① Electric polarisation of 1D insulators

$$\boxed{\underbrace{\underline{P}}_{\text{defined modulo } e} = \frac{e}{2\pi} \sum_{n \in occ} \underbrace{\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} A_n(k)\, dk}_{\text{gauge-invariant modulo } 2\pi}} \quad (1)$$

* Argument of plausibility for (1):

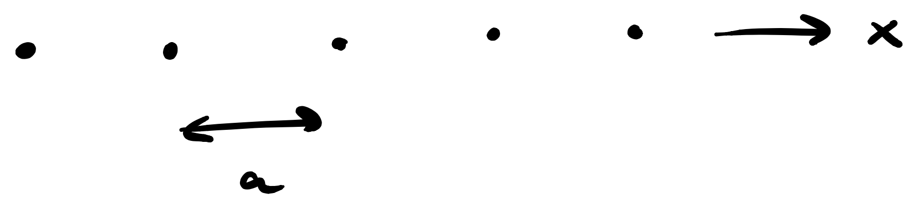
We introduce "Wannier functions".

In 1D:

$$\boxed{\underbrace{|l, n\rangle}_{\text{Wannier function}} = \frac{1}{\sqrt{N}} \sum_{k \in 1BZ} e^{-ikla} \underbrace{|\psi_{kn}\rangle}_{\text{Bloch state}}}$$

where

l = unit cell label



Lattice vectors: $\vec{l} = l\, a\, \hat{x}$

where $l \in \mathbb{Z}$

n = band label.

N = # of unit cells.

$|l, n\rangle$ is not an eigenstate of the Hamiltonian.

Some properties of $|l, n\rangle$:

(i) $\langle l, n | l', n' \rangle = \delta_{ll'}\, \delta_{nn'}$

$$\langle l, n \mid l', n' \rangle =$$

$$= \frac{1}{N} \sum_{k k'} e^{ikla} \, e^{-ik'l'a} \underbrace{\langle \psi_{kn} \mid \psi_{k'n'} \rangle}_{\delta_{kk'} \, \delta_{nn'}}$$

$$= \frac{1}{N} \delta_{nn'} \sum_{k \in 1BZ} e^{ik(l-l')a}$$

$$= \frac{1}{N} \delta_{nn'} \frac{\overset{Na}{L}}{2\pi} \underbrace{\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \, e^{ik(l-l')a}}_{\frac{2\pi}{a} \delta_{ll'}}$$

$$= \delta_{nn'} \, \delta_{ll'}$$

$$\sum_{\ell m} |\ell, m\rangle\langle \ell, m| = \mathbb{1}$$

Also, charge density (per unit length) at point x:

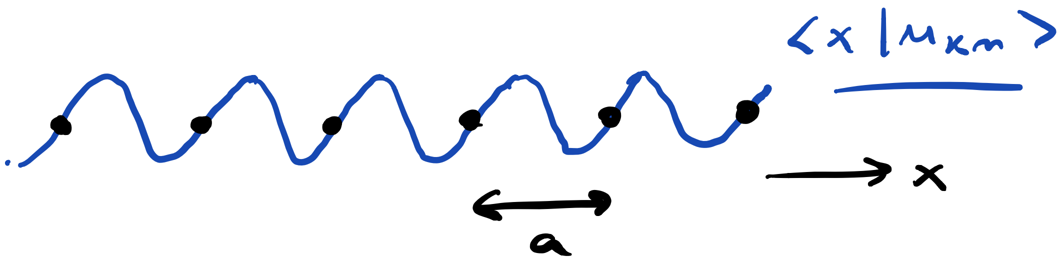
$$\sum_{k} \sum_{m} |\langle x | \psi_{km}\rangle|^2$$

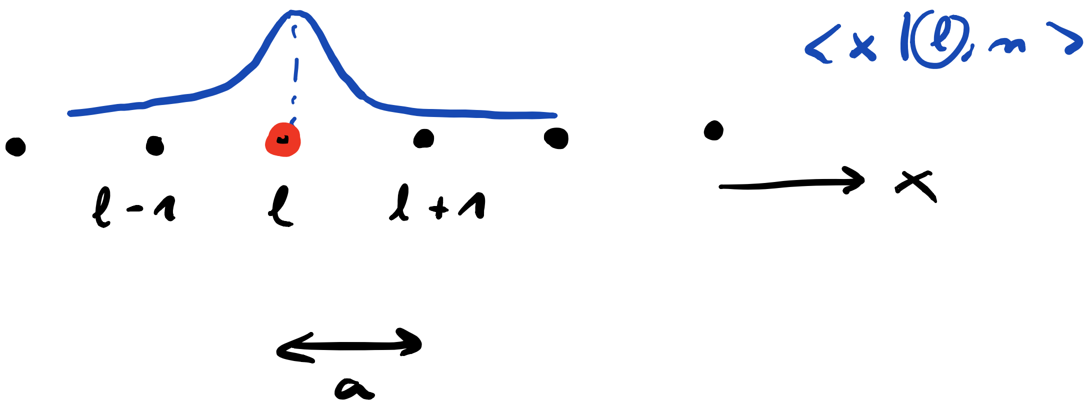
$$= \sum_{\ell} \sum_{m} \underbrace{|\langle x | \ell, m\rangle|^2}$$

$$\boxed{\langle x|\ell, m\rangle} = \frac{1}{\sqrt{N}} \sum_{k} e^{-ik\ell a} \langle x|\psi_{km}\rangle$$

$$\boxed{= \frac{1}{\sqrt{N}} \sum_{k} e^{+ik(x-\ell a)} \langle x|u_{km}\rangle}$$

$$\langle x|\psi_{km}\rangle = e^{ikx} \langle x|u_{km}\rangle$$





Let us "calculate"

$A_n(k)$ using Wannier functions.

$$A_n(k) = i \langle u_{kn} | \frac{d}{dk} | u_{kn} \rangle$$

We need to write $|u_{kn}\rangle$

in terms of Wannier functions.

$$|\underline{\underline{l}}, \underline{\underline{n}}\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-ikla} e^{ikx} |u_{kn}\rangle$$

operator.

Invert this to get

$$\boxed{|u_{kn}\rangle = \frac{1}{\sqrt{N}} \sum_l e^{ikla} e^{-ikx} |l, n\rangle}$$

operator.

Then,

$$A_n(k) = i \langle u_{kn}| \frac{d}{dk} |u_{kn}\rangle$$

$$= \frac{i}{N} \sum_l \sum_{l'} e^{-ikl'a} e^{ikla}$$

$$\langle l', n| e^{ikx} \frac{d}{dk} \left(e^{-ikx} \right) \underline{\underline{|l, n\rangle}}$$

$$= \frac{1}{N} \sum_{\ell\ell'} e^{i k (\ell - \ell') a}$$

$$\langle \ell', n | (x - \ell a) | \ell, n \rangle$$

Now,

$$\int_{BZ} dk\, A_n(k) =$$

$$= \frac{1}{N} \sum_{\ell\ell'} \underbrace{\left[\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk\, e^{i k (\ell - \ell') a} \right]}_{2\pi/a \ \delta_{\ell\ell'}}$$

$$\langle \ell', n | (x - \ell a) | \ell, n \rangle$$

operator

times identity op.

$$= \frac{2\pi}{Na} \sum_{\ell} \langle \ell, n | (x - \ell a) | \ell, n \rangle$$

$$= \frac{2\pi}{Na} \left(\sum_{\ell} \langle \ell, m | x | \ell, m \rangle - a \sum_{\ell} \ell \underbrace{\langle \ell, m | \ell, m \rangle}_{1} \right)$$

$$= \frac{2\pi}{Na} \sum_{\ell} \langle \ell, m | x | \ell, m \rangle$$

$$\sum_{\ell} \ell = 0$$

Then,

$$\frac{e}{2\pi} \sum_{m \in occ} \int_{BZ} A_m(k)\, dK =$$

$$= \frac{e}{Na} \sum_{m \in occ} \sum_{\ell} \langle \ell, m | x | \ell, m \rangle$$

length of crystal

$$= \frac{e}{Na} \underbrace{\sum_{n \in occ} \sum_{l} \int dx\, x\, \underbrace{|\langle x | l, n \rangle|^2}}_{\text{dipole moment of the crystal}}$$

1.1 Link between Berry phase and the "Wannier center"

$$\overbrace{\langle l, n | x | l, n \rangle}^{\text{Wannier center.}} =$$

$$= \langle 0, n | x | 0, n \rangle + la$$

exercise

unit cell at the origin.

$\Rightarrow$

$$P = \frac{e}{Na} \sum_{m \in occ} \sum_{l} \langle l, m | x | l, m \rangle$$

$$= \frac{e}{Na} \sum_{m \in occ} \sum_{l} \underbrace{\langle 0, m | x | 0, m \rangle}_{\text{independent of } l}$$

$$\sum_{l} l = 0$$

$$= \frac{e}{\cancel{N}a} \cancel{N} \sum_{m \in occ} \underline{\langle 0, m | x | 0, m \rangle}$$

But, we also have

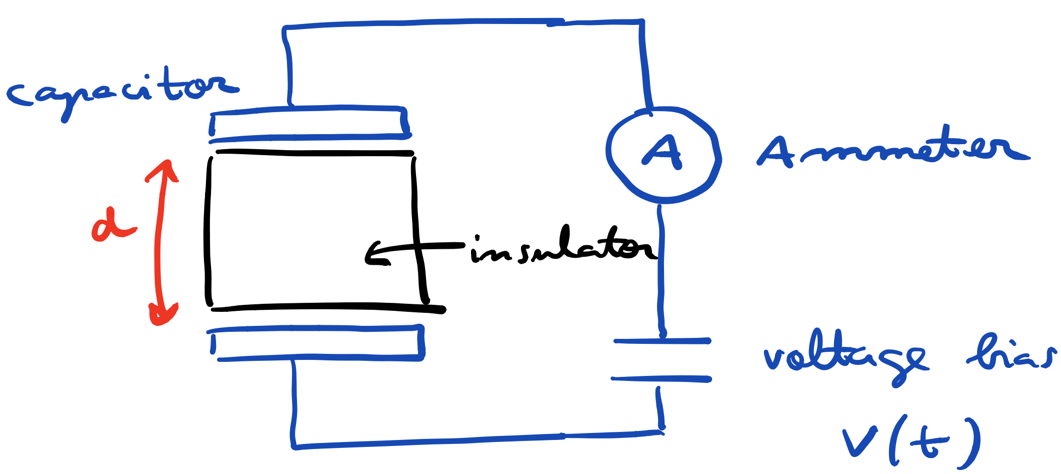
$$P = \frac{e}{2\pi} \sum_{m \in occ} \int_{BZ} dk \, A_{km}(k)$$

It follows that

$$\boxed{\begin{aligned}&\langle 0,n | x | 0,n \rangle \\ &= \frac{a}{2\pi} \int_{BZ} dk\, A_n(k)\end{aligned}}$$

$$\boxed{\underline{P} = \frac{e}{a} \sum_{n \in occ} \underline{\langle 0,n | x | 0,n \rangle}}$$

1.2 Experimental measurement of $\underline{P}$



Electric field in the insulator :

$$\mathcal{E} = \frac{V}{d} .$$

$V \rightarrow \mathcal{E} \longrightarrow$ changes $\underline{P}$

$$\longrightarrow \vec{J} = \frac{\partial \vec{P}}{\partial t}$$

$\rightarrow$ current through ammeter

What is measured :

$$\underbrace{\Delta \vec{P}} = \underbrace{\int \vec{J}\, dt}_{\text{experimentally measured.}}$$

② Thouless charge pump

[PRB 27, 6083 (1983)]

Suppose a 1D insulator, subjected to a $\underbrace{\text{(adiabatic)}}$ time-periodic perturbation.

slow compared to gap of insulator.

$$\mathcal{H}(\underbrace{k, t})$$

2D parameter space.

$$\mathcal{H}(k, t + \underbrace{T}) = \mathcal{H}(k, t)$$

period of the perturbation.

Charge pumped in a cycle :

$$= \int_0^T \frac{d\underline{P}}{dt}\, dt$$

$$= \underline{P}(t=T) - \underline{P}(t=0)$$

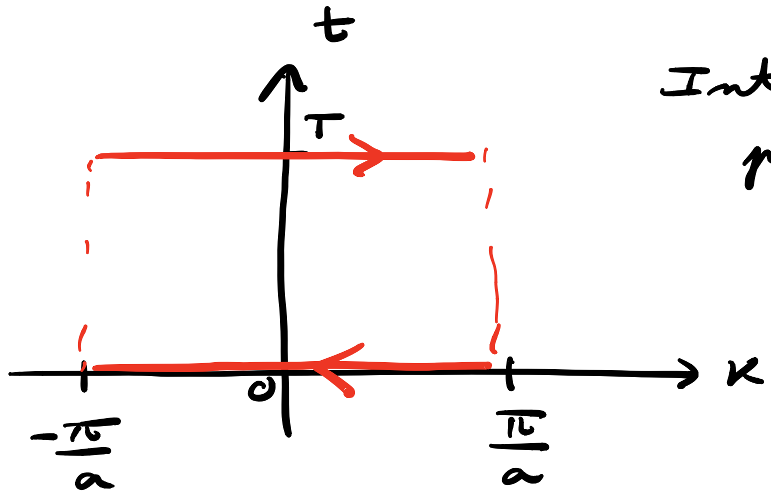
$$\equiv \Delta \underline{P} .$$

$\Delta \underline{P} = e \times \text{integer} . !$

Proof :

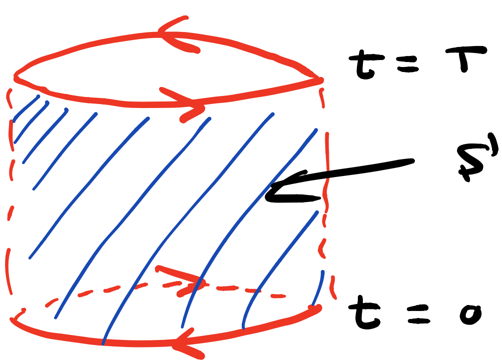
$$\Delta \underline{P} = \frac{e}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \sum_{n \in occ} A_n(k,T)$$

$$- \frac{e}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \sum_{n \in occ} A_n(k,0)$$



Integration path

Because $-\frac{\pi}{a}$ and $\frac{\pi}{a}$ are equivalent, we may redraw the preceding picture as



The closed loop is the boundary of a cylinder.

Stokes theorem:

$$\oint dk \; A_n(k,T) - \oint dk \; A_n(k,0)$$

$$= \int_{S} B_n(k,t) \, dk \, dt$$

surface of cylinder, parametrized by (k,t), which is delimited by the loops.

$B_n(k,t)$ = Berry curvature

$$= \underline{\frac{\partial}{\partial k}} \left[i \langle u_{kn} | \underline{\underline{\frac{\partial}{\partial t}}} | u_{kn} \rangle \right]$$

$$
-\frac{\partial}{\partial t}\left[i \left\langle u_{km} \middle| \frac{\partial}{\partial k} \middle| u_{km} \right\rangle \right]
$$

$$
= i \left[\left\langle \frac{\partial u_{km}}{\partial k} \middle| \frac{\partial u_{km}}{\partial t} \right\rangle - \left\langle \frac{\partial u_{km}}{\partial t} \middle| \frac{\partial u_{km}}{\partial k} \right\rangle \right]
$$

$$
= 2 \, \mathrm{Im} \left[\left\langle \frac{\partial u_{km}}{\partial t} \middle| \frac{\partial u_{km}}{\partial k} \right\rangle \right]
$$

Then,

$$
\Delta P = \frac{e}{2\pi} \sum_{n \in occ} \int_0^T dt \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk \; B_n(k, t)
$$

Because $t = 0$ and $t = T$ are equivalent times, S is a closed surface.
(surface of a torus)

$$\Rightarrow \frac{1}{2\pi}\int_0^T dt \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk\ B_n(k,t)$$

$= C_n =$ Chern # of band n

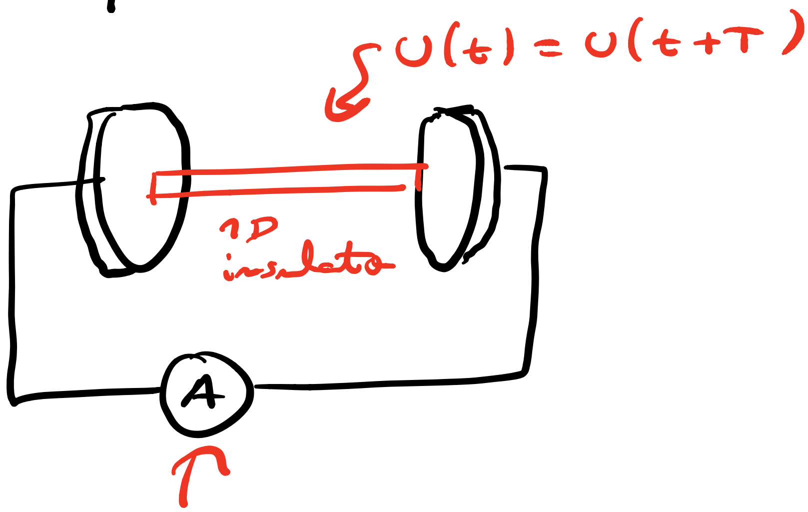
integer and topological invariant.

Then,

$\boxed{\Delta P}$ = charge pumped in a cycle $= \boxed{e \sum_{n \in occ} C_n}$ ←

Quantization of pumped charge!

Note: the pumped charge is quantized only in insulators.



How does one calculate ΔP ?

(i) Solve $\mathcal{H}(k,t)\,|u_{kn}(t)\rangle$

$$= E_{kn}(t)\,|u_{kn}(t)\rangle$$

$$\Rightarrow \text{get} \begin{cases} |u_{kn}(t)\rangle \\ E_{kn}(t) \end{cases}$$

(ii) Calculate Berry curvature

(iii) Calculate Chern #

Alternative way to calculate C_n :

$$\underline{P} = \frac{e}{2\pi} \sum_{n \in occ} \langle 0,n | x | 0,n \rangle$$

$$\Delta \underline{P} = \underline{P}(t=T) - \underline{P}(t=0)$$

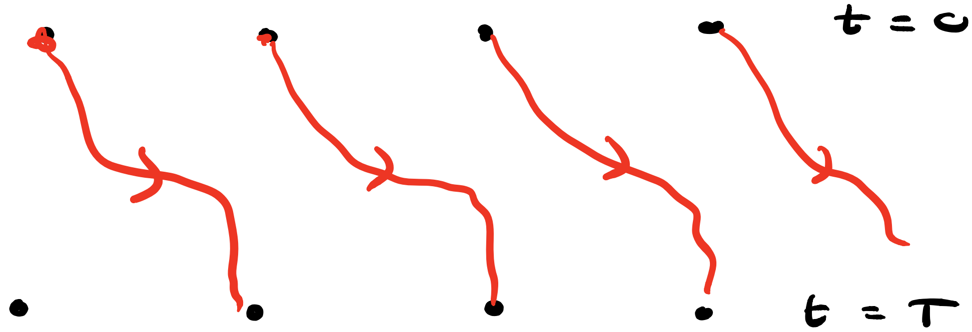
$$= \frac{e}{a} \sum_{n \in occ} \Big[\langle 0,n | x | 0,n \rangle \Big|_{t=T} - \langle 0,n | x | 0,n \rangle \Big|_{t=0} \Big]$$

$$= e \sum_{n \in occ} c_n$$

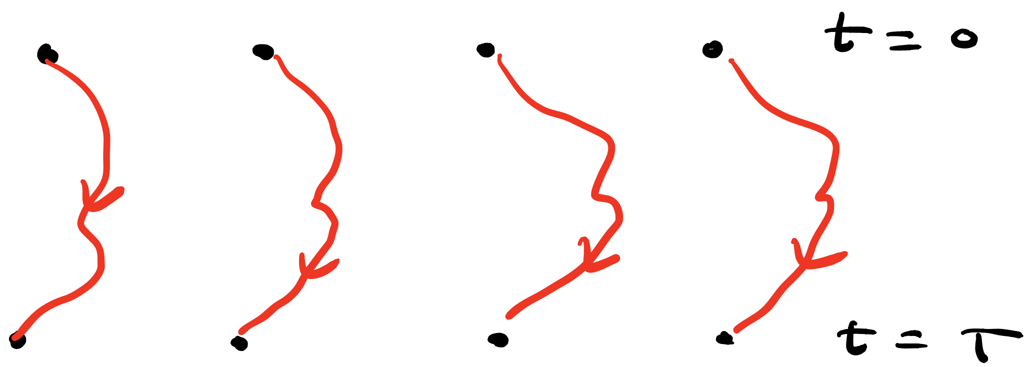
$$\Rightarrow \boxed{c_n =}$$

$$= \frac{\langle 0, n | x | 0, n \rangle \big|_{t=T} - \langle 0, n | x | 0, n \rangle \big|_{t=0}}{a}$$

$c_n = 1$ is equivalent to the Wannier center advancing one unit cell between $t = 0$ and $t = T$.



$C_n = 1$



$C_n = 0$.