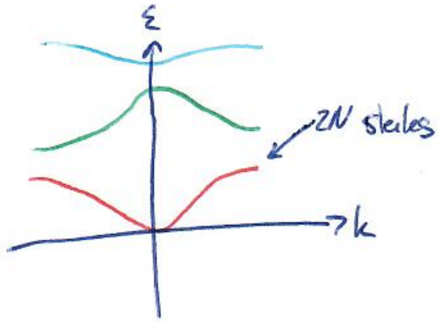
The Mott insulator



Band theory ⇒ $\begin{cases} \text{metal} & \#e^-/uc \text{ odd} \\ \text{insulator} & \#e^-/uc \text{ even} \end{cases}$

Problem CoO, $\frac{\#e^-}{uc}$ odd but insulator. → Mott Insulator

Assume half filling:

$$\mathcal{H} = \underbrace{\sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma}}_{\mathcal{H}_{Band}} + \underbrace{U \sum_{j} n_{j\uparrow} n_{j\downarrow}}_{\mathcal{H}_{Coulomb}}$$

antiferromagnet in insulator → $\mathcal{H}_{Band}$

$\mathcal{H}_{Coulomb}$ ← ferromagnetism of Fermi liquid

$|FS\rangle$ v.s. localized

Mott-Hubbard transition

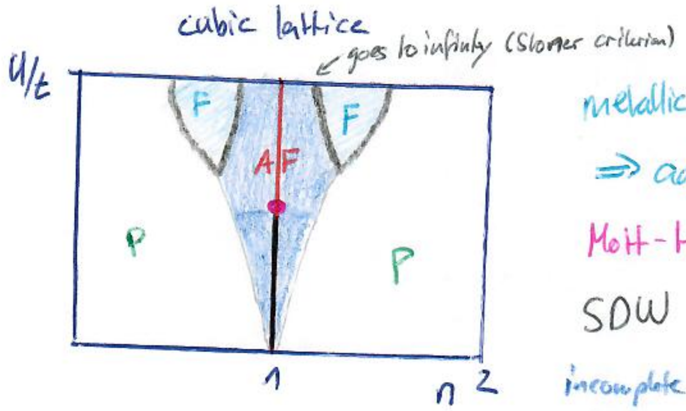
Mott insulators have a single e^- per unit cell ⇒ antiferromagnet

re-inforces insulator $\begin{cases} \cdot \text{ doubling unit cell} \Rightarrow 2e^- \text{ per unit cell} \\ \cdot \text{ SDW band gap} \end{cases}$

Away from half-filling:

$n \neq 1 \overset{?}{\Rightarrow}$ metal, No! impurities localize (Anderson localization)

cubic lattice



metallic Ferromagnet, large U ⇒ polarized spins
⇒ added spins form a band with different polarization

Mott-Hubbard transition

SDW

Mott insulator, U strong ⇒ localization of e^-

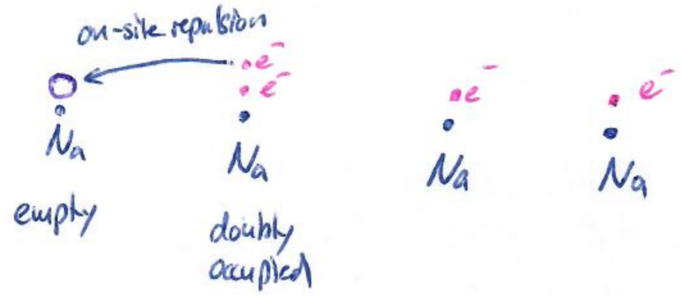
incomplete SDW, metallic

The Mott insulator

Problem: • CuO has an odd $\#e^-$ but is an insulator

• Na remains a metal even for $a \to \infty$

Resolution: Coulomb interaction between e^- with different spin



However, opening a gap allows storage of kinetic energy.

⇒ a large ⇒ Coulomb repulsion strong ⇒ insulator

for $\frac{\#e^-}{\text{unit cell}}$ odd but still insulator are called Mott insulator

⇒ a small ⇒ formation of band structure ⇒ metal

⇝ Mott-Hubbard transition predicts that for high pressure any Mott insulator becomes a metal.

discontinuous, formation of excitons, suddenly break free
(e^--hole pair)

Hubbard Model

$$\mathcal{H} = \mathcal{H}_{Band} + \mathcal{H}_{Coulomb}$$

antiferromagnetism in insulators → $\mathcal{H}_{Band}$

Fermi liquid ferromagnetism → $\mathcal{H}_{Coulomb}$

Fermi sea: likes $\mathcal{H}_{Band}$, hates $\mathcal{H}_{Coulomb}$

fully localized: 0

Compare Fermi sea vs. fully localized ⇒ phase transition

Fermi sea ← uncorrelated: don't care about up e^- if e^- down present (p. 358 GMB/Wlr footnote)

fully localized ← correlated: $e_\uparrow$ avoid $e_\downarrow$

The Mott-Hubbard transition is a collective localization of e^- due to their Coulomb repulsion.

SDW instability

An antiferromagnetically ordered state reinforces its insulating nature by doubling the magnetic period compared to structural.

⇒ $2e^-$ per unit cell ⇒ insulator

<u>Example</u> cubic lattice $\overset{\text{perfect nesting}}{\Rightarrow}$ SDW antiferromagnetic at $q = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$ $\overset{\text{Gap}}{\Rightarrow}$ insulator

at half filling + antiferromagnet ⇒ Mott insulator

(band theory predicts metal, but it's insulator ⇓)

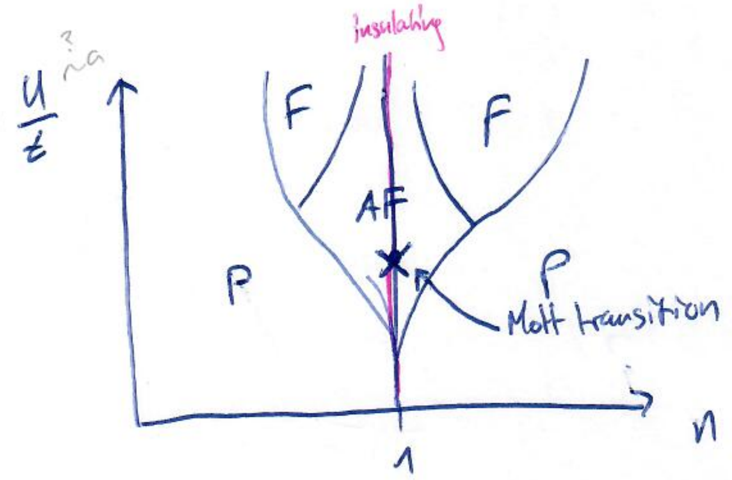
(this is however justified)

Away from half filling

$n = \frac{\#e^-}{\text{unit cell}}$, $\underbrace{n \sim 1, n \neq 1}_{\text{impurities, dislocations}} \Rightarrow$ metal ↯

However, scattering of e^- at impurities. lowest energy single e^- are localized at scattering centers, and not propagating. ← Anderson localization

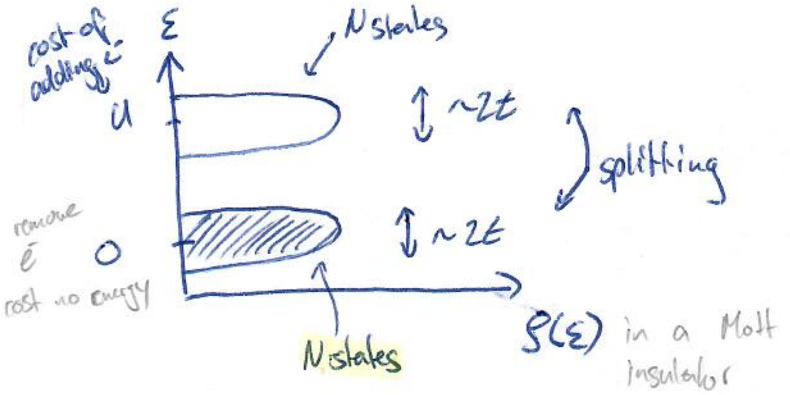
⇒ Mott insulator robust even for slight deviation from half-filling.

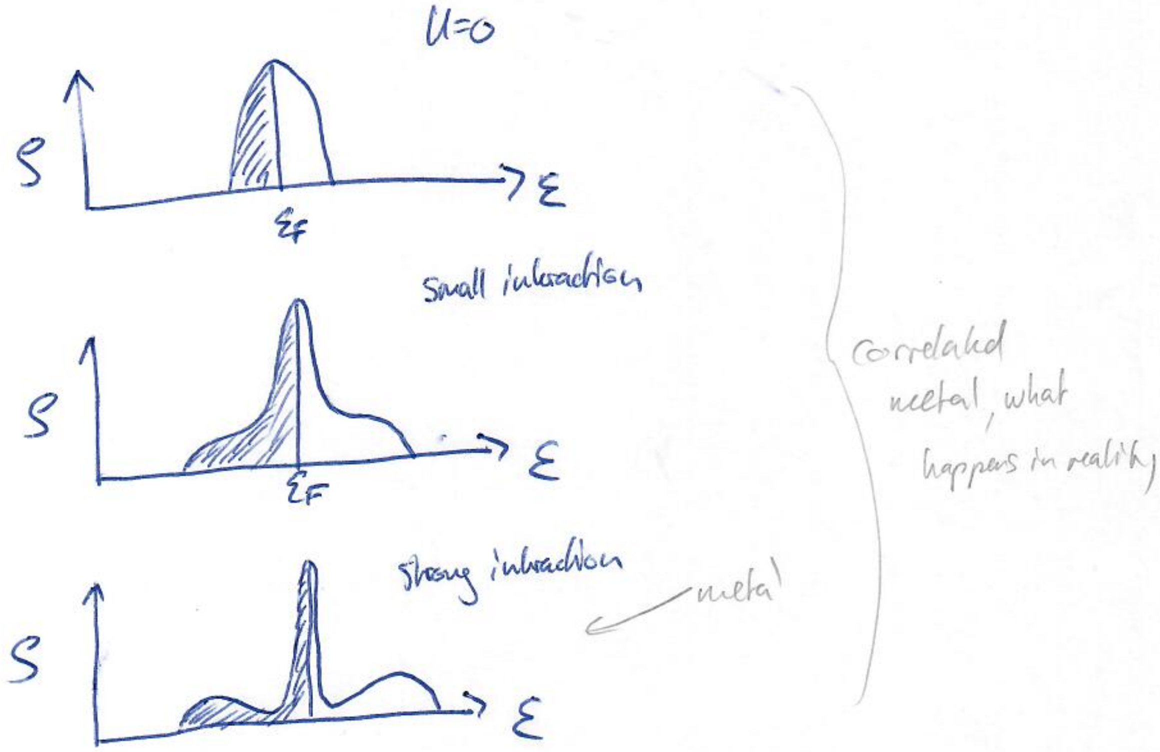


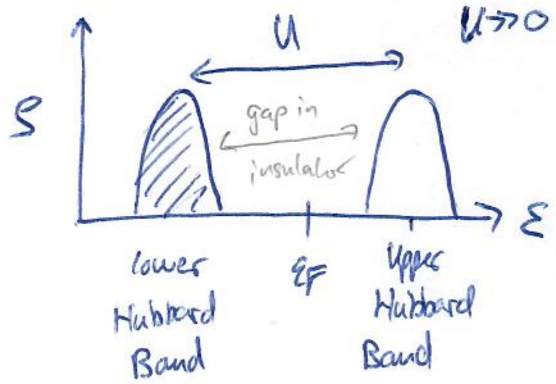
cubic lattice
(particle hole symmetry)

Hubbard subbands

next level excitations in addition to spin dof







Mott-Hubbard insulator

In real materials not the case, excitons due to long range Coulomb

⇒ BEC of excitons ⇒ excitonic insulator