Pancharatnam-Zak phase*

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*With D. Roy & J. Samuel (based on arXiv:1909.00818)

Zak phase

- Thouless (1982 - 1983) discover the topological invariant - TKNN - Chern class in condensed matter systems

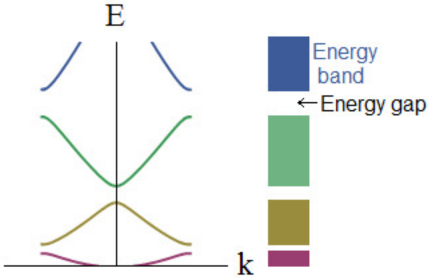
$$\int d^2k \ (\partial_{k_1} A_{k_2} - \partial_{k_2} A_{k_1})$$

- Berry (1983-1984) shows the origin of geometric phase in adiabatic quantum evolution

$$\oint d\vec{R} \cdot \vec{A}$$

- Barry Simons (1983) points out the mathematical connection between the above
- First condensed matter manifestation of geometrical phase was shown

- Motivated by Berry (1984), Zak (1989) shows another manifestation of geometric phase in 1D periodic lattice system
- Considers the adiabatic motion of electron in Bloch state ψ_{nk} influenced by a weak tangential electric field
- Argues that $k \to k + eA(t)$ causes a circuit in FBZ, which can be understood as a circle
- Possibility of adiabatic cyclic geometric phase - (Berry kind)



- The Hamiltonian Bloch eigenstates $\psi_{nk}(x)$ can be written as:

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x), \qquad u_{nk}(x+a) = u_{nk}(x)$$

  in terms of cell periodic Bloch states $u_{nk}(x)$
- Considers the Hamiltonian: $\hat{H} = \frac{1}{2\mu}\left(\hat{p} - eA(t)\right)^2 + V(\hat{x})$
- Zak shows that the geometric phase acquired during the circuit is

$$\gamma_{Zak} = i \int_0^{\frac{2\pi}{a}} dk \, \langle u_n(k) | \frac{\partial}{\partial k} | u_n(k) \rangle$$

- Argues existence of a notion of position: Band center $x_c = \frac{a}{2\pi}\gamma_{Zak}$
- Later Resta, Vanderbilt and others show that change in electric polarisation is

$$\Delta P = e \Delta x_c$$

- The modern understanding of polarisation in dielectrics is based upon this notion
- Celebrated piece of work: many applications

Problems with Zak

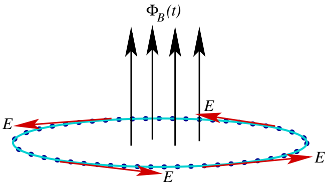
- Derivation is unsatisfactory, k is treated as a continuous variable, and changes as a function of time,
$$\text{BUT } [\hat{H}, \hat{T}_x(a)] = 0 \qquad \text{implying } \Delta k = 0$$
selection rule !
- The expression for γ_{Zak} is NOT gauge invariant
- Known to change its value under unit cell reparametrisation
- For SSH model, several values of γ_{Zak} are quoted in the literature
- General agreement that γ_{Zak} itself is a unphysical, unobservable quantity; only $\Delta\gamma_{Zak}$ matters

Kinematics

- Consider 1D lattice system with the existence of periodic boundary condition (PBC)
- The system can be thought of as a periodic lattice forming a ring
- We allow a linearly time-varying magnetic flux $\Phi_B(t)$ to pierce the ring, while giving rise to a weak tangential electric field E
- A system described by the Hamiltonian:

$$\hat{H}_{\alpha(t)} = \frac{1}{2\mu}\left(\hat{p} + \hbar\alpha(t)\right)^2 + V(\hat{x}),$$

where the time-dependent vector potential $A(t) = -Et$ and $\alpha(t) = -eA(t)/\hbar$.



- Hamiltonian admits normalized instantaneous eigenstates $|\Psi_{nk_m\alpha}\rangle$ which solve:

$$\hat{H}_\alpha|\Psi_{nk_m\alpha}\rangle = E_{nk_m\alpha}|\Psi_{nk_m\alpha}\rangle$$
$$\hat{T}_x(a)|\Psi_{nk_m\alpha}\rangle = e^{ik_m a}|\Psi_{nk_m\alpha}\rangle$$

- Owing to PBC, we have $\Psi_{nk_m\alpha}(x+Na) = \Psi_{nk_m\alpha}(x)$, so that each band consists of exactly N states with quantum number $k_m = \frac{2\pi}{Na}m$, where $m = 0, 1, \cdots, N-1$
- So the states $\Psi_{nk_m\alpha}$ and $\Psi_{nk_{m+N}\alpha}$ are colinear:

$$|\Psi_{nk_{m+N}\alpha}\rangle = e^{i\chi}|\Psi_{nk_m\alpha}\rangle$$

  where χ is some arbitrary real number
- The states $\Psi_{nk_{m+N}\alpha}(x)$ and $\Psi_{nk_m\alpha}(x)$ describe the same physical state, as the corresponding density matrices are identical
- It is often assumed that $\chi = 0$, a choice of convention which is referred to as the *periodic gauge* condition
- Clearly, all the physical observables must be insensitive to the value of the unphysical phase χ

- The vector potential at any time t can be written as a gauge transformation:

$$A(t) = A(0) + \frac{i\hbar}{e} U^\dagger(x,t)\partial_x U(x,t),$$

where $U(x,t) = \exp\left(\frac{i}{\hbar} eEtx\right)$

- Under such a transformation, the momentum operator transforms as: $\hat{p} - eA(t) = U^\dagger(x,t)\hat{p}\,U(x,t)$, which allows the Hamiltonian at some time t and at $t = 0$ to be unitarily connected:

$$\hat{H}(t) = U^\dagger(x,t)\hat{H}(0)U(x,t)$$

- The operator $U(x,t)$ must respect the PBC: $U(x,t) = U(x+L,t)$ in order to be a well defined operator
- Only for time $t = j\tau$ (j is an integer), PBC is respected, where

$$\tau = \frac{2\pi\hbar}{eEL}$$

- The Hamiltonians $\hat{H}(j\tau)$ (for different js) are physically the same (they are *gauge equivalent*), their spectra are identical
- Their instantaneous eigenstates are related to each other by the gauge transformation:

$$\begin{aligned}|\Psi_{nk_m\alpha(j\delta)}\rangle &= U^\dagger(x,j\tau)|\Psi_{nk_{m+j}\alpha(0)}\rangle \\ &= \exp\left(-i\frac{2\pi xj}{L}\right)|\Psi_{nk_{m+j}\alpha(0)}\rangle,\end{aligned}$$

as also the energies $E_{nk_m\alpha(j\delta)} = E_{nk_{m+j}\alpha(0)}$.

- The transformation factor $U(x, j\tau) = e^{i\frac{2\pi x}{L}j}$ has a very interesting topological property
- It is a function of x, albeit with the PBC, implying that the points $x = 0$ and $x = L$ are identified since $U(0, j\tau) = U(L, j\tau)$
- It lives on a circle with circumference L
- $U(x, j\tau)$ by definition is a phase and takes values only on the unit circle in the complex plane
- So $U(x, j\tau)$ is a map from one circle (with circumference L) to the unit circle, are classified in terms of homotopy classes, with each of them characterized by an integer called the *winding number*, which measures the number of times one circle is winded on another
- Incidentally $e^{ik_jx} = e^{i\frac{2\pi x}{L}j}$ also appears while defining cell periodic Bloch states - encountered earlier

Dynamics

- Initial state is $|\Phi(0)\rangle = |\Psi_{nk_l\alpha(0)}\rangle$, then it is constrained to evolve with the same quantum number k_l at any other time t (No transitions within the band !)
- The system's state $|\Phi(t)\rangle$ essentially evolves *adiabatically* in the presence of a weak electromagnetic field (no interband transitions)

$$|\Phi(t)\rangle = e^{i\phi(t)}|\Psi_{nk_l\alpha(t)}\rangle$$

- The phase factor is given by $\phi(t) = i\int_0^t ds\, \langle\Psi_{nk_l\alpha(s)}|\frac{\partial}{\partial s}|\Psi_{nk_l\alpha(s)}\rangle - \frac{1}{\hbar}\int_0^t ds\, E_{nk_l\alpha(s)}$.
- At time $j\tau$ this takes the form:

$$|\Phi(j\tau)\rangle = e^{i\phi(j\tau)}\hat{U}^\dagger(x, j\tau)|\Psi_{nk_{l+j}\alpha(0)}\rangle$$

- After time $N\tau$, the state of the system is:

$$|\Phi(N\tau)\rangle = e^{i\chi}e^{i\phi(N\tau)}\hat{U}^\dagger(x, N\tau)|\Psi_{nk_l\alpha(0)}\rangle,$$

  indicating that the system returns to the initial state with a large gauge transformation
- It may be noted that in general, $|\langle\Psi_{nk_l\alpha(0)}|\hat{U}^\dagger(x, N\tau)|\Psi_{nk_l\alpha(0)}\rangle| \neq 1$ which indicates that the initial and final states are NOT colinear:

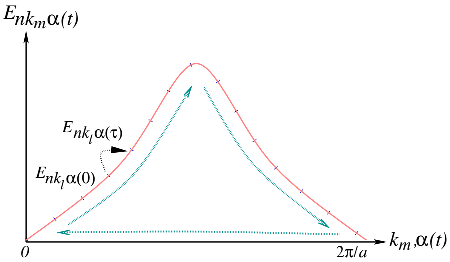
$$|\Phi(N\tau)\rangle \neq e^{i\theta}|\Phi(0)\rangle,$$

  and the corresponding density matrices are NOT identical

- Strictly speaking the system does not return to its initial state after time $N\tau$
- However, owing to the gauge transformation factor $U^\dagger(x, N\tau)$ it is straightforward to see that the average of any observable $\hat{F}(\hat{x}, \hat{p} - eA(t))$ returns after time $N\tau$:

$$\langle \Psi_{nk_l\alpha(0)}|\hat{F}(\hat{x}, \hat{p} - eA(0))|\Psi_{nk_l\alpha(0)}\rangle$$
$$= \langle \Psi_{nk_l\alpha(N\tau)}|\hat{F}(\hat{x}, \hat{p} - eA(N\tau))|\Psi_{nk_l\alpha(N\tau)}\rangle$$

- So the states $|\Phi(0)\rangle$ and $|\Phi(N\tau)\rangle$ while being non-colinear, nevertheless represent the same physical state of the system, albeit expressed in different gauges
- The time evolution of the system in this case is found to be *adiabatic* and *cyclic* kind
- It must be mentioned that this notion of cyclicity generalizes the existing notion in the literature based on the requirement of returning of the density matrix



Geometric phase

- The geometric phase gained by the system reads:

$$\gamma_g(n) = \text{Arg}\langle\Psi_{nk_l\alpha(0)}|\Psi_{nk_l\alpha(N\tau)}\rangle + i\int_0^{N\tau} dt\, \langle\Psi_{nk_l\alpha(t)}|\partial_t|\Psi_{nk_l\alpha(t)}\rangle$$

  This expression can be simplified by working with the cell periodic Bloch states $|u(k_l + \alpha(t))\rangle$ which are defined as:

$$|\Psi_{nk_l\alpha}\rangle = e^{ik_l\hat{x}}|u_n(k_l + \alpha)\rangle$$

- A crucial relation for these Bloch states follows:

$$|u_n(q + \frac{2\pi}{a})\rangle = e^{i\chi}e^{-i\frac{2\pi}{a}\hat{x}}|u_n(q)\rangle$$

  showing that the ray space for these states is NOT closed

- We set $k_l = 0$, and employ the reparametrization invariance of the geometric phase, which enables us to express $\gamma_g(n)$ in terms of $|u_n(\alpha)\rangle$ while treating α as a parameter
- This leads us to the expression for Pancharatnam-Zak phase $\gamma_g(n)$:

$$\gamma_g(n) = \text{Arg}\langle u_n(0)|u_n(2\pi/a)\rangle + i\int_0^{\frac{2\pi}{a}} d\alpha\, \langle u_n(\alpha)|\partial_\alpha|u_n(\alpha)\rangle$$

Pancharatnam-Zak phase

- This geometric phase correctly and consistently characterizes the band
- The Pancharatnam-Zak phase so obtained above is independent of the total number of cells N in the system, as it should be, since it captures the curvature of the state space of the system, which is solely determined by the Hamiltonian
- It follows that one can write the amplitude $\text{Arg}\langle u_n(0)|u_n(2\pi/a)\rangle$ as a line integral over the natural connection $\mathcal{A}_n(l) = i\langle u_n(l)|\partial_l|u_n(l)\rangle$:

$$\text{Arg}\langle u_n(0)|u_n(2\pi/a)\rangle = \int_{2\pi/a}^{0} dl\, \mathcal{A}_n(l)\Big|_{geodesic\,/\,Nullcurve},$$

  which is to be evaluated along the shortest geodesic (null curve) connecting $|u_n(2\pi/a)\rangle$ to $|u_n(0)\rangle$
- The Pancharatnam-Zak phase thus takes a manifestly gauge invariant form

$$\gamma_g(n) = \oint_C dl\, \mathcal{A}_n(l).$$

- The state $|u_n(q)\rangle$ and $e^{i\Lambda(q)}|u_n(q)\rangle$, represent the same physical state of the system, since the corresponding density matrices are identical, one demands that a physically observable quantity must remain invariant under such a gauge transformation for any choice of $\Lambda(q)$
- The Pancharatnam-Zak phase is indeed insensitive to such a transformation

- The Pancharatnam-Zak phase is also expressible as an argument of Bargmann invariant Δ_M:

$$\Delta_M = \langle u_{n,0}|u_{n,M}\rangle\langle u_{n,M}|u_{n,M-1}\rangle\cdots\langle u_{n,2}|u_{n,1}\rangle\langle u_{n,1}|u_{n,0}\rangle,$$

  where $|u_{n,i}\rangle \equiv |u_n(\frac{2\pi i}{Ma})\rangle$
- $\langle u_{n,0}|u_{n,M}\rangle$ missing in the Zak definition, fact not appreciated in the literature
- Here the variable M is not to be confused with the number of unit cells N. In large M limit:

$$\gamma_g(n) = \lim_{M\to\infty} \text{Arg}\, \Delta_M.$$

- This crucially shows that the value of $\gamma_g(n)$ *can not* be altered by changing the gauge convention and by translating the origin of the unit cell $|u_{n,i}\rangle \to e^{-i\frac{\varepsilon}{\hbar}\hat{p}}|u_{n,i}\rangle$ by distance ε
- For inversion symmetric lattices, $V(-\hat{x}) = \hat{\Pi}\, V(\hat{x})\hat{\Pi}^\dagger = V(\hat{x})$, one finds that $|u_n(-\kappa)\rangle = \hat{\Pi}|u_n(\kappa)\rangle$, one finds that the Pancharatnam-Zak phase for such a system is quantized:

$$\gamma_g(n) = 0 \text{ or } \pi$$

- The Pancharatnam-Zak phase in inversion symmetric lattices becomes a topological index, whose non-zero value corresponds to a topologically non-trivial band

Filled band case

- Most condensed matter systems studied in this context are filled bands
- The many-particle wavefunction $\bar{\Psi}$ representing such a filled band at any time t in the adiabatic approximation is given by the Slater determinant:

$$\bar{\Phi}_n(x_1, x_2, \cdots, x_N; \alpha(t)) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_{nk_0\alpha(t)}(x_1) & \Phi_{nk_1\alpha(t)}(x_1) & \cdots & \Phi_{nk_{N-1}\alpha(t)}(x_1) \\ \Phi_{nk_0\alpha(t)}(x_2) & \Phi_{nk_1\alpha(t)}(x_2) & \cdots & \Phi_{nk_{N-1}\alpha(t)}(x_2) \\ \vdots & \vdots & & \vdots \\ \Phi_{nk_0\alpha(t)}(x_N) & \Phi_{nk_1\alpha(t)}(x_N) & \cdots & \Phi_{nk_{N-1}\alpha(t)}(x_N) \end{vmatrix}$$

- $\Phi_{nk_l\alpha(t)}(x_i)$ represents the i^{th} particle wave function adiabatically evolving
- The many-particle wavefunction at time $j\tau$ can be straightforwardly written as:

$$\bar{\Phi}_n(\cdots; \alpha(j\tau)) = \frac{e^{i\Gamma(j\tau)}}{\sqrt{N!}} \hat{G} \begin{vmatrix} \Psi_{nk_j\alpha(0)}(x_1) & \Psi_{nk_{j+1}\alpha(0)}(x_1) & \cdots & \Psi_{nk_{N+j}\alpha(0)}(x_1) \\ \Psi_{nk_j\alpha(0)}(x_2) & \Psi_{nk_{j+1}\alpha(0)}(x_2) & \cdots & \Psi_{nk_{N+j}\alpha(0)}(x_2) \\ \vdots & \vdots & & \vdots \\ \Psi_{nk_j\alpha(0)}(x_N) & \Psi_{nk_{j+1}\alpha(0)}(x_N) & \cdots & \Psi_{nk_{N+j}\alpha(0)}(x_N) \end{vmatrix}$$

- The N-particle large gauge transformation G is given by the product:

$$G(x_1, x_2, \cdots, x_N; \tau) = \prod_{j=1}^{N} U^\dagger(x_j, j\tau),$$

whereas the phase factor $\Gamma(j\tau)$ reads:

$$\Gamma(j\tau) = \sum_{l=0}^{N-1} \left(i \int_{k_l}^{k_{l+j}} d\alpha \, \langle u_n(\alpha) | \partial_\alpha | u_n(\alpha) \rangle - \frac{1}{\hbar} \int_0^{j\tau} dt \, E_{nk_l\alpha(t)} \right)$$

- Generalizing the geometric phase expression for a filled band scenario, one finds that the geometric phase acquired by the band fermions evolving adiabatically till time $j\tau$ reads:

$$\begin{aligned}\Gamma_g(j\tau) =& (j(N-j) \bmod 2)\pi \\ &+ \sum_{l=0}^{N-1} \left(\mathrm{Arg}\langle u_n(k_l)|u_n(k_{l+j})\rangle + i\int_{k_l}^{k_{l+j}} d\alpha \, \langle u_n(\alpha)|\partial_\alpha|u_n(\alpha)\rangle \right)\end{aligned}$$

- Interestingly the geometric phase acquired by the band fermions after evolution till time τ is purely statistically in nature: $\Gamma_g(\tau) = ((N-1) \bmod 2)\pi$, sensitive to the odd/even nature of N
- Whereas the phase acquired after evolution till time $N\tau$ is solely geometric and it reads:

$$\Gamma_g(N\tau) = N\gamma_g(n).$$

This is an expected result since each of the fermion is evolving independently in this non-interacting system, giving rise to Pancharatnam-Zak phase $\gamma_g(n)$, which all add up to yield this result

Summary

- Provide a proper description of the (simplest) geometric phase in a condensed matter system: Single and Many particle case
- A gauge and reparametrisation invariant definition of band center
- Particle statistics manifestation in this formulation
- Paves the foundation for a more satisfactory understanding of electric polarisation
- Correct counting of edge states in topological models
- Connection of TKNN-Chern class and this Pancharatnam-Zak phase needs to be clarified

THANK YOU FOR YOUR ATTENTION