Theory of correlated fermionic condensed matter

2. Electronic correlations - from models to materials

a. DMFT and the Mott-Hubbard metal-insulator transition

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 6, 2009

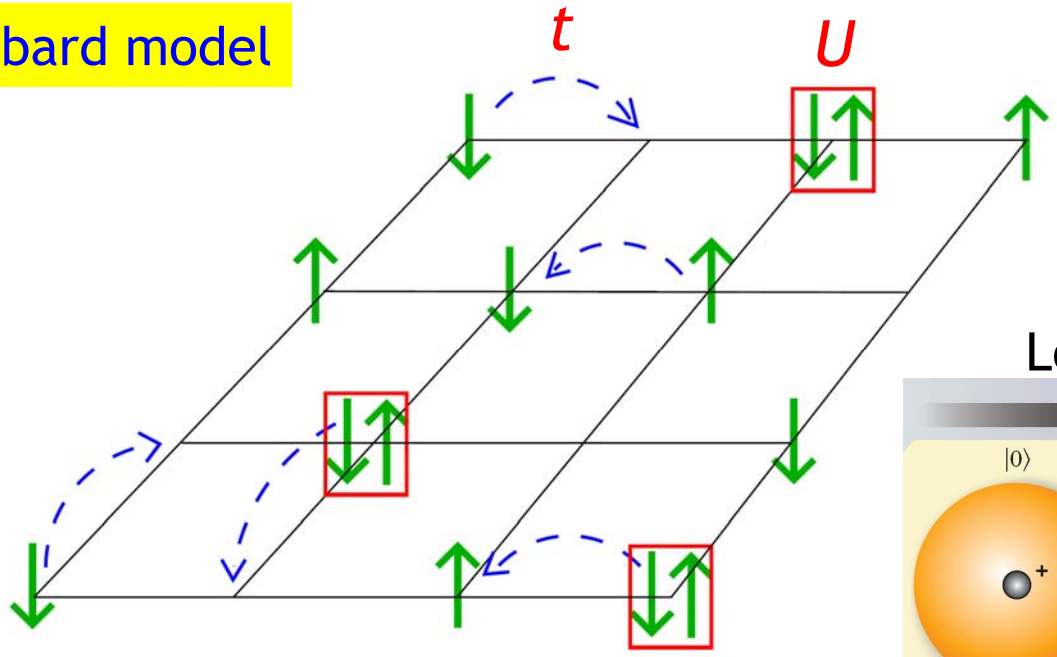
Dieter Vollhardt

Supported by Deutsche Forschungsgemeinschaft through SFB 484

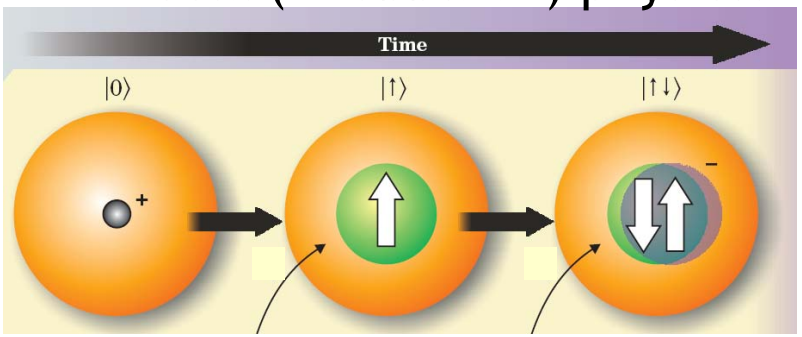
Outline:

- Dynamical mean-field theory (DMFT) for correlated electrons and " single-impurity" physics
- The DMFT self-consistency equations
- Application: Mott-Hubbard metal-insulator transition

Hubbard model



Local ("Hubbard") physics:



$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$\left\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle \neq \left\langle n_{\mathbf{i}\uparrow} \right\rangle \left\langle n_{\mathbf{i}\downarrow} \right\rangle$$

Correlation phenomena:

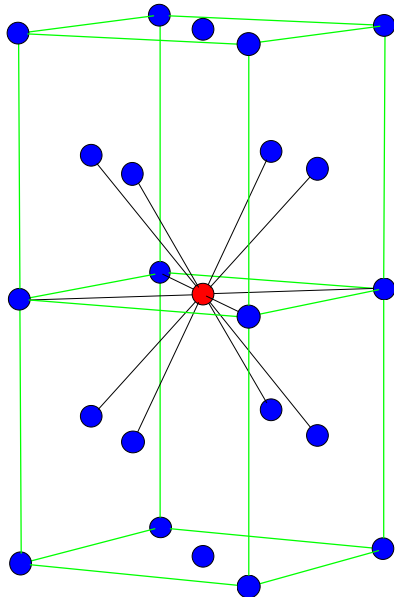
- Metal-insulator transition

$d \to \infty$ mean-field theory: Hubbard model

$$\langle H_{\text{kin}} \rangle = -\underbrace{t}_{\frac{1}{\sqrt{Z}}} \sum_{i\sigma} \underbrace{\sum_{j(NN\ i)}}_{Z} \underbrace{\langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle}_{\frac{1}{\sqrt{Z}}}$$

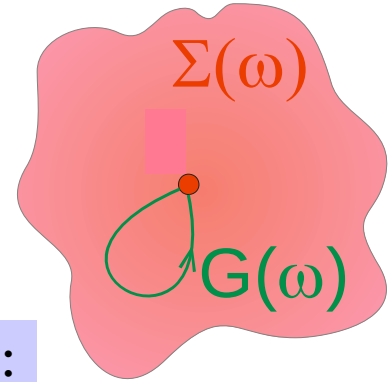
Metzner, DV (1989)

Quantum rescaling $t = \frac{t^*}{\sqrt{Z}}$



Z=12

Z or $d \to \infty$

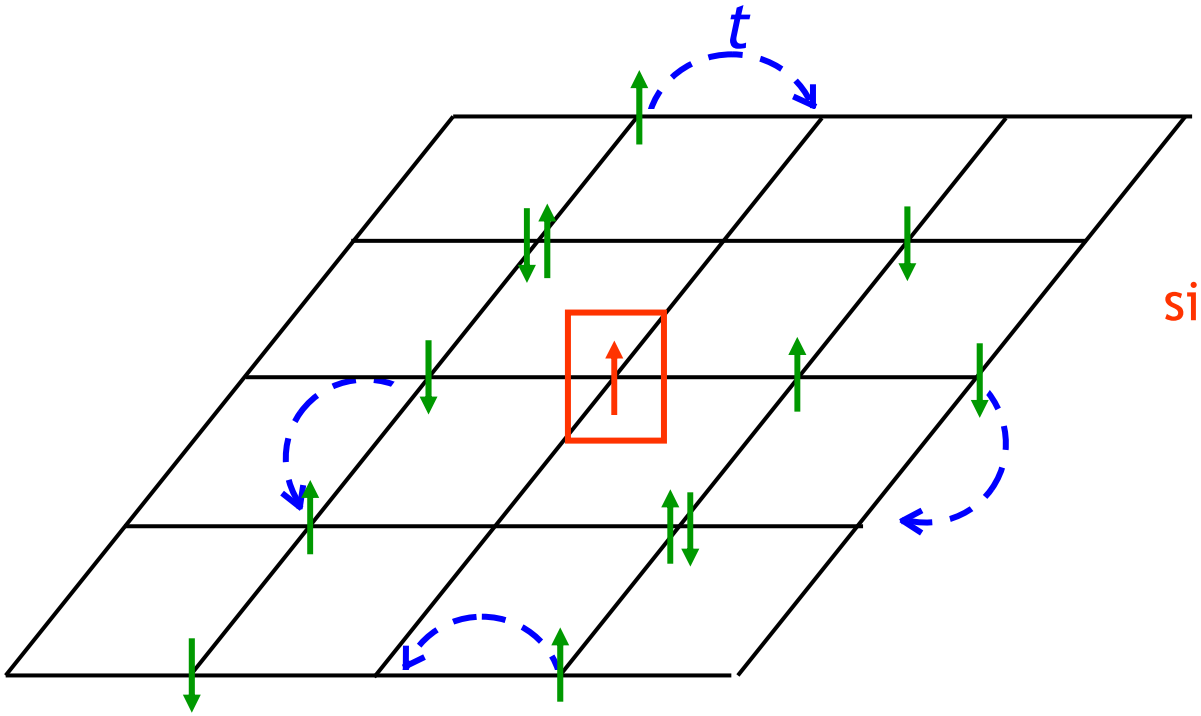


Useful *interpretation*:

Single-impurity Anderson model
+ self-consistency

Georges and Kotliar (1992), Jarrell (1992)

Excursion: Single-impurity Anderson model



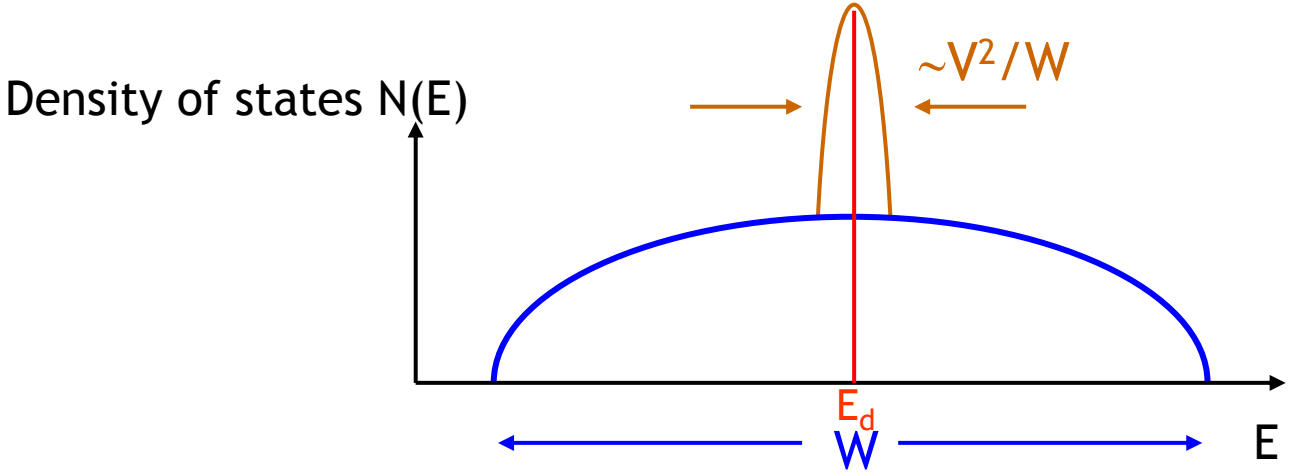
Non-interacting
conduction (*s*-) electrons

+

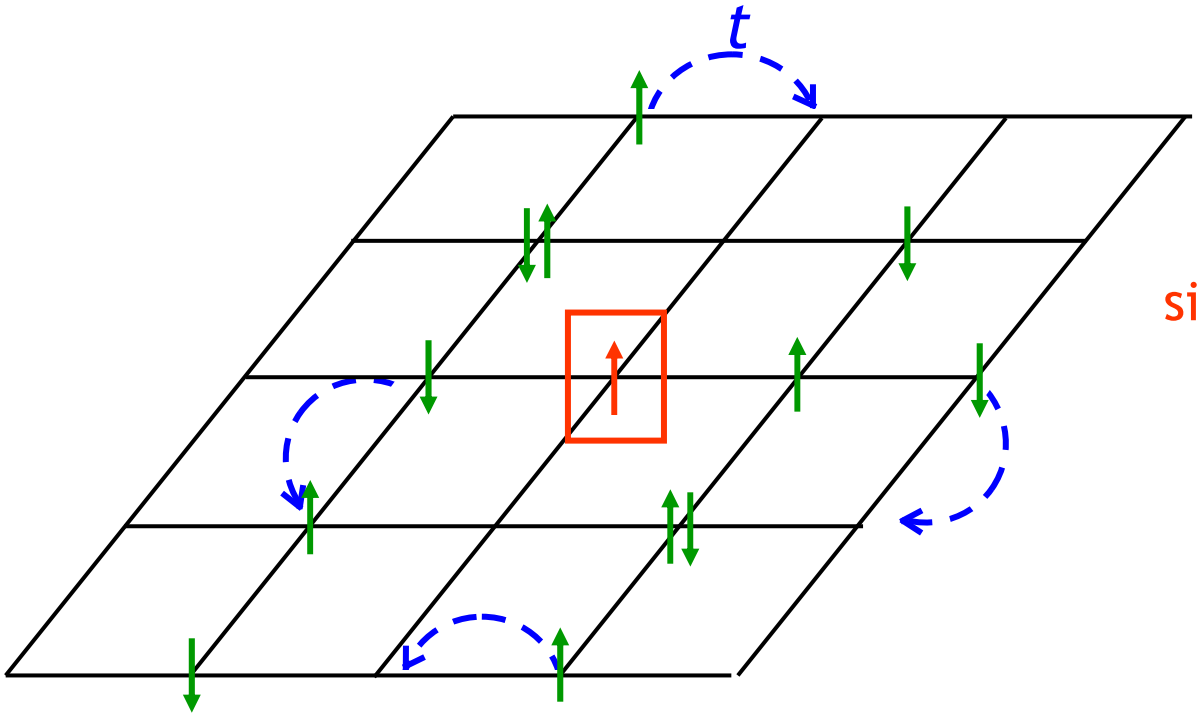
single *d*-orbital ("impurity")

+

s,*d*-hybridization V



Excursion: Single-impurity Anderson model



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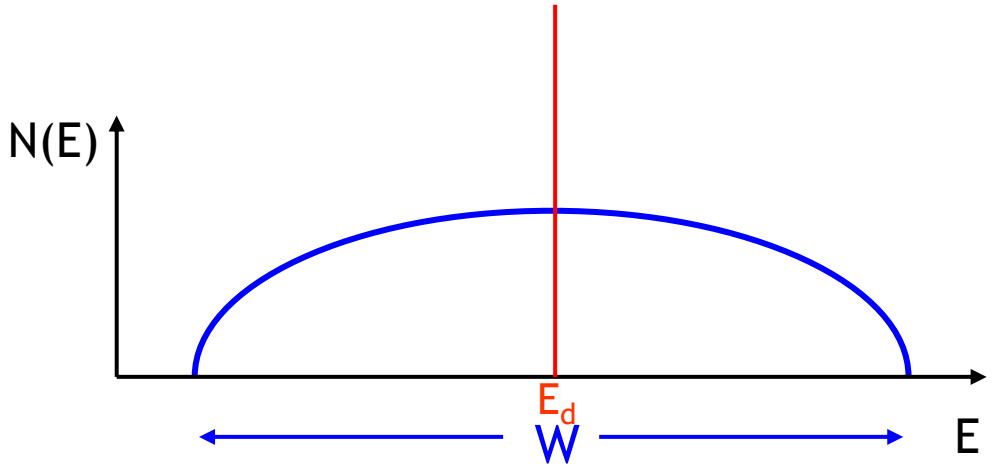
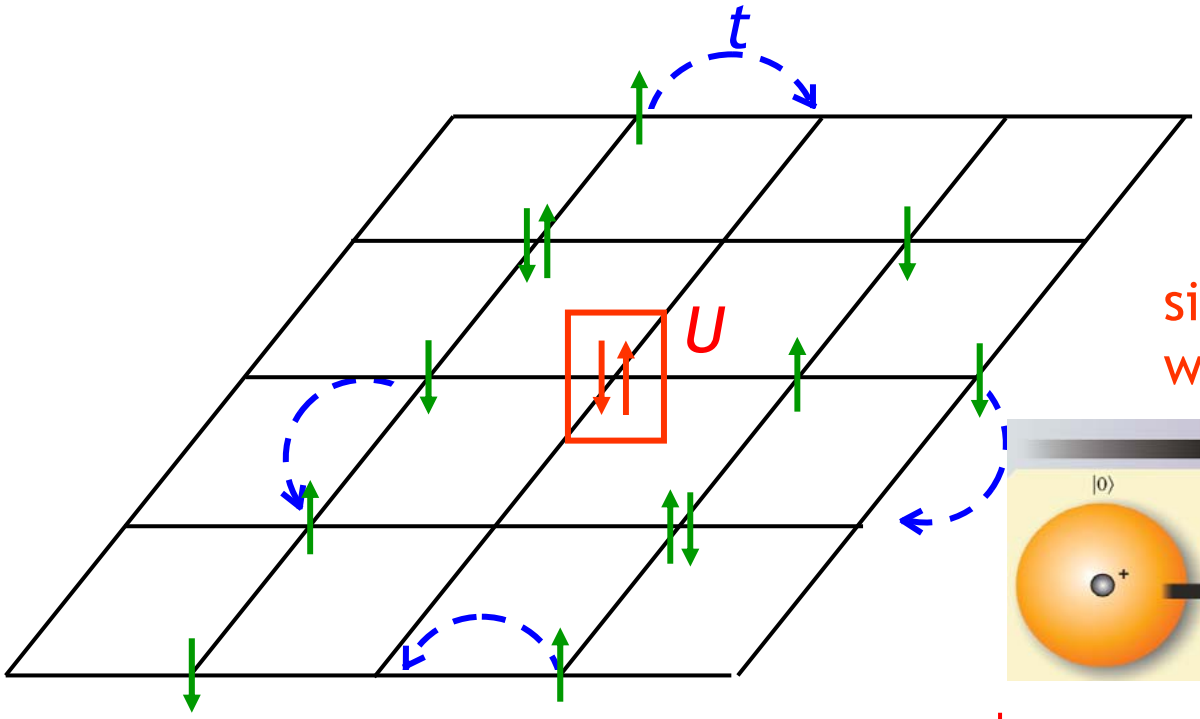


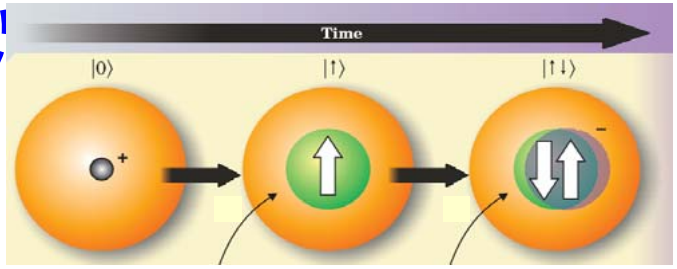
Excursion: Single-impurity Anderson model

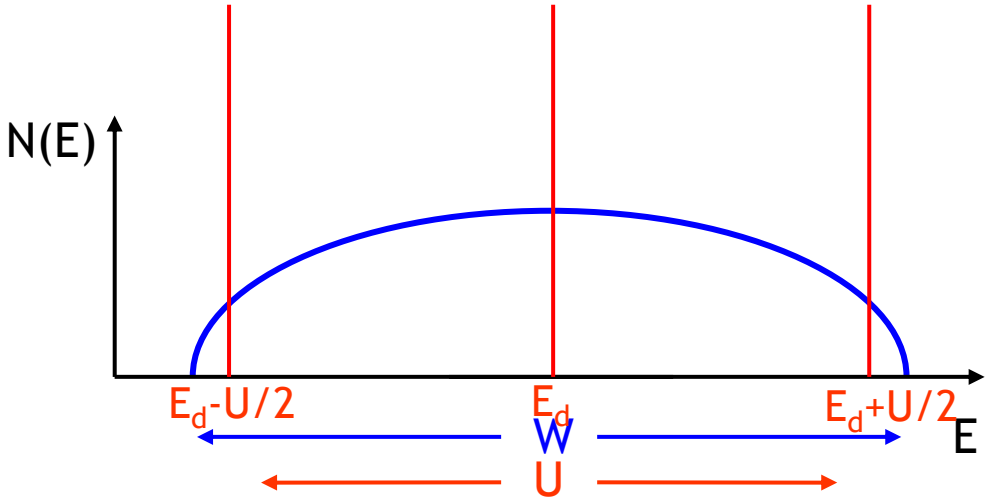


Non-interacting
conduction (*s*-) electrons

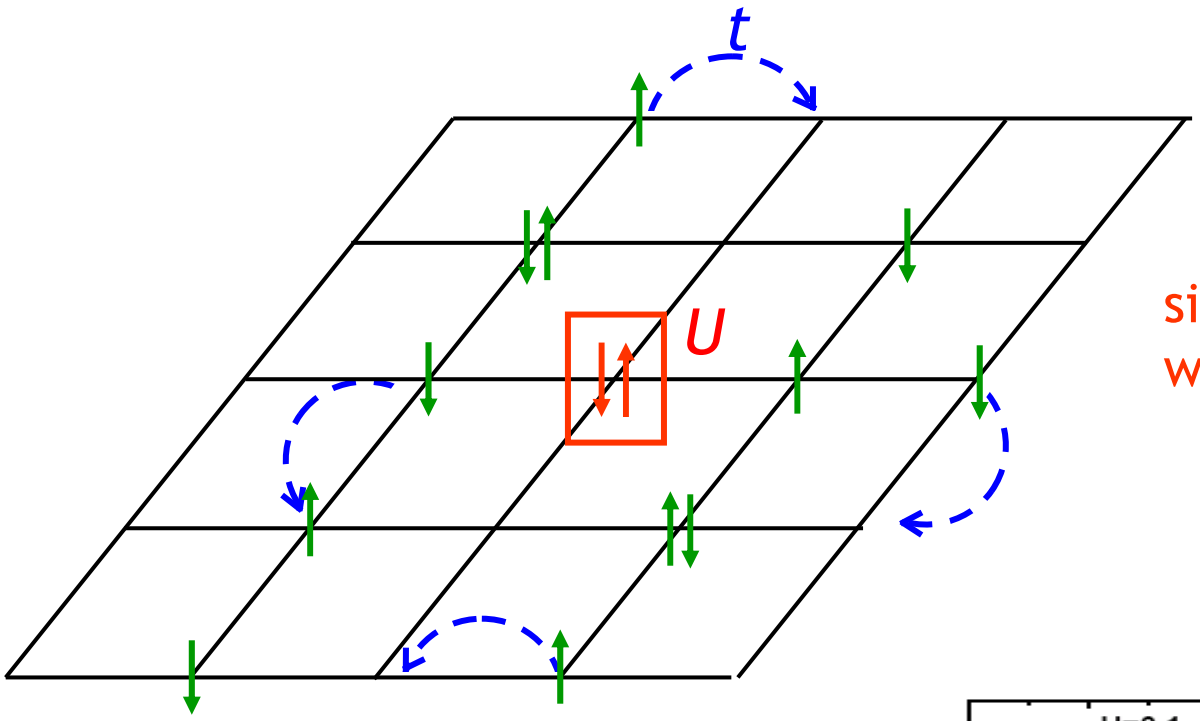
+

single *d*-orbital ("impurity")
with **interaction** *U*





Excursion: Single-impurity Anderson model



Non-interacting
conduction (*s*-) electrons

+

single *d*-orbital ("impurity")
with **interaction** *U*

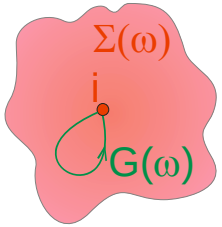
+

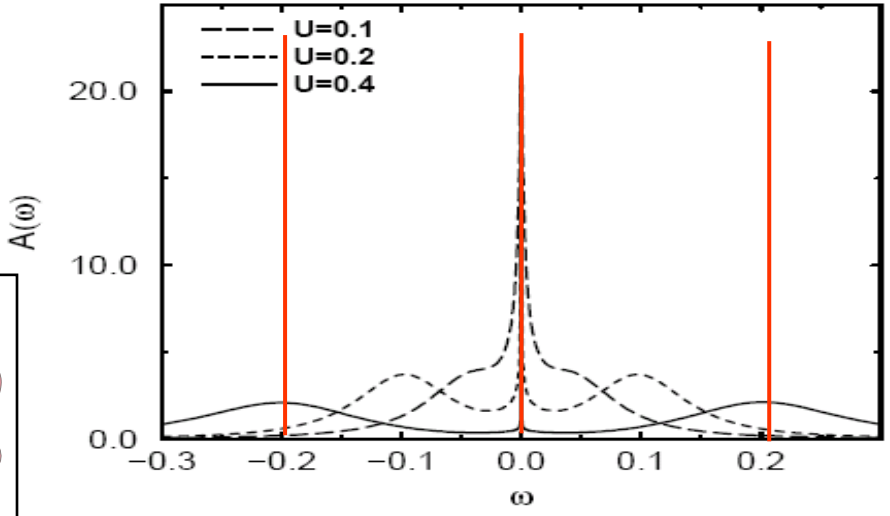
s,*d*-hybridization V

- Characteristic 3-peak structure
- *non-perturbative* energy scale ("Kondo physics")

Connection with

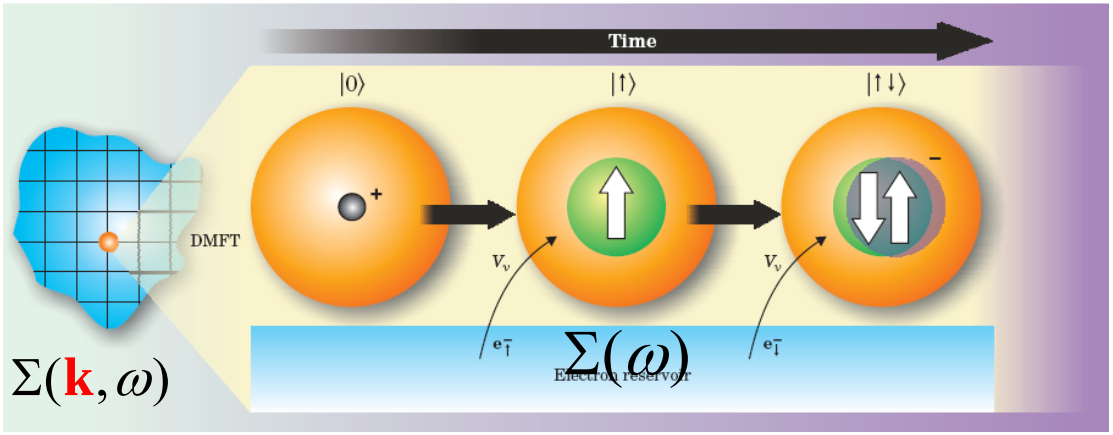
lattice fermions in Z→∞:





Useful *interpretation*:

Hubbard model $\xrightarrow{d\to\infty}$ single-impurity Anderson model + self-consistency



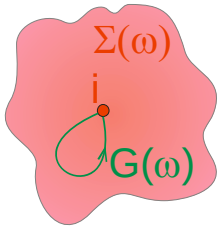
Kotliar, DV (**Physics Today**, March 2004)

Proper time resolved treatment of local electronic interactions

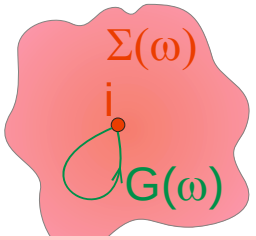
→ includes all many-body correlations

"Dynamical Mean-Field Theory (DMFT)"

Local many-body problem with full dynamics $\Sigma(\omega)$



DMFT self-consistency equations



Σ(ω): "effective medium"

(i) Effective single impurity problem: "local propagator"

$$G = -\frac{1}{Z}\int \mathcal{D}[\psi,\psi^*]\psi\psi^* e^{\psi^*[G^{-1}+\Sigma]\psi - U\psi^*\psi\psi^*\psi + J\psi^*\psi\psi^*\psi}$$

single-site (impurity) action A

(ii) *k*-integrated Dyson equation ("lattice Green function": lattice enters)

$$G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \Sigma(\omega) - \varepsilon} = G^0(\omega - \Sigma(\omega))$$

→ free electrons in a dynamic potential Σ(ω)

Solve with an „impurity solver", e.g., QMC, NRG, ED,...

T=0

Lattice Green function in real frequencies

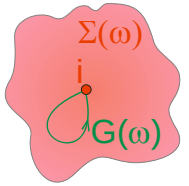
$$G_\sigma(\omega) \equiv G_{ii,\sigma}(\omega) = \frac{1}{V_B}\sum_{\boldsymbol{k}} \frac{1}{\omega+\mu-\epsilon_{\boldsymbol{k}}-\Sigma_\sigma(\omega)}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{N^0(\varepsilon)}{\omega+\mu-\epsilon-\Sigma_\sigma(\omega)} \,.$$

DMFT-propagator has *k*-dependence!

$$G_{\vec{k}}(\omega) = \frac{1}{\omega-\epsilon_{\vec{k}}+E_F-\Sigma(\omega)}$$

Σ(ω): "effective medium"



→free electrons in a dynamic potential Σ(ω)

T>0

In Matsubara frequencies

self-energy $\Sigma_{\sigma n} \equiv \Sigma_\sigma(i\omega_n)$

Green function $G_{\sigma n} \equiv G_\sigma(i\omega_n)$

$$G_{\sigma n} = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \frac{N^0(\varepsilon)}{i\omega_n+\mu-\Sigma_{\sigma n}-\varepsilon}$$

$$G_{\sigma n} = -\langle \psi_{\sigma n}\psi^*_{\sigma n}\rangle_{\mathcal{A}}.$$

Coherent state path integral formulation

Fermionic operator $\hat{c}$ → Grassmann variable ψ

Thermal average

$$\langle \hat{C} \rangle_{\mathcal{A}} = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\, \mathcal{D}[\psi^*]\, C[\psi, \psi^*]\, \mathrm{e}^{\mathcal{A}[\psi, \psi^*, \mathcal{G}]}$$

Partition function

$$\mathcal{Z} = \int \mathcal{D}[\psi]\, \mathcal{D}[\psi^*]\, \mathrm{e}^{\mathcal{A}[\psi, \psi^*, \mathcal{G}]}$$

Single-site ("impurity") action

$$\mathcal{A}[\psi, \psi^*, \mathcal{G}] = \sum_{\sigma, n} \psi^*_{\sigma n} \mathcal{G}^{-1}_{\sigma n} \psi_{\sigma n} - \frac{U}{2} \sum_{\sigma \sigma'} \int_0^\beta \mathrm{d}\tau\, \psi^*_\sigma(\tau) \psi_\sigma(\tau) \psi^*_{\sigma'}(\tau) \psi_{\sigma'}(\tau)$$

Example: local propagator

$$G = -\frac{1}{Z} \int \mathcal{D}[\psi, \psi^*] \psi \psi^* e^{(\psi^* [G^{-1} + \Sigma] \psi - U \psi^* \psi \psi^* \psi + J \psi^* \psi \psi^* \psi)}$$

Effective local propagator (bath Green function=Weiss mean-field)

$$\mathcal{G}^{-1}_{\sigma n} = G^{-1}_{\sigma n} + \Sigma_{\sigma n}$$

Explain the form of the DMFT equations → black board

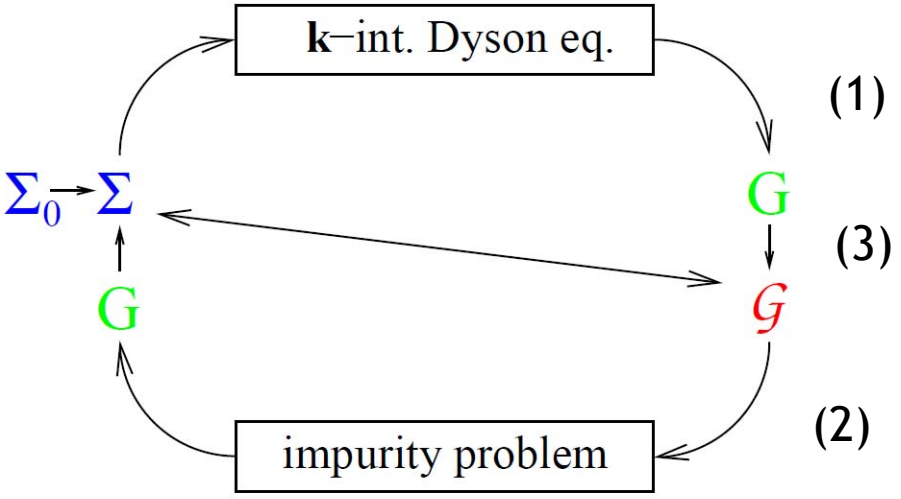
Derivation of DMFT self-consistency eqs. by cavity method
→ Training session (Anna Kauch)

DMFT self-consistency cycle

$$G_{\sigma n} = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, \frac{N^0(\varepsilon)}{i\omega_n + \mu - \Sigma_{\sigma n} - \varepsilon} \qquad (1)$$

$$G_{\sigma n} = -\langle \psi_{\sigma n} \psi^*_{\sigma n} \rangle_{\mathcal{A}}. \qquad (2)$$

$$\mathcal{G}^{-1}_{\sigma n} = G^{-1}_{\sigma n} + \Sigma_{\sigma n} \qquad (3)$$



hard part!

Blümer (2003)

Application of DMFT: Mott-Hubbard metal-insulator transition

Insulator: $\sigma^{DC}_{\alpha,\beta}(T=0) = \lim_{T\to 0^+} \lim_{\omega\to 0} \lim_{|\mathbf{q}|\to 0} \Re[\sigma_{\alpha,\beta}(\mathbf{q},\omega)] = 0$

Classification of insulators:

single-particle effects vs. many-particle effects

Band filling (Bloch-Wilson)
Lattice deformations (e.g., Peierls)
Disorder/randomness (Anderson)

Electronic correlations (Mott-Hubbard)
Long-range order (Slater, Heisenberg,...)

qualitatively different?

Band insulator ⟷ Mott insulator

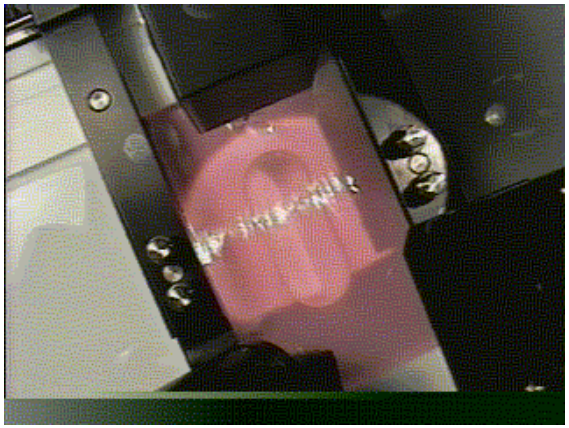
Need better understanding of insulators

Two-band Hubbard model (analytic): Smooth crossover Rosch (2006)

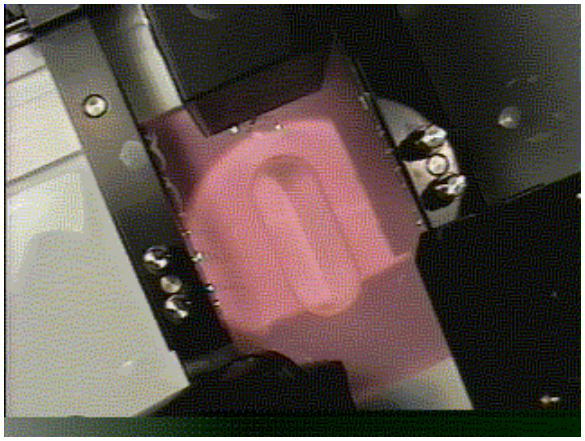
Correlation-induced metal-insulator transitions: Examples

1. Squeezable nanocrystal film switching between metal and insulator

Compressed film: metal
(metallic sheen)



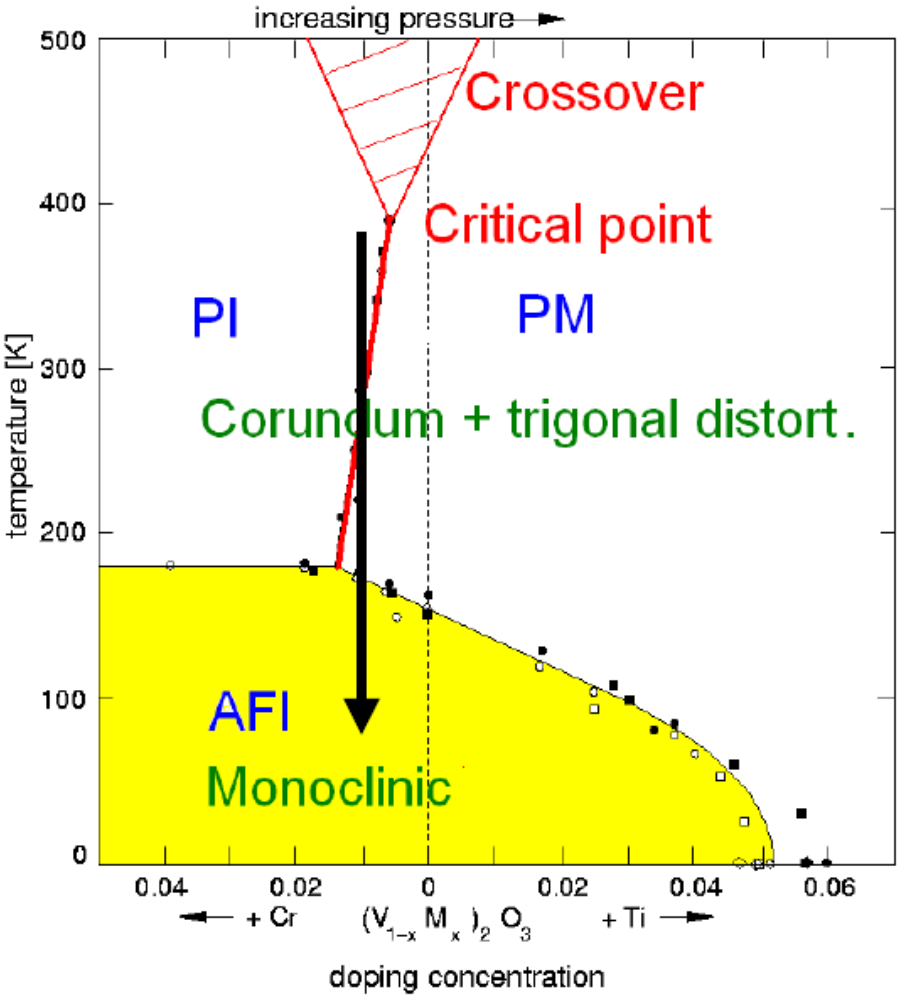
Uncompressed film: insulator
(shininess is gone)



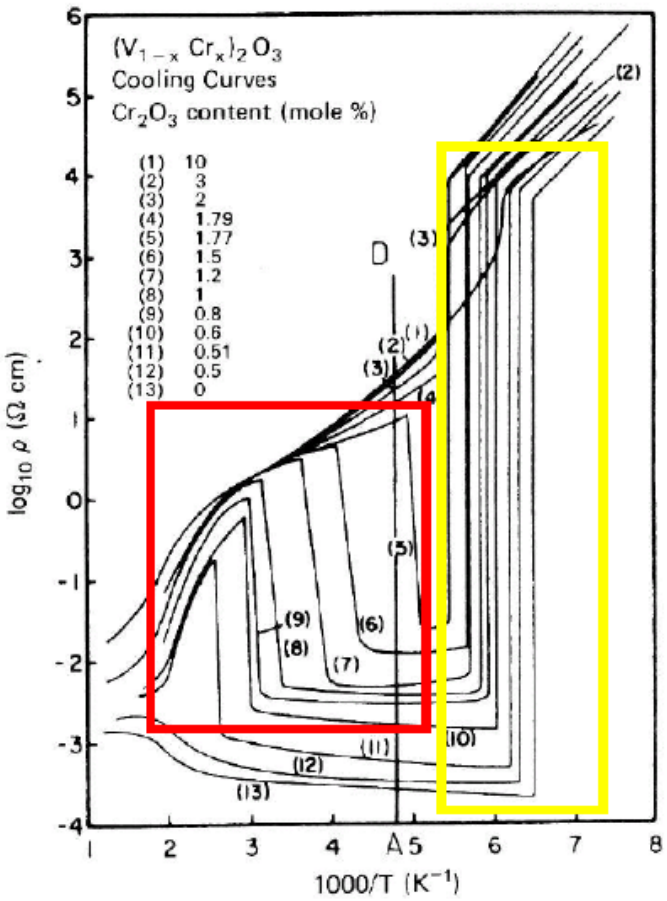
Discontinuous transition

Collier, Saykally, Shiang, Henrichs, Heath (1997)

2. Mott metal-insulator transition in V_2O_3 (interaction/correlation induced)



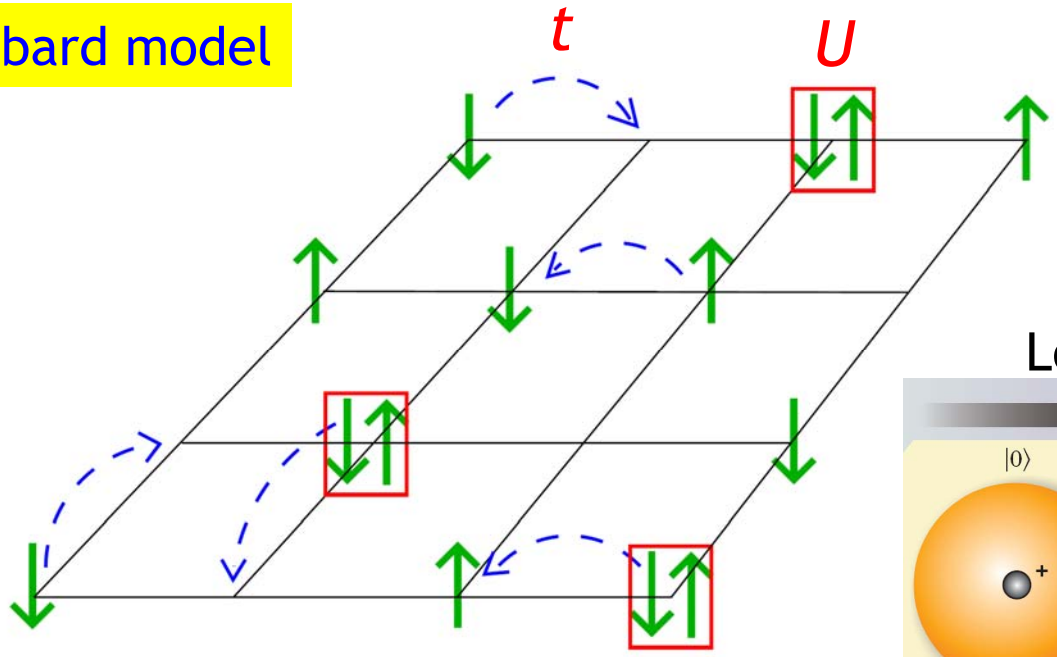
McWhan *et al.* (1971)



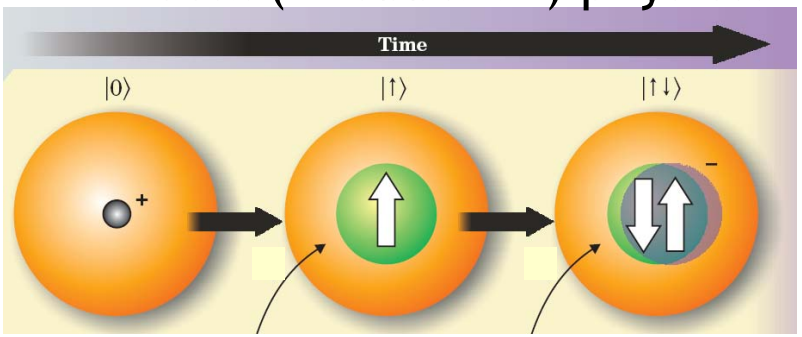
Kuwamoto, Honig, Appel (1980)

Theory of correlation-induced metal-insulator transitions

Hubbard model



Local ("Hubbard") physics:



$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$\left\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle \neq \left\langle n_{\mathbf{i}\uparrow} \right\rangle \left\langle n_{\mathbf{i}\downarrow} \right\rangle$$

$n_\uparrow = n_\downarrow, \; n = n_\uparrow + n_\downarrow = \frac{N}{L}$

$n = 2$ filled band

$n = 1$, "half-filled band"

N=# particles
L=# lattice sites

Correlation phenomena:
$n=1$, $U>U_c$: Metal-insulator transition

Gutzwiller-Brinkman-Rice theory

$$\hat{H} = \sum_{i,j,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \underbrace{\sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{D}}$$

Gutzwiller (1963)
Hubbard (1963)
Kanamori (1963)

Gutzwiller wave function $|\psi_G\rangle = e^{-\lambda \hat{D}} |\psi_0\rangle$

One-particle wave function
(Hartree-Fock, BCS, etc.)

$$= \prod_{\vec{R}_i} [1 - (1-g)\hat{D}_i] \, |\psi_0\rangle$$

$$\hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Gutzwiller-Brinkman-Rice theory

$$\hat{H} = \sum_{i,j,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \underbrace{\sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{D}}$$

Gutzwiller (1963)
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Gutzwiller wave function $|\psi_G\rangle = e^{-\lambda \hat{D}} |\psi_0\rangle$

Expectation values, e.g.:

Energy density

$$E_G = \frac{1}{L} \frac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$$

L: # lattice sites

Density of doubly occupied sites

$$d = \frac{D}{L} = \frac{1}{L} \frac{\langle \psi_G | \hat{D} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$$

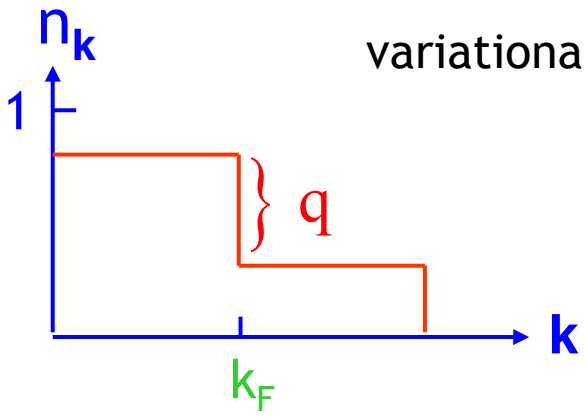
d=1,∞: exact analytic evaluation possible

Metzner, DV (1988/89)

Gutzwiller approximation (GA) (1963/65)

$$\frac{E_G}{L} \overset{GA}{=} q(d)\bar{\varepsilon}_0 + Ud,$$

variational parameter $\frac{\partial E}{\partial d} = 0$



$n_\sigma = \frac{1}{2}$ (half-filled band)

$$d = \frac{1}{4}\left[1 - \frac{U}{U_c}\right],$$

$$q = 1 - \left[\frac{U}{U_c}\right]^2,$$

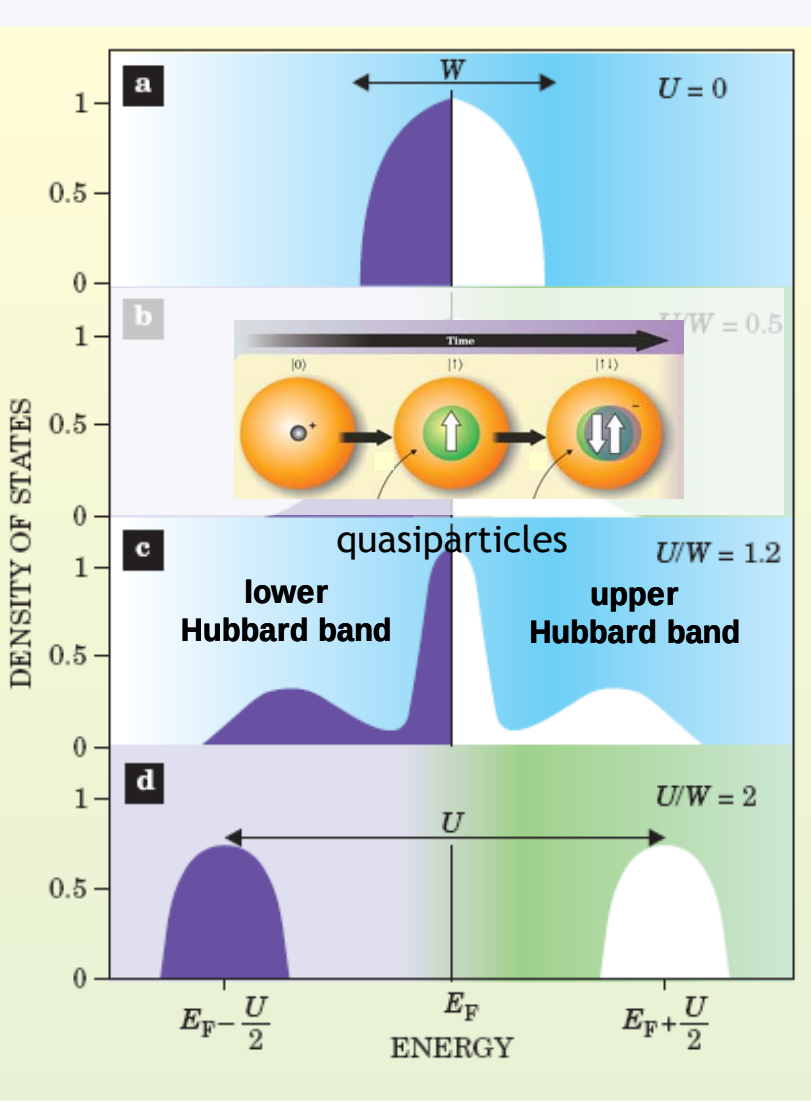
$$E_g/L = -|\bar{\varepsilon}_0|\left[1 - \frac{U}{U_c}\right]^2$$

$$U_c = 8|\bar{\varepsilon}_0|$$

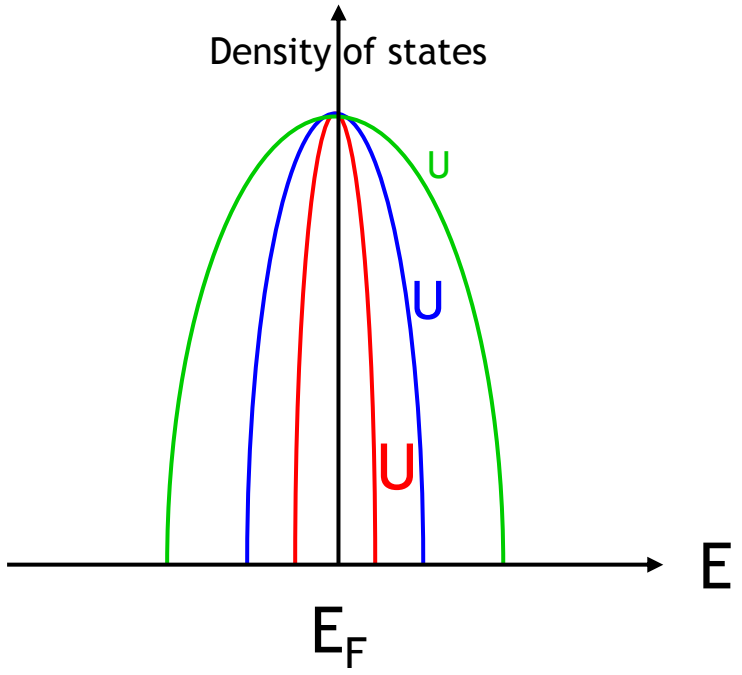
Brinkman, Rice (1970): $\frac{m^*}{m} = q^{-1} \equiv Z^{-1} \xrightarrow{U \to U_c} \infty$

describes metal-insulator ("Mott") transition, e.g., V_2O_3

Application of DMFT: Mott-Hubbard metal-insulator transition



Hubbard model, n=1

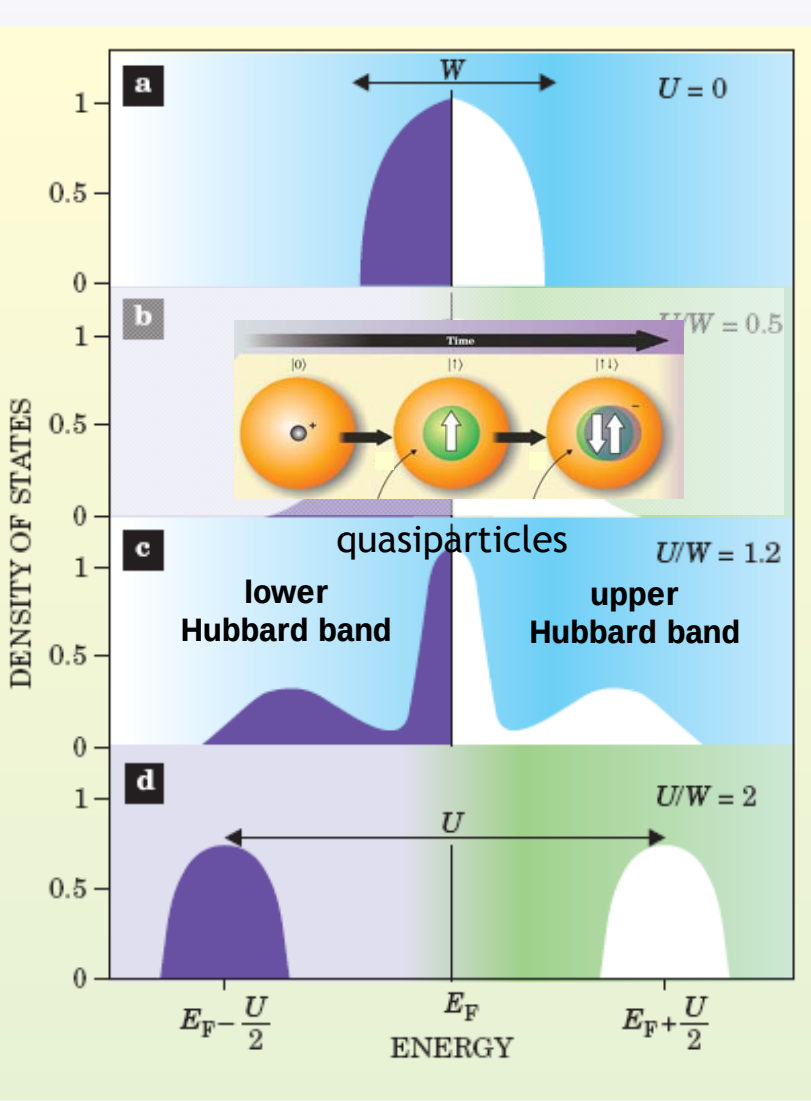


Quasiparticle renormalization , $Z^{-1} = \frac{m^*}{m} \to \infty$

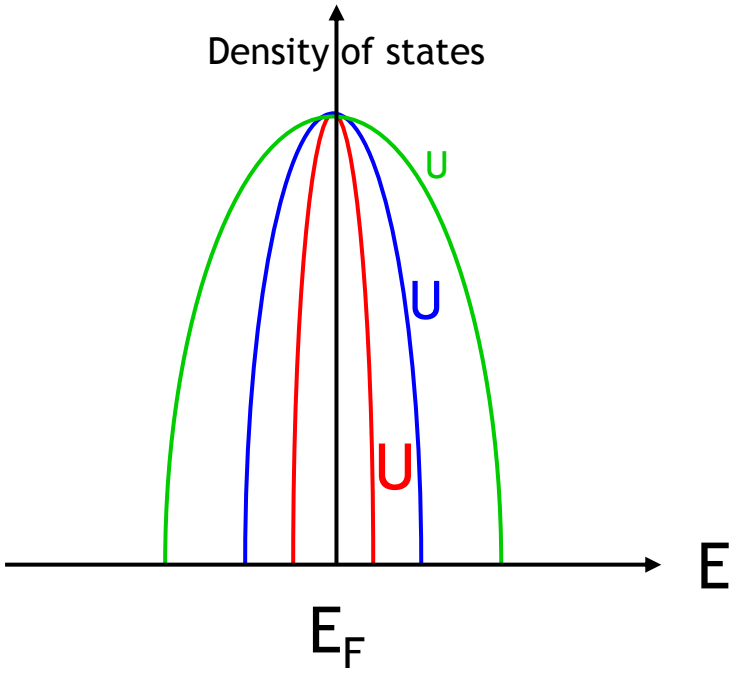
←→ Gutzwiller-Brinkman-Rice theory

"Hubbard bands" ←→ Hubbard I approximation (1963)

Application of DMFT: Mott-Hubbard metal-insulator transition

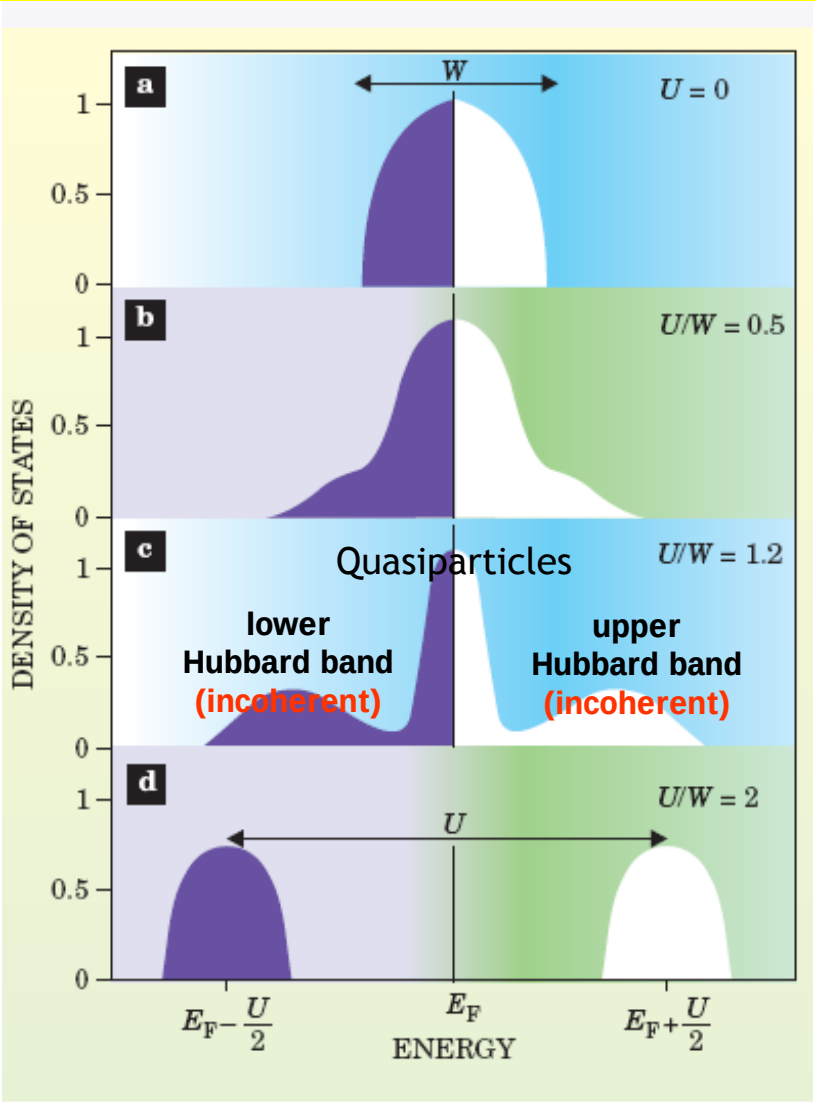


Hubbard model, n=1



Correlations lead to transfer of spectral weight

Application of DMFT: Mott-Hubbard metal-insulator transition



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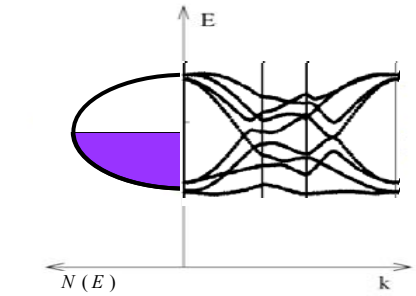
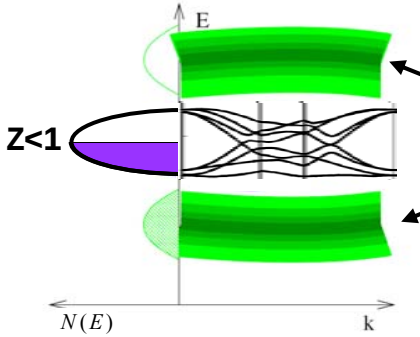
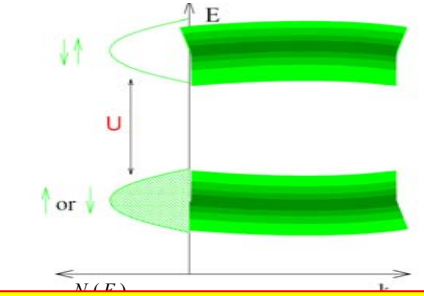


Coherent (**k**-) states:
Quasiparticles



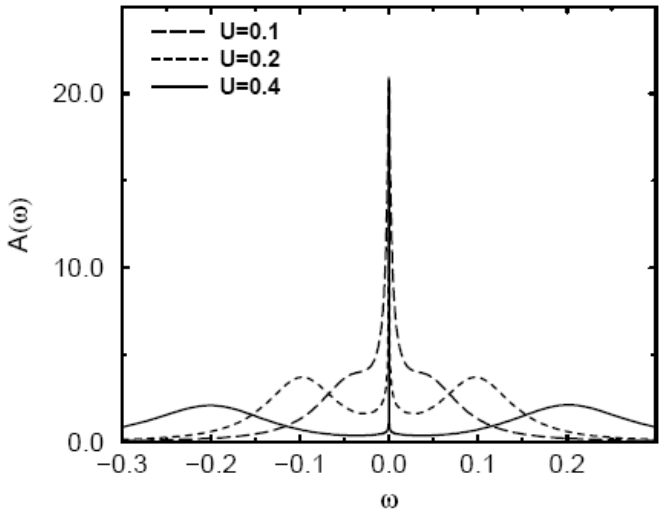
Incoherent
states
(Hubbard bands)



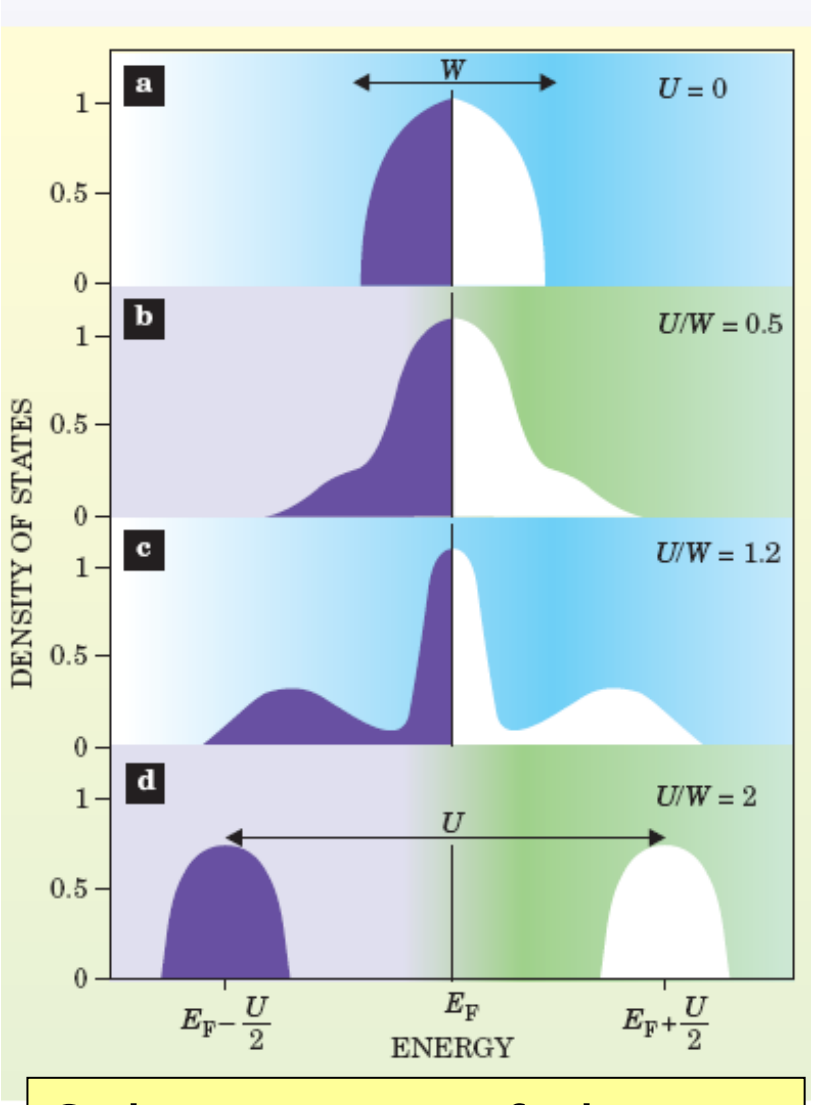
Only
incoherent
states

Correlations lead to transfer of spectral weight

Characteristic three-peak structure



Single-impurity Anderson model



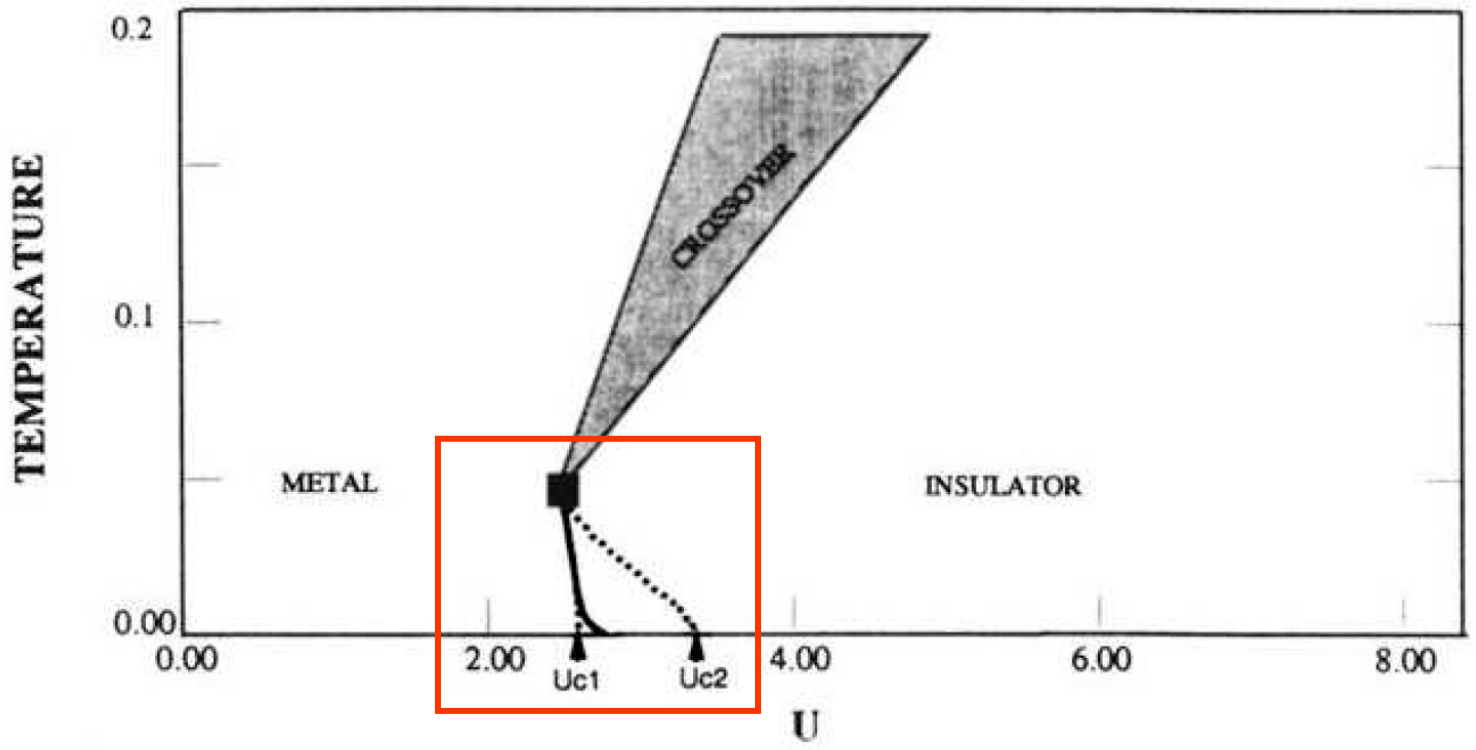
Two types of electrons

Only one type of electron

Experimentally detectable?

Metal-insulator transition in the one-band Hubbard model

1994

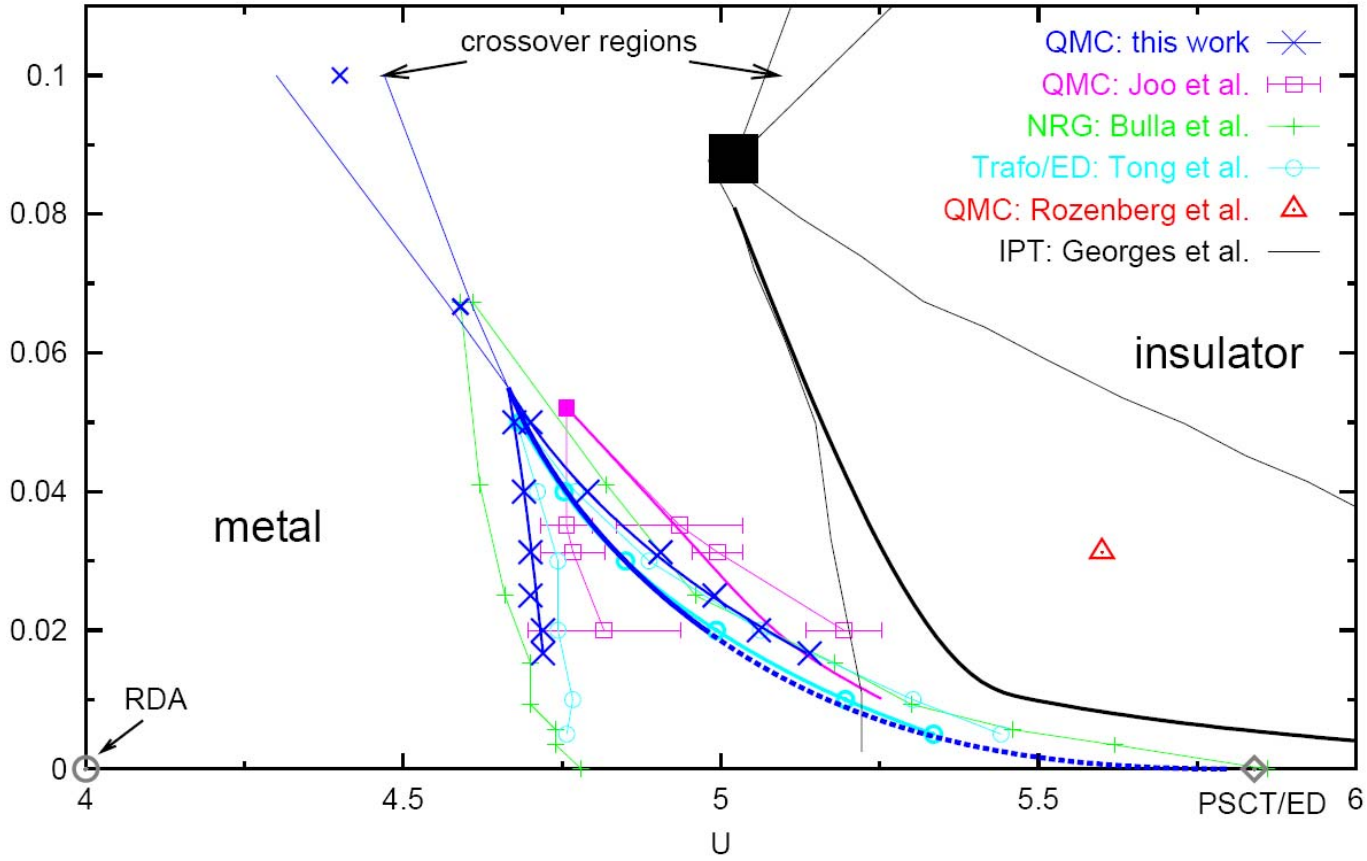


Iterated perturbation theory Rozenberg *et al.* (1994)

Explanation of IPT → blackboard

Metal-insulator transition in the one-band Hubbard model

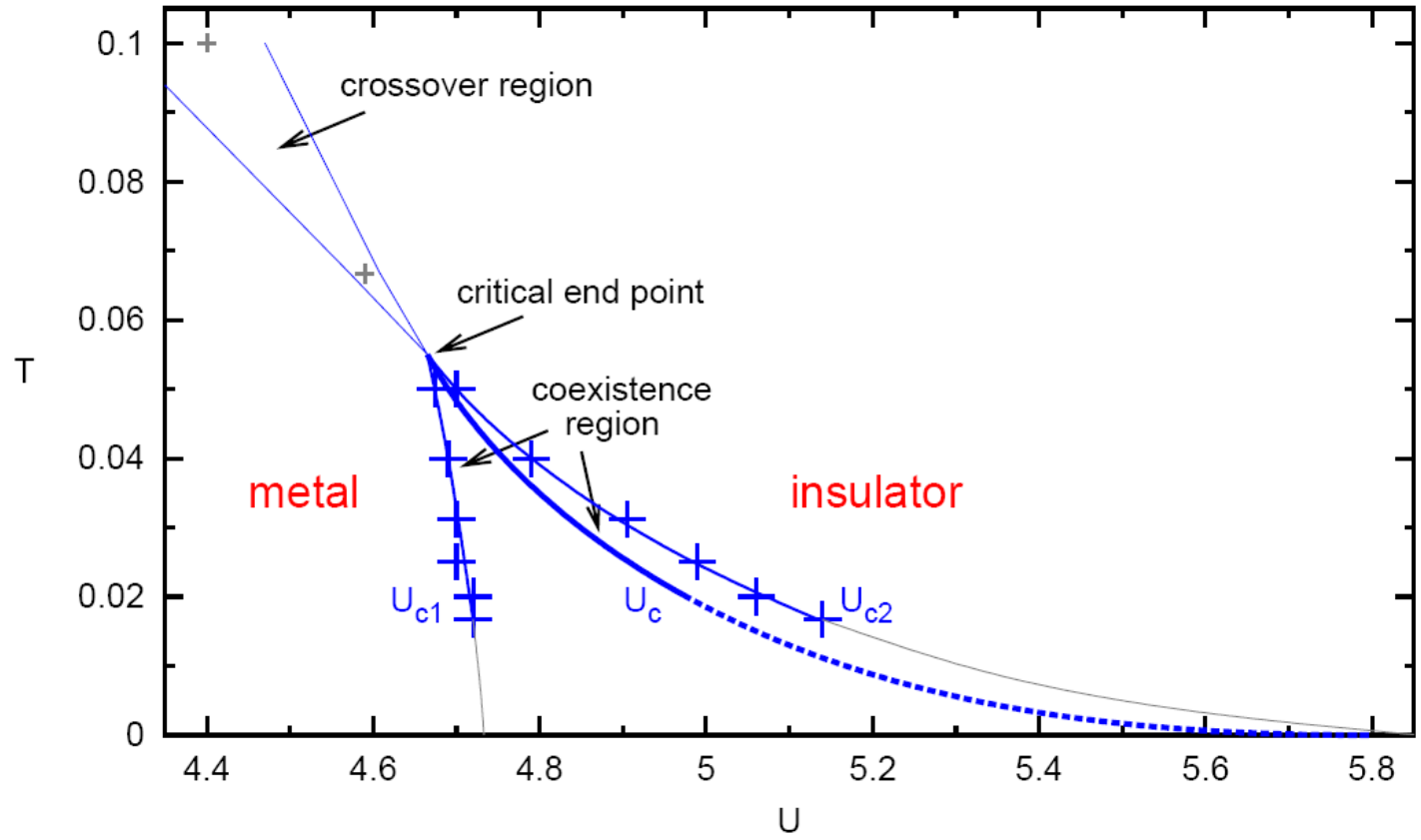
2000



Blümer, Dissertation 2002

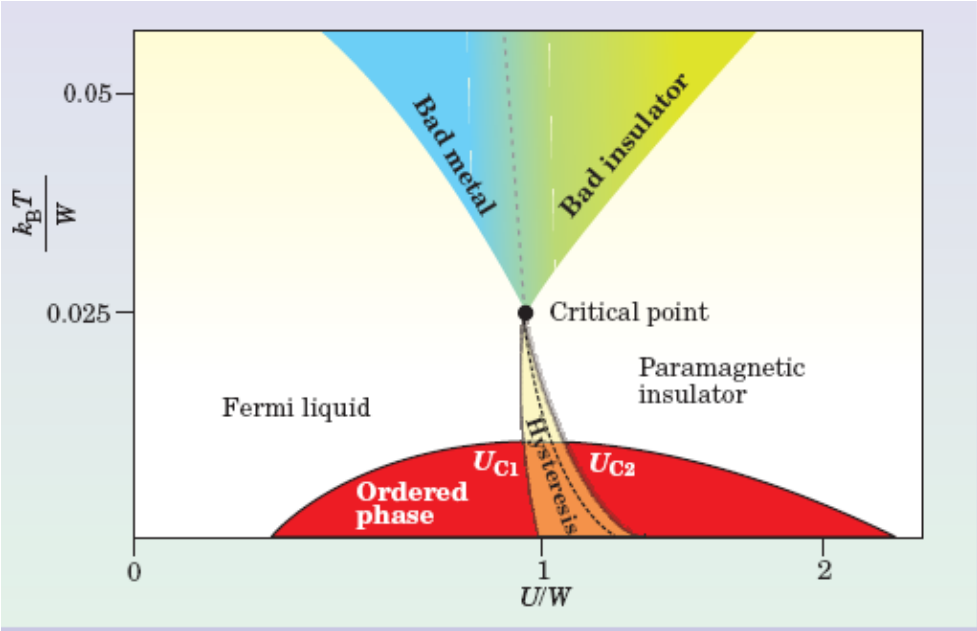
Metal-insulator transition in the one-band Hubbard model
High precision phase diagram

2002



Blümer, Dissertation 2002

Hubbard model (n=1): DMFT phase diagram



Strongly correlated electron materials

V_2O_3
$NiSe_{2-x}S_x$
κ-organics, ...

Kotliar, DV (2004)

Reason for the anomalous slope of $T(U)$?

One-band Hubbard model +

- next-neighbor hopping t_1
- bipartite lattice
- half-filling (n=1)

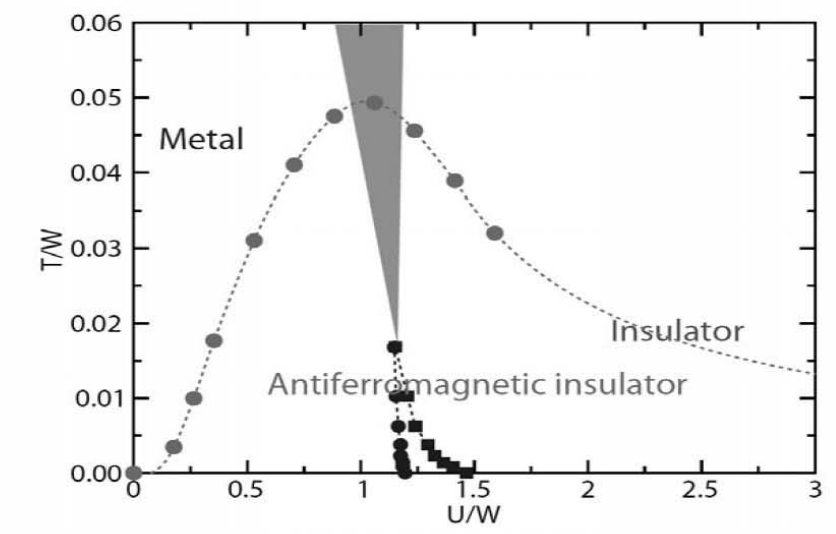
$\Rightarrow$ „perfect nesting“

$\Rightarrow$ antiferromagnetic (AF) order

- further-range hopping t_2, t_3,...
- and/or non-bipartite lattices

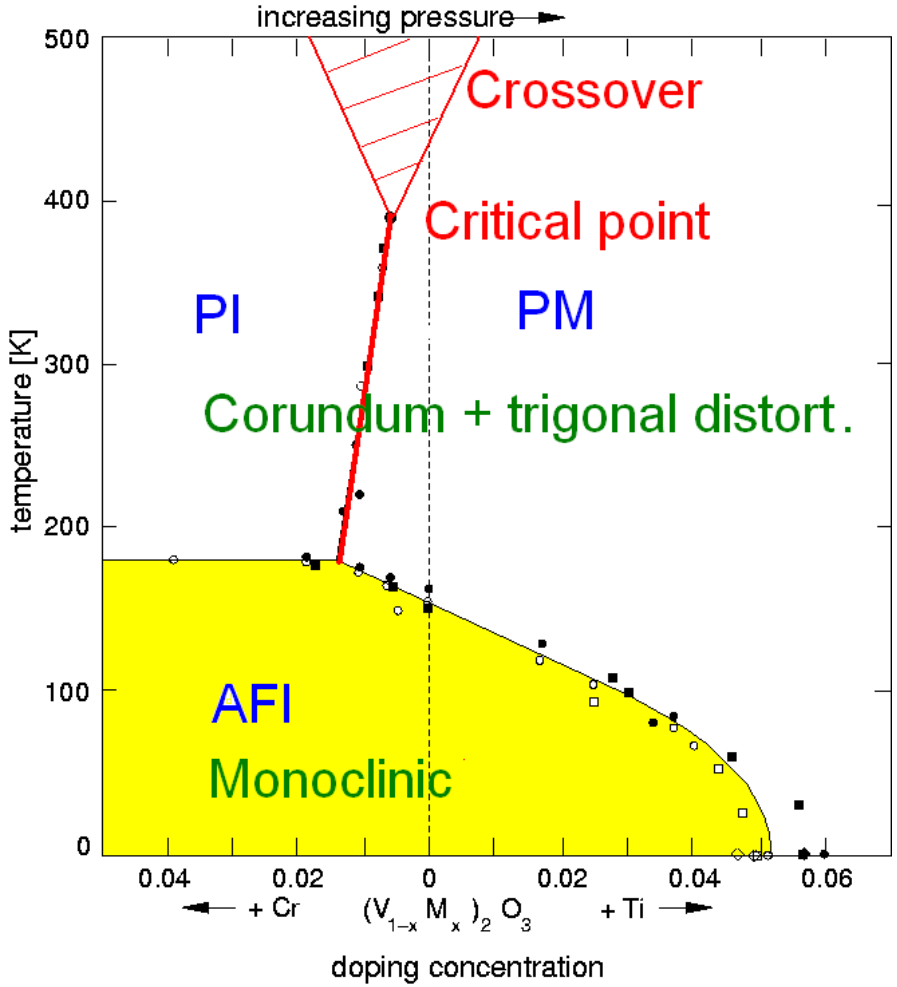
$\Rightarrow$ magnetic „frustration“

Zitzler *et al.* (2004), Pruschke (2005)



Mott-Hubbard metal-insulator transition in V_2O_3

Mott-Hubbard metal insulator transition in V_2O_3



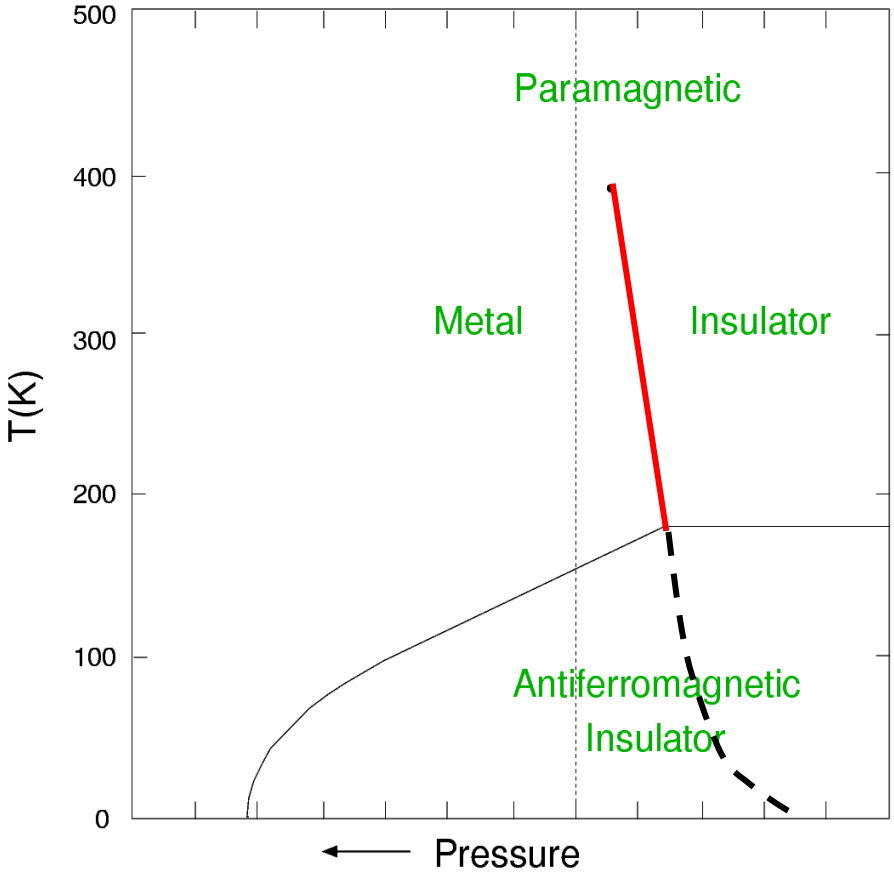
pressure P

interaction U

Rice, McWhan (1970);
McWhan *et al.* (1973)

- PI ⟷ PM: 1. order transition without lattice symmetry change
- Anomalous slope of P(T)

Mott-Hubbard metal insulator transition in V_2O_3



Interaction U

Rice, McWhan (1970);
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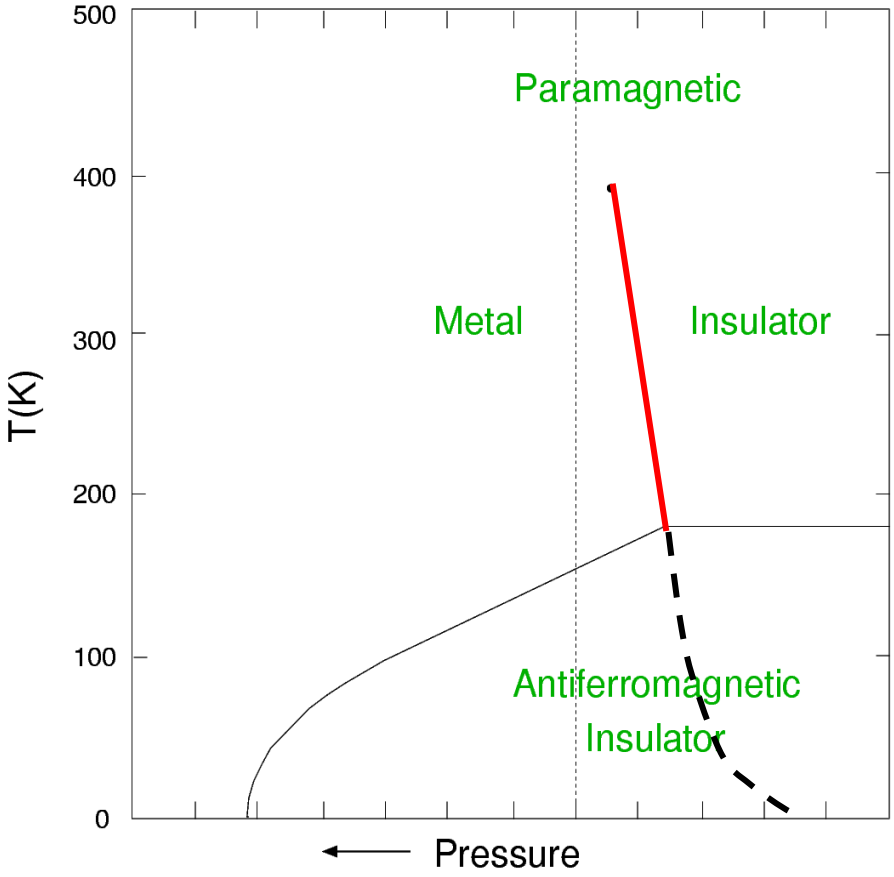
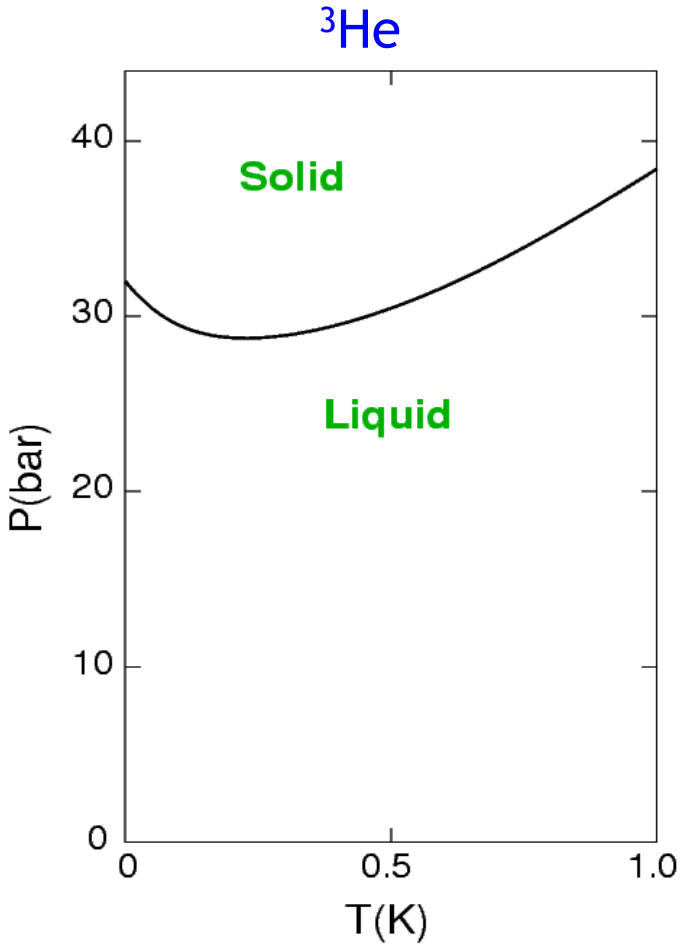
- PI ⟷ PM: 1. order transition without lattice symmetry change
- Anomalous slope of P(T)

→ Pomeranchuk effect in ^{3}He

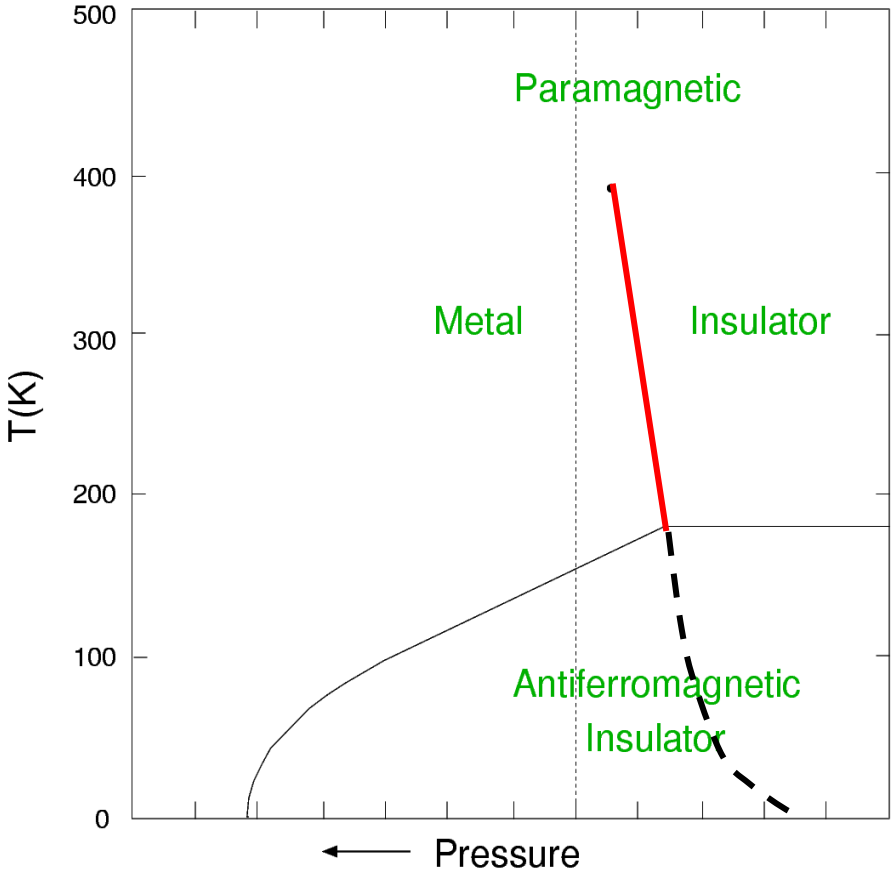
Mott-Hubbard metal insulator transition in V_2O_3



Interaction U

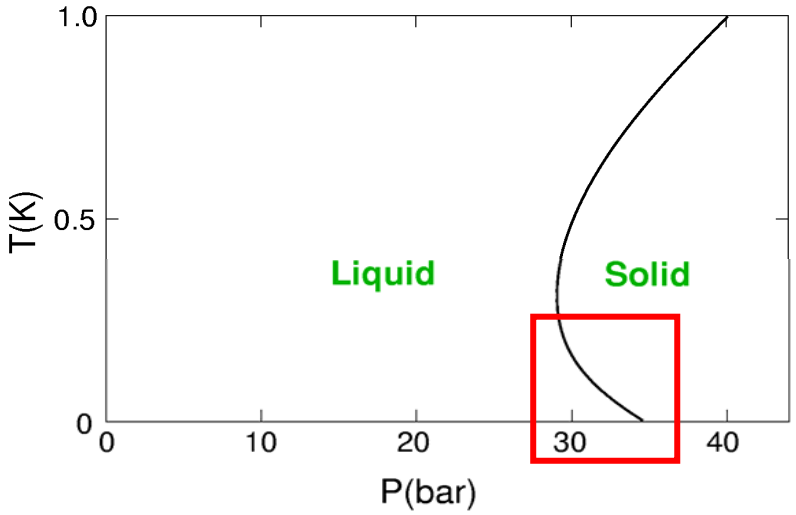


Mott-Hubbard metal insulator transition in V_2O_3



Interaction U

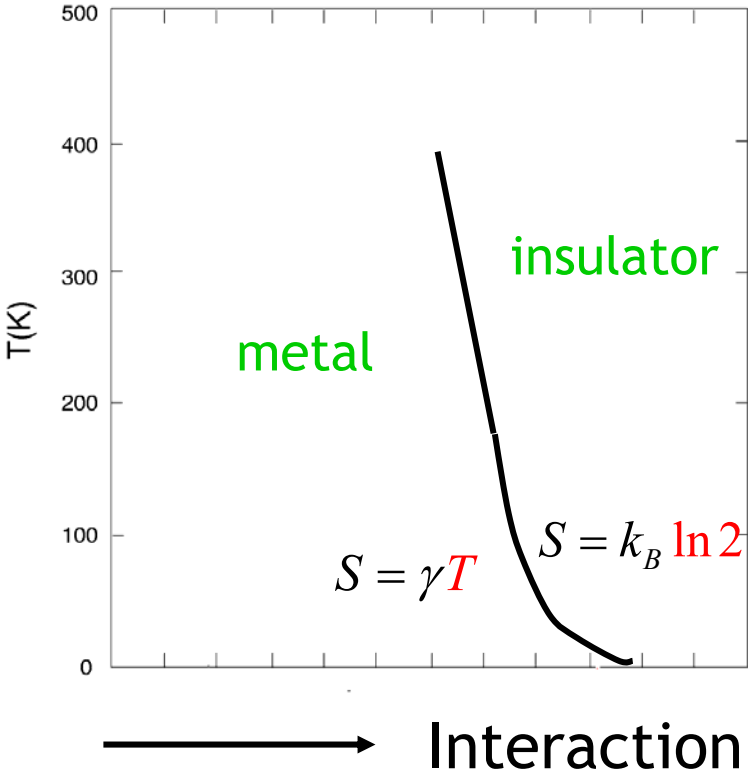
^3He



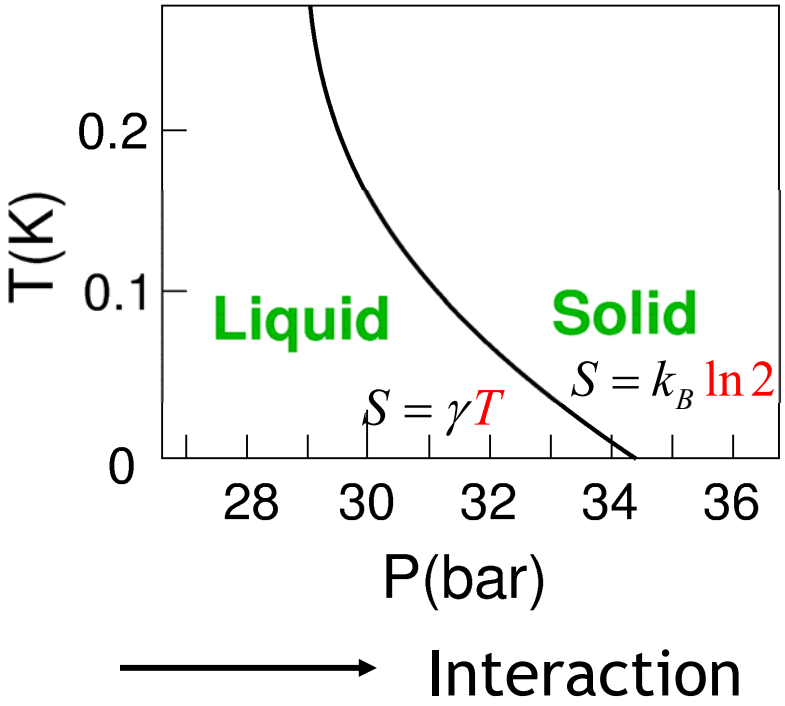
Interaction U

Mott-Hubbard metal insulator transition in V_2O_3

V_2O_3: metal-insulator transition

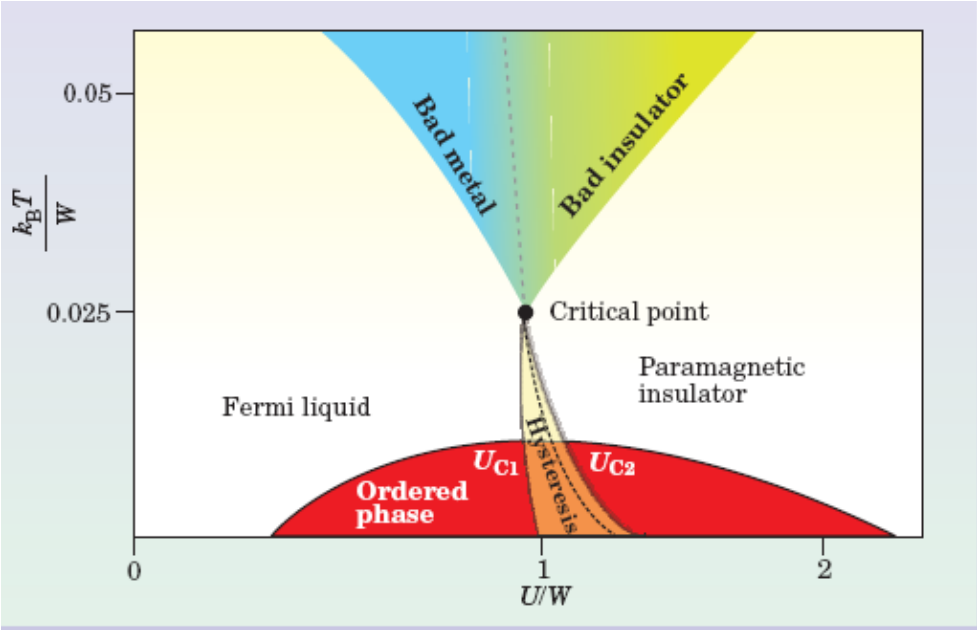


^3He: liquid-solid transition



Fermionic **correlation** effect

Hubbard model (n=1): DMFT phase diagram



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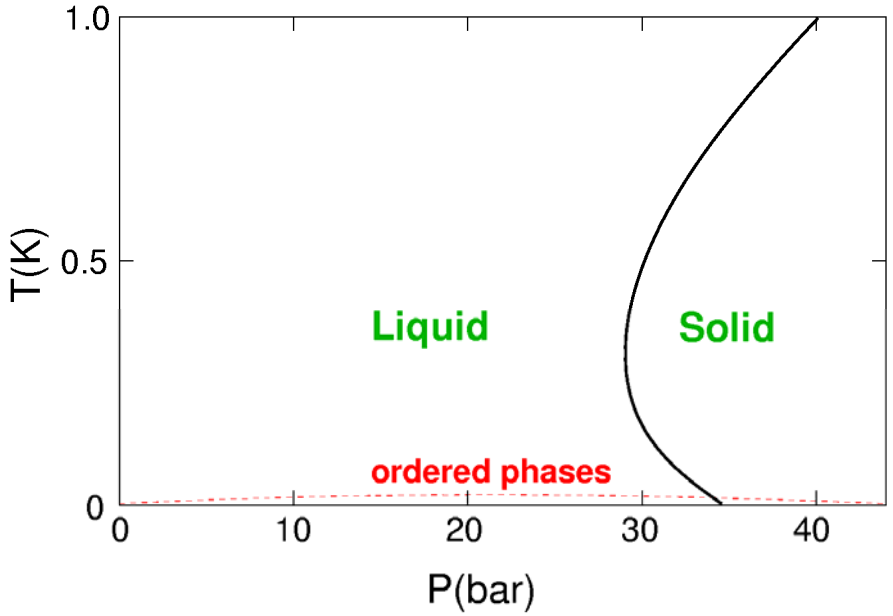

Helium-3

Universality due to Fermi statistics

Beyond DMFT: Cluster Extensions

Dynamical cluster approx. (DCA) Jarrell *et al.* (2000)
Cluster DMFT (CDMFT) Kotliar *et al.* (2001)
Self-energy functional theory Potthoff (2003)