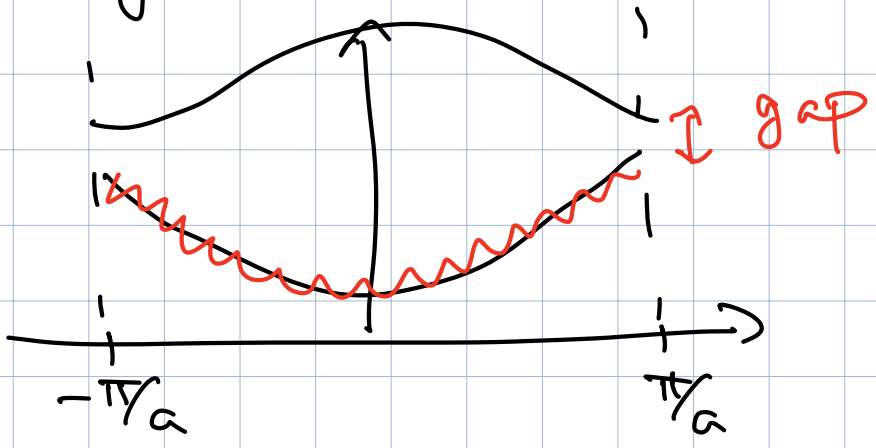
Band theory



filled band (+gap) = insulator / semiconductor
(large gap) (small gap)

highest filled band = valence band

lowest empty " = conduction band

Counting e^- : N unit cells → N $\vec{k}$ states
× 2 spin states
→ 2N e^- fill band

any even number of e^- per unit cell will fill integer number of bands

SiC: valence = 4
→ 8 e^- / unit cell
→ $\frac{8}{2} = 4$ bands filled

metals : odd # e^- / unit cell

⟶ partially filled bands

How big gaps between bands

Tight binding : each band form atomic orbitals.

Bandwidth related hopping t

Nearly free e^- : gaps open at BZ boundary due to periodic $V(x)$

if V strong ⟶ gaps are big

States in 1st BZ are pushed down in E when $V(x)$ is applied

states in 2nd BZ are pushed up in E

Monovalent : $1e^-$ / unit cell

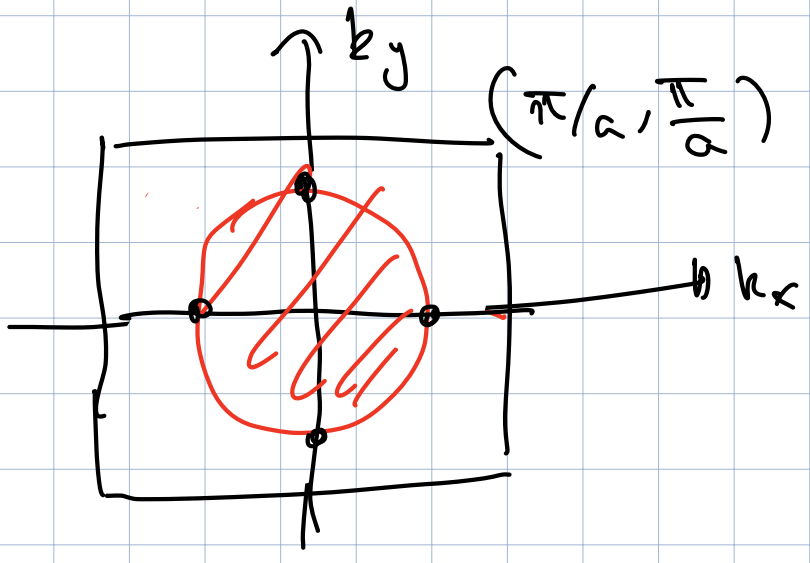
2D / square lattice

- $V(x) \to 0$

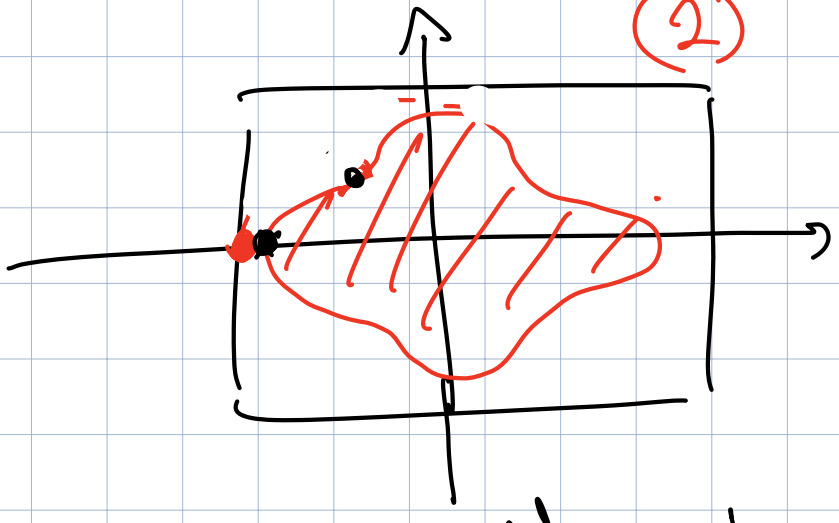
$A_{Fermi} = \frac{1}{2} A_{BZ}$

$= \frac{1}{2}\left(\frac{2\pi}{a}\right)^2$

No periodic potential

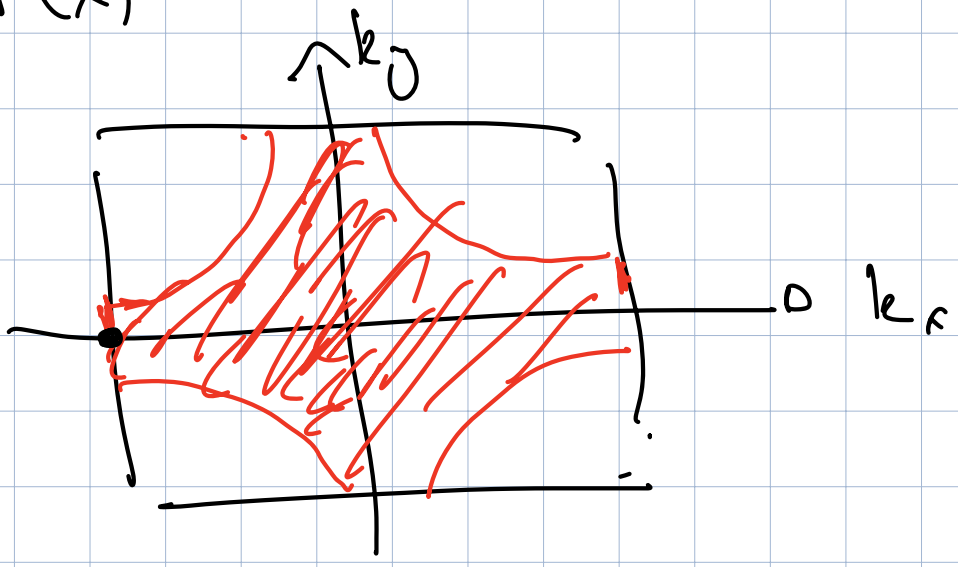


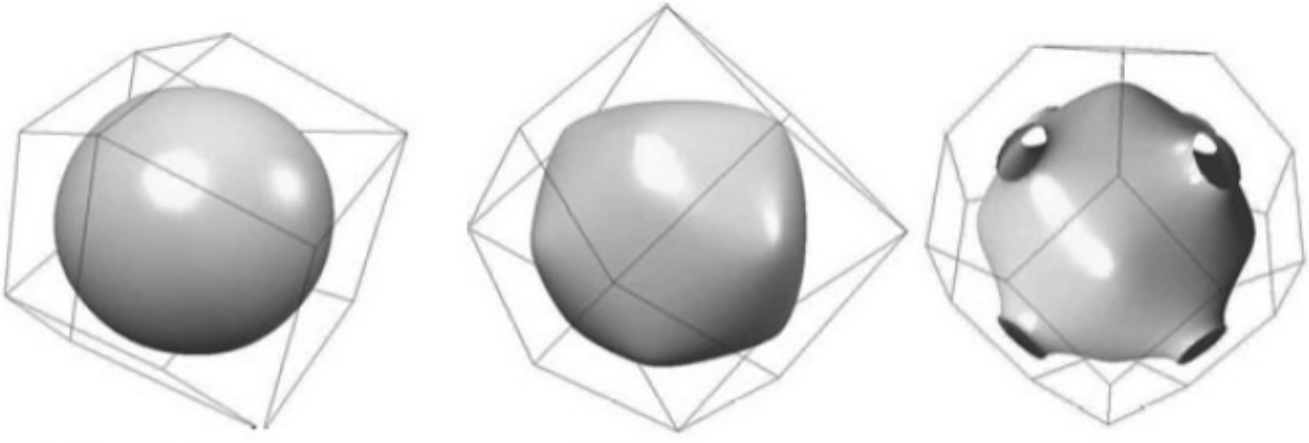
- Intermediate $V(x)$



States to the boundary have smaller energy

- Very strong $V(x)$

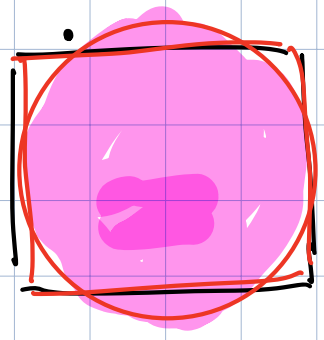




Potassium Lithium Copper

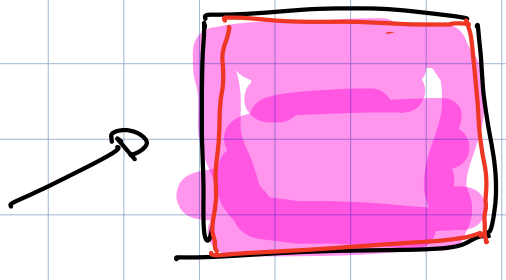
2 e^- / unit cell

$V(x) \to 0$

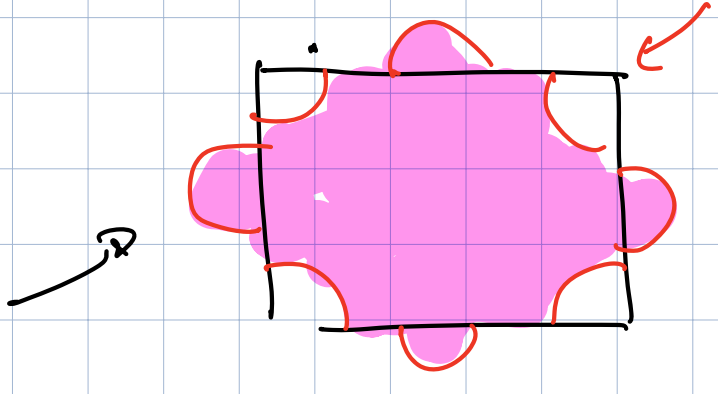


$A_{Fermi} = A_{BZ}$

Strong $V(x)$ very large



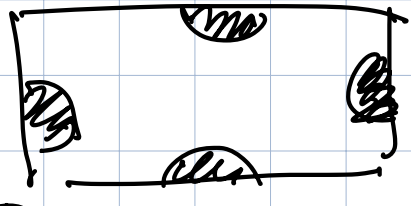
intermediate $V(x)$



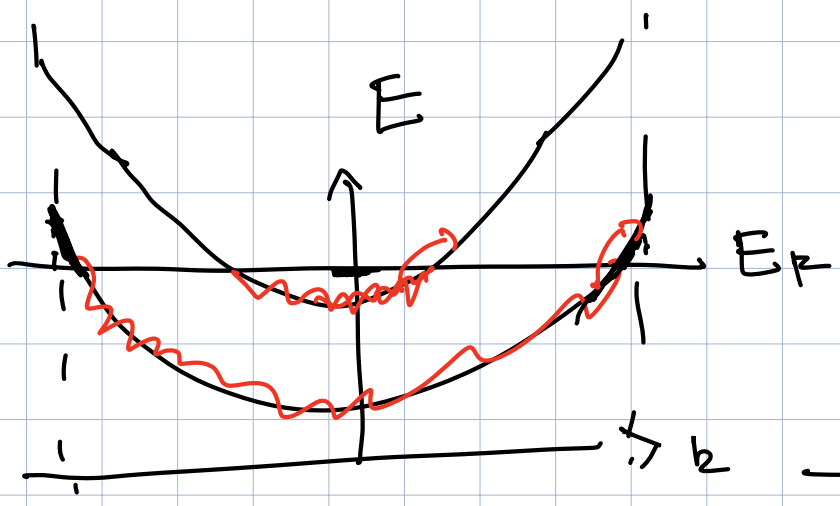
Extended zone

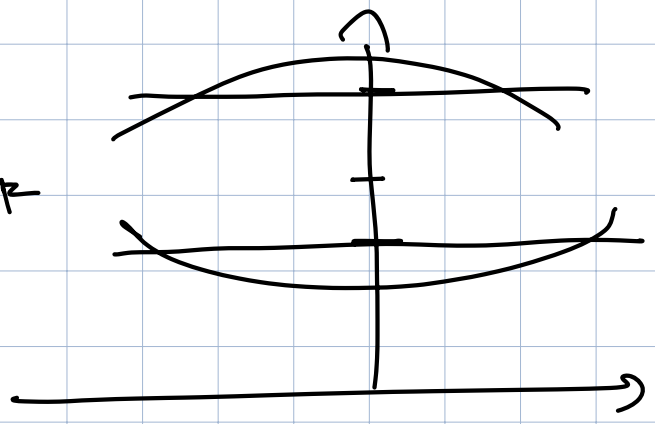
First band

Second band



Reduced zone





Not overlapping

Overlapping band

↓ Reduce zone scheme

First zone

Second zone