Introduction to Zak phase

Fun with periodic 2×2 matrices

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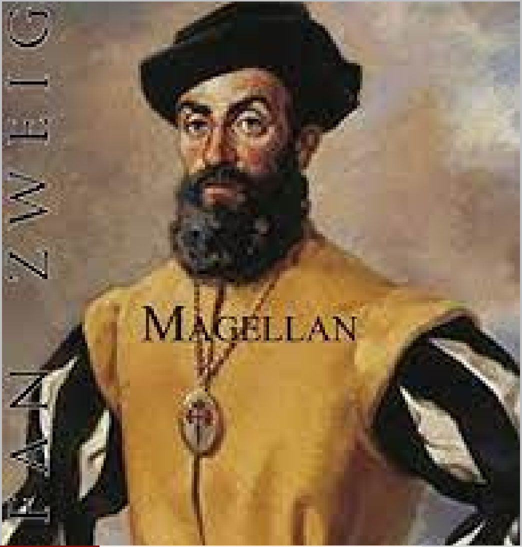
A topological invariant from the 16 century

Discoverer: Antonio Pigafetta



Joshua Zak

Technion

- Born 1929 (age 93)
- 1940-1945 Labor and death camps
- 1946-1949 Red army
- 1951 Silver medal (physics)
  Gold medal (Kayaking)
- Known for:
  - Zak transfrom
  - Magnetic translations
  - Zak phase

Geometry of 2×2 hermitian matrices

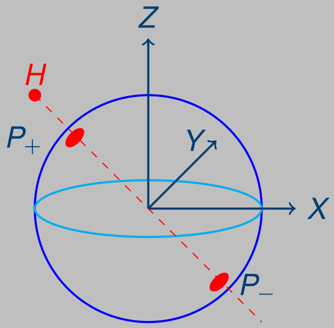
Hamiltonians & states

- $H = xX + yY + zZ, \quad x, y, z \in \mathbb{R}^3$
- X, Y, Z Pauli matrices.

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Eigen-projections

$$P_\pm = \frac{\mathbb{1} \pm \hat{H}}{2}, \quad \hat{H} = \frac{H}{|H|}$$



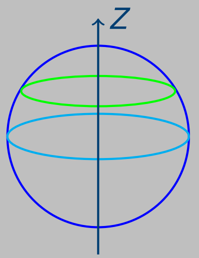
Bloch sphere

Parallel transport

Keeping normalization and phase

Parallel transport $\langle\psi|d\psi\rangle = 0$

- $\mathrm{Re}\langle\psi|d\psi\rangle = 0$
  constant normalization (exact)
- $\mathrm{Im}\langle\psi|d\psi\rangle = 0$
  constant phase (leading order)
- Rigid rotation
  - $|\psi_\theta\rangle = e^{-iZ\theta/2}\,|\psi\rangle$
  - $i\langle\psi_\theta|d\psi_\theta\rangle = \frac{1}{2}\,\langle\psi|\,Z\,|\psi\rangle\,d\theta$



Equator: $\langle\psi|\,Z\,|\psi\rangle = 0$

Berry's phase

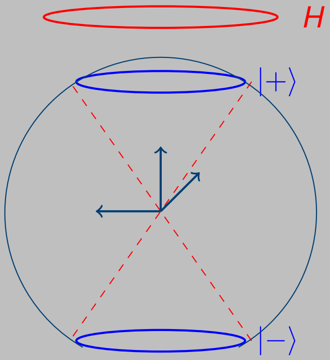
Berry's gauge potential

Berry's 1-form

$$A = -\mathrm{Im}\langle\psi|d\psi\rangle$$

Berry's phase

$$\beta = \left(\oint A\right) \mod 2\pi$$



$\beta =$ (spherical angle)$/2$

$$\beta_+ + \beta_- = 0 \mod 2\pi$$

What does Berry's phase measure?

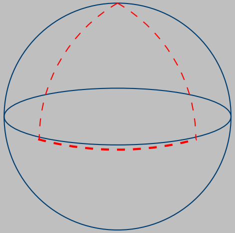
Deviation from parallel transport

- $|\varphi\rangle$ parallel transported
- $|\psi\rangle$ smooth normalized section

$$|\psi\rangle = e^{-i\beta}\,|\varphi\rangle$$

- Berry's connection

$$i\langle\psi|d\psi\rangle = d\beta$$



Berry's phase for a closed path

Holonomy of parallel transport

The mother of $\mathbb{Z}_2$ phases

Topology associated with periodic real symmetric matrices

- Real symmetric:

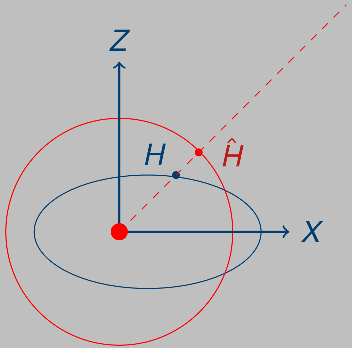
$$H(x,z) = \begin{pmatrix} z & x \\ x & -z \end{pmatrix}$$

- Spectral projections

$$P_\pm = \frac{\mathbb{1} \pm \hat{H}}{2}, \quad \hat{H} = \frac{H}{|H|}$$

- $P_\pm$ smooth on punctured plane

$$\mathbb{R}^2/0$$



Winding of H

Much ado about nothing

A circle of real smooth eigenfunction must vanish

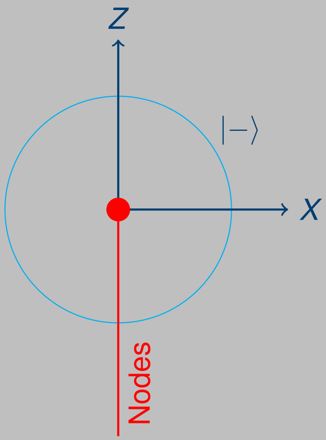
- Real and smooth eigenfunction

$$|\psi_-\rangle = \begin{pmatrix} -x \\ z + \sqrt{x^2 + z^2} \end{pmatrix}$$

- Not normalizable

$$|\psi_-\rangle \Big|_{x=0, z<0} = 0$$

- Node: Movable, but indelible



A tail of discontinuity

A circle parallel transported state must fail to be smooth

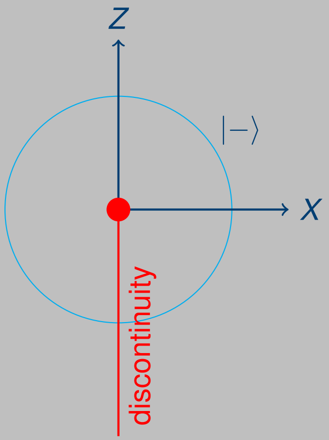
- Real and normalized

$$|\psi_-\rangle = -\sin(\theta/2)\,|0\rangle + \cos(\theta/2)\,|1\rangle$$

- Discontinuity

$$|\psi_-(0)\rangle = -\,|\psi_-(2\pi)\rangle$$

- Discontinuity: Movable but indelible
- Holonomy of parallel transport.



Freedom is complex

A circle of smooth eigen-function must fail parallel transport

- Smooth, normalized but complex

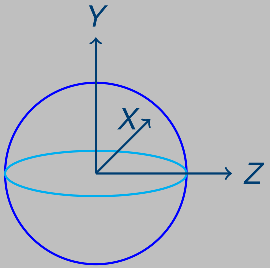
$$|\psi_-\rangle = (1 - e^{i\theta})\,|0\rangle + (e^{i\theta} + 1)\,|1\rangle$$

- Fails parallel transport.

$$A = i\langle\psi|d\psi\rangle = -\frac{d\theta}{2},$$

- Berry's phase = holonomy

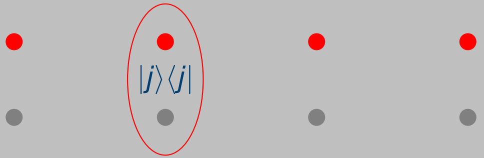
$$\oint A = -\pi$$



π=half spherical angle

Periodic matrices from periodic Hamiltonians

Unit cell with 2 atoms (or spin)



- $H = \sum_{j,\ell \in \mathbb{Z}} |j+\ell\rangle\langle j| \otimes H_\ell, \quad H_\ell = H^*_{-\ell} = \begin{pmatrix} \bullet & \bullet \\ \bullet & \bullet \end{pmatrix}$
- Bloch Hamiltonian:

$$H(k) = \sum_{\ell \in \mathbb{Z}} e^{ik\ell} H_\ell, \quad H(k) = H^*(k) = \begin{pmatrix} z_k & \zeta_k \\ \bar{\zeta}_k & -z_k \end{pmatrix}$$

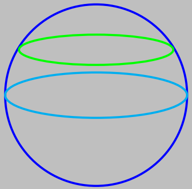
Two bands

Gapped: $z_k^2 + |\zeta_k|^2 > 0$

Zak phase

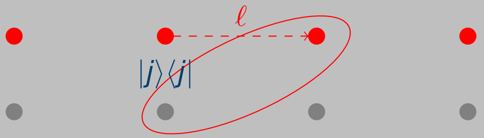
Berry's phase for a full band

- Berry's phase for a full band
- Not quantized (in general)
- Quantization: Symmetry protected
- Depends on the choice of unit cell
- Related to polarization



Choice of Unit cell as Gauge freedom

Spectrum: independent of the choice of unit cell, Zak phase depends on the choice



- Change of unit cell

$$H(k) \mapsto G_k H(k) G_k^*$$

- G:

$$G_k = e^{ik\ell}\,|0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} e^{ik\ell} & 0 \\ 0 & 1 \end{pmatrix}$$

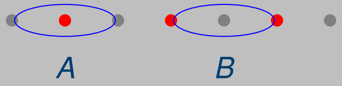
- Transformation of Berry's 1-form:

$$A_\ell - A_0 = i\ell\,\langle\psi_k|\,G^*\dot{G}\,|\psi_k\rangle = -\ell|\langle\psi_k|0\rangle|^2$$

Physical properties that depends on unit cell

- Red atom: center of unit cell A
- Red atom: edges of unit cell B
- Total charge in unit cell:

$$N_- = \int_{-\pi}^{\pi} \frac{dk}{2\pi} |\psi_k\rangle\langle\psi_k|$$



- Comparing Zak phases

Polarization of dielectrics
Resta & Vanderbilt

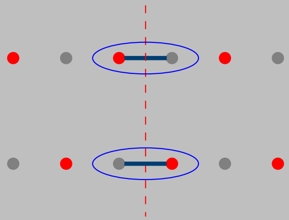
$$\beta_\ell - \beta_0 = -2\pi\ell \langle 0| N_- |0\rangle \overset{\text{mod } 2\pi}{=} \underbrace{\pi\ell\Big(\langle 1| N_- |1\rangle - \langle 0| N_- |0\rangle \Big)}_{\text{polarization}}$$

Symmetry-I

Reflection about a bond

- Reflection of cells

$$R\Big(\,|j\rangle\langle j|\,\Big) = |-j\rangle\langle -j|$$



- Reflection in cell

$$R\Big(\,|a\rangle\langle a|\,\Big) = X\,|a\rangle\langle a|\,X, \quad a \in 0, 1$$

$$R(H(k)) = XH(-k)X$$

- Bond reflection invariance

$$z_k = -z_{-k}, \quad \zeta_k = \bar{\zeta}_{-k}$$

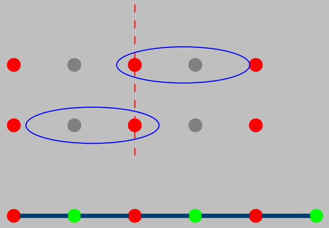
Symmetry-II

Reflection about an atom

- Reflection$\Longrightarrow$ k-dependent gauge:

$$R(H(k)) = G_k\Big(H(-k)\Big)G_k^*$$

- $G_k = \begin{pmatrix} e^{ik} & 0 \\ 0 & 1 \end{pmatrix}$



Reflection invariance: $\zeta_k = \bar{\zeta}_{-k}$

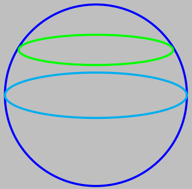
$$H(k) = \begin{pmatrix} 1 & 1+e^{ik} \\ 1+e^{-ik} & -1 \end{pmatrix}, \quad \zeta = e^{i\theta}$$

Symmetry protected $\mathbb{Z}_2$ phase

Berry's 2-nd gauge

- $\lambda_k \, |\psi_{-k}\rangle = G_k \, |\psi_k\rangle$
- Covariant connection

$$\mathcal{A} = \mathrm{Im}\langle\psi|D\psi\rangle, \quad D = d + \underbrace{\frac{1}{2} G^* dG}_{2-\text{gauge}}$$



Green: Berry's phase
Cyan: STP phase

- Symmetry implies

$$\mathcal{A}_{-k} + \mathcal{A}_k = i d \log \lambda$$

SPT Zak phase

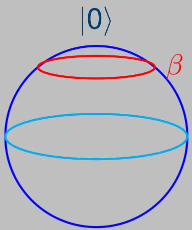
$$2 \int_{-\pi}^{\pi} \mathcal{A} \, dk \in 2\pi\mathbb{Z} \Longrightarrow \int_{-\pi}^{\pi} \mathcal{A} \, dk \in \pi\mathbb{Z}$$

Deformation

Gapped

- Take: $G_k = e^{ikA}$
- $U_\pi = U_{-\pi} \Longrightarrow \text{spect}(A) \in \mathbb{Z}$
- Covariant connection $D = d + \frac{i}{2}A$
- If $z < 0$, deform $z \to -\infty$

$$|\psi\rangle \to |0\rangle\,, \quad \beta \to 0$$



Red: General case
Cyan: STP phase

Index and phase

$$\int_{-\pi}^{\pi} \mathcal{A}\, dk \overset{\text{mod } 2\pi}{=} \pi \langle 0| A |0\rangle$$

Symmetry protected $\mathbb{Z}_2$ index

Invariant points

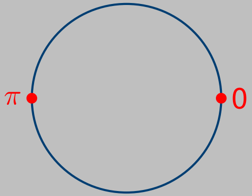
- Symmetry:

$$G_k H_k = H_{-k} G_k,$$

- Involution: $G_{-k} G_k = \mathbb{1}$
- Continuous:

$$G_\pi = G_{-\pi}$$

- Ambiguity: $G \mapsto \pm e^{ink} G$



- $[H_0, G_0] = [H_\pi, G_\pi] = 0$
- $G_0^2 = G_\pi^2 = \mathbb{1}$

Index of invariant points (disambiguous)

$$\frac{\langle\psi_0|\, G_0\, |\psi_0\rangle}{\langle\psi_\pi|\, G_\pi\, |\psi_\pi\rangle} \in \pm 1$$

Example: SSH model

Su Schriefer Heeger

- SSH Hamiltonian

$$H(k) = \begin{pmatrix} 0 & s + te^{ik} \\ s + te^{-ik} & 0 \end{pmatrix}$$

SSH model

- Symmetry $H(-k) = XH(k)X$
- Gapped: $|s| \neq |t|$
- $H_{0,\pi} = (s \pm t)X$

$$\text{Index} = \frac{\langle\psi_0|\, X \,|\psi_0\rangle}{\langle\psi_\pi|\, X \,|\psi_\pi\rangle} = \text{sgn}(|s| - |t|)$$

$$\text{Index}\Big(0 - \text{Cell}\Big) = (-)^\ell \ \text{Index}\Big(\ell - \text{Cell}\Big)$$

Kitaev chain

A model without particle conservation

- Periodic Kitaev Chain:

$$H(k) = \varepsilon_k a_k^* a_k + \underbrace{\left(e^{ik} a^*{}_k a^*{}_{-k} + h.c.\right)}_{\text{particle non-conserving}}, \quad \varepsilon_k = \mu + t \cos k$$

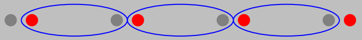
- Majorana:

$$\gamma_{2j+1} = a_j + a_j^*, \quad \gamma_{2j+2} = -i(a_j - a_j^*)$$

- μ term: $2a_j^* a_j = i\gamma_{2j+1}\gamma_{2j+2}$

- Hopping & super-conductivity:

$$i\gamma_{2j+2}\gamma_{2j+3} = a_j a_{j+1} + a_j a_{j+1}^* + h.c.$$



Reduction to 2×2 matrices

Fermionic Bloch-Fock space

- $$H(k) + H(-k) = \varepsilon_k \left(a_k{}^* a_k + a_{-k}{}^* a_{-k} \right) + 2i \sin k \left(a^*{}_k a^*{}_{-k} - a_{-k} a_k \right)$$
- Fock-Bloch basis

$$|0\rangle \,,\ a^*{}_k\,|0\rangle \,,\ a^*{}_{-k}\,|0\rangle \,,\ a^*{}_k a^*{}_{-k}\,|0\rangle$$

- 4×4 matrix

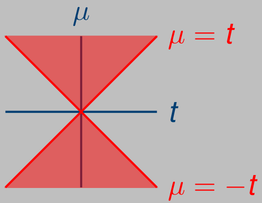
$$H_k + H_{-k} - \varepsilon_k = \begin{pmatrix} -\varepsilon_k & 0 & 0 & -2i \sin k \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2i \sin k & 0 & 0 & \varepsilon_k \end{pmatrix}$$

2×2: Span $|0\rangle$ and $a_k^* a_{-k}^*\,|0\rangle$

Bands in the vacuum-Cooper pairs sector

$\mathbb{Z}_2$ Index

- 2-Bands
  $H(k) = Z\varepsilon_k + 2Y \sin k$
- $H_{0,\pi} = (\mu \pm t)Z$
- Gapped: $\mu \neq \pm t$
- Symmetry: $H(-k) = ZH(k)Z$



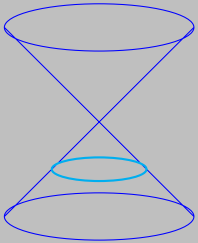
Topological phase diagram

$$\text{Index} = \frac{\langle \psi_0 | Z | \psi_0 \rangle}{\langle \psi_\pi | Z | \psi_\pi \rangle} = \text{sgn}(\,|\mu| - |t|)$$

Short history of Zak phase

Mother of SPT

- 1979: Mead and Truhlar: Conics crossing, molecules
- 1982: TKNN: Topology for 2-D bands
- 1984: M. Berry: adiabatic connection & curvature
- 1983: B. Simon: "Berry's phase", "Chern bundle"
- 1989: J. Zak, Geometry & topology of 1-D bands
- 1993: Resta & Vanderbilt, Zak phase=Polarization,
- 2013: Bloch: Measurement of Zak phase
- Kitaev, Gu & Wen, Pollmann
- Graf, Shapiro, Schultz-Baldes, Ogata



Reference

Review

- JK Asbóth, L Oroszlány, A Pályi, A short course on topological insulators