Parametric dependence on $\underline{k}$

∴ Can define Berry connection and phase in BZ:

$$A_{n\underline{k}} = i\langle u_{n\underline{k}} | \frac{d}{d\underline{k}} u_{n\underline{k}}\rangle, \quad \phi_n(P) = \oint_P A_{n\underline{k}} \cdot d\underline{k}$$

Basic ingredients of "topological band theory"

<u>DISCRETIZED BERRY PHASE</u> (Numerics)



$|u_N\rangle = |u_0\rangle$ $\quad N = 6$

(Dropped index n)

Def.: $$\boxed{\phi = -\operatorname{Im}\ln\left[\langle u_0|u_1\rangle\langle u_1|u_2\rangle \cdots \langle u_{N-1}|u_0\rangle\right]}$$

For $z = |z|e^{-i\phi}$, $\quad \phi = -\operatorname{Im}\ln z \pmod{2\pi}$

Thus, our def. takes the complex phase of the product of overlaps, and discards the magnitude

<u>COMMENTS</u>:

(i) If the $|u_j\rangle$ are <u>real</u> vectors, $\phi = 0$ or π depending on the sign of the product of overlaps. Generic values of ϕ require a <u>complex</u> vector space

(ii) ϕ is unaffected by $|u_j\rangle \to e^{-i\beta_j}|u_j\rangle$, since every $|u_j\rangle$ appears twice, once as a ket and once as a bra

(iii) Continuum limit : $|u_j\rangle \to |u_\lambda\rangle$, $\lambda \in [0,1]$

Assume smooth (differentiable)

$$\Rightarrow \ln \langle u_\lambda | u_{\lambda+\Delta\lambda}\rangle = \ln \langle u_\lambda | \left(|u_\lambda\rangle + \Delta\lambda \frac{d|u_\lambda\rangle}{d\lambda} + \dots \right)$$

$$= \ln\left(1 + \Delta\lambda \langle u_\lambda | \partial_\lambda u_\lambda\rangle + \dots\right)$$

$\ln(1+\delta) \simeq \delta$

$$= \Delta\lambda \langle u_\lambda | \partial_\lambda u_\lambda \rangle + \dots$$

$$\phi = -\operatorname{Im} \ln \prod_{j=0}^{N-1} \langle u_j | u_{j+1}\rangle$$

$$= -\operatorname{Im} \sum_{j=0}^{N-1} \ln \langle u_j | u_{j+1}\rangle$$

$$\simeq -\operatorname{Im} \sum_{j=0}^{N-1} \Delta\lambda \langle u_\lambda | \partial_\lambda u_\lambda\rangle$$

$\Delta\lambda \to 0$

$$= -\operatorname{Im} \int_0^1 \langle u_\lambda | \partial_\lambda u_\lambda \rangle \, d\lambda$$

$\langle u_\lambda | \partial_\lambda u_\lambda\rangle$ purely imag.

$$= \int_0^1 i \langle u_\lambda | \partial_\lambda u_\lambda\rangle \, d\lambda$$

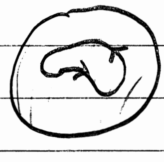
$$= \oint \underline{A}(\underline{\lambda}) \cdot d\underline{\lambda} \quad //$$

· **Example : spin in magnetic field** $\underline{B} = B\hat{\underline{n}}$

$$H = -\gamma \underline{B} \cdot \underline{S} = -\frac{\gamma \hbar B}{2} \hat{\underline{n}} \cdot \underline{\sigma} \qquad \text{(spin 1/2)}$$

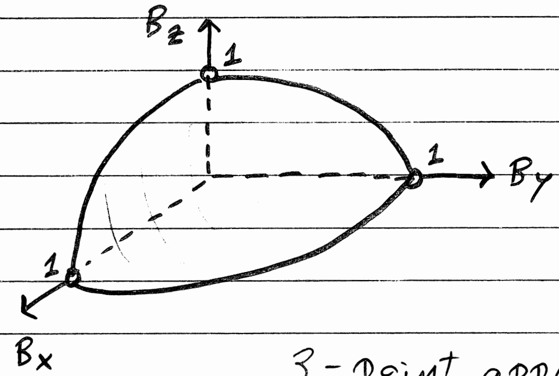
GS is a spin eigenstate of $\hat{\underline{n}} \cdot \underline{\sigma}$, indep. of magnitude B

$\rightarrow$ write as $|u_{\hat{\underline{n}}}\rangle$



Berry phase of $|u_{\hat{\underline{n}}}\rangle$ as $\hat{\underline{n}}$ is carried around a loop in $\hat{\underline{n}}$-space, i.e. a closed path on the surface of unit sphere

Let $\hat{n}$ start along $\hat{z}$, then rotate it to $\hat{x}$, then to $\hat{y}$, and then back to $\hat{z}$, thereby tracing out an octant of the unit sphere



3-point approx.:

$$\phi \approx -\mathrm{Im}\ln\left[\langle\uparrow_z|\uparrow_x\rangle\langle\uparrow_x|\uparrow_y\rangle\langle\uparrow_y|\uparrow_z\rangle\right]$$

"spin up in direction $\hat{y}$"
(GS is "up" for $\gamma > 0$)

QM textbooks:

$$|\uparrow_{\hat{n}}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{pmatrix}, \quad (\theta,\varphi) \text{ are polar and azimuthal angles of } \hat{n}$$

$$\Rightarrow \quad |\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |\uparrow_z\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\boxed{\phi \approx -\mathrm{Im}\ln\left[(1)\times(1+i)\times(1)\right] = -\frac{\pi}{4}}$$

Berry phase of an octant of the unit sphere

This result happens to be exact: it does not change if one uses a dense mesh of intermediate points along each great-circle arc.

(see p. 10 for exact calc.)

BERRY CURVATURE: $\underline{\Omega}(\underline{\lambda}) \equiv \underline{\nabla} \times \underline{A}(\underline{\lambda})$

"Berryology" table:

	DEF.	GAUGE TRANSF.
CONNECTION	$\underline{A} = i\langle u \vert \underline{\nabla} u\rangle$	$\tilde{\underline{A}} = \underline{A} + \underline{\nabla}\beta$
PHASE	$\phi = \oint \underline{A}\cdot d\underline{\lambda}$	$\tilde{\phi} = \phi + 2\pi l$
CURVATURE	$\underline{\Omega} = \underline{\nabla}\times\underline{A}$	$\tilde{\underline{\Omega}} = \underline{\Omega}$

$\underline{\nabla}\times(\underline{\nabla}\beta) = 0$

$$\boxed{\underline{\Omega} = i\langle \underline{\nabla} u \vert \times \vert \underline{\nabla} u\rangle = -\,\mathrm{Im}\langle \nabla u \vert \times \vert \nabla u\rangle}$$

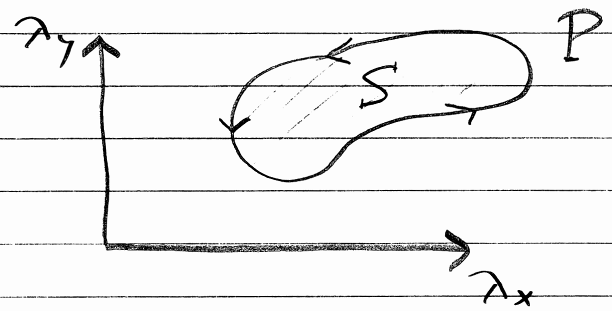
3D: $\underline{\lambda} = (\lambda_x, \lambda_y, \lambda_z)$

$\Omega_x = -2\,\mathrm{Im}\langle \partial_y u \vert \partial_z u\rangle$, etc (vector)

2D: $\underline{\lambda} = (\lambda_x, \lambda_y)$, $\underset{\text{(scalar)}}{\Omega \equiv \Omega_z} = -2\,\mathrm{Im}\langle \partial_x u \vert \partial_y u\rangle$

- Relation to Berry phase

2D:



$$\underbrace{\phi(P) \equiv \oint_P \underline{A}\cdot d\underline{\lambda}}_{\substack{\text{Berry phase} \\ (\mathrm{mod}\ 2\pi)}} \underset{\wedge}{=} \underbrace{\int_S \Omega\, dS \equiv \Phi(S)}_{\text{Berry flux}}$$

Stokes, $\Omega = (\underline{\nabla}\times\underline{A})_z$

Comments:

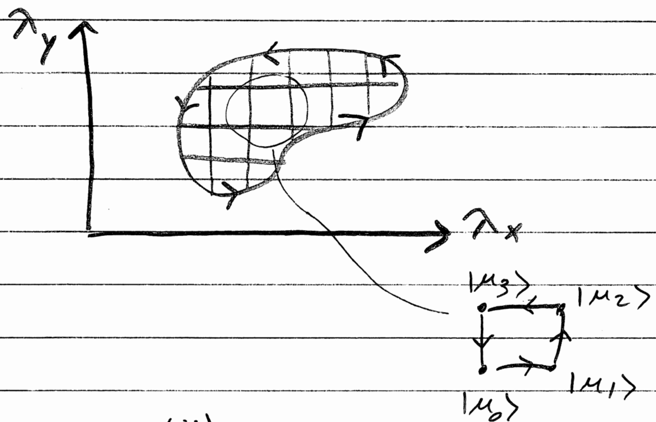
(i) Stokes' thm. assumes a smooth gauge everywhere on region S. From one smooth gauge to another, LHS may change by $2\pi l$, while RHS remains inv.

(ii) For a small loop P s.t. $\Omega \approx$ const. in S,

$$\phi(P) \approx \Omega \times \text{Area}(S)$$

$\therefore$ $\boxed{\text{Berry curv.} = \text{Berry phase density}}$

(iii) Discretized Berry curv.:



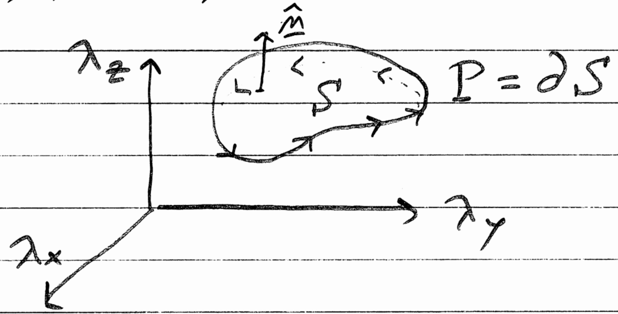
Discretized plaquette Berry phase

$$\Omega \overset{(ii)}{\approx} -\frac{1}{\text{Area}(\square)} \text{Im} \ln \left[\langle u_0|u_1\rangle \langle u_1|u_2\rangle \langle u_2|u_3\rangle \langle u_3|u_0\rangle \right]$$

with $\text{Im} \ln[\ldots] \in [-\pi, \pi[$ (why?)

Becomes exact as $\text{Area}(\square) \to 0$

(iv) Stokes' thm in 3D



$$\phi(P) = \oint_P \underline{A} \cdot d\underline{\lambda} = \int_S \underline{\Omega} \cdot \underline{\hat{n}}\, dS \equiv \Phi(S)$$

Spinor in a B field revisited

$$\underline{\Omega}(\hat{\underline{n}}) = -\,\mathrm{Im}\,\langle \underline{\nabla} \uparrow_{\hat{\underline{n}}} | \times | \underline{\nabla} \uparrow_{\hat{\underline{n}}} \rangle$$

$$|\uparrow_{\hat{\underline{n}}}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)\, e^{i\varphi} \end{pmatrix}$$

Around the "north pole" of the unit sphere $(\theta \approx 0)$

$$\cos\left(\frac{\theta}{2}\right) \approx 1 \,, \quad \sin\left(\frac{\theta}{2}\right) e^{i\varphi} \approx \frac{\theta}{2} e^{i\varphi} \approx \frac{1}{2} \sin\theta (\cos\varphi + i \sin\varphi)$$

$$= \frac{1}{2}(n_x + i n_y)$$

$$\Rightarrow \quad |\uparrow_{\hat{\underline{n}}}\rangle \approx \begin{pmatrix} 1 \\ \frac{1}{2}(n_x + i n_y) \end{pmatrix} \quad \text{near } \hat{\underline{n}} = \hat{\underline{z}}$$

$$\Omega_z = -2\,\mathrm{Im}\,\langle \partial_{n_x} \uparrow_{\hat{\underline{n}}} | \partial_{n_y} \uparrow_{\hat{\underline{n}}} \rangle, \text{ etc}$$

$$|\partial_{n_x} \uparrow_{\hat{\underline{n}}}\rangle\Big|_{\theta=0} = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\partial_{n_y} \uparrow_{\hat{\underline{n}}}\rangle\Big|_{\theta=0} = \frac{1}{2}\begin{pmatrix} 0 \\ i \end{pmatrix}$$

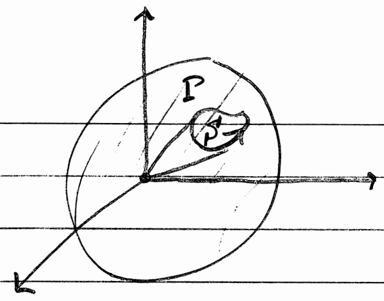
$$\Rightarrow \Omega_z(\hat{\underline{z}}) = -2 \times \frac{1}{2} \times \frac{1}{2}\,\mathrm{Im}\left[\begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ i \end{pmatrix}\right] = -\frac{1}{2}$$

$$\Omega_x(\hat{\underline{z}}) = \Omega_y(\hat{\underline{z}}) = 0$$

$$\text{i.e.} \quad \underline{\Omega}(\hat{\underline{n}} = \hat{\underline{z}}) = -\frac{1}{2}\hat{\underline{z}}$$

But since physics of spinor in free space is isotropic

$$\boxed{\underline{\Omega}(\hat{\underline{n}}) = -\frac{1}{2}\hat{\underline{n}}} \quad (\text{arbitrary } \hat{\underline{n}})$$



$$\phi_P = \Phi_S = \int_S \underline{\Omega} \cdot \hat{\underline{n}}\, dS$$
$$= -\frac{1}{2} \int_S dS$$

surface patch of unit sphere enclosed by P

$$\therefore \boxed{\phi(P) = -\frac{1}{2} \times (\text{solid angle})}$$

subtended at origin by S

If S = octant, then solid angle $= \frac{1}{8} \times 4\pi = \frac{\pi}{2}$

$\Rightarrow \phi(P) = -\frac{1}{2} \times \frac{\pi}{2} = -\frac{\pi}{4}$ agrees w/ 3-point discretized Berry-phase result // (p.6)

CHERN THEOREM

Here $C = -1$

Φ (unit sphere) $= -\frac{1}{2} \times 4\pi = -2\pi$

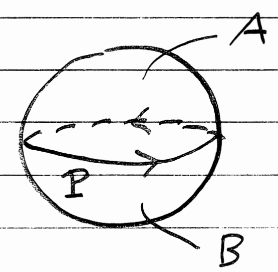
Integer Chern number

More generally,

$$\boxed{\oint_S \underline{\Omega} \cdot \hat{\underline{n}}\, dS = 2\pi C}$$

for any closed surface S (w/o edges)

Proof by division:



Will apply Stokes to regions A and B:
need to choose smooth gauges for each of them

In region A, use $|\uparrow_{\hat{\underline{n}}}\rangle_A = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)\, e^{i\varphi} \end{pmatrix}$

This gauge is not smooth everywhere in B: it has a singularity at the South pole $\theta = \pi$, where the phase of

$$|\uparrow_{-\hat{z}}\rangle = \begin{pmatrix} 0 \\ e^{i\varphi} \end{pmatrix}$$

depends on the azimuthal direction along which the limit $\theta \to \pi$ is taken

A smooth gauge in B can be obtained as follows:

$$|\uparrow_{\hat{\underline{n}}}\rangle_B = e^{-i\varphi}\, |\uparrow_{\hat{\underline{n}}}\rangle_A = \begin{pmatrix} \cos(\theta/2)\, e^{-i\varphi} \\ \sin(\theta/2) \end{pmatrix}$$

This gauge transformation transfers singularity to North pole

$$\Phi(\text{unit sphere}) = \int_A \underline{\Omega} \cdot \hat{\underline{n}}\, dS + \int_B \underline{\Omega} \cdot \hat{\underline{n}}\, dS$$

Stokes

$$= \oint_P \underline{A}_A \cdot d\underline{l} - \oint_P \underline{A}_B \cdot d\underline{l}$$

But these both measure ϕ_P, (in different gauges)
which is well-defined mod 2π

$$\therefore \oint_{\substack{\text{unit}\\ \text{sphere}}} \underline{\Omega} \cdot \hat{\underline{n}}\, dS = 2\pi \times \underbrace{(\text{integer})}_{C}$$

$$2\pi C = \oint_S \underline{\Omega} \cdot \hat{\underline{m}}\, dS \overset{\text{Gauss}}{=} \int_V \underline{\nabla} \cdot \underline{\Omega}\, dV \overset{\underline{\nabla}\cdot(\underline{\nabla}\times\underline{A}) = 0}{=} 0 \;!$$

How can C be nonzero ?!

Consider $\underline{\Omega}(\underline{B})$ instead of $\underline{\Omega}(\hat{\underline{m}})$ $\quad (\underline{B} = B\hat{\underline{m}})$

$$\Omega_z(\underline{B} = B\hat{\underline{z}}) = -2\,\mathrm{Im}\langle \partial_{B_x} \uparrow_z | \partial_{B_y} \uparrow_z \rangle$$

$$\partial_{B_x} = \frac{1}{B}\partial_{m_x} \qquad = \frac{1}{B^2}\left(-2\,\mathrm{Im}\langle \partial_{m_x} \uparrow_z | \partial_{m_y} \uparrow_z \rangle\right)$$

$$= -\frac{1}{2B^2}\hat{\underline{z}}$$

$$\therefore \quad \boxed{\underline{\Omega}(\underline{B}) = -\frac{\underline{B}}{2B^3}}$$ Monopole at $\underline{B} = 0$!

Identity: $\underline{\nabla} \cdot \dfrac{\underline{r}}{r^3} = 4\pi\delta^3(\underline{r})$

$$\Rightarrow \quad \boxed{\underline{\nabla} \cdot \underline{\Omega} = -2\pi\delta^3(\underline{B})}$$ Divergence-free except at $\underline{B} = 0$

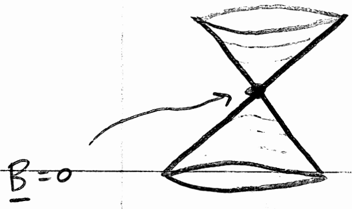
$$2\pi C = \int_V \underline{\nabla} \cdot \underline{\Omega}\, d^3B = -2\pi, \text{ i.e. } C = -1$$

Comments:

(i) $H = -\left(\dfrac{\gamma\hbar B}{2}\right)\hat{\underline{m}} \cdot \underline{\sigma} \Rightarrow \begin{cases} E_\uparrow = -\dfrac{\gamma\hbar B}{2} \\ E_\downarrow = +\dfrac{\gamma\hbar B}{2} \end{cases}$

$\Delta E = \gamma\hbar B$ (Zeeman splitting)

At $B = 0$, states $|\uparrow\rangle$ and $|\downarrow\rangle$ are degenerate, and the two levels split linearly w/ B away from degeneracy point



(school logo!)

$\boxed{\text{Isolated degeneracies in a 3D parameter space act as monopole sources/sinks of Berry curvature}}$

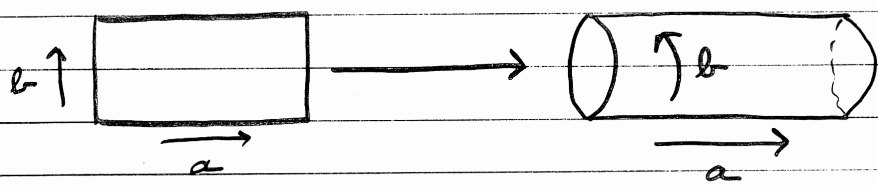
"Weyl points" or "Diabolical points"

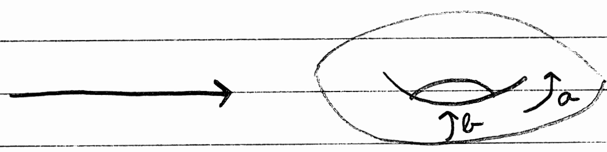
(ii) When $C \neq 0$ for some closed surface S, it is impossible to construct a smooth gauge over the entire surface: If such a gauge existed, then we could apply Stokes' thm. directly to S and conclude that $C = 0$:

$$2\pi C = \oint_S \underline{\Omega} \cdot \hat{\underline{n}}\, dS = \oint_{\partial S = 0} \underline{A} \cdot d\underline{\lambda} = 0 \;//$$

$\boxed{\text{C(S)} \neq 0 \text{ presents a "Topological obstruction" to the construction of a globally smooth gauge}}$

- <u>Chern number of a 2-Torus</u> (e.g. 2D BZ)

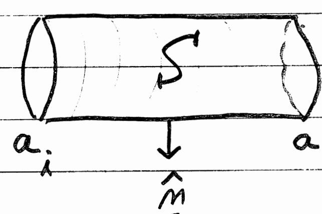




closed surf.

(i) Berry flux through cylindrical surface

(a, b) param. space, w/ $b \in [0, 1]$ cyclic:



$$|u_{a, b=1}\rangle = |u_{a, b=0}\rangle$$

$$A_a = i\langle u|\partial_a u\rangle, \quad A_b = i\langle u|\partial_b u\rangle$$

$$\underline{\Omega}\cdot\underline{n} = \partial_a A_b - \partial_b A_a$$

$$\Phi(S') = \int_{a_i}^{a_f} da \int_0^1 db\,(\partial_a A_b - \partial_b A_a)$$

$$2^{nd}\text{ term} = -\int_{a_i}^{a_f} da\,[A_a(a, b=1) - A_a(a, b=0)]$$

$= 0$ because $|u(a,b)\rangle$ is cyclic in b

$$\Rightarrow \Phi(S') = \int_{a_i}^{a_f} da\,\frac{\partial}{\partial a}\underbrace{\int_0^1 A_b\,db}_{\phi^{(b)}}$$

$\phi^{(b)}$ = Berry phase along b-loop at fixed a

$$\Phi(S') = \phi^{(b)}(a_f) - \phi^{(b)}(a_i)$$

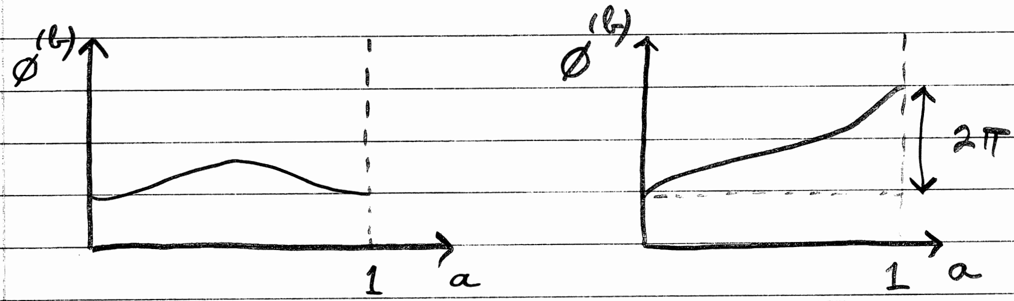
no 2π jumps (assuming continuous evolution of $\phi^{(b)}$ between a_i and a_f)

(ii) Chern number of the torus

For S' = torus, $a_i = 0$ and $a_f = 1$ are also identified

$$\boxed{2\pi C = \Phi(S') = \phi^{(b)}(a=1) - \phi^{(b)}(a=0)}$$

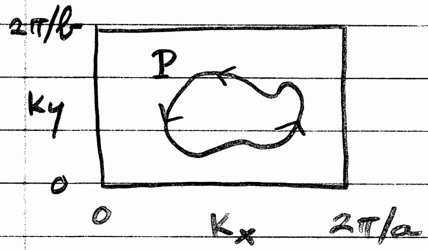
$\therefore$ $\boxed{C = \text{winding number of } \phi^{(b)} \text{ as we evolve around cycle in } a}$



$\boxed{C=0}$ $\boxed{C=1}$

ZAK PHASE

We saw earlier that Berry phases can be defined for closed loops in a 2D BZ



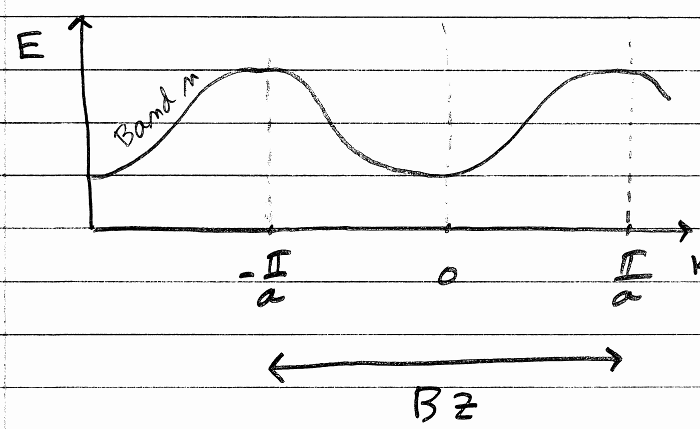
cell-periodic

$$\underline{A}_{\underline{k}} = i \langle u_{\underline{k}} | \frac{d}{d\underline{k}} u_{\underline{k}} \rangle$$

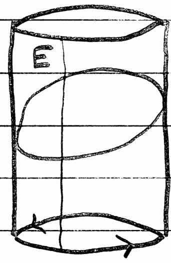
$$\phi = \oint_P \underline{A}_{\underline{k}} \cdot d\underline{k}$$

What about a $\underline{1D\ BZ}$?

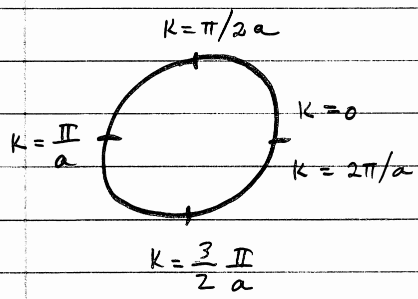
$$E_{n,k+\frac{2\pi}{a}} = E_{nk}$$



(conventional view)



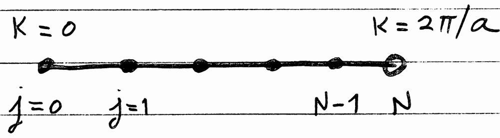
BZ wrapped into a circle, bands plotted on a cylinder (topological view)



$$\boxed{\phi_n = \int_0^{2\pi/a} A_{nk}\, dk}$$

Zak phase of band n (assumed isolated)

Discretization:



$$k_j = \frac{j}{N}\frac{2\pi}{a}$$

Let $|\mu_j\rangle \equiv |\mu_{k_j}\rangle$

$$\phi \overset{?}{=} -\mathrm{Im}\ln\left[\langle\mu_0|\mu_1\rangle\langle\mu_1|\mu_2\rangle\cdots\langle\mu_{N-1}|\mu_0\rangle\right]$$

This would be correct if $|\mu_{k=2\pi/a}\rangle = |\mu_{k=0}\rangle$

But we already imposed $|\psi_{k=2\pi/a}\rangle = |\psi_{k=0}\rangle$ (p. 3)

Since $\psi_k(x) = \exp(ikx)\,\mu_k(x)$

$$\Rightarrow \boxed{\underbrace{|\mu_{k=2\pi/a}\rangle}_{|\mu_N\rangle} = \exp\left(-i\frac{2\pi}{a}x\right)\underbrace{|\mu_{k=0}\rangle}_{|\mu_0\rangle}}$$

$$\boxed{\phi = -\mathrm{Im}\ln\left[\langle\mu_0|\mu_1\rangle\langle\mu_1|\mu_2\rangle\cdots\langle\mu_{N-1}|e^{-i\frac{2\pi}{a}x}\mu_0\rangle\right]}$$

Discretized Zak phase

While the Berry phase only depends on the wavefunctions along the loop, the Zak phase also depends on the coordinate operator x, i.e on the "real-space embedding" of wavefcts.

WANNIER FUNCTIONS

Def.: $$|W_R\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk\, e^{-ikR}\,|\psi_k\rangle$$

lattice vec. $R = ja$

$\updownarrow$ FOURIER

$$|\psi_k\rangle = \sum_R e^{+ikR}\,|W_R\rangle$$

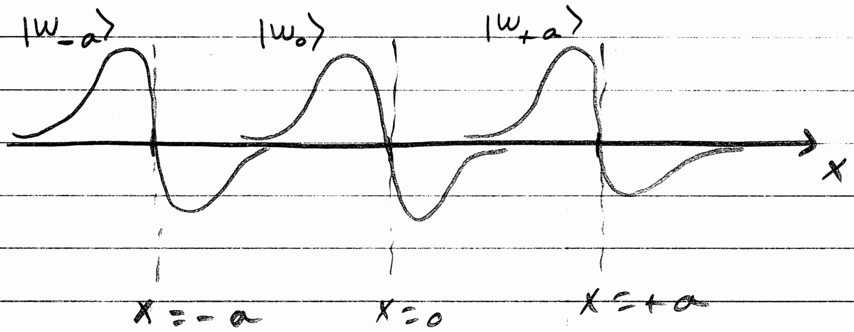
(assuming isolated band, dropped index n)

If $\psi_k(x)$ is a smooth fct. of k, then
$w_R(x)$ is a localized fct. centered near R

Properties:

① WFs w/ different R are periodic images of one another:

$$\boxed{w_R(x) = w_0(x-R)}$$



② WFs form an orthonormal set:

$$\boxed{\langle w_R | w_{R'} \rangle = \delta_{R,R'}}$$

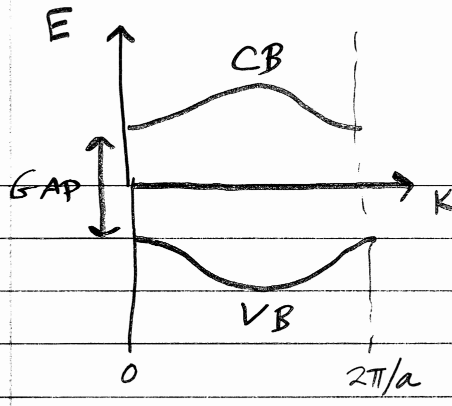
③ WF centers are given by the Zak phase ϕ

$$\bar{x}_R \equiv \langle w_R | \hat{x} | w_R \rangle \overset{①}{=} \bar{x}_0 + R$$

$$\boxed{\bar{x}_0 = a\,\frac{\phi}{2\pi}}$$

Physical interpretation: For a valence band in an insulator, $\bar{x}_0$ is the center of mass of all electrons in that band, in the $R=0$ cell

("intracell electronic coord.")



One valence band

$\Rightarrow$ $2e^-$s / cell ($\uparrow$ and $\downarrow$ spin)

$Z_{ion} = +2e$ / cell

Intracell dipole : $d_{cell} = 2e(z_{ion} - \bar{x}_0)$

Electric polarization: $P_{el} = d_{cell}/a$

$$\therefore \quad \boxed{P_{el} = 2e\left(\frac{z_{ion}}{a} - \frac{\phi}{2\pi}\right)}$$

"Berry-phase polarization"

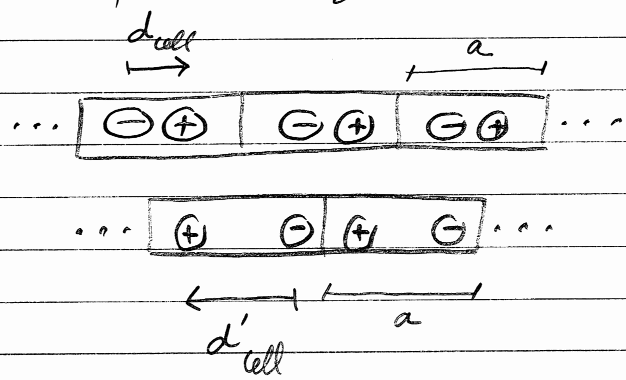
Comments :

(i) This is not the same as the dipole/cell calculated from the bulk charge density $\rho(x)$, which has contribs. from tails of WFs centered on neighboring cells, and whose value depends (continuously) on choice of cell

Ill-defined! $\longrightarrow$

(ii) Since ϕ is only defined mod 2π, bulk P_{el} is only defined mod $2e$ ("quantum of indeterminacy")

But same is true for a periodic chain of classical point charges!



$d_{cell} - d'_{cell} = ea$

($\times 2$ for spin degen.)

(iii) Quantum of indeterminacy does not affect the calculation of the change in P as a function of some param. λ (e.g. strain, phonon amplitude)

$$P_{el}'(\lambda) = P_{el}(\lambda) - 2e$$

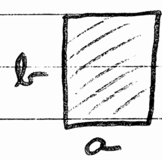
$$\frac{dP_{el}'}{d\lambda} = \frac{dP_{el}}{d\lambda}$$

$$\Rightarrow \quad \Delta P_{el} = \int_{\lambda_i}^{\lambda_f} \frac{dP_{el}}{d\lambda}\, d\lambda \text{ is uniquely defined}$$

Exp't'ly one always measures this //

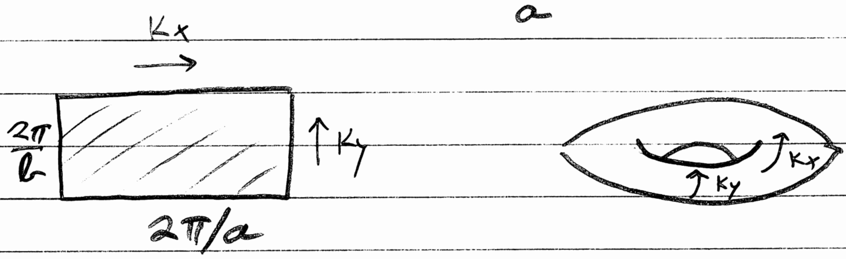
QUANTUM ANOMALOUS HALL EFFECT IN 2D

2D insulator w/ one valence band (spinless).
Rectangular lattice



unit cell

BZ:



CONVENTIONAL VIEW TORUS TOPOLOGY

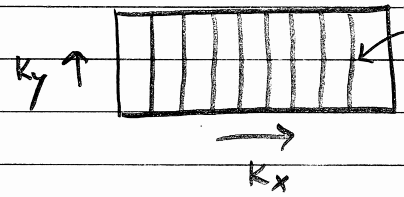
$$\Omega(k_x, k_y) = -2\,\mathrm{Im}\,\langle \partial_{k_x} u \,|\, \partial_{k_y} u \rangle$$

$$C = \frac{1}{2\pi} \int_0^{2\pi/a} dk_x \int_0^{2\pi/b} dk_y\, \Omega(k_x, k_y)$$

Integer Chern number

Recall that $C(\text{torus})$ = winding # of the Berry phase (p. 14)

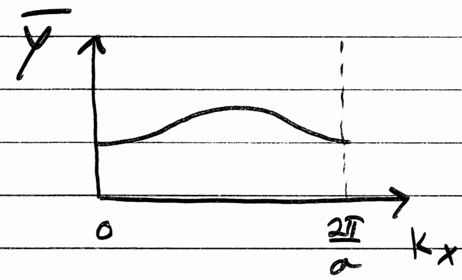
Same here, but with Zak phase of BZ strings at fixed k_x:



$$\phi^{(y)}(k_x) = \int_0^{2\pi/b} i\langle u|\partial_{k_y} u\rangle \, dk_y$$

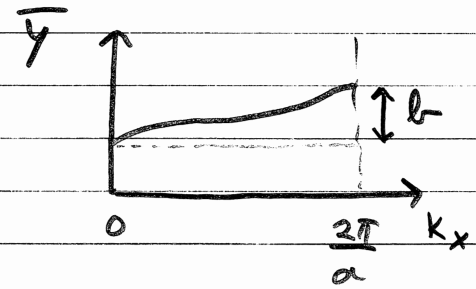
$$\bar{y}(k_x) = b\,\frac{\phi^{(y)}(k_x)}{2\pi}$$

= "hybrid WF center"



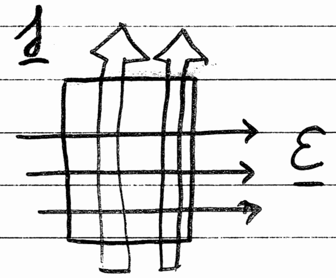
$\boxed{C=0}$

ordinary insulator



$\boxed{C=1}$

"Chern/QAH insulator"



$$\boxed{j_y = +C\,\frac{e^2}{h}\,\mathcal{E}_x}$$

QAH effect

Proof: $\hbar \dot{k}_x = -e\,\mathcal{E}_x \;\Rightarrow\; \hbar\,\Delta k_x = -e\,\mathcal{E}_x\,\Delta t$ $\quad (e>0)$

$(\mathcal{E}_x > 0)$ For $\Delta k_x = -\frac{2\pi}{a}$, $\begin{cases} \Delta t = \dfrac{h}{e a \mathcal{E}_x} = T_{\text{Bloch}} \\ \Delta \bar{y} = -C b \end{cases}$

$$\langle v_y \rangle = \frac{\Delta \bar{y}}{T_{\text{Bloch}}} = -C\,\frac{e}{h}\,a b\,\mathcal{E}_x$$

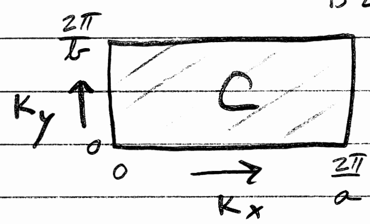
$$j_y = \underbrace{\frac{-e}{ab}}_{\rho_{el}} \langle v_y \rangle = +C\,\frac{e^2}{h}\,\mathcal{E}_x \;//$$

Hall conductivity : $\sigma_{Hall} \equiv \frac{j_y}{\mathcal{E}_x} = C \frac{e^2}{h}$ ← quantum of conductance

Like IQHE, but at $\underline{B} = 0$! $\Rightarrow$ "Anomalous" (QAHE)

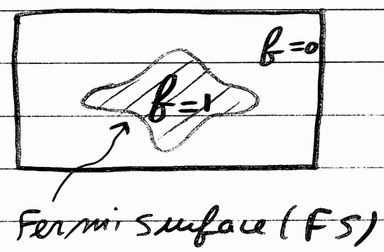
$\therefore$ $\boxed{\text{For a 2D insulator, anomalous Hall conductivity must be quantized in units of } e^2/h}$

$$\sigma_{AH} = \frac{e^2}{2\pi h} \int_{BZ} \Omega(k_x, k_y)\, d^2k$$



• AHC of a 2D metal

(Fermi level cuts through valence band)



$$\sigma_{AH} = \frac{e^2}{2\pi h} \int_{BZ} f(k_x, k_y)\, \Omega(k_x, k_y)\, d^2k$$

$$= \frac{e^2}{2\pi h} \int_{\substack{\text{occ. BZ} \\ \text{region}}} \Omega(k_x, k_y)\, d^2k$$

Stokes
$\Omega = (\nabla \times \underline{A})_z$

$$= \frac{e^2}{2\pi h} \oint_{FS} \underline{A}(\underline{k}) \cdot d\underline{k}$$

Berry phase of FS contour

$$\boxed{\sigma_{AH} = \frac{e^2}{h} \frac{\phi_{FS}}{2\pi}}$$

(mod e^2/h)

Amazing!