Correlated Insulators

Mott – Hubbard insulator

Nevill Francis Mott

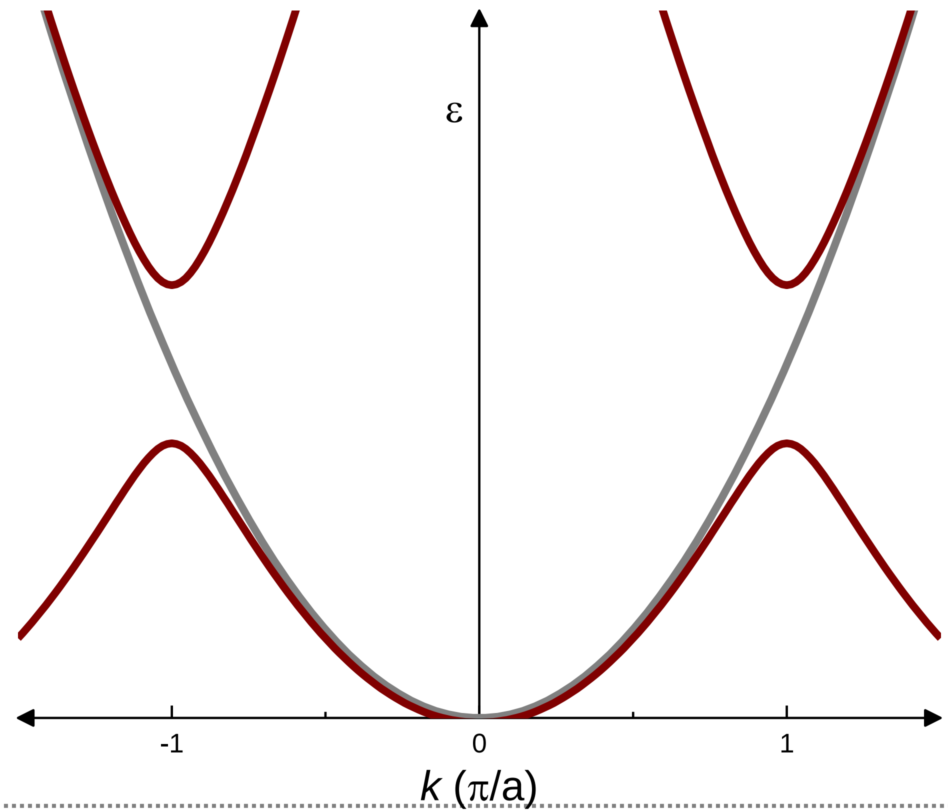
M. Imada, A. Fujimori, Y. Tokura, Metal-insulator transitions. *Rev. Mod. Phys.* **70**, 1039–1263 (1998).

So far: Nearly free electron – band theory

$$\epsilon^{\pm}(k) = \frac{\hbar^2}{2m}\frac{1}{2}\left(k^2 + \left(k - \frac{2\pi}{a}\right)^2\right) \pm \sqrt{\left(\frac{\hbar^2}{2m}k^2 - \frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}\right)^2\right)^2 + 4V_{2\pi/a}^2}$$

Single-electron states in periodic potential

Correction of free electron model by considering lattice potential $V_{2\pi/a}$



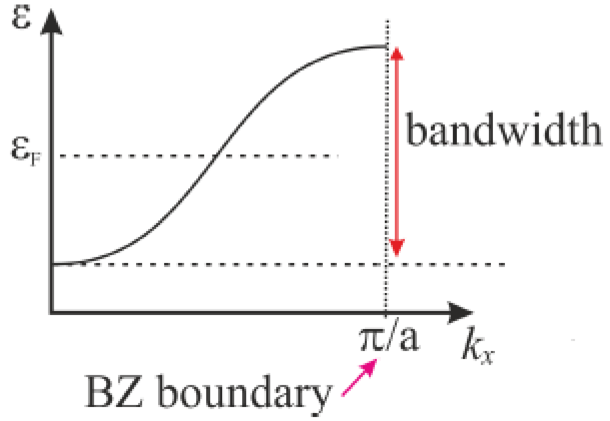
Alternative: Tight Binding Approximation

- First order $\epsilon(k) = \epsilon_0 + t\sum_j \exp(-ik \cdot r_j)$
- Hoping constant t

Simple cubic structure $r = (\pm a, 0,0)\ (0, \pm a, 0)\ (0,0, \pm a)$

$$\epsilon(k) = \epsilon_0 - 2t\left(\cos k_x a + \cos k_y a + \cos k_z a\right)$$

Band width $w = 12t$

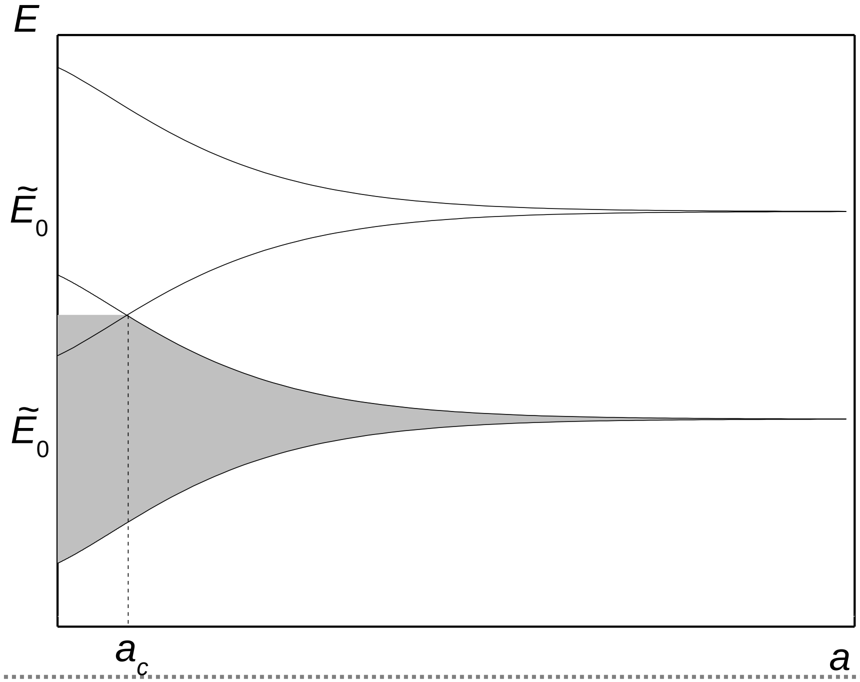


Hopping Integrals

$$t = -\int \phi_{i+1} H \phi_i \, dr$$

S-orbitals:

$$\mathrm{t} = \left\{\frac{3}{2}(1+\mathrm{a}) + \frac{1}{6}\mathrm{a}^2\right\} \mathrm{e}^{-\mathrm{a}}$$



Metal-Insulator transition at a_c

Not a correlation effect

Tight binding in reciprocal and real space

Reciprocal space

$$\epsilon(k) = \epsilon_0 - t\sum_j e^{ikr_j}$$

2nd quantisation

$$H = \sum_{k,s} \epsilon_k a_{ks}^{+} a_{ks}$$

Real Space

Wannier operators (Fourier transform of Bloch operators)

$$c_n = \frac{1}{\sqrt{N}}\sum_k e^{ikna} a_k$$

$$c_n^{+} = \frac{1}{\sqrt{N}}\sum_k e^{-ikna} a_k^{+}$$

Electron hopping Hamiltonian

$$H = -\sum_{i\,j} t_{ij} c_i^{+} c_j$$

Hopping

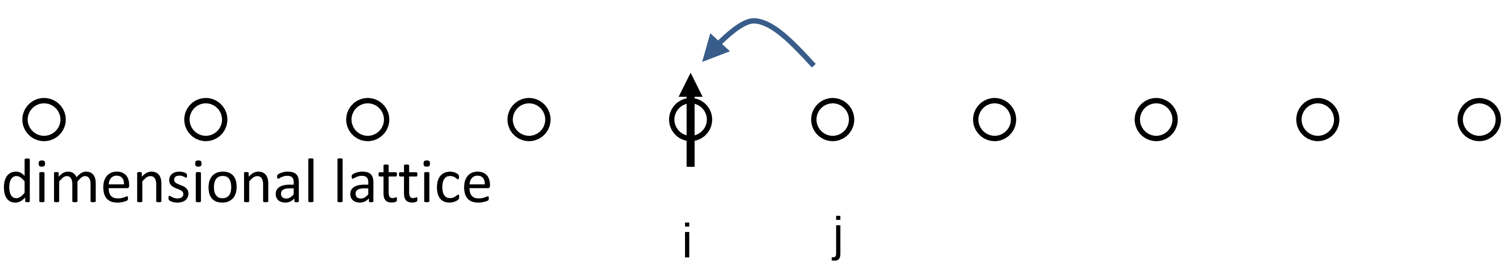
$$H = -\sum_{i\,j} t_{ij} c_i^+ c_j$$

c_i^+ creates electron on site i

c_j annihilates electron on site j

t_{ij} hopping integral calculated from orbital overlap (analoge to exchange interaction)

Non-interacting single-particle states



One-dimensional lattice

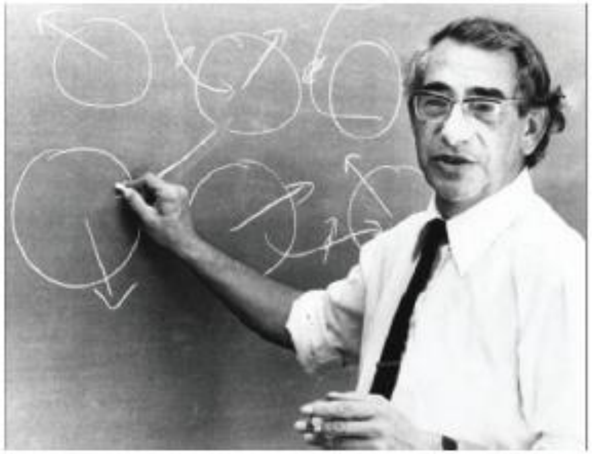
Hubbard model

The „hydrogen atom“ of correlated Electron Physics

$$H = -\sum_{i\,j\,s} t_{ij} c_{is}^{+} c_{js} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$n_{i\uparrow} = c_{is}^{+} c_{is}$ number of electrons on site i

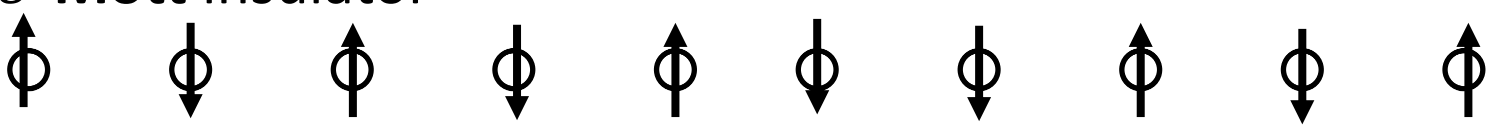
U energy cost for 2 electrons on same site



John Hubbard

Half-Filling (1 electron per site)

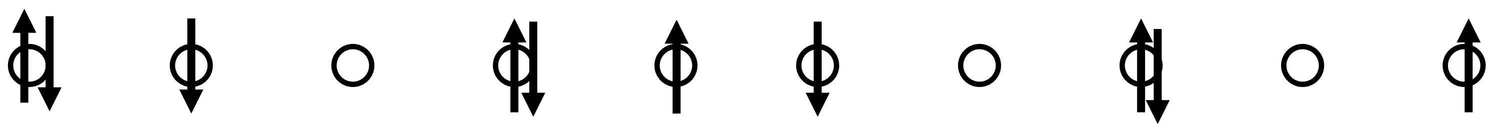
- $t \gg U$ metal
- $t \ll U$ **Mott** insulator



Limiting Case U=0

$$H = t\sum_{ijs} c_{is}^{+}c_{js}$$

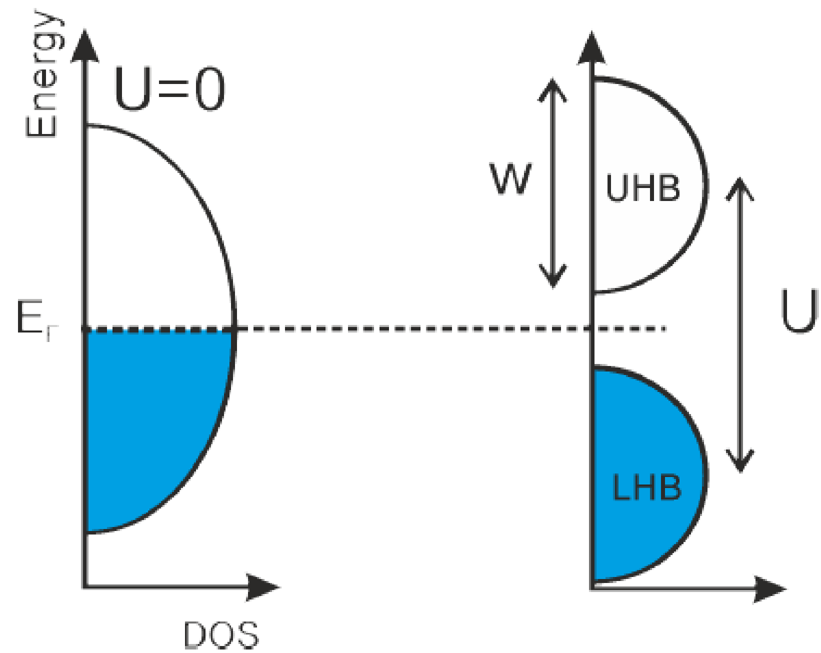
- Back to non-correlated
- Metal

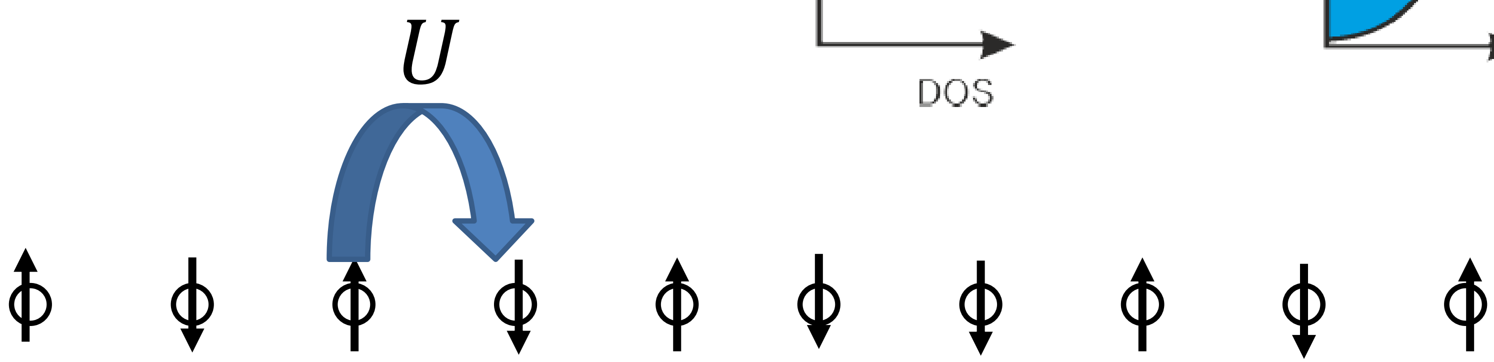


Limiting Case $t = 0$

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- Insulator
- One electron fixed per site
- No hopping



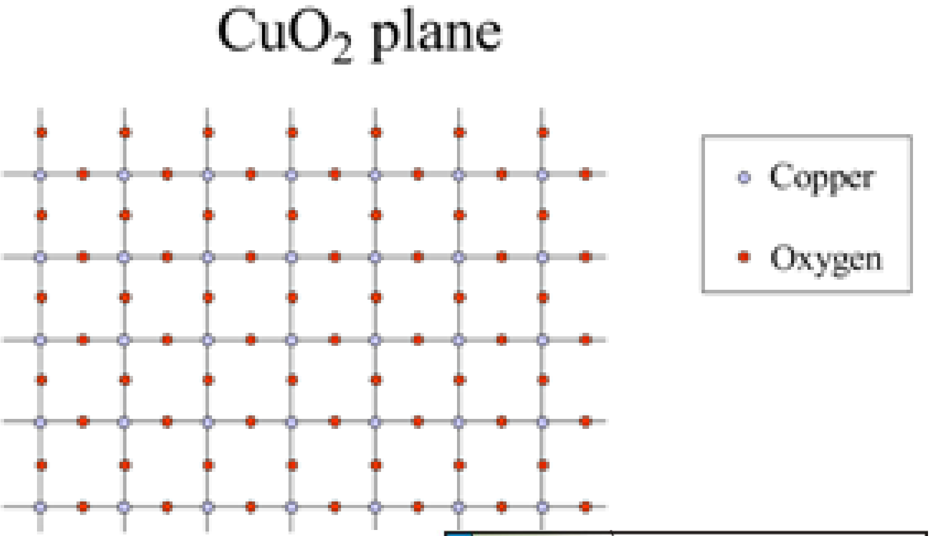


Antiferromagnetic Insulator at Half-Filling

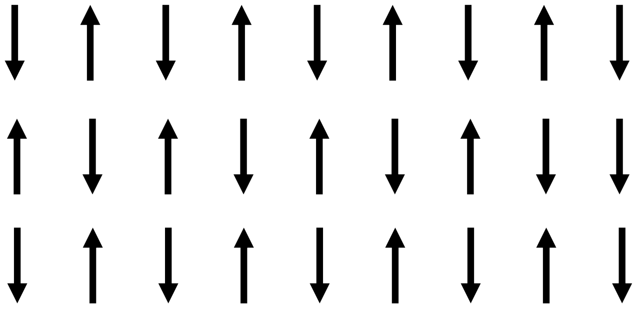
- Hubbard model at half filling can be approximated by Heisenberg for $\boldsymbol{U} \gg \boldsymbol{t}$

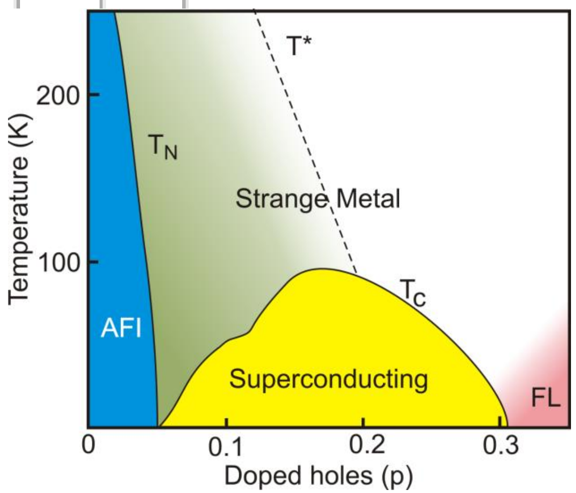
$$H_J = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

$$J_{ij} = \frac{4t_{ij}^2}{U}$$



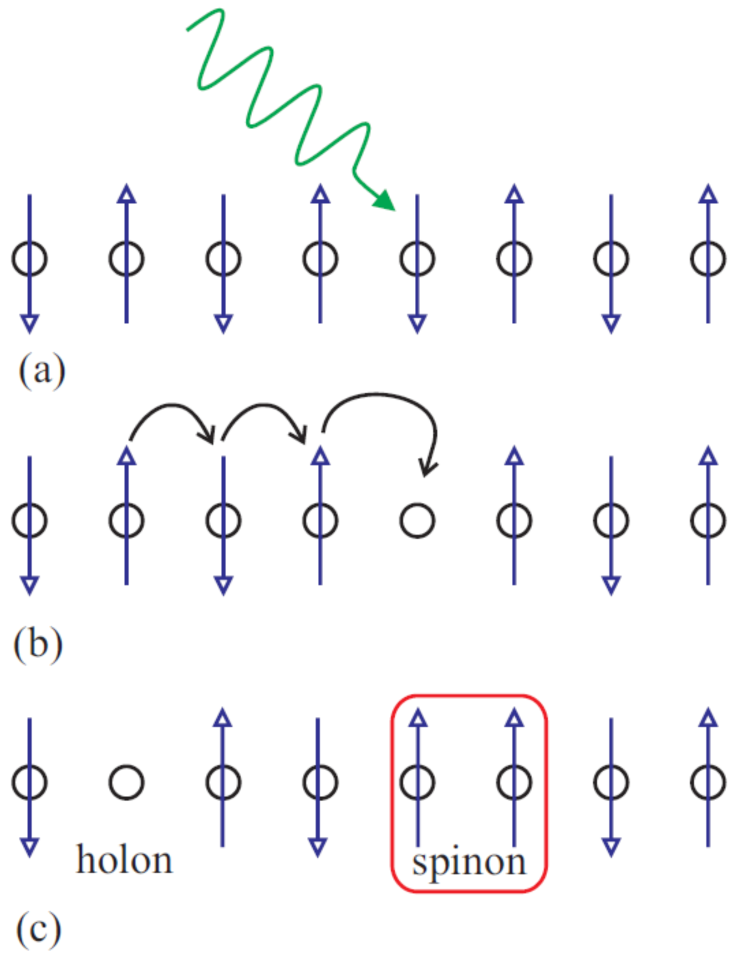
Leads to antiferromagnetic order





Emergent quasiparticles

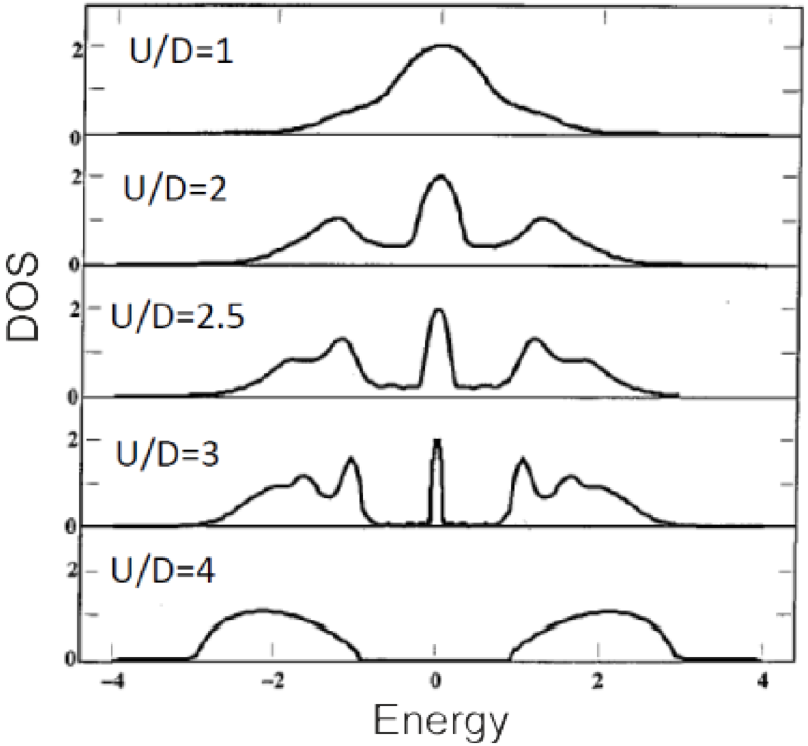
- Fractional quantum hall effect
- New quasiparticles with fractionalised charge
- Many-body phenomen



- Spin and charge separation
- New quasiparticles
- Spinon and holon
- Observed in $SrCuO_2$
- New physics and applications

Highly correlated metal close to Mott state

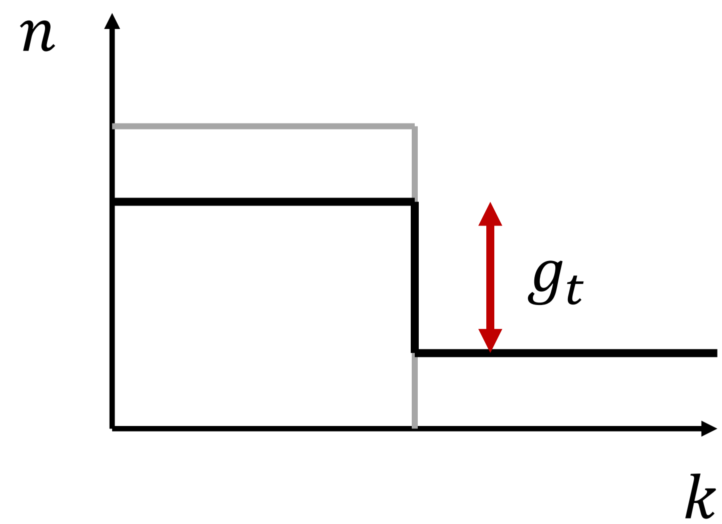
- Around $t \sim U$
- Emergent narrow band at ϵ_F
- Highly correlated
- Large $D(\epsilon_F)$
- Novel states



A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).

The metallic state

- Gutzwiller approximation
- Renormalisation $g_t = 8d(1-2d)$
- Vanishing Quasiparticle Weight
- Quasiparticle ceases to exist
- Fermi liquid ground state
- Strong renormalisations (divergences)



$$\frac{m^*}{m} = \frac{1}{g_t} = \frac{1}{1 - U^2/U_c^2}$$

$$F_0^s = \frac{U\,g(E_F)}{4}\frac{2U_c - U}{(U-U_c)^2}U_c \qquad \kappa$$

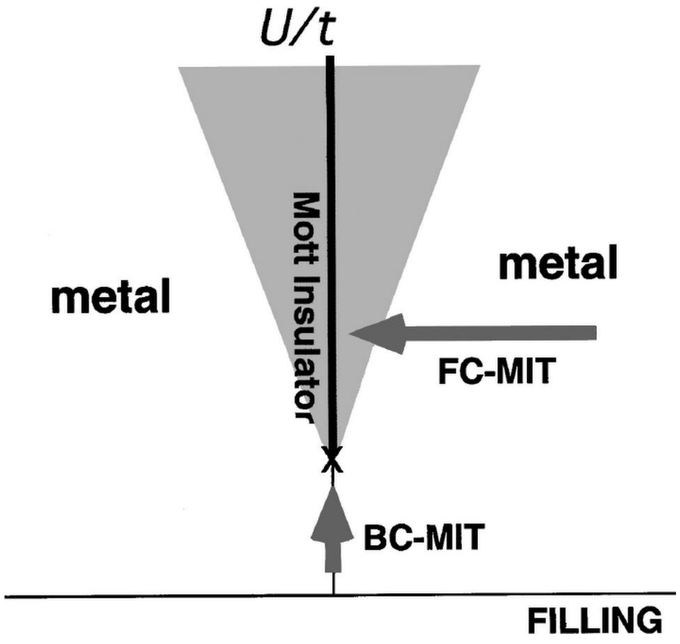
$$F_1^s = \frac{3U^2}{U_c^2 - U}$$

$$F_0^a = -\frac{U\,g(E_F)}{4}\frac{2U_c + U}{(U+U_c)^2}U_c \qquad \chi$$

The Phase diagram

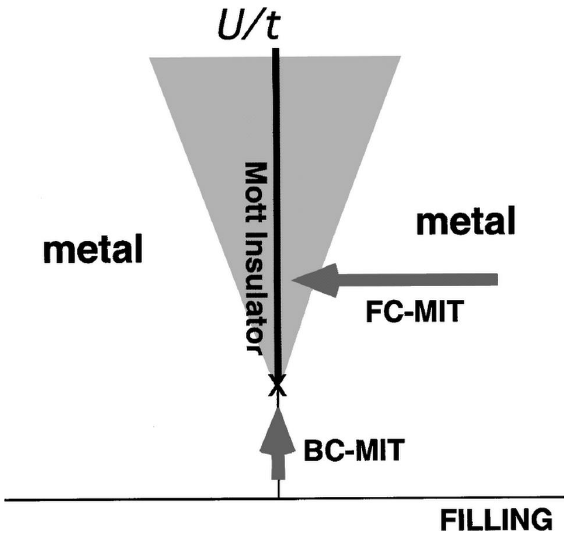
- Band width control $\frac{U}{t}$
- Can be realised with pressure

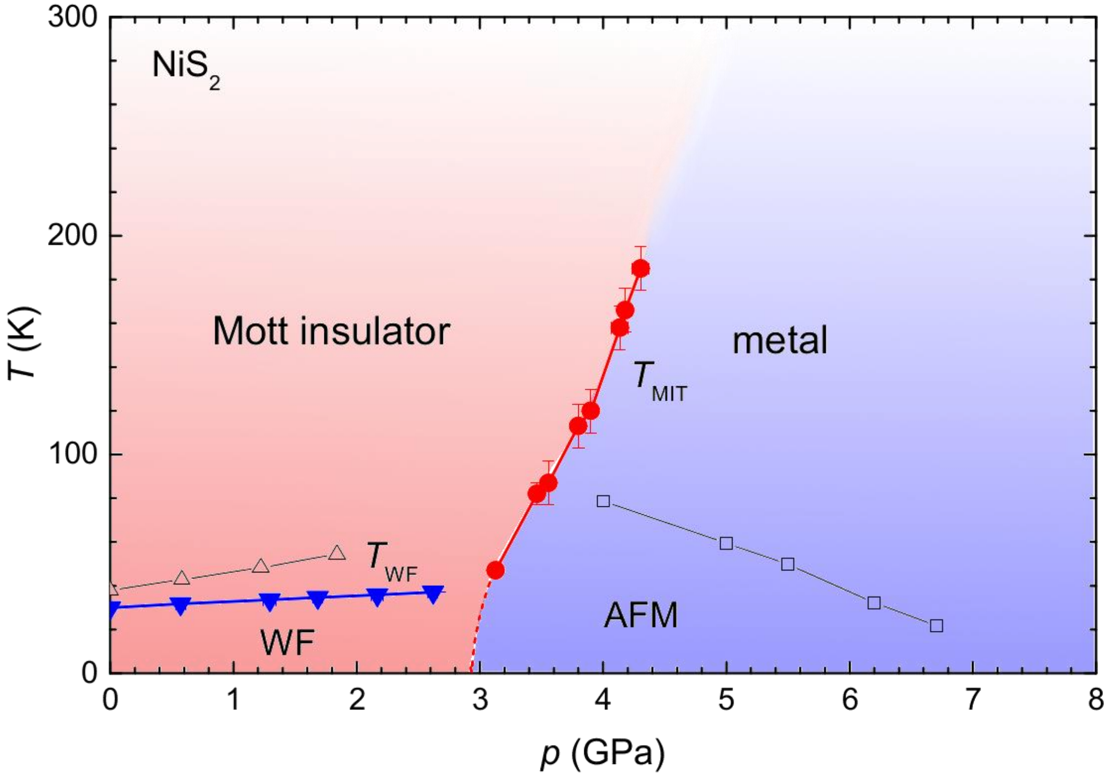
  (changing the overlap)
- E.g. NiS_2
- Filling control n
- Can be realised with doping
- E.g. cuprates



NiS_2 under pressure

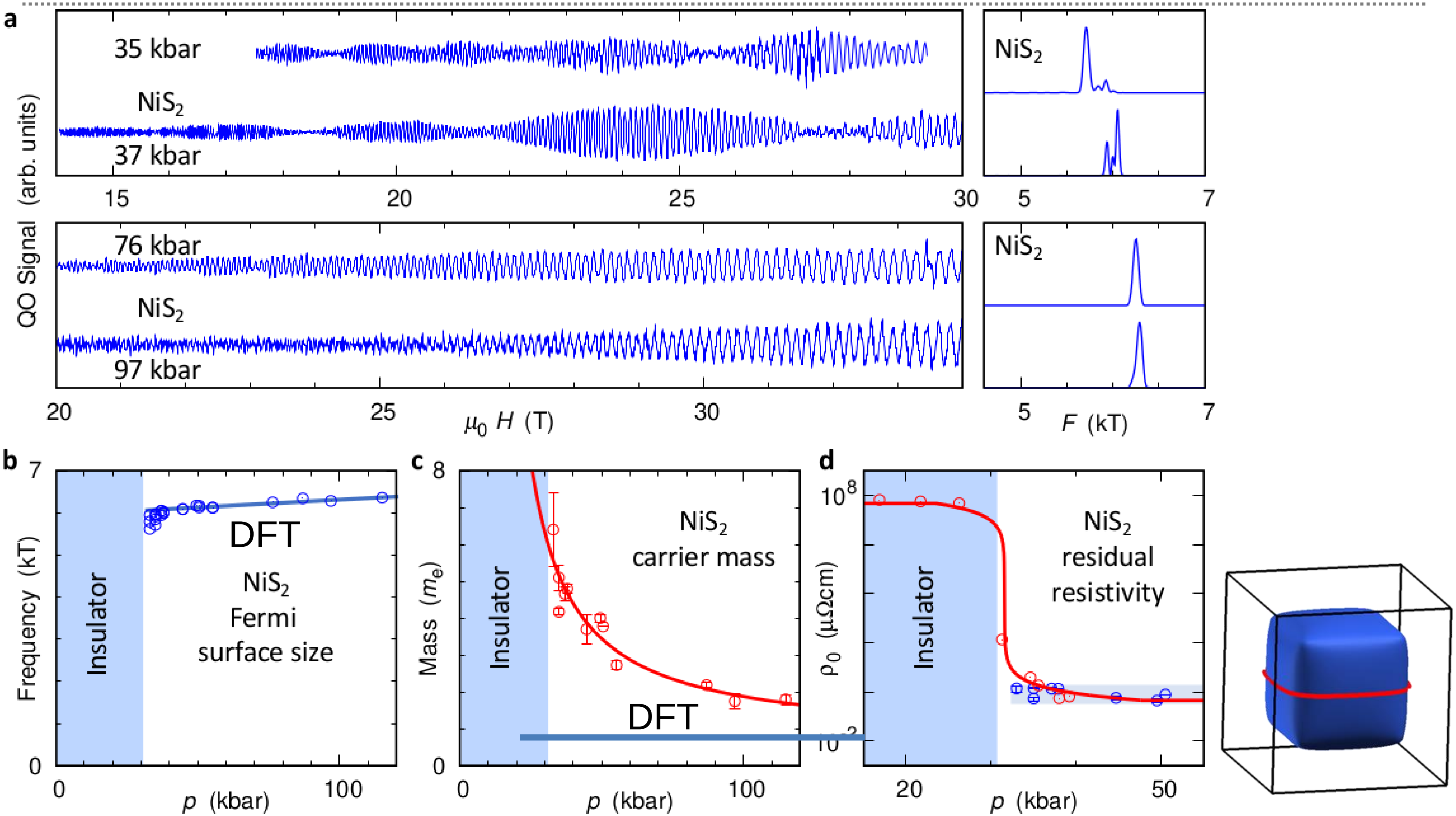
- Band-width control





arXiv:1509.00397

Mott transition: Mass Divergence



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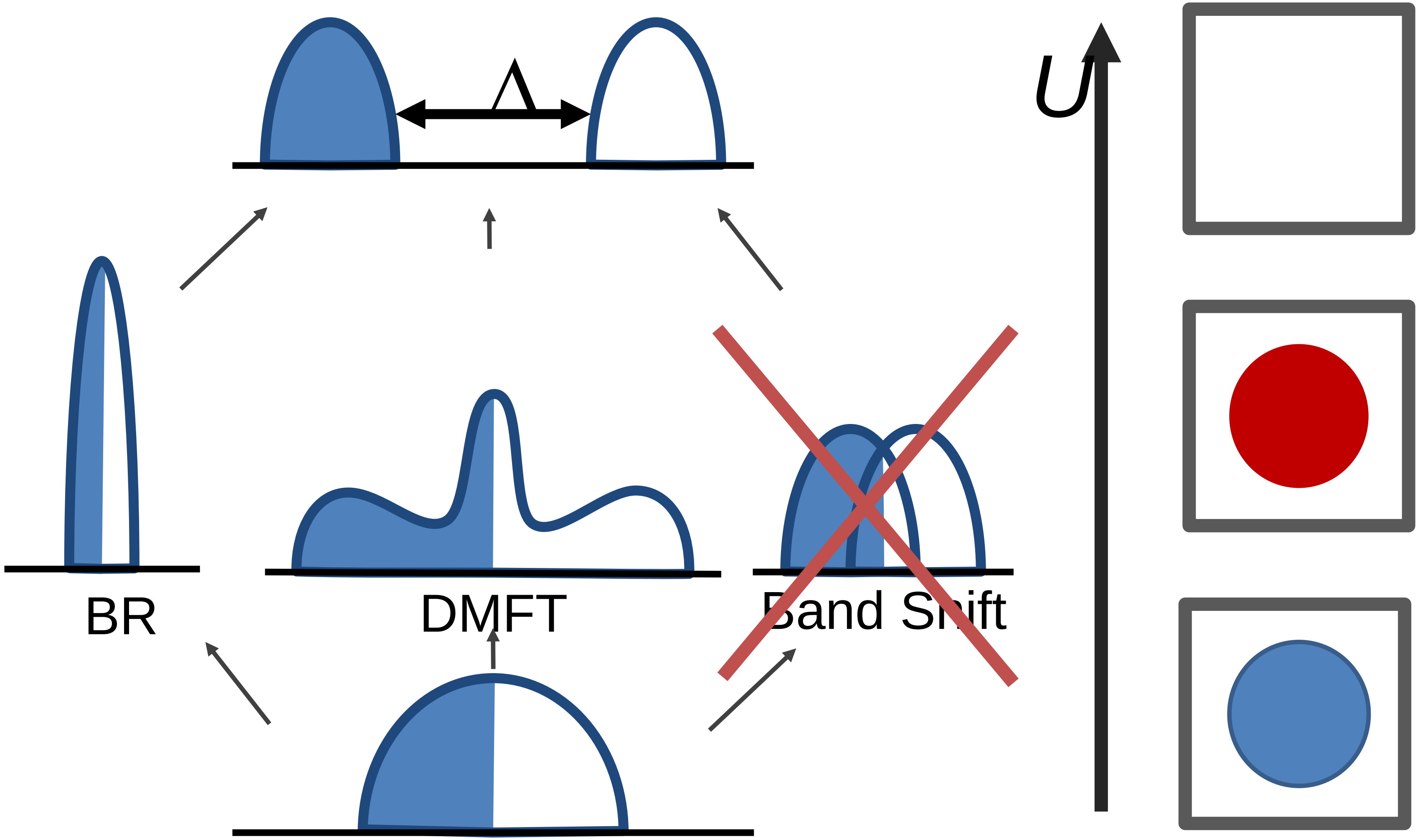
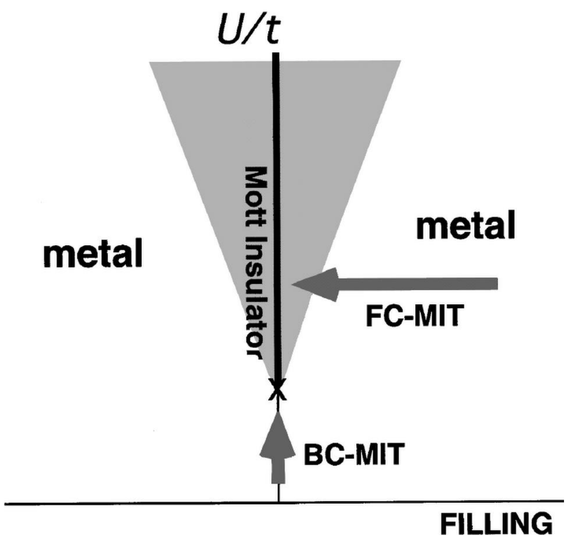
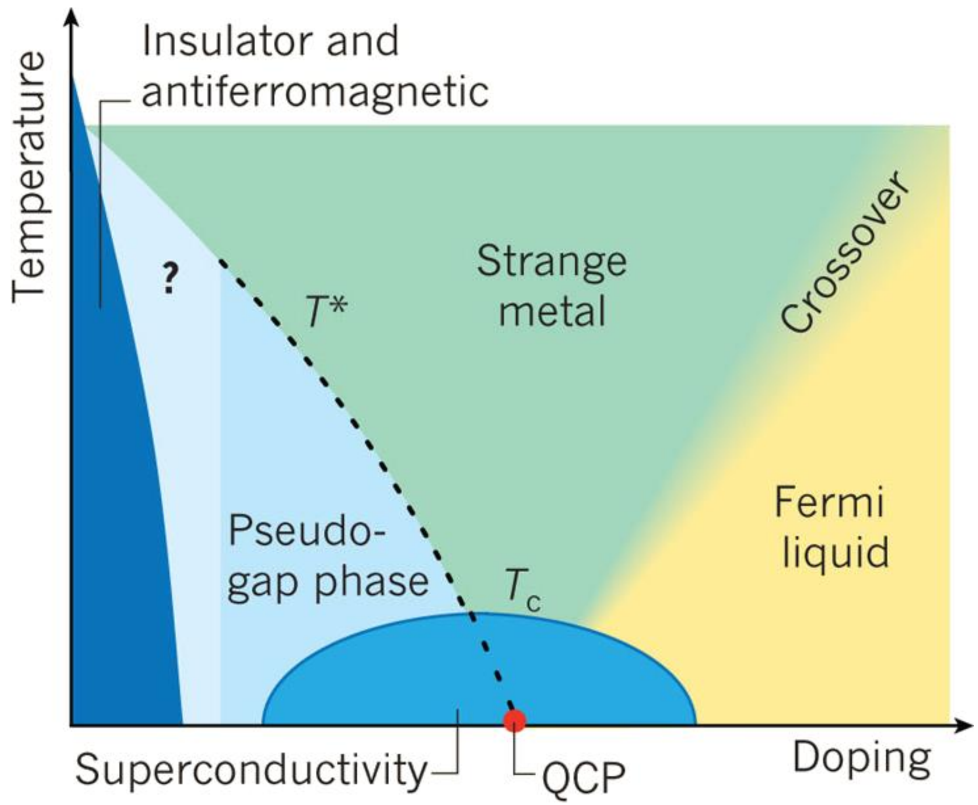
Mott transition: Emergent Fermi surface



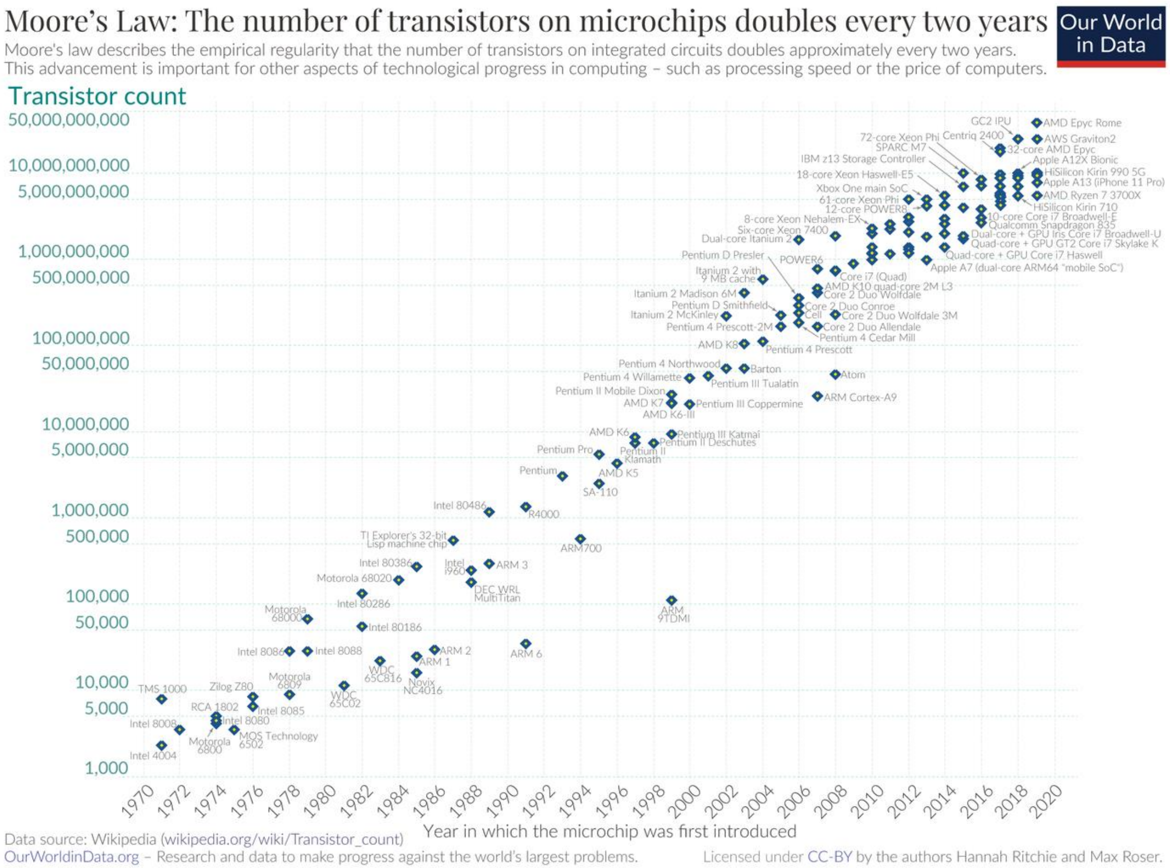
Experimental examples

- Cuprates
- Doping
- Filling control
- Very challenging to understand





Applications of Mott insulators



- Field-effect transistors
- Photovoltaics
- Magnetic cooling