Topological Invariants in Crystalline Insulators
following Hasan & Kane, RMP

Mappings (topology): H_k is a mapping from BZ (i.e. k) to band structures (ε_k) and eigenstates (u_k.)

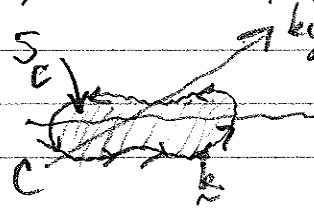
Crucial to understand: BZ is a torus topologically, due to it periodicity.
2D BZ is topologically a usual donut (torus).
3D BZ is " a straightford generalization.

Gapped band structures can be classified into equivalence classes whose members can be deformed into each other without closing the energy gap (filled bands; empty bands). These classes are characterized by a "topological invariant" $n \in \mathbb{Z}$ (an integer) called the CHERN INVARIANT.
[In mathematical topology, this is the theory of "fiber bundles."]

Consider u_{km} as a fn of $\underset{\sim}{k}$. If k is transported around a closed loop, it picks up a "Berry phase" from a "vector potential"

$$\underset{\sim}{A}_{km} = i\langle u_{km}|\nabla_k|u_{km}\rangle \equiv i\langle u_{km}|\nabla_k u_{km}\rangle$$

If no accidental degeneracy is encountered,



$$\phi_m = \int_C \underset{\sim}{A}_m \cdot d\underset{\sim}{l}$$

This can be transformed to $\phi_m = \int_{S_C} \underset{\sim}{\nabla} \times \underset{\sim}{A}_m \cdot d\underset{\sim}{S}$ over the "surface".

$\underset{\sim}{\nabla} \times \underset{\sim}{A}_m \equiv \underset{\sim}{F}_m$ = "Berry flux".

The "Chern invariant" is the total flux in the BZ (2D) expressed as

$$n_m = \frac{1}{2\pi}\int (F_m)_z \, d^2k$$

n_m is quantized due to the periodicity constraints on the BZ.

The total Chern number, when n_m is summed over all m occupied bands,

$$N = \sum_m^{occ} n_m$$

is an invariant even if bands cross (degeneracies)

$N = 0$ "trivial insulator"
$N = \pm 1$ "topological insulator"

Thouless et al. (TKKN, 1982) calculated the Hall conductivity for an insulator and found the quantized result

$$\sigma_{xy} = N\frac{e^2}{h}$$ where N is the Chern number just discussed.

This is the "quantum Hall effect" (QHE), where a large magnetic field applied to an electron gas turns the continuous spectrum into a ladder of discrete Landau levels.

$$E_n = (n+\tfrac{1}{2})\hbar\omega_c, \quad \omega_c = \frac{eB}{mc} \quad (\hbar\omega_c = 2\mu_B B)$$

Hamiltonian for $u_k(r)$, etc.

$H = \frac{\hat{p}^2}{2m} + V$, $\quad H\psi_k = \varepsilon_k \psi_k$. suppress band index

$\psi_k(r) = e^{ik\cdot r} u_k(r)$. Set $\hbar = 1$.

$$\hat{p}\, e^{ik\cdot r} u_k(r) = \underset{\sim}{k}\, e^{ik\cdot r} u_k(r) + e^{ik\cdot r} \underset{\sim}{p}\, u_k(r)$$

$$\hat{p}^2 \psi_k = \hat{p}_k \cdot \hat{p}_k \psi_k = p_k \cdot \left(\underset{\sim}{k} \psi_k + e^{ik\cdot r} \underset{\sim}{p}\, u_k(r) \right)$$

$$= \underset{\sim}{k} \cdot \underset{\sim}{p}_k \psi_k + \underset{\sim}{k}\, e^{ik\cdot r} \cdot \underset{\sim}{p}\, u_k(r) + e^{ik\cdot r} \underset{\sim}{p}^2 u_k(r)$$

$$= \underset{\sim}{k} \cdot \left(\underset{\sim}{k} \psi_k + e^{ik\cdot r} \underset{\sim}{p}\, u_k \right) + \underset{\sim}{k}\, e^{ik\cdot r} \cdot \underset{\sim}{p}\, u_k(r) + e^{ik\cdot r} \underset{\sim}{p}^2 u_k$$

$$= \underset{\sim}{k}^2 \psi_k + 2 e^{ik\cdot r}\, \underset{\sim}{k} \cdot \underset{\sim}{p}\, u_k + e^{ik\cdot r} \underset{\sim}{p}^2 u_k$$

$$= e^{i\underset{\sim}{k}\cdot \underset{\sim}{r}} \left[\underset{\sim}{k}^2 + 2\underset{\sim}{k}\cdot \underset{\sim}{p} + \underset{\sim}{p}^2 \right] u_k$$

Then $\left\{ \hat{p}^2/2m + V = \varepsilon_k \right\} e^{ik\cdot r} u_k(r)$

can be divided through by $e^{ik\cdot r}$ (it is never zero) to give

$$\boxed{\left(\frac{(\underset{\sim}{p} + \underset{\sim}{k})^2}{2m} + V \right) u_k(r) = \varepsilon_k u_k(r)}$$ Eq'n for $u_k(r)$.

More abstractly:

$$\left[\frac{(\underset{\sim}{p} + \underset{\sim}{k})^2}{2m} + V(r) \right] |u_k\rangle = \varepsilon_k |u_k\rangle . \qquad \boxed{u_k(r) = \langle r | u_k \rangle}$$

Apply ∇_k to this eq'n:

$$\nabla_k \frac{(\underset{\sim}{p} + \underset{\sim}{k})^2}{2m} = \frac{\underset{\sim}{p} + \underset{\sim}{k}}{m} . \qquad \underset{\sim}{\nabla}_k \varepsilon_k = \underset{\sim}{v}_k$$ band velocity (recall $\hbar = 1$).

Then applyeng ∇_k to the $\underset{\sim}{k}\cdot p$ eq'n: add bandindex

$$\frac{p+\underset{\sim}{k}}{m}|u_{kn}\rangle + H_k|\nabla_k u_{kn}\rangle = v_{kn}|u_{kn}\rangle + \varepsilon_{kn}|\nabla_k u_{kn}\rangle$$

Take scalar product with $\langle u_{km}|$:

$$\langle u_{km}|\frac{p+k}{m}|u_{kn}\rangle + \varepsilon_{kn}\cancel{\langle u_{km}|\nabla_k u_{kn}\rangle} = v_{kn}\,\delta_{nm} + \varepsilon_{kn}\cancel{\langle u_{km}|\nabla u_{kn}\rangle}$$

$$\langle u_{km}|\frac{p}{m}|u_{kn}\rangle + \frac{\underset{\sim}{k}}{m}\delta_{m,n} = v_{kn}\,\delta_{m,n}$$

$$\boxed{\underline{\underline{m=n}}:\ \frac{1}{m}\langle p^{k}_{m,n}\rangle + \frac{k}{m} = \underset{\sim}{v}_{kn} = \nabla_{\underset{\sim}{k}}\varepsilon_{kn}}$$

$$(H_k-\varepsilon_{kn})|\nabla_k u_{kn}\rangle = \left(v_{kn} - \frac{p+k}{m}\right)|u_{kn}\rangle$$

Apply $\langle u_{km}|$ to this eqn:

$$\langle u_{km}|(\varepsilon_{km}-\varepsilon_{kn})|\nabla_k u_{kn}\rangle = \langle u_{km}|\left(v_{kn}-\frac{p+k}{m}\right)|u_{kn}\rangle$$

$\varepsilon_m \neq \varepsilon_n$, $\langle u_{km}|\nabla_k u_{kn}\rangle = \dfrac{\langle u_{km}|p|u_{kn}\rangle/m}{\varepsilon_{kn}-\varepsilon_{km}} = \dfrac{p^{k}_{m,n}/m}{\varepsilon_{kn}-\varepsilon_{kn}}$

Now: $\langle u_{km}|\nabla_k|u_{kn}\rangle = \langle u_{km}|-i\underset{\sim}{R}_{(k)}|u_{kn}\rangle$ $\qquad \underset{\sim}{R} = i\nabla_{\underset{\sim}{k}}$ in k-representation

so $\underset{\sim}{A}_k \equiv -i\langle u_{km}|\nabla_k|u_{kn}\rangle = -\langle u_{km}|\underset{\sim}{R}|u_{kn}\rangle$

(dipole operator
matrix element
(off-diagonal in bands)