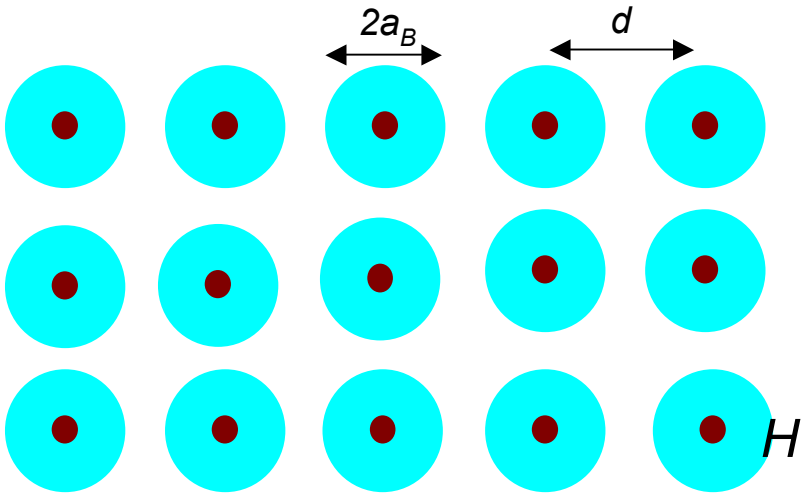
Mott insulators

Atomic limit - view electrons in real space

Virtual system: lattice of H-Atoms: $a_B << d$



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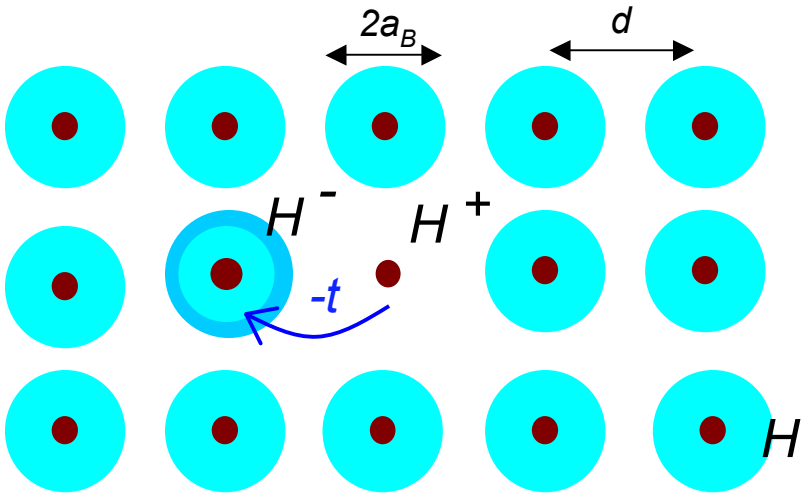

- hopping - electron transfer

$$-t|\{H^+\}_i,\{H^-\}_j\rangle\langle\{H\}_i\{H\}_j| + h.c.$$

- ionization energy

$$U = E(H^+) + E(H^-) - 2E(H)$$

delocalization

$-2tz$

kinetic energy

metal

localization

U

charge excitation energy

Mott insulator

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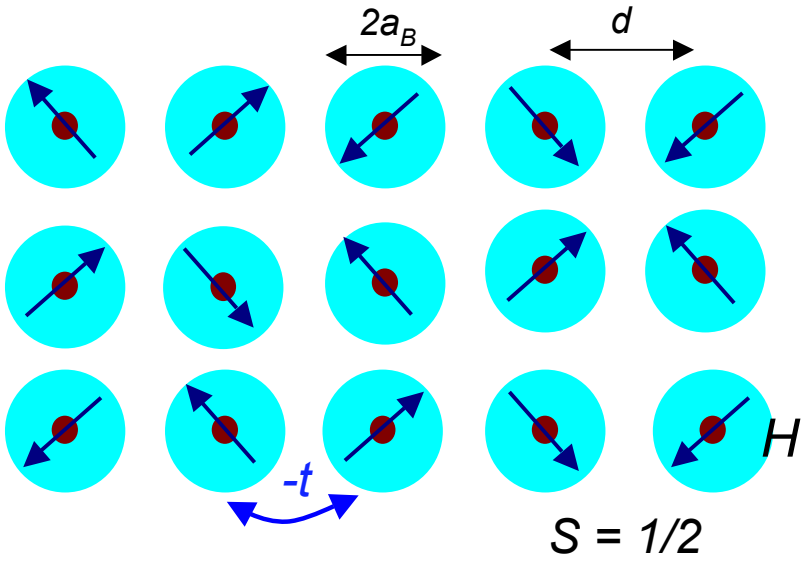

- hopping - electron transfer

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- ionization energy

$$U = E(H^+) + E(H^-) - 2E(H)$$

Mott isolator

low-energy physics

no charge fluctuation
only spin fluctuation

effective low-energy model

$$H_{\text{Heisenberg}} = J\sum_{i,j}\vec{S}_i\cdot\vec{S}_j$$

Mott insulators

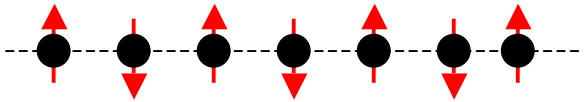
Metal-insulator transition from the insulating side

Hubbard-model:

$$H = -t \underbrace{\sum_{\langle i,j\rangle,s} \left\{ c_{is}^{\dagger} c_{js} + c_{js}^{\dagger} c_{is} \right\}}_{\text{n.n. hopping}} + \underbrace{U \sum_{i} n_{i\uparrow} n_{i\downarrow}}_{\text{onsite repulsion}} = \sum_{\vec{k},s} \epsilon_{\vec{k}} c_{\vec{k}s}^{\dagger} c_{\vec{k}s} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

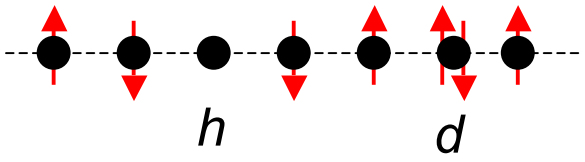
density: *n=1*

„ground state“

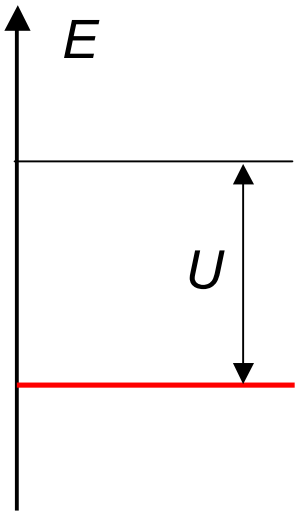


t = 0

charge excitation



$$E = U$$



Mott insulators

Metal-insulator transition from the insulating side

Hubbard-model:

$$H = -t \underbrace{\sum_{\langle i,j\rangle,s} \left\{ c_{is}^{\dagger} c_{js} + c_{js}^{\dagger} c_{is} \right\}}_{\text{n.n. hopping}} + U \underbrace{\sum_{i} n_{i\uparrow} n_{i\downarrow}}_{\text{onsite repulsion}} = \sum_{\vec{k},s} \epsilon_{\vec{k}} c_{\vec{k}s}^{\dagger} c_{\vec{k}s} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

density: *n=1*

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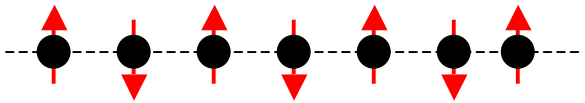
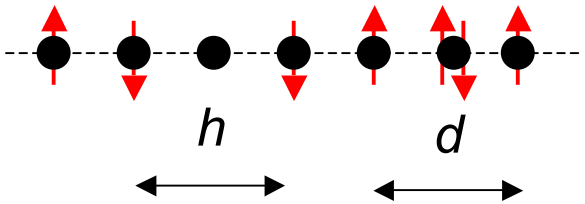
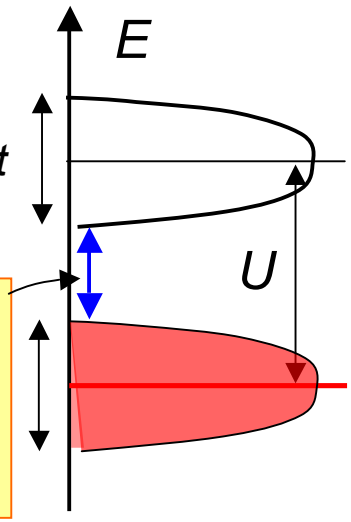


charge excitation



t > 0



$$E_{\vec{k},\vec{k}'} = U + \epsilon_{\vec{k}} + \epsilon_{\vec{k}'} \geq U - 4dt$$

metal-insulator transition: $U_c = 4dt$

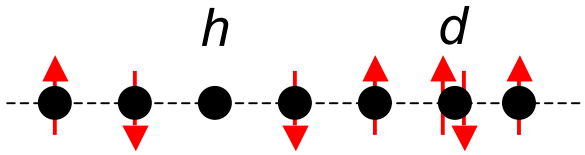
Mott insulators

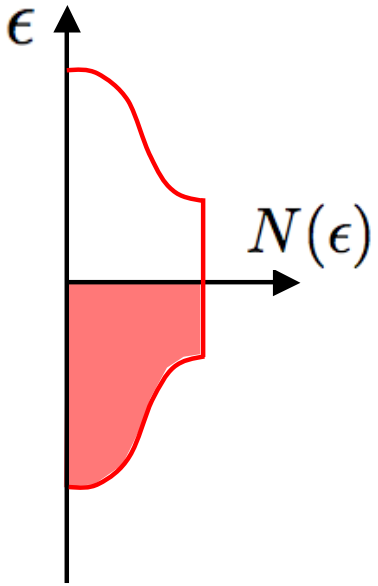
Metal side

$$H = -t \sum_{\langle i,j \rangle, s} \left\{ c_{is}^{\dagger} c_{js} + c_{js}^{\dagger} c_{is} \right\} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} = \sum_{\vec{k},s} \epsilon_{\vec{k}} c_{\vec{k}s}^{\dagger} c_{\vec{k}s} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$\epsilon_{\vec{k}} = -2t(\cos k_x a + \cos k_y a + \cos k_z a)$$

$U = 0$ tight-binding model





half-filled conduction band

	density
empty sites	*h = 1/4*
doubly occupied sites	*d = 1/4*
singly occupied sites	*s = 1/2*

$U > 0$ ➡ $\begin{cases} h = d \to 0 \\ s \to 1 \end{cases}$

reducing mobility

Mott insulators

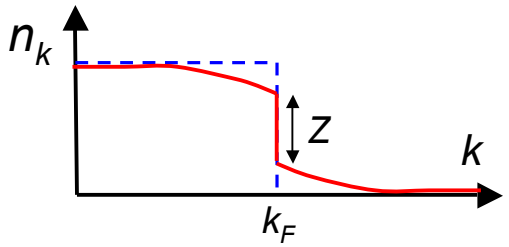
Metal-insulator transition from the metallic side

Gutzwiller approximation

$$\mathcal{H}_{eff} = g_t \sum_{\vec{k},s} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} \qquad g_t = 1 - \left(\frac{U}{U_c}\right)^2$$

Fermi liquid property

renormalized momentum distribution



quasiparticle weight: $Z = g_t$

at MIT $U \to U_c$

$$\begin{cases} \dfrac{m^*}{m} \to \infty \\ Z \to 0 \end{cases}$$