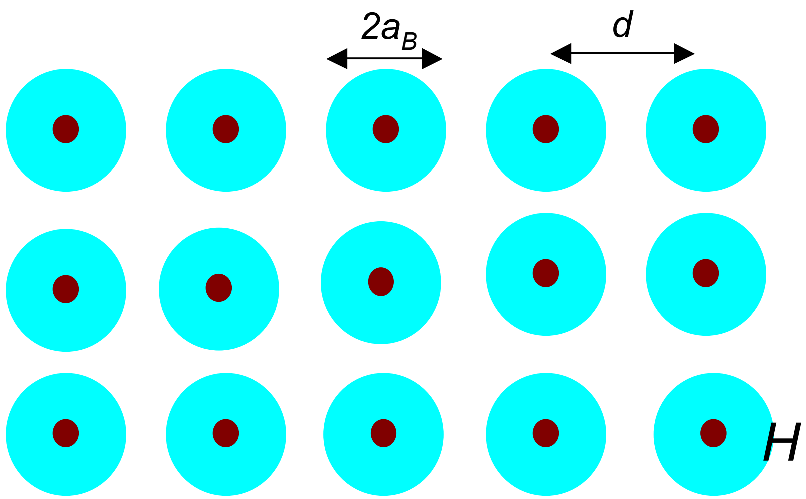
Mott insulators

Atomic limit - view electrons in real space

Virtual system: lattice of H-Atoms: $a_B \ll d$



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Atomic limit - view electrons in real space

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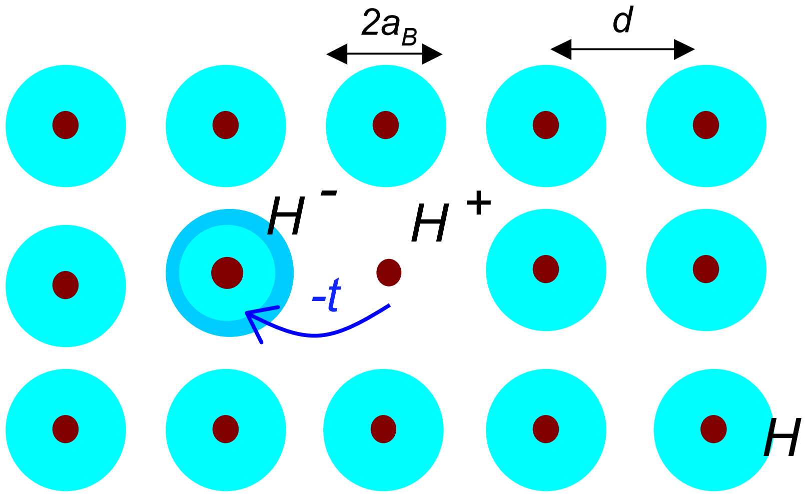

- hopping - electron transfer

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

- 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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Atomic limit - view electrons in real space

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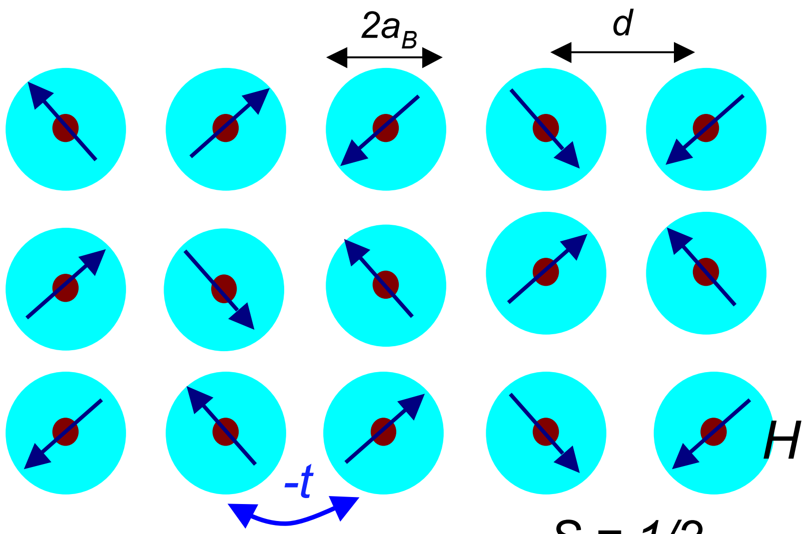


$S = 1/2$

- hopping - electron transfer

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

- ionization energy

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

Mott isolator

low-energy physics

no charge fluctuation
only spin fluctuation

effective low-energy model

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

Mott insulators

Metal-insulator transition from the insulating side

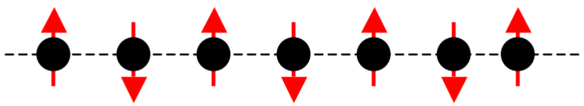
Hubbard-model:

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

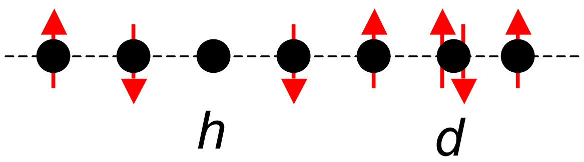
density: *n=1*

$\boxed{t = 0}$

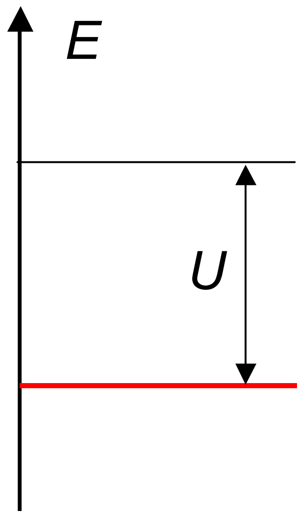
„ground state“



charge excitation



$$\boxed{E = U}$$



Mott insulators

Metal-insulator transition from the insulating side

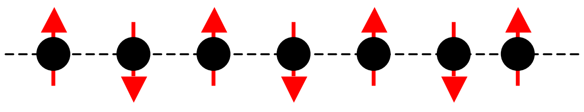
Hubbard-model:

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

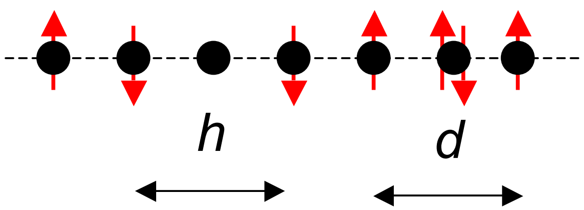
density: *n=1*

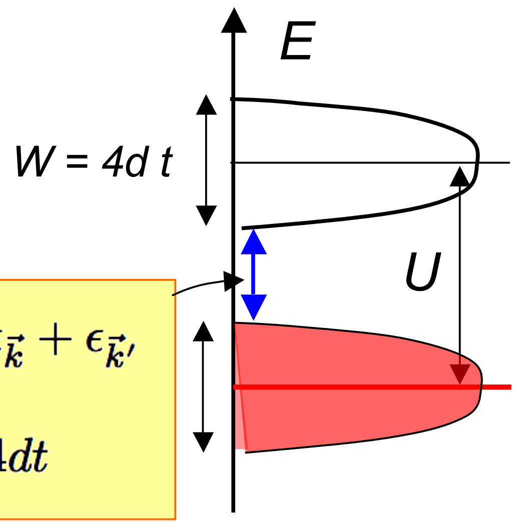
$\boxed{t > 0}$

„ground state“



charge excitation





$$\boxed{\begin{aligned} E_{\vec{k},\vec{k}'} &= U + \epsilon_{\vec{k}} + \epsilon_{\vec{k}'} \\ &\geq U - 4dt \end{aligned}}$$

metal-insulator transition: $U_c = 4dt$

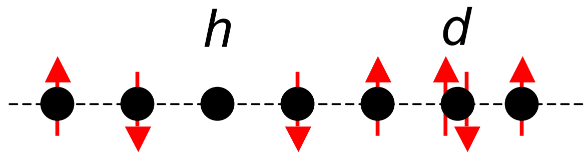
Mott insulators

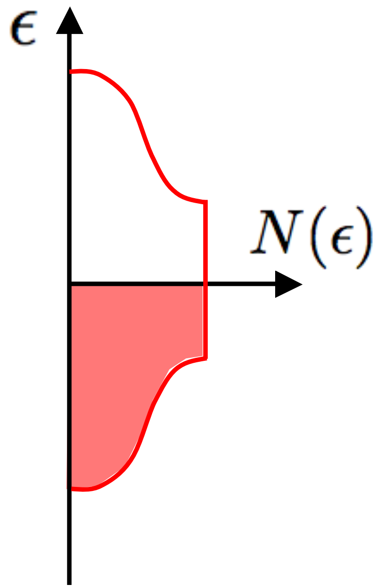
Metal-insulator transition from the metallic side

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

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

$U = 0$ 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

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

reducing mobility

Metal-insulator transition from the metallic side

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

Gutzwiller-approach: variational

diminish double-occupancy

$$|\Psi_{GW}\rangle = \prod_{i} \left(1 - (1-g) n_{i\uparrow} n_{i\downarrow}\right) |\Psi_0\rangle$$

uncorrelated state

variational groundstate

$$E_g = \frac{\langle \Psi_{GW} | H | \Psi_{GW} \rangle}{\langle \Psi_{GW} | \Psi_{GW} \rangle} \Rightarrow E_g = \langle \Psi_0 | H_{eff} | \Psi_0 \rangle + U d N$$

density of doubly occupied sites

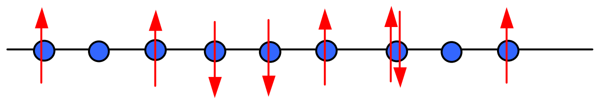
$$\boxed{H_{eff} = -g_t t \sum_{\langle i,j \rangle, s} \left\{ c_{is}^{\dagger} c_{js} + c_{js}^{\dagger} c_{is} \right\} = \sum_{\vec{k},s} g_t \epsilon_{\vec{k}} c_{\vec{k}s}^{\dagger} c_{\vec{k}s}}$$

renormalized hopping

Metal-insulator transition from the metallic side

densities:

1	electron density
$s_\uparrow$	density of singly occupied sites with spin $\uparrow$
$s_\downarrow$	density of singly occupied sites with spin $\downarrow$
d	density of doubly occupied sites
h	density of empty sites



no spin polarization

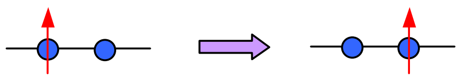
$$s_\downarrow = s_\uparrow = s/2$$

half-filling $h = d$

sum rule $1 = s + h + d = s + 2d$

Metal-insulator transition from the metallic side

hopping probability: sector of fixed *d*



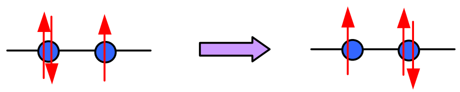
correlated renormalization factor *uncorrelated*

$$P(\uparrow 0) + P(\downarrow 0) = g_t \left\{ P_0(\uparrow 0) + P_0(\downarrow 0) \right\}$$

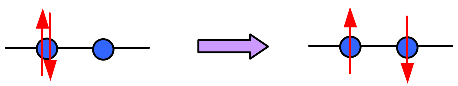
$$P(\uparrow 0) + P(\downarrow 0) = hs = ds = d(1-2d)$$

$$P_0(\uparrow 0) = n_{i\uparrow}(1-n_{i\downarrow})(1-n_{j\uparrow})(1-n_{j\downarrow}) = \frac{1}{16}$$

$$\boxed{g_t = 8d(1-2d)}$$



analogous with same g_t



d changed, not in sector

Metal-insulator transition from the metallic side

$$H_{eff} = -g_t t \sum_{\langle i,j\rangle,s} \left\{ c_{is}^\dagger c_{js} + c_{js}^\dagger c_{is} \right\} = \sum_{\vec{k},s} g_t \epsilon_{\vec{k}} c_{\vec{k}s}^\dagger c_{\vec{k}s}$$

$$E_g = \langle \Psi_0 | H_{eff} | \Psi_0 \rangle + UdN$$

minimize w.r.t. *d*

$$E(d) = g_t \epsilon_{kin} + Ud = 8d(1-2d)\epsilon_{kin} + Ud$$

per site

$$\epsilon_{kin} = \int_{-W}^{0} d\epsilon \, N(\epsilon)\epsilon$$

$$U_c = 8|\epsilon_{kin}| \approx 16t = 4W$$

Brinkmann-Rice (1970)

$$d = \frac{1}{4}\left(1 - \frac{U}{U_c}\right)$$

$$g_t = 1 - \left(\frac{U}{U_c}\right)^2$$

Mott insulators

Gutzwiller approximation

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

optical conductivity:

$$\sigma_1(\omega) = \frac{\omega_p^{*2}}{4}\delta(\omega) + \sigma_1^{reg}(\omega) \qquad \frac{\omega_p^{*2}}{\omega_p^2} = \frac{m}{m^*} = g_t$$

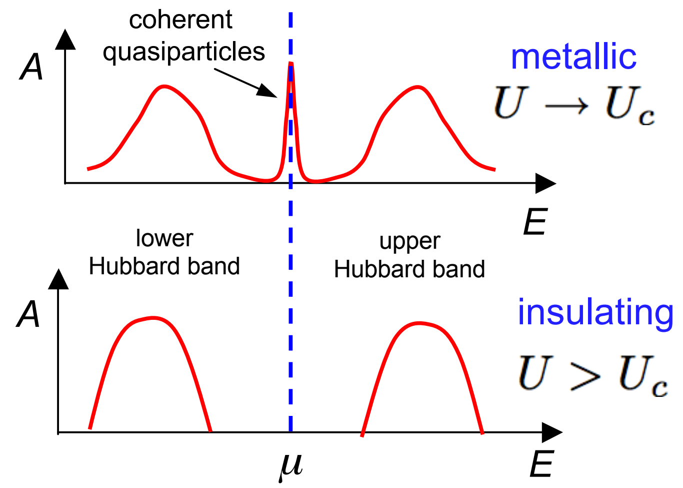
Drude weight

quasiparticle weight: $Z = g_t$

at MIT
$U \to U_c$

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

single particle spectral function



Mott insulators

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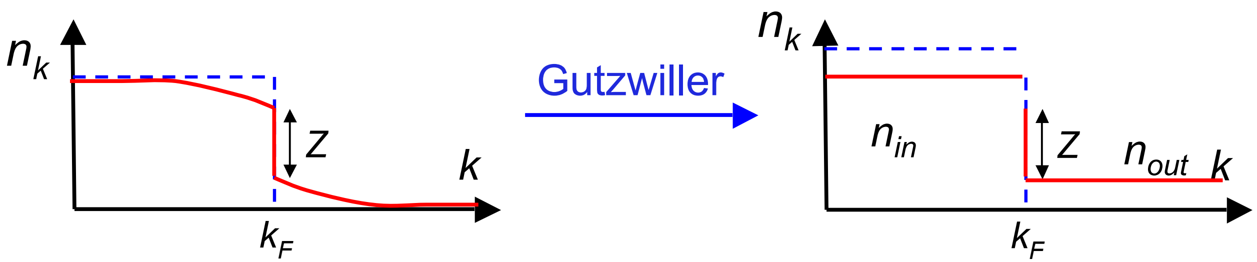
$$\mathcal{H}_{eff} = g_t \sum_{\vec{k},s} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} \qquad g_t = 1 - \left(\frac{U}{U_c}\right)^2$$

Fermi liquid properties within Gutzwiller approximation:

renormalized momentum distribution



$$\frac{1}{2} = \frac{1}{N}\sum_{\vec{k}\in FS} n_{in} + \frac{1}{N}\sum_{\vec{k}\notin FS} n_{out} = \frac{1}{2}(n_{in}+n_{out})$$ half-filling

$$g_t \epsilon_{kin} = \frac{1}{N}\sum_{\vec{k}\in FS} n_{in}\epsilon_{\vec{k}} + \frac{1}{N}\sum_{\vec{k}\notin FS} n_{out}\epsilon_{\vec{k}}$$ renormalized hopping

$$0 = \frac{1}{N}\sum_{\vec{k}\in FS} \epsilon_{\vec{k}} + \frac{1}{N}\sum_{\vec{k}\notin FS} \epsilon_{\vec{k}}$$ particle-hole symmetry

$$\epsilon_{kin} = 2\sum_{\vec{k}\in FS} \epsilon_{\vec{k}}$$

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

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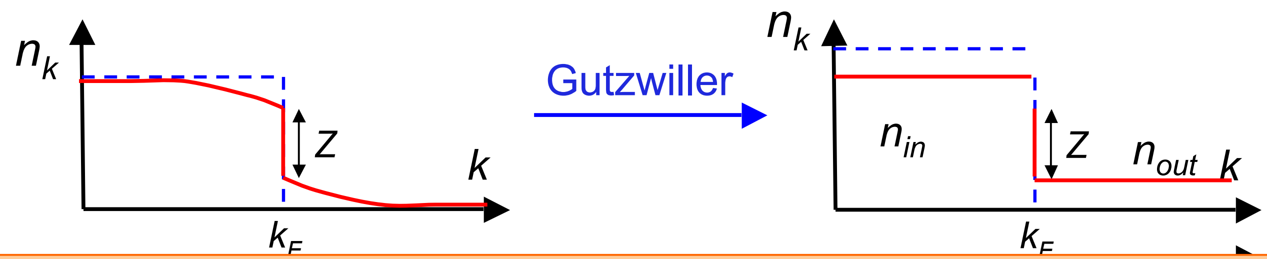

$$\frac{1}{2} = \frac{1}{N} \sum_{\vec{k}\in F}$$

$$g_t \epsilon_{kin} =$$

$$0 = \frac{1}{N} \sum_{\vec{k}\in}$$

quasiparticle weight

$$n_{in} = \frac{1}{2}(1+g_t)$$

$$n_{out} = \frac{1}{2}(1-g_t)$$

$$\Rightarrow \quad Z = g_t$$

compressibility

$$\kappa = \frac{N(\epsilon_F)^*}{1+F_0^s} \propto g_t$$

$$N(\epsilon_F)^* = N(\epsilon_F)/g_t$$

$$F_0^s = \frac{U N(\epsilon_F)}{4} \frac{2U_C - U}{(U-U_c)^2}$$