(5) Berry phase in crystals

Single electron in a periodic potential:

$$* \quad \mathcal{H} = \frac{p^2}{2m} + V(\vec{r}) + \lambda_{so}\, \vec{p} \cdot (\vec{\sigma} \times \vec{\nabla} V)$$

λ_{so}: spin-orbit coupling; $\vec{\sigma}$: spin

$$V(\vec{r}) = V(\vec{r} + \vec{\ell})$$

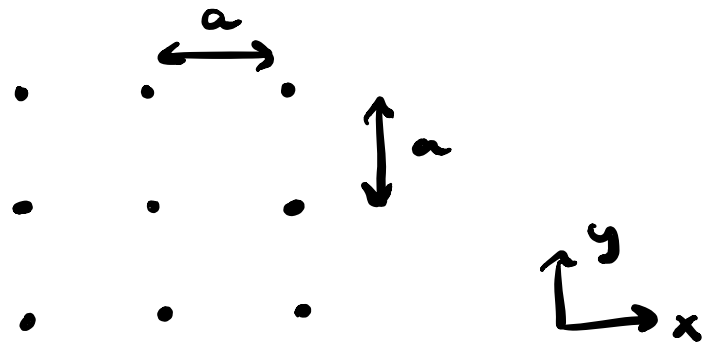
$\vec{\ell}$: lattice vector

1D:

$$\vec{\ell} = a\, \ell\, \hat{x}$$

$$\ell \in \mathbb{Z}$$

2D:



$$\vec{\ell} = a(\ell_1, \ell_2)$$

$$\ell_1, \ell_2 \in \mathbb{Z}$$

3D cubic crystal:

$$\vec{\ell} = a(\ell_1, \ell_2, \ell_3)$$

$$\ell_i \in \mathbb{Z}$$

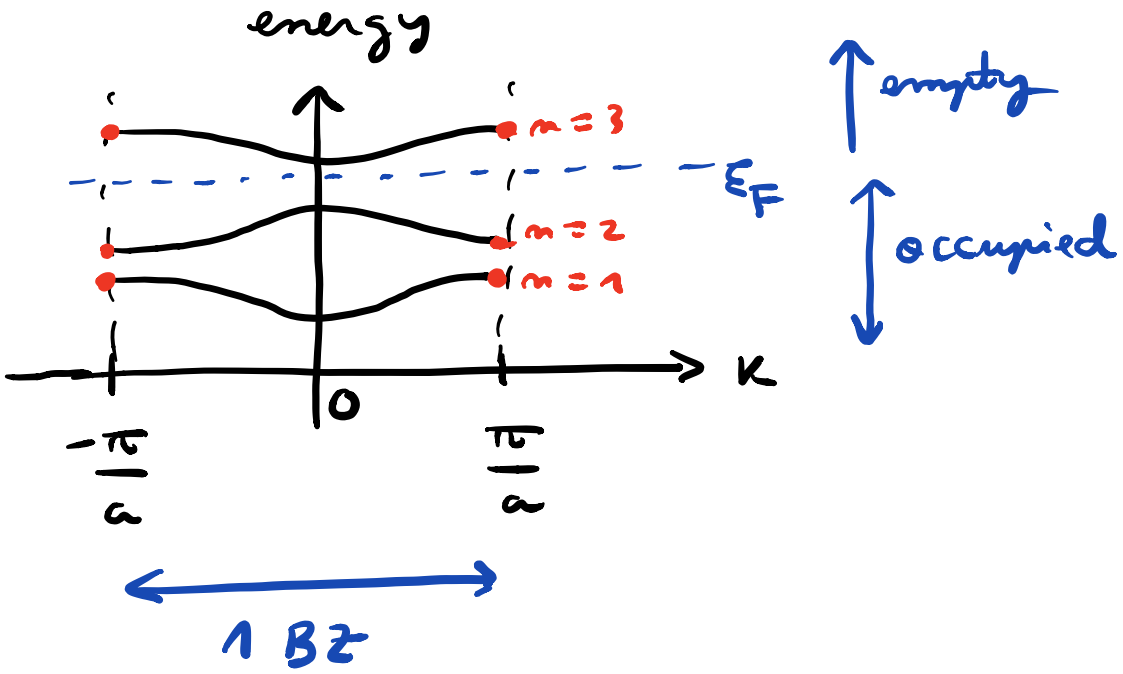
* $\mathcal{H} \, |\psi_{\vec{k}n}\rangle = E_{\vec{k}n} \, |\psi_{\vec{k}n}\rangle$

$\vec{k}$ = crystal momentum
(good quantum # b/c of

periodicity of crystal)

n = band index

example of a 1D crystal w/ lattice constant a



$$E_{\vec{k}+\vec{G}\,n} = E_{\vec{k}\,n}$$

"periodic gauge"

$$|\psi_{\vec{k}+\vec{G},n}\rangle = |\psi_{\vec{k}\,n}\rangle$$

where $\vec{G}$ is a reciprocal lattice vector.

$$\vec{G} \cdot \vec{\ell} = 2\pi \times \text{integer}.$$

1D: $\vec{G} = \frac{2\pi}{a} m \hat{x}$, $m \in \mathbb{Z}$

2D square lattice:

$$\vec{G} = \frac{2\pi}{a} (m_1, m_2)$$

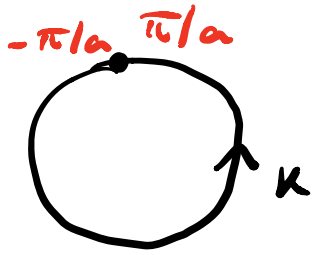
$m_1, m_2 \in \mathbb{Z}$

3D cubic lattice:

$$\vec{G} = \frac{2\pi}{a} (m_1, m_2, m_3)$$

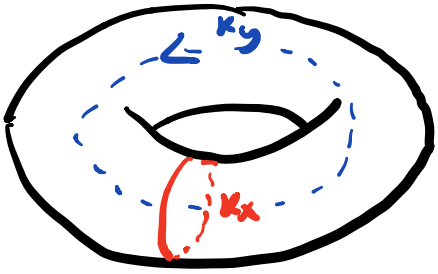
* Topology of BZ:

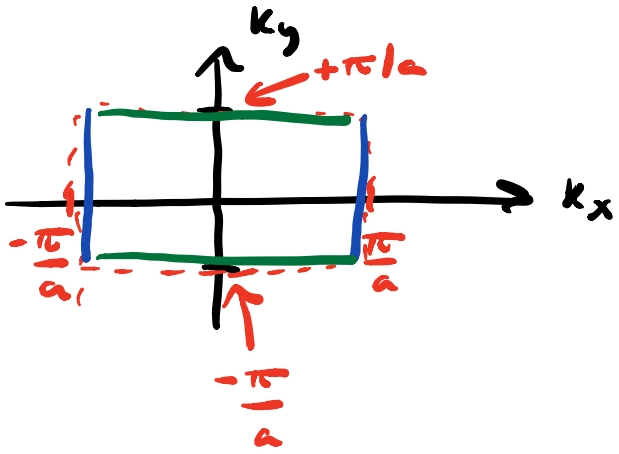
(i) 1D:



circle

(ii) 2D : torus





(iii) 3D : higher dimensional tori.

* $|\psi_{\vec{k}m}\rangle$ = eigenstates

$$\langle \psi_{\vec{k}m} | \psi_{\vec{k}'m'} \rangle = \delta_{\vec{k}\vec{k}'} \delta_{mm'}$$

$$\sum_{\vec{k}m} |\psi_{\vec{k}m}\rangle \langle \psi_{\vec{k}m}| = \mathbb{1}$$

* Bloch's theorem:

$$\langle \vec{r} | \psi_{\vec{k}m} \rangle = \psi_{\vec{k}m}(\vec{r})$$

$$= \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}m}(\vec{r})$$

N = # of unit cells

$$u_{\vec{k}m}(\vec{r}) = \langle \vec{r} | u_{\vec{k}m} \rangle$$

$$u_{\vec{k}m}(\vec{r}+\vec{l}) = u_{\vec{k}m}(\vec{r})$$

Note: in the periodic gauge,

$$u_{\vec{k}+\vec{G},m}(\vec{r}) = e^{-i\vec{G}\cdot\vec{r}}\, u_{\vec{k}m}(\vec{r}).$$

$$\langle u_{\vec{k}m} | u_{\vec{k}m'} \rangle = \delta_{mm'}$$

but,

$$\langle u_{\vec{k}m} | u_{\vec{k}'m'} \rangle \not= \delta_{mm'}$$

$$\sum_m |u_{\vec{k}m}\rangle\langle u_{\vec{k}m}| = \mathbb{1}$$

$$* \quad \mathcal{H}\,|\psi_{\vec{k}m}\rangle = E_{\vec{k}m}\,|\psi_{\vec{k}m}\rangle$$

$\Rightarrow$

Bloch's thm

$$\mathcal{H}\, e^{i\vec{k}\cdot\vec{r}}\, |u_{\vec{k}m}\rangle = E_{\vec{k}m}\, e^{i\vec{k}\cdot\vec{r}}\, |u_{\vec{k}m}\rangle$$

$$\underbrace{e^{-i\vec{k}\cdot\vec{r}}\, \mathcal{H}\, e^{i\vec{k}\cdot\vec{r}}}_{\mathcal{H}(\vec{k})}\, \underbrace{|u_{\vec{k}m}\rangle}_{} = E_{\vec{k}m}\, \underbrace{|u_{\vec{k}m}\rangle}_{}$$

$$\mathcal{H}(\vec{k}) = \frac{(\vec{p} + \hbar\vec{k})^2}{2m} + V(\vec{r})$$

$$+ \lambda_{so}\, (\vec{p} + \hbar\vec{k}) \cdot (\vec{\sigma} \times \vec{\nabla} V)$$

$$= \text{"Bloch Hamiltonian"}$$

$$* \quad \mathcal{H}(\vec{k})\, |u_{\vec{k}m}\rangle = E_{\vec{k}m}\, |u_{\vec{k}m}\rangle$$

One Hamiltonian for each $\vec{k}$.

This has the same form as

$$\mathcal{H}(\vec{R})\, |m, \vec{R}\rangle = E_m(\vec{R})\, |m, \vec{R}\rangle$$

(section 2)

Correspondence :

$$\mathcal{H}(\vec{k}) \longleftrightarrow \mathcal{H}(\vec{R})$$

$$E_m(\vec{k}) \longleftrightarrow E_m(\vec{R})$$

$$|u_{\vec{k}m}\rangle \longleftrightarrow (m, \vec{R})^*$$

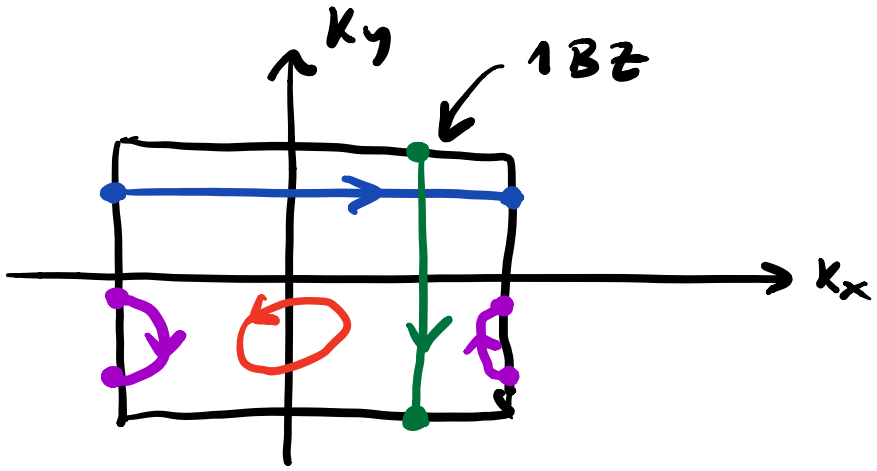
$$\vec{k} \longleftrightarrow \vec{R}$$

* watch out with the fact that $|u_{\vec{k}m}\rangle$ need not be single-valued.

$\Rightarrow$ physical quantities depending on closed paths in $\vec{k}$-space will be influenced by Berry phase.

Some possible closed paths in $\vec{k}$ - space :

(example of 2D)



* Berry (Zak) phase :

$$\gamma_m(C) = \oint_C \vec{A}_m(\vec{k}) \cdot d\vec{k}$$

where

$$\vec{A}_m(\vec{k}) = i \langle u_{\vec{k}m} | \frac{d}{d\vec{k}} | u_{\vec{k}m} \rangle$$

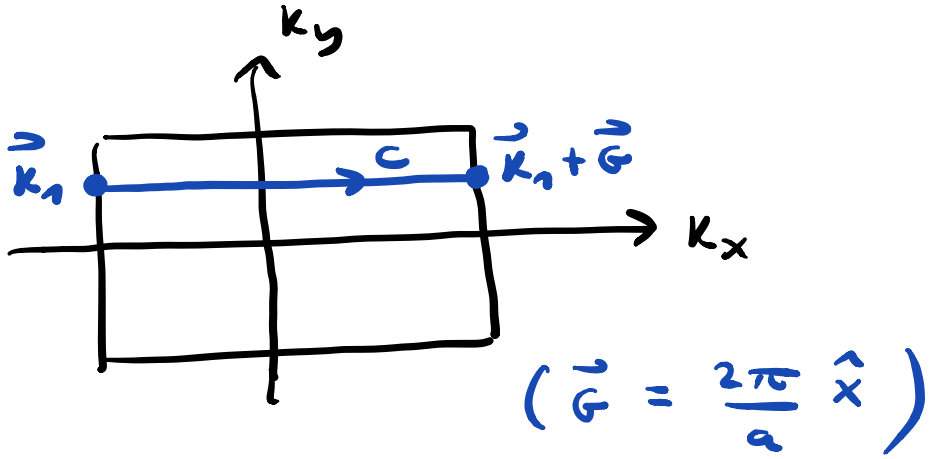
is the Berry connection.

Note: in the periodic gauge,

$u_{\vec{k}n}(\vec{r}) \neq u_{\vec{k}+\vec{G}n}(\vec{r})$

$\Rightarrow$ if the path C involves connecting $\vec{k}$ and $\vec{k}+\vec{G}$, we need to adjust the Berry phase formula to a non single-valued basis.

Example:



$\left(\vec{G} = \frac{2\pi}{a}\hat{x}\right)$

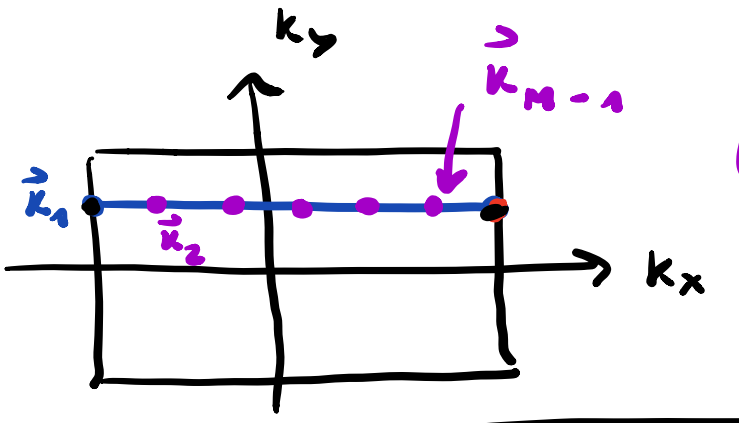
$$\gamma_m = \oint_C \vec{A}_m(\vec{k}) \cdot d\vec{k}$$

$$- i \ln \left[\langle u_{\vec{k}_1 m} | u_{\vec{k}_1 + \vec{G} m} \rangle \right]$$

If $|u_{\vec{k}_1 + \vec{G} m}\rangle = |u_{\vec{k}_1 m}\rangle$,

we recover the old expression.

Numerical calculation:



$(M \gg 1)$

$$\gamma_m = - \mathrm{Im} \ln \left[\langle u_{\vec{k}_1 m} | u_{\vec{k}_2 m} \rangle \right.$$

$$\left. \langle u_{\vec{k}_2 m} | u_{\vec{k}_3 m} \rangle \cdots \right.$$

$$\cdots \langle u_{\vec{k}_{M-1},m} | \underbrace{e^{-i\vec{G}\cdot\vec{r}} | u_{\vec{k}_1 m}\rangle}_{| u_{\vec{k}_M, m}\rangle}$$

Again, if we had chosen a gauge in which $|u_{\vec{k}}\rangle = |u_{\vec{k}+\vec{G}}\rangle$ we would recover the old formula (from a few lectures ago).

* Berry curvature:

(i) 1D: none (unless we apply a time-periodic perturbation)

(ii) 2D:

$$\vec{B}_m(\vec{k}) = \hat{z}\left(\frac{\partial A_{m,x}}{\partial y} - \frac{\partial A_{m,y}}{\partial x}\right)$$

where

$$A_{m,j} = i \langle u_{\vec{k}m} | \frac{\partial}{\partial k_j} | u_{\vec{k}m} \rangle$$

$j = x, y.$

(iii) 3D:

$$\vec{B}_m(\vec{k}) = \vec{\nabla}_{\vec{k}} \times \vec{A}_m(\vec{k}),$$

where $\vec{\nabla}_{\vec{k}} = \frac{\partial}{\partial \vec{k}}$

When do we expect $\vec{B}_m(\vec{k}) \neq 0$?

Symmetry constraints:

(1) If the crystal is centrosymmetric,

$$\vec{B}_n(\vec{k}) = \vec{B}_n(-\vec{k})$$

(2) If the system has time-reversal symmetry,

$$\vec{B}_n(\vec{k}) = -\vec{B}_n(-\vec{k})$$

(3) If the crystal has both time-reversal and spatial inversion symmetry,

$$\vec{B}_n(\vec{k}) = \vec{B}_n(-\vec{k}) = -\vec{B}_n(\vec{k})$$

(1) (2)

$$\Rightarrow \vec{B}_n(\vec{k}) = 0 .$$

/

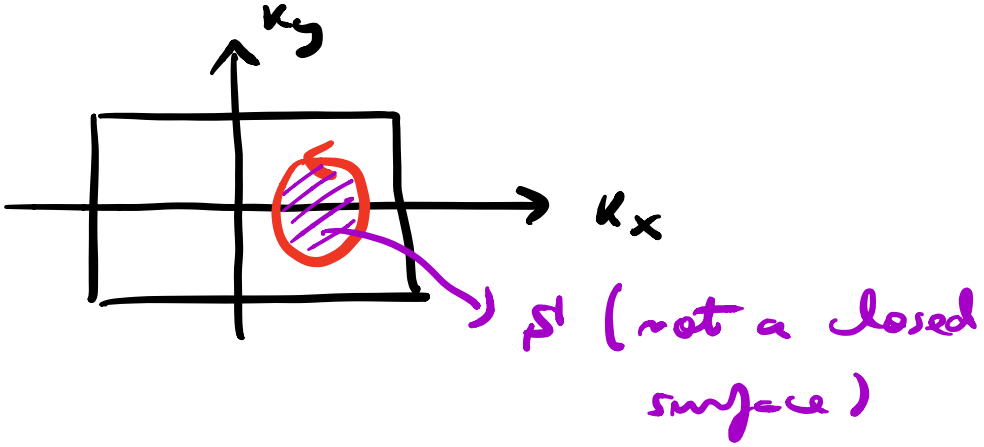
also applies if the crystal has only the product of space-inversion and time-reversal symmetries

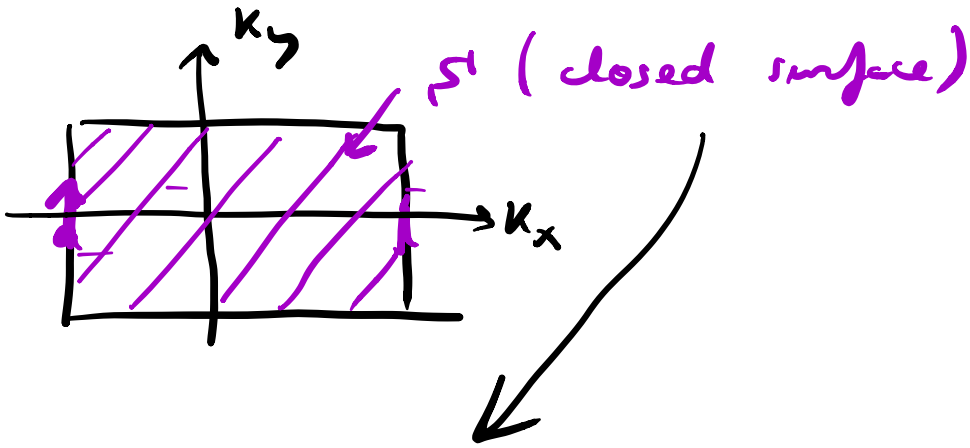
* Chern # of electronic bands:

Need a 2D closed surface.

(i) 1D: none (unless we add some other external parameter, like time).

(ii) 2D:





$$C_n = \frac{1}{2\pi} \oint_{S'} \vec{B}_n(\vec{k}) \cdot d\vec{S}$$

$\vec{B}_n(\vec{k}) \parallel \hat{z}$

= integer.

(iii) 3D :

e.g. a Fermi surface.

Can also define C_n

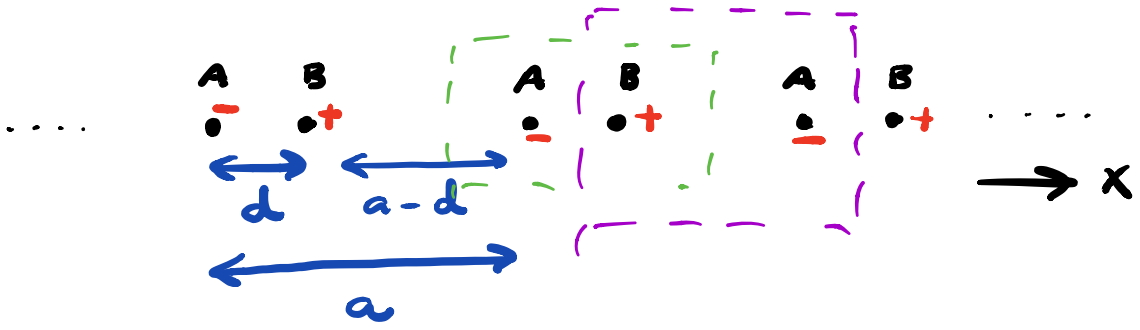
CH. 2: TOPOLOGICAL BAND THEORY IN 1D

① Electric polarisation of an insulator

$\vec{P}$ = electric dipole moment per unit volume

In a periodic crystal, the definition of $\vec{P}$ is subtle. This is partly due to the fact that $\vec{P}$ has a fundamental ambiguity.

* example

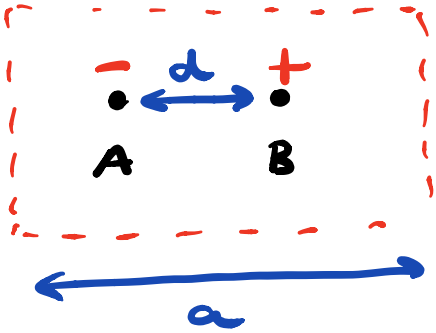


$q_A = -q$ (localised charges)

$q_B = +q$

q is a multiple of e.

Choice #1 for unit cell:



$$\vec{P} = \frac{1}{L} \sum_i \vec{p}_i$$

L: length of crystal

$\sum_i$: sum over unit cells

$\vec{p}_i$: dipole moment of unit cell

$L = Na$, where

N = # of unit cells.

$$\vec{r}_i = q\,(x_B - x_A)\,\hat{x}$$

$$= q\,d\,\hat{x} \quad , \text{ for } \forall\, i$$

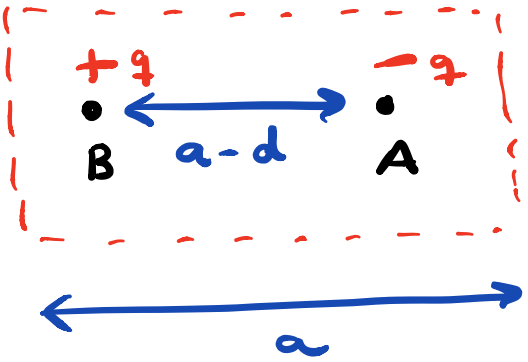
Then,

$$\vec{P} = \frac{1}{Na}\, N\, q\, d\, \hat{x}$$

$$= \frac{q\,d}{a}\,\hat{x}$$

Note: in 1D, $\vec{P}$ has the units of charge.

Choice #2 for unit cell:



$$\vec{P} = \frac{1}{Na} \sum_i \vec{r}_i$$

$$= \frac{1}{Na} N q (d-a) \hat{x}$$

$$\vec{r}_i = q (x_B - x_A) \hat{x}$$

$$= q (d-a) \hat{x}$$

$$= \underbrace{\frac{q d}{a} \hat{x}} - \underbrace{q \hat{x}}$$

Different choices of unit cell lead to different $\vec{P}$!

$$|\Delta \vec{P}| = q = n e$$

where $n \in \mathbb{Z}$

In 1D, bulk polarisation is defined only modulo e.

In 2D, $\vec{P}$ is defined modulo $\frac{e \vec{l}}{A_{cell}}$

A_{cell}: area of unit cell

In 3D, $\vec{P}$ is defined modulo $\frac{e \vec{l}}{V_{cell}}$

* "Modern theory of electric polarization" (Resta, Vanderbilt)

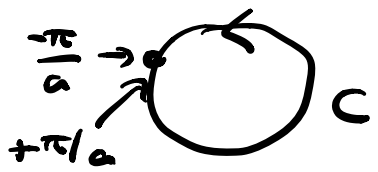
In 1D :

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

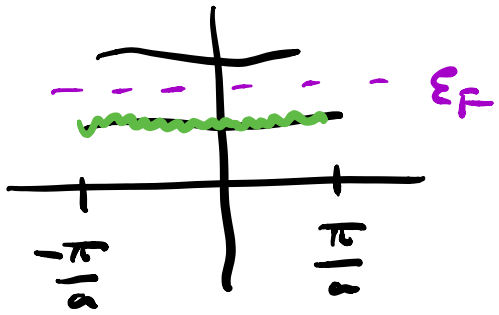
sum over occupied bands

$$i \langle u_{kn} | \frac{d}{dk} | u_{kn} \rangle$$

$$\boxed{P} = \frac{e}{2\pi} \sum_{n \in occ} \gamma_n(C)$$



In an insulator, each band is either fully occupied (i.e. occupied for all $k \in 1BZ$) or fully empty, at $T = 0$.



Recall from ch. 1 :

γ_n is defined modulo 2π

$\Rightarrow$ P is defined modulo

$$\frac{e}{2\pi} \, 2\pi$$