Mott – Hubbard metal – insulator transition in binary – alloy systems

Krzysztof Byczuk

Instytut Fizyki Teoretycznej

Uniwersytet Warszawski

February 27, 2004

Collaboration:

- Walter Hofstetter - Harvard University, USA
- Martin Ulmke - FGAN - FKIE, Wachtberg, Germany
- Dieter Vollhardt - Augsburg University, Germany

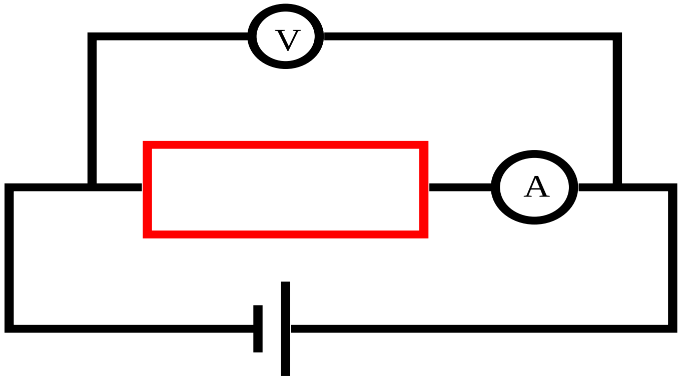
Plan of the talk:

1. Introduction
   - Basic definitions
   - Gap in insulators
   - Phase transitions from conductors to insulators
2. Single – particle insulators
3. Many – body insulators
4. Mott - Hubbard MIT at integer filling
   - physical view
   - MIT according to DMFT
5. Mott - Hubbard MIT at noninteger fillings
6. Conclusions

Conductors and Insulators – definitions:

Basic physical property of a system: how good/bad the charges (masses) are transported through it.

School knowledge



$$R = \frac{U}{I}$$

$$R = \rho \frac{L}{A} \quad [\rho] = \left[\Omega \cdot \mathrm{m}^{\mathrm{d}-2}\right]$$

Transport occurs in a nonequilibrium processes.

Transport can be disturbed by: ions, electron – electron interactions,external fields, etc.

Conductors and Insulators – definitions:

Exact definitions of a conductor or an insulator possible only at $T = 0$ within linear response theory.

weak external field – Ohm's law

$$j_\alpha(\mathbf{q},\omega) = \sum_\beta \sigma_{\alpha,\beta}(\mathbf{q},\omega) E_\beta(\mathbf{q},\omega)$$

$\sigma_{\alpha,\beta}(\mathbf{q},\omega)$ – conductivity tensor

Definition:
Insulator is a system where

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

Conductors and Insulators – definitions:

Drude law for typical metal

$$\Re[\sigma_{\alpha,\beta}(T=0,\omega\to 0)] = (D_c)_{\alpha,\beta}\frac{\tau}{\pi(1+\omega^2\tau^2)}$$

$(D_c)_{\alpha,\beta} = \frac{\pi e^2 n}{m^*}\delta_{\alpha,\beta}$ – Drude weight

τ – relaxation time for electron scattering, i.g. with ions

Definition:
Ideal conductor is a system where

$$\Re[\sigma_{\alpha,\beta}(T=0,\omega\to 0)] = (D_c)_{\alpha,\beta}\delta(\omega)$$

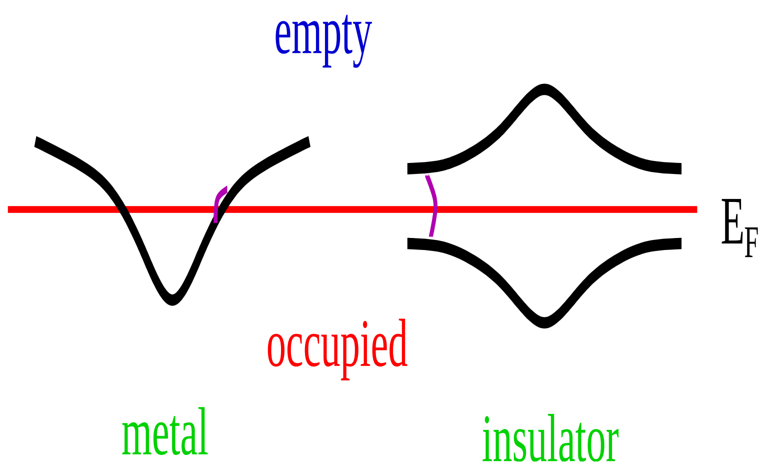
For a translationally invariant system $\tau^{-1}\to 0$

Warning: superconductor $\equiv$ ideal conductor $+$ ideal diamagnet

Gap in the Insulator

To get a charge transport in a conductor:

- There are low – energy excitations (electron – hole) above the ground – state
- Excited states must be extended



$$\mu^+(\lambda) = E_0(N+1,\lambda) - E_0(N,\lambda)$$

$$\mu^-(\lambda) = E_0(N,\lambda) - E_0(N-1,\lambda)$$

Gap: $\Delta(\lambda) = [\mu^+(\lambda) - \mu^-(\lambda)]_{\mathrm{extended}}$

$\lambda = \lambda(p, x, n)$ – control parameter

There is a gap $\Delta(\lambda) > 0$ in the single – particle spectrum in an insulator

Insulator at finite T

Experiment $\Delta(\lambda) \gg k_B T > 0$

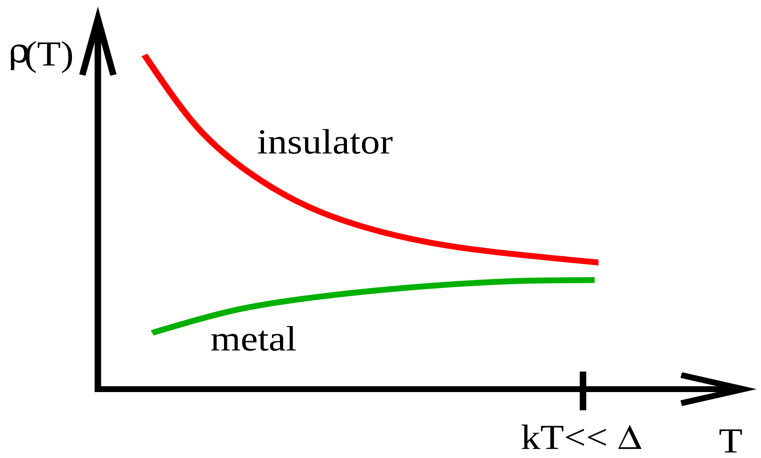
good – bad conductor – obscure meaning

E.g.
semiconductor: $\rho_{\rm semi-cond} \sim 10^{-3} - 10^{9}\ \Omega cm$
semimetal: $\rho_{\rm semi-metal} \sim 10^{-5} - 10^{-4}\ \Omega cm$

However, $\rho_{\rm semi-cond} = \infty$ and $\rho_{\rm semi-metal} = 0$ at $T = 0$!

activation energy $\Delta(\lambda)$:

$$\Re[\sigma_{\alpha,\beta}(k_B T \ll \Delta(\lambda), \omega \to 0)] \sim e^{-\frac{\Delta(\lambda)}{k_B T}}$$

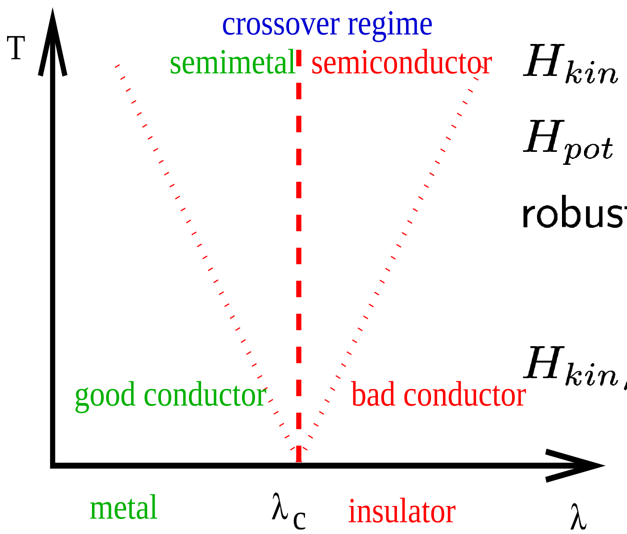


Gap at finite T

robust gap – exists for all temperature
soft gap – vanishes for $T > T_c$

Roots to form a gap

- quantum phase transition – competition between E_{kin} and E_{pot}
- thermodynamic phase transitions – competition between U and S



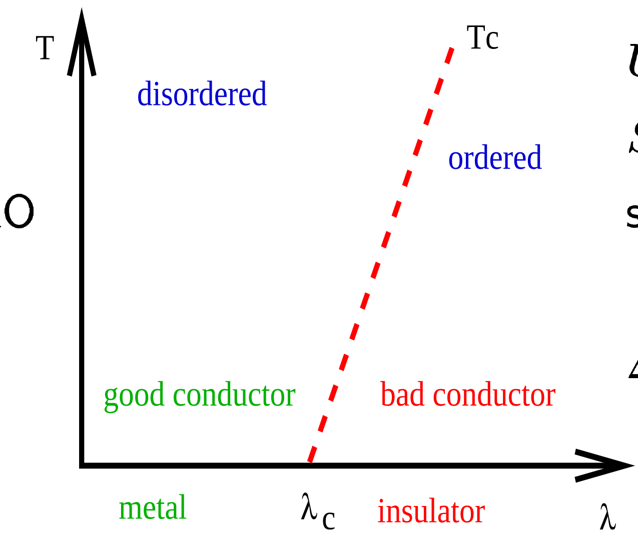
H_{kin} – delocalized

H_{pot} – localized

robust gap without LRO

$H_{kin}/H_{pot} = \lambda$

$H = H_0 + H_1$, $[H_0, H_1] \neq 0$



U – ordered

S – disordered

soft gap with LRO

$\Delta(\lambda, T < T_c) \neq 0$

SSB with LRO below $T < T_c$

Types of insulators

- single – particle: due to electron – ion interactions
  - Bloch – Wilson (band) insulators
  - Peierls (lattice deformation) insulators
  - Anderson (lattice randomness) insulators (!)
- many – particle: due to electron – electron interactions
  - Slater (SDW) insulators
  - Mott – Hubbard (PM) insulators (!!)
  - Mott – Heisenberg (localized AF) insulators

Band insulators

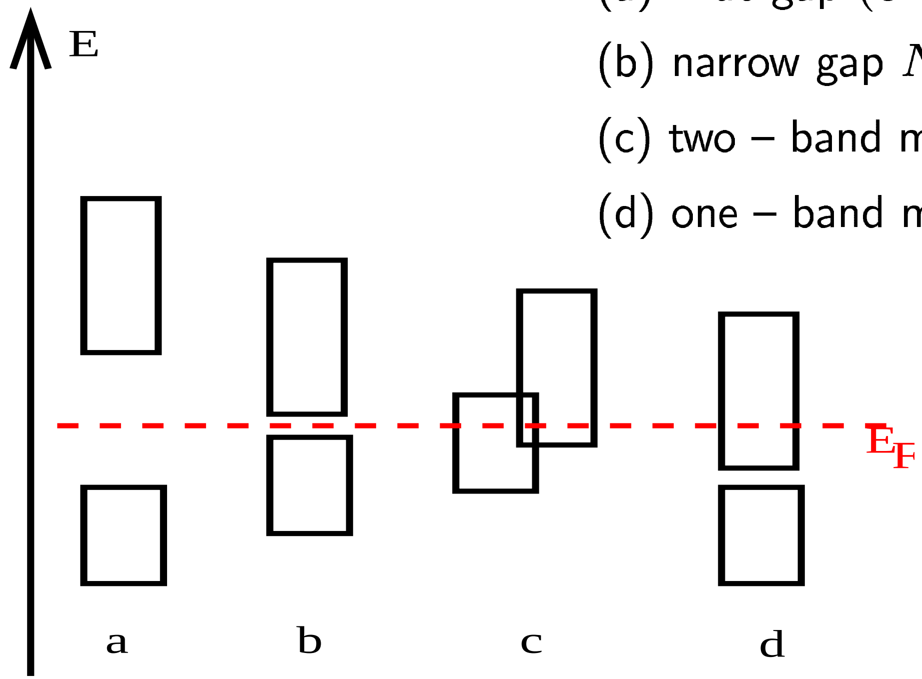
ideal lattice – $\Psi_{\mathbf{k},n}(\mathbf{r})$, $E_{\mathbf{k},n}$ – Bloch states, $2N$ states in a band, completely filled bands do not participate in transport, robust gap in a single – particle spectrum

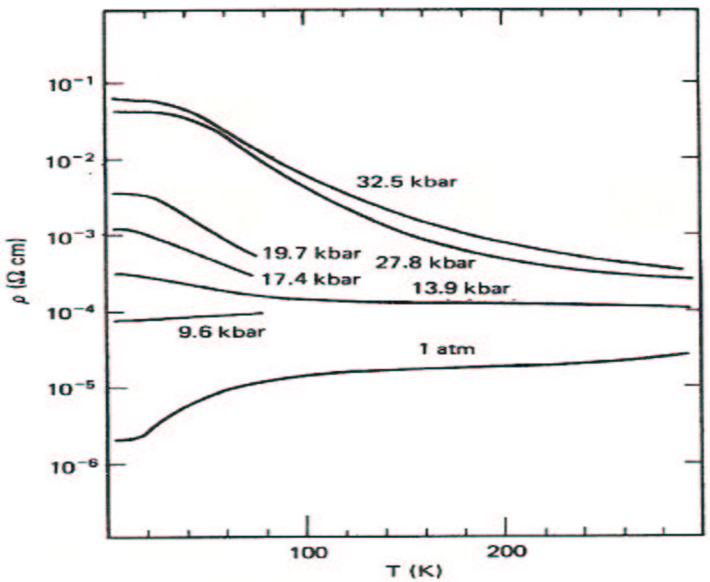
(a) wide gap $(5-10eV)$ insulator (diamond, noble atom crystals)

(b) narrow gap $N_e = 2N$ $(0,1-1eV)$ insulator (Si)

(c) two – band metal $N_e = 2N$ (As, Sb, Bi)

(d) one – band metal $N_e = N$ (Na, K, Ca, ...)

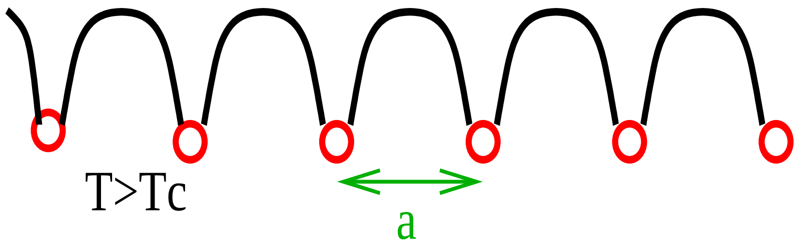




quantum MIT in Yb (iterb) at $p_c = 13kbar$

Peierls insulators

Coupling electron – phonon leads to formation of lattice deformation

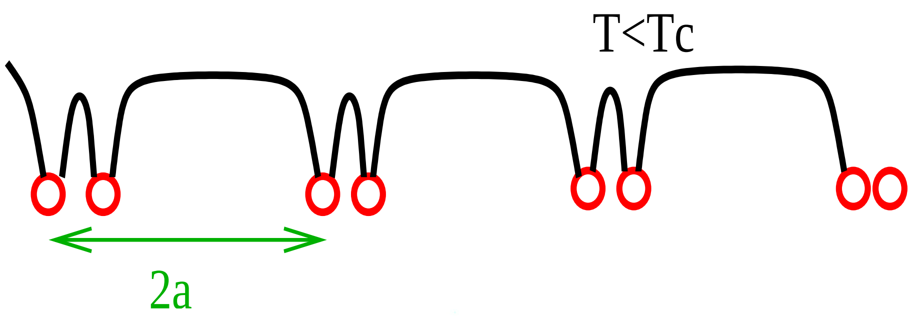


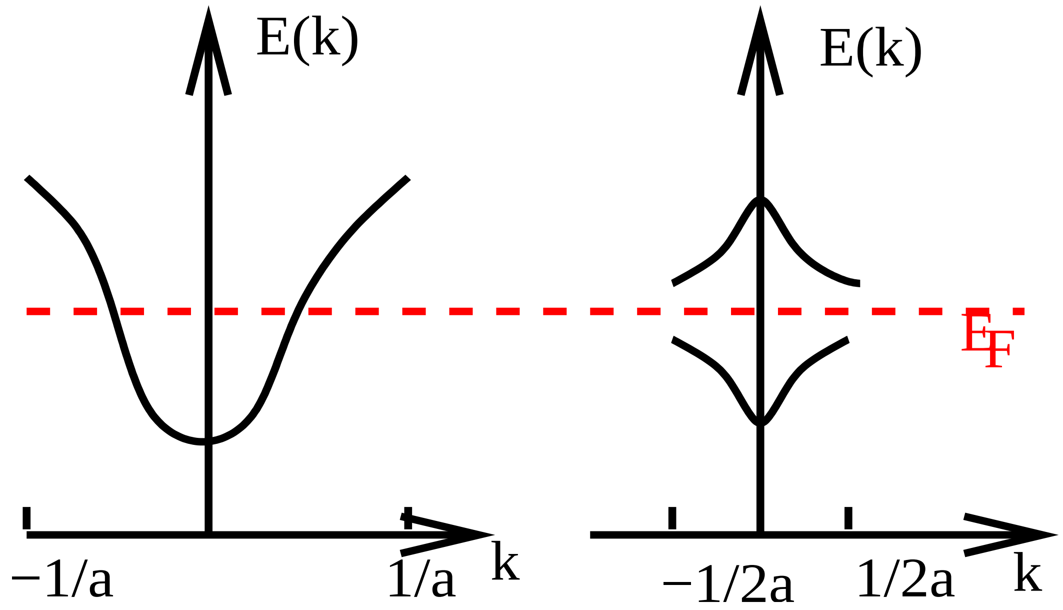
soft – gap in SSB at $T < T_c$

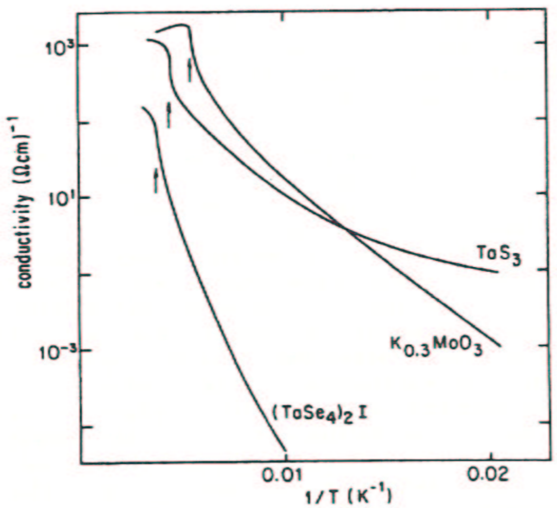
charge – density wave (CDW)

$n(x) \sim \Delta \cos(2k_F x)$

$E(k) = E_F \pm \sqrt{\epsilon_k^2 + \Delta^2}$, $\Delta(T) \sim \sqrt{T_c - T}$







thermodynamic MITs

Mott insulators – when interaction becomes important

Compare the kinetic energy

$$t_{ij} = \int d_3r \; \Phi_i(\mathbf{r})^* \left[-\frac{\nabla^2}{2m} + V(\mathbf{r}) \right] \Phi_j(\mathbf{r})$$

with the potential energy

$$U = \int d_3r d_3r' \; \Phi_i^*(\mathbf{r}) \Phi_i^*(\mathbf{r}') \frac{e}{|\mathbf{r} - \mathbf{r}'|} \Phi_i(\mathbf{r}') \Phi_i(\mathbf{r})$$

on a lattice of ions labeled by $i (\equiv \mathbf{R}_i)$ and j.

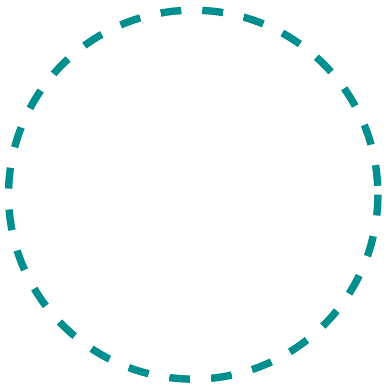
When

$$\frac{U}{|t_{ij}|} \gtrsim 1 \quad ?$$

Material ingredient

s and p valence orbitals have large effective radius

d and f valence orbitals have small effective radius



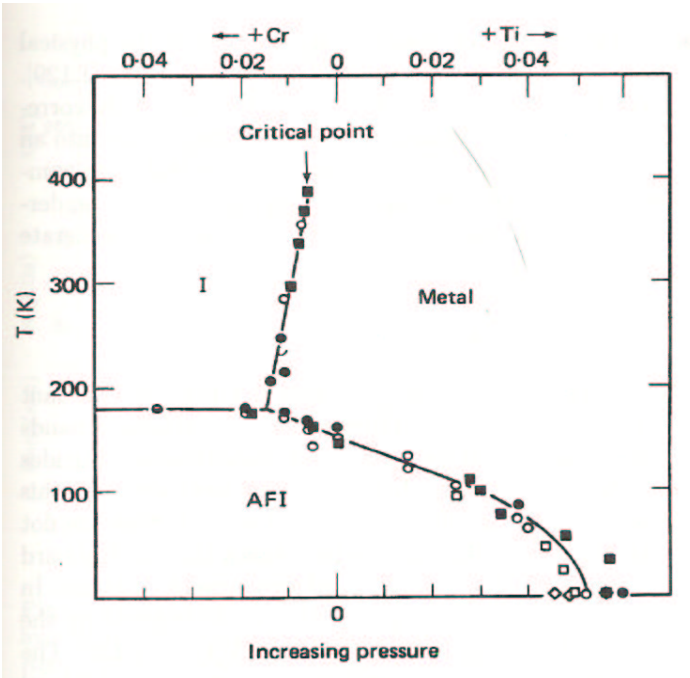
$$\frac{U}{|t_{ij}|} \ll 1$$

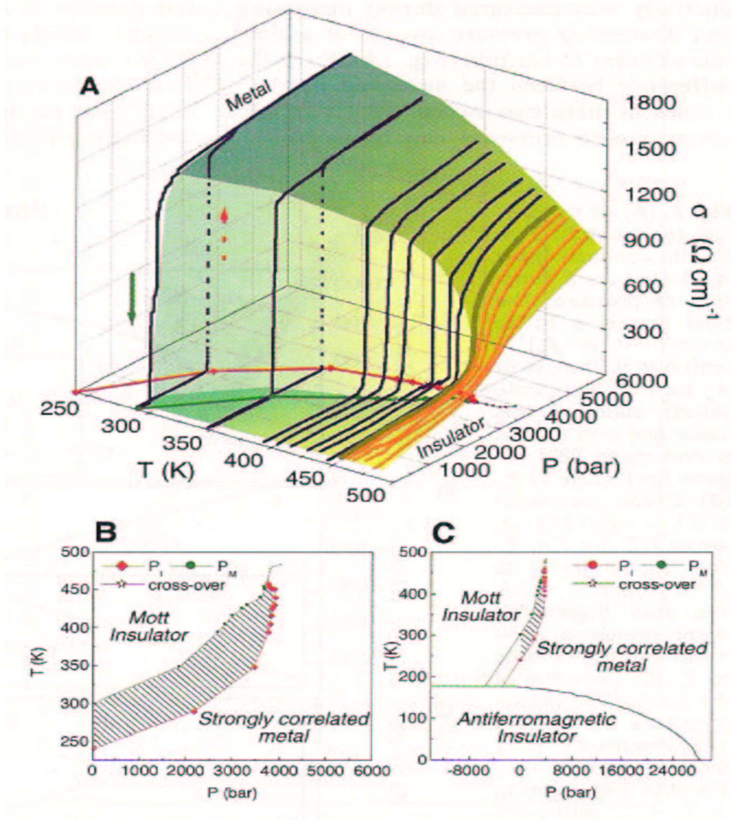
$$\frac{U}{|t_{ij}|} \gtrsim 1$$

Compounds with transition metal or rare earth elements are strongly correlated electron systems

Canonical example: V_2O_3

$V \quad ([Ar]3d^2 4s^2)$ gives V^{+3} valence band partially filled
should be metal?





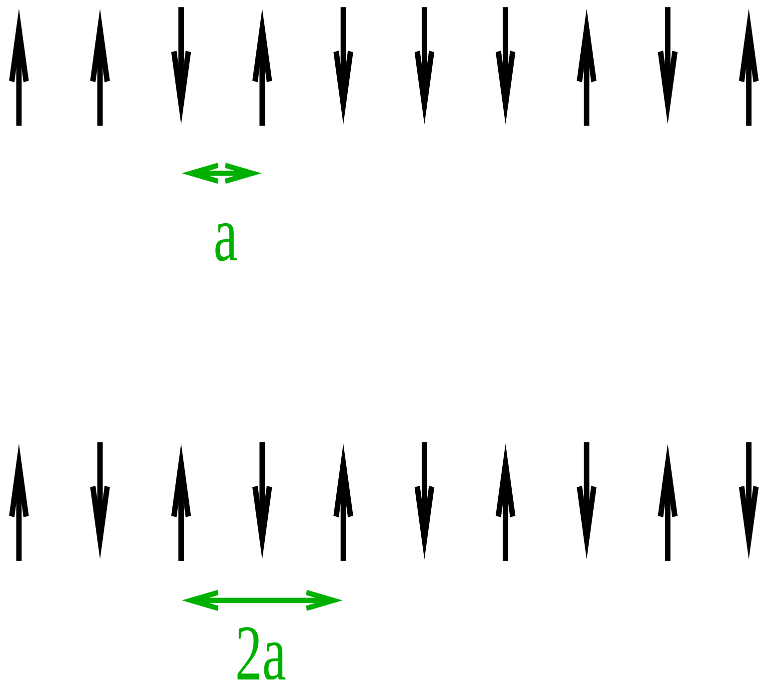
True Mott insulator

persists above T_N

Mott – Hubbard Insulator, Mott – Heisenberg Insulator, and Slater Insulator

Peierls insulators

Coupling electron – phonon leads to formation of lattice deformation

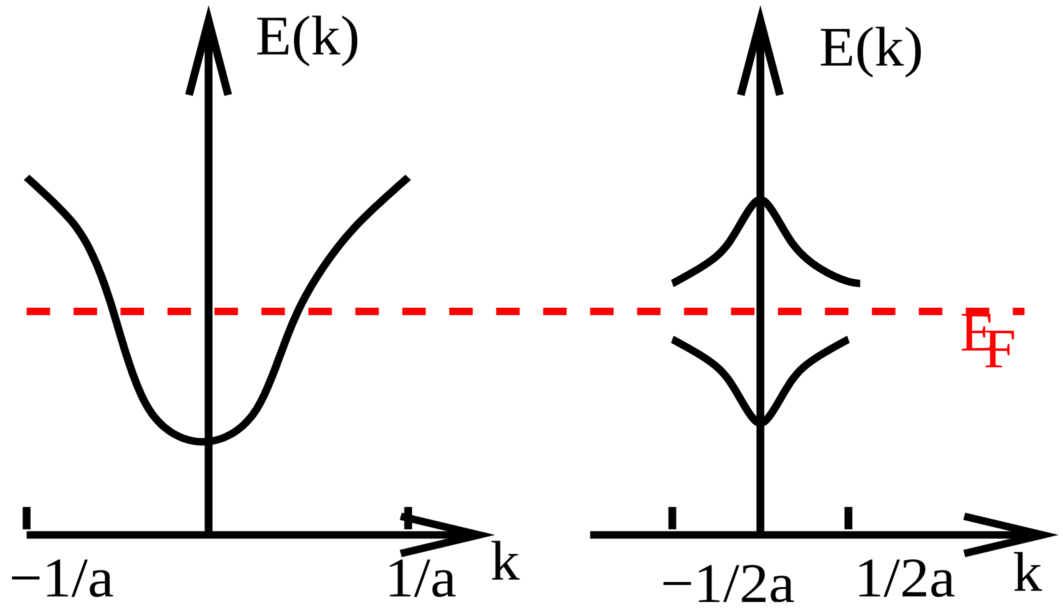


soft – gap in SSB at $T < T_c$

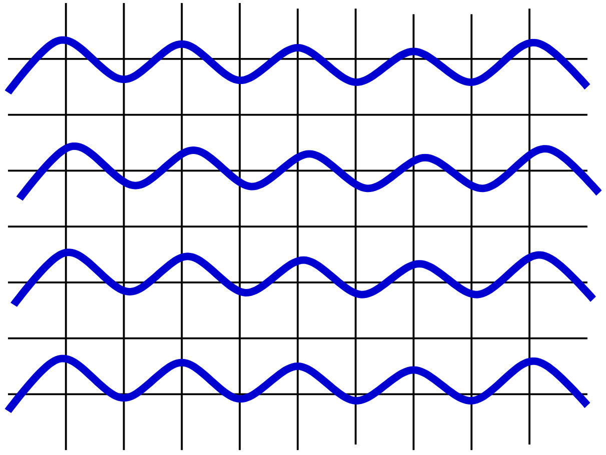
spin – density wave (SDW)

$\langle S^z(x) \rangle \sim \Delta \cos(2k_F x)$

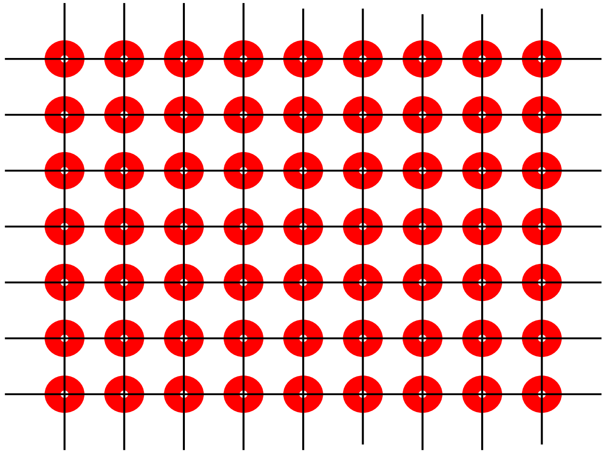
$E(k) = E_F \pm \sqrt{\epsilon_k^2 + \Delta^2}$, $\Delta(T) \sim \sqrt{T_c - T}$



Mott-Hubbard metal-insulator transition at $n = 1$

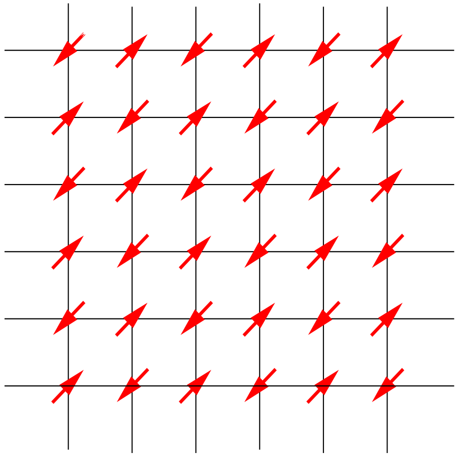


$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$



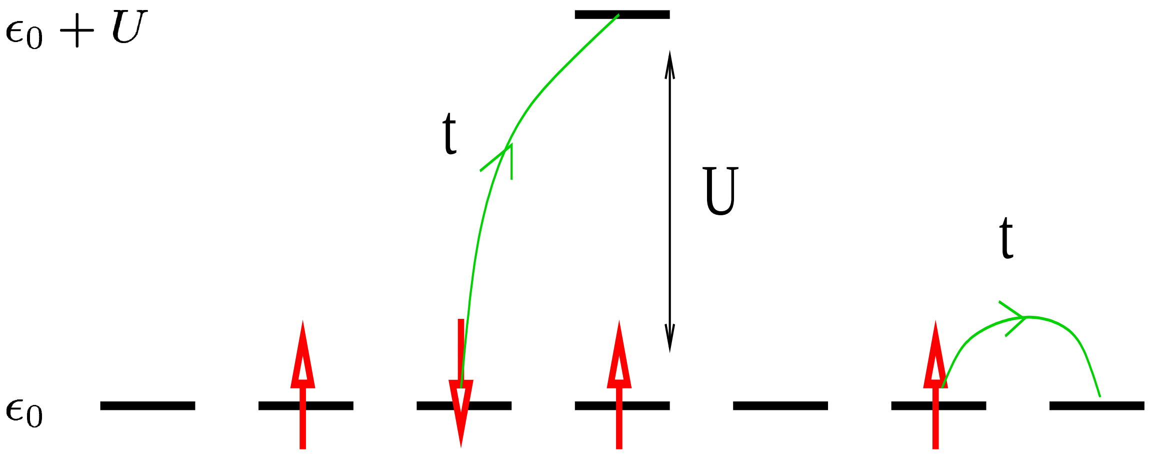
$U \gg |t_{ij}|$, $\Delta\mathbf{r} = 0$

Antiferromagnetic Mott insulator



typical intermediate coupling problem $U_c \approx |t_{ij}|$

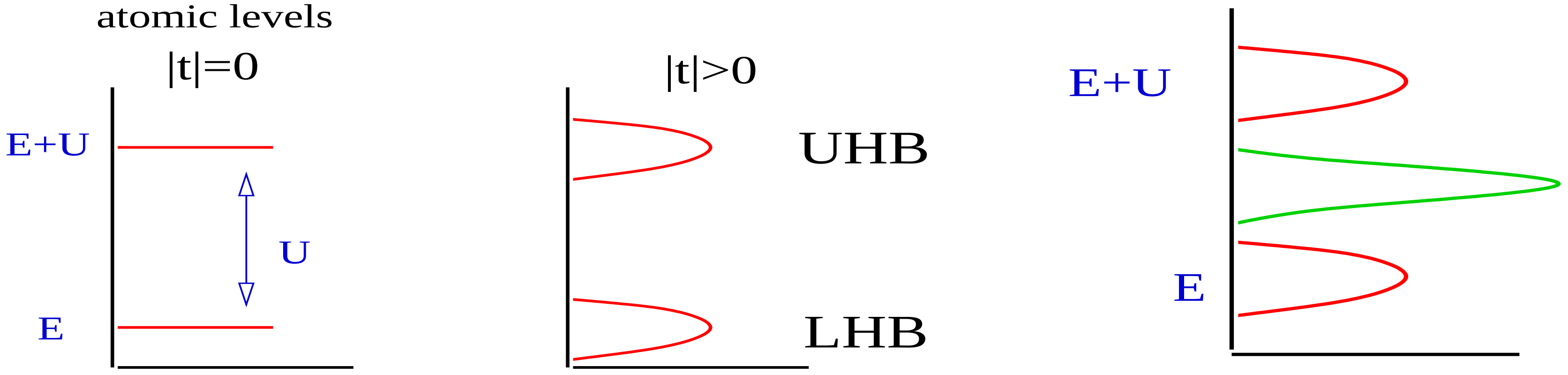
Hubbard model to capture right physics



$$H = \sum_{i\sigma} \epsilon_0 n_{i\sigma} + \sum_{ij\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- long history, many contradictions
- exactly solvable in $d = 1$
- exactly solvable in $d = \infty$
- how to approximate in $1 < d < \infty$?

Physical picture, $n = 1$



spin flip on central site

at $U = U_c$ resonance disapears
gaped insulator

dynamical processes with spin-flips inject states into correlation gap giving a quasiparticle resonance

From $d = \infty$ to DMFT

Mezner, Vollhardt 89

To have well defined limit $d = \infty$ we have to rescale

$$t \to \frac{t^*}{\sqrt{2d}}$$

$$t' \to \frac{t'^*}{2d}$$

etc., BUT

$$U \to U$$

Then the propagator (Green function)

$$G^0_{ij} \sim O\left(\frac{1}{d^{\frac{||R_i - R_j||}{2}}}\right)$$

- **simplification in $d = \infty$ because all connected, irreducible perturbation theory diagrams in position space collapse**

- **self-energy**

$$\Sigma_{ij}(\omega) = \delta_{ij}\Sigma_{ii}(\omega)$$

  local quantity depending only on time (frequency)

- **in momentum space**

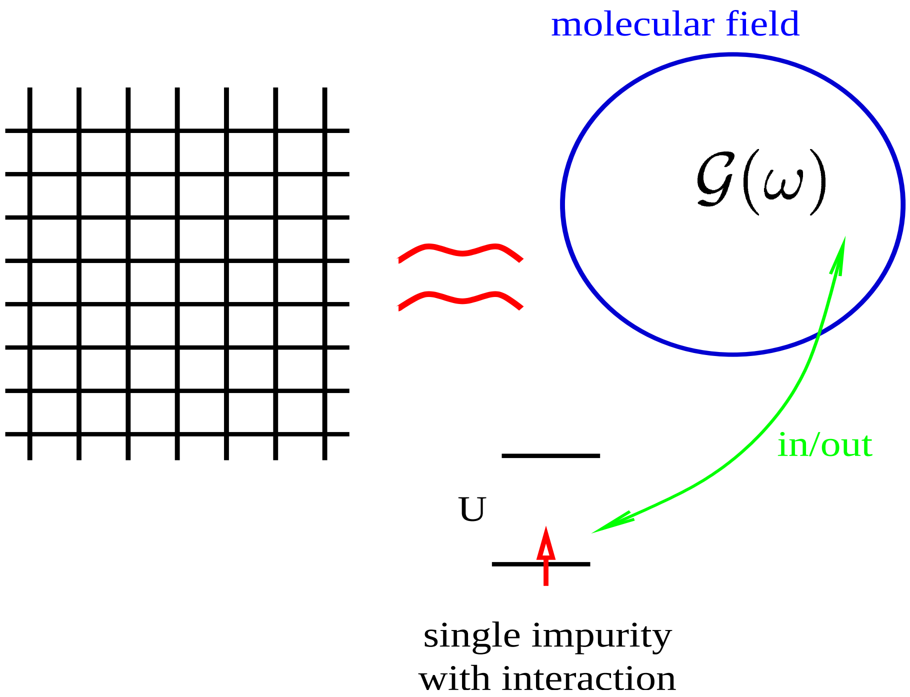
$$\Sigma(\mathbf{k}, \omega) = \Sigma(\omega)$$

- **quantum (local) dynamics survives**

Dynamical mean-field theory

Kotliar et al., Vollhardt et al.

Lattice problem of interacting particles is mapped onto a single impurity (single atom) coupled to the molecular bath



Molecular (Weiss) function $\mathcal{G}(\omega)$ is a dynamical quantity, determined self-consistently

Dynamical mean-field equations

$$G_\sigma(\tau) = -\frac{1}{Z}\int D[c^*,c]c(\tau)c^*(0)e^{-S_{\mathrm{eff}}[c^*,c]}$$

where

$$S_{\mathrm{eff}}[c^*,c] =$$
$$-\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^*_\sigma(\tau)\mathcal{G}(\tau-\tau')c_\sigma(\tau')$$
$$+U\int_0^\beta d\tau n_\uparrow(\tau)n_\downarrow(\tau)$$

and $\mathcal{G}(i\omega_n)^{-1} = G_\sigma(i\omega_n)^{-1} + \Sigma_\sigma(i\omega_n)$

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - E(\mathbf{k}) - \Sigma_\sigma(i\omega_n)}$$

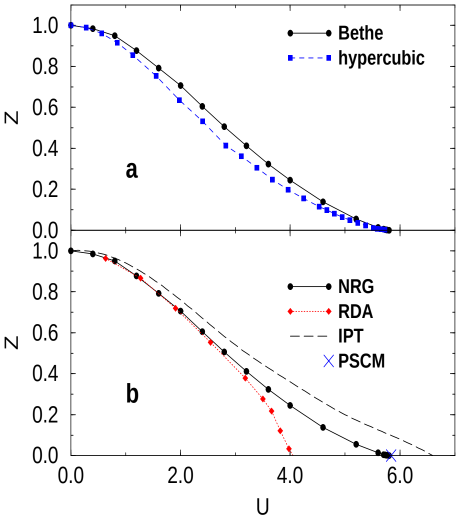
T=0 Mott transition according to DMFT

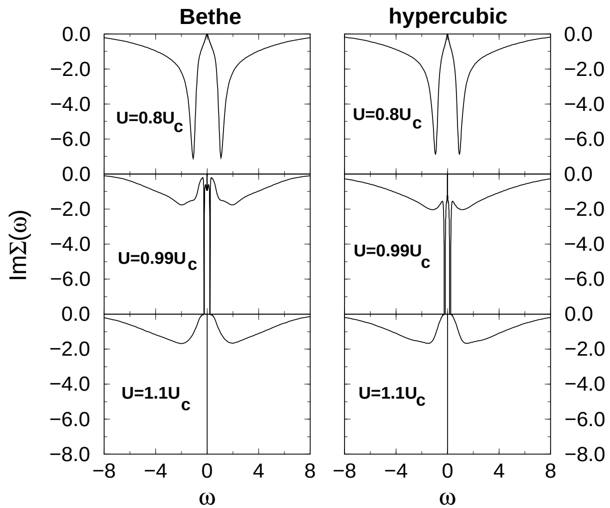
Kotliar et al. 92-96, Bulla, 99

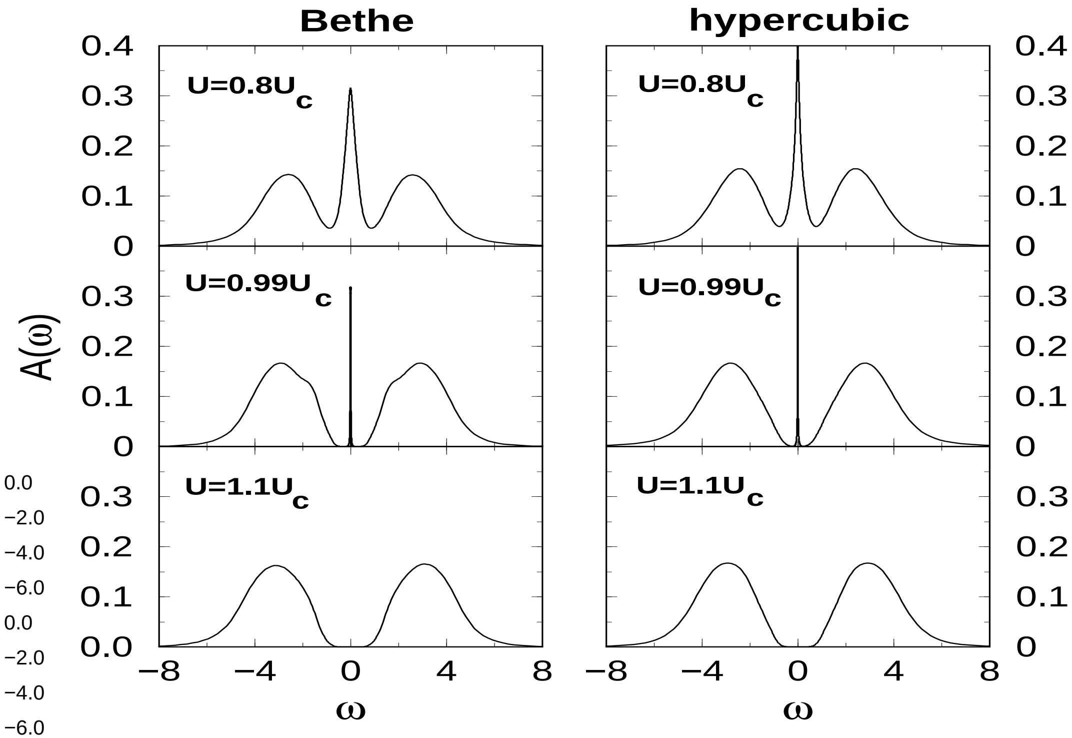
quantity to be determined

$$A(\omega) = -\frac{1}{\pi}\Im G(\omega)$$

spectral density function



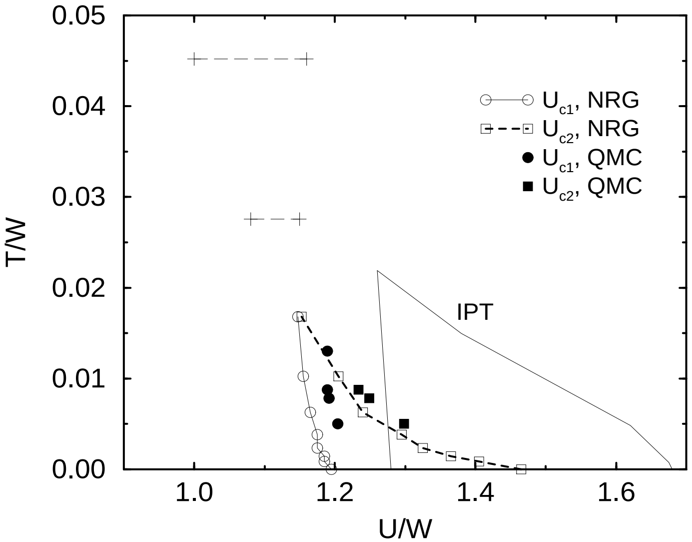


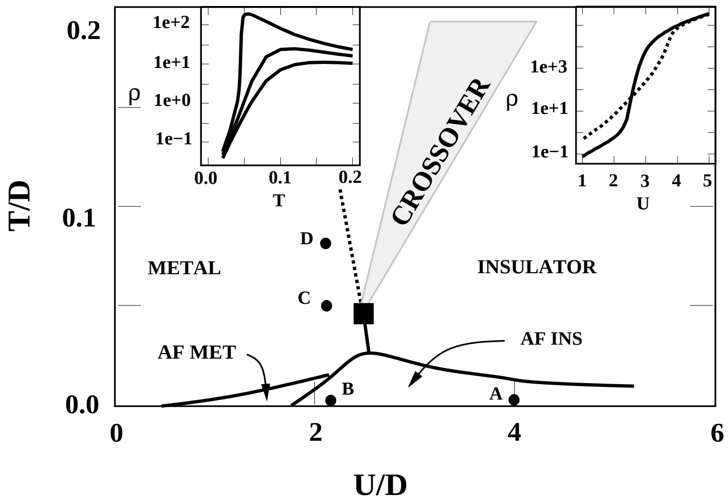


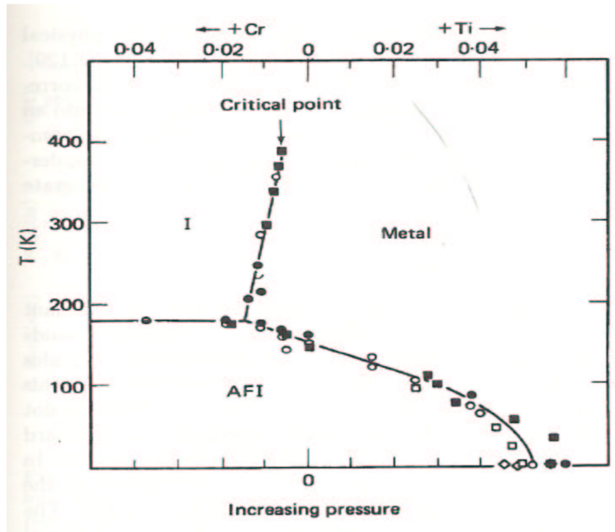
$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$

Mott transition at $T > 0$

Kotliar et al. 92-96, Bulla et al. 01, also Spalek 87







1^{st}-order transition

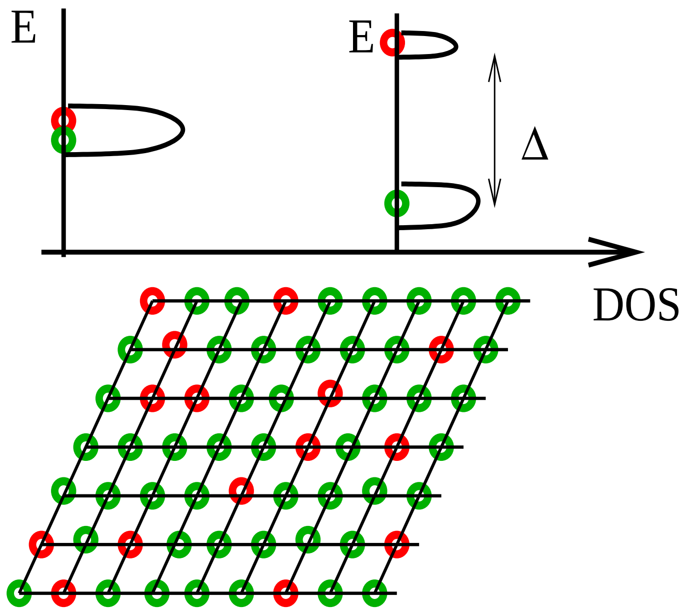
Mott MIT in binary alloy

Byczuk et al., PRL03, PRB04

Disordered alloy $A_x B_{1-x}$

$$\mathcal{P}(\epsilon_i) = x\delta(\epsilon_i + \frac{\Delta}{2}) + (1-x)\delta(\epsilon_i - \frac{\Delta}{2})$$

When $\Delta \gg |t_{ij}|$ **the spectral function splits into lower and upper alloy subbands**



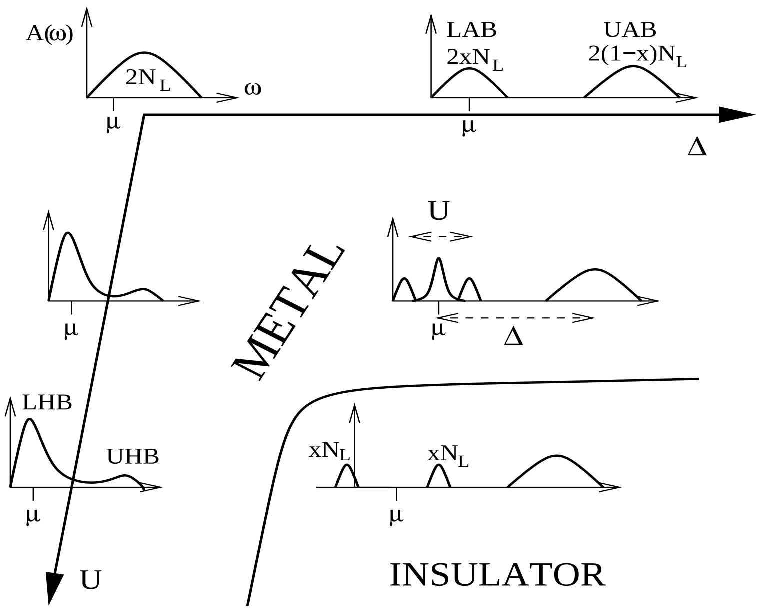
Is there Mott MIT at $n \neq 1$**?**

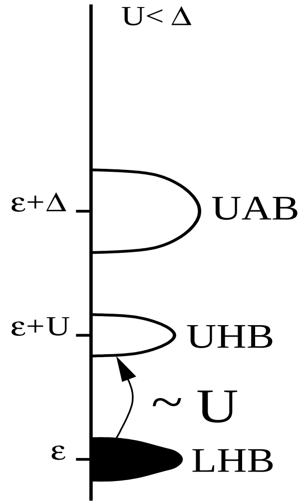
DMFT + $G(\omega) = \int d\epsilon_i \mathcal{P}(\epsilon_i) G(\omega, \epsilon_i)$

Mott MIT in binary alloy at $n \neq 1$

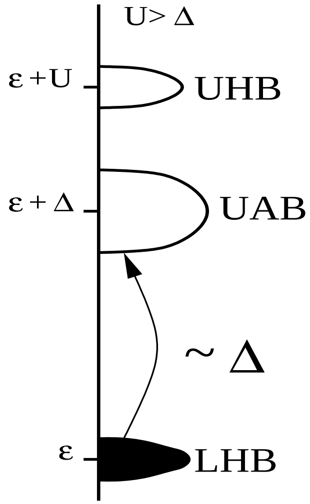
Byczuk et al., PRL03, PRB04

$$n = x \text{ or } n = 1 + x$$

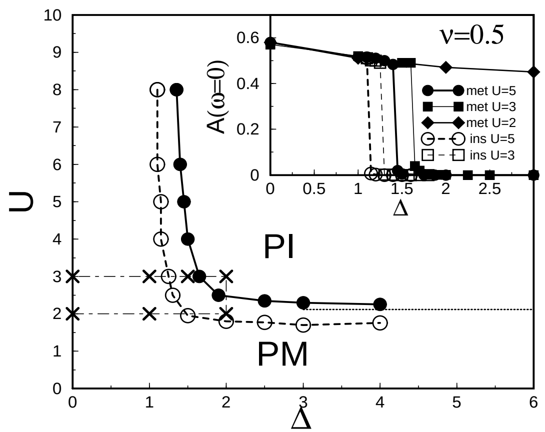




alloy Mott insulator



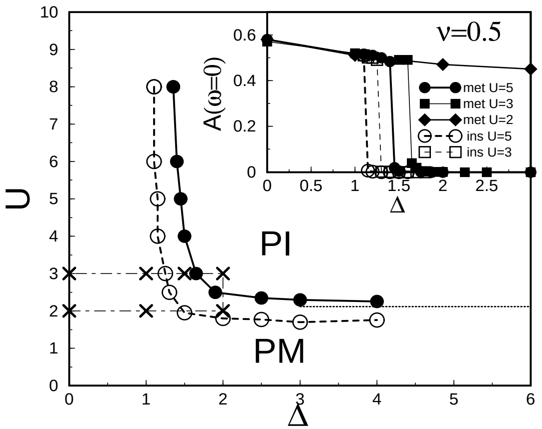
alloy charge transfer insulator

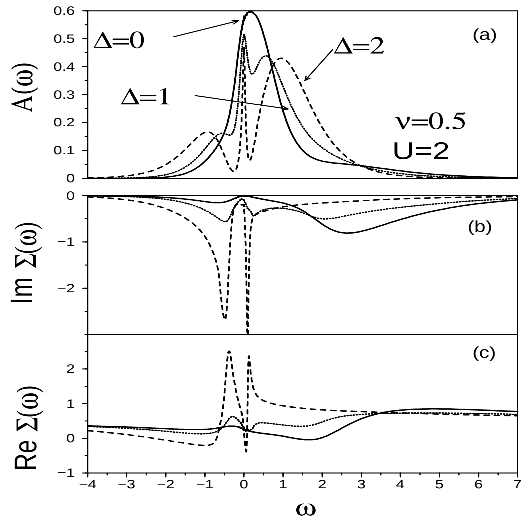


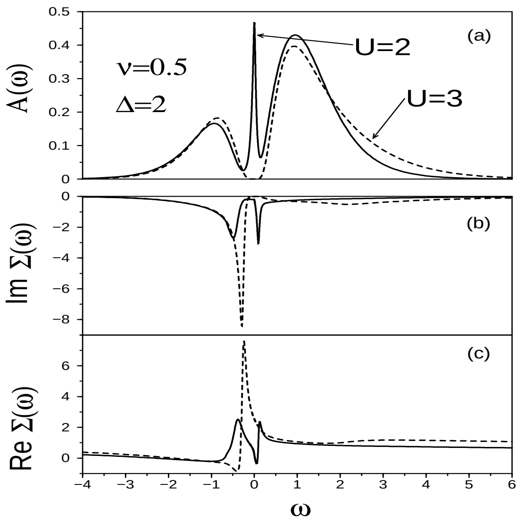
$$U_c^{\Delta \to \infty} = 6t^* \sqrt{x}$$

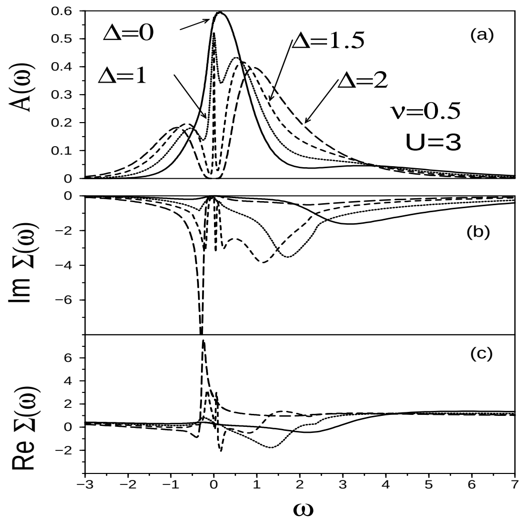
Mott MIT in binary alloy at $\nu = x = 0.5$

Byczuk et al., PRL03, PRB04





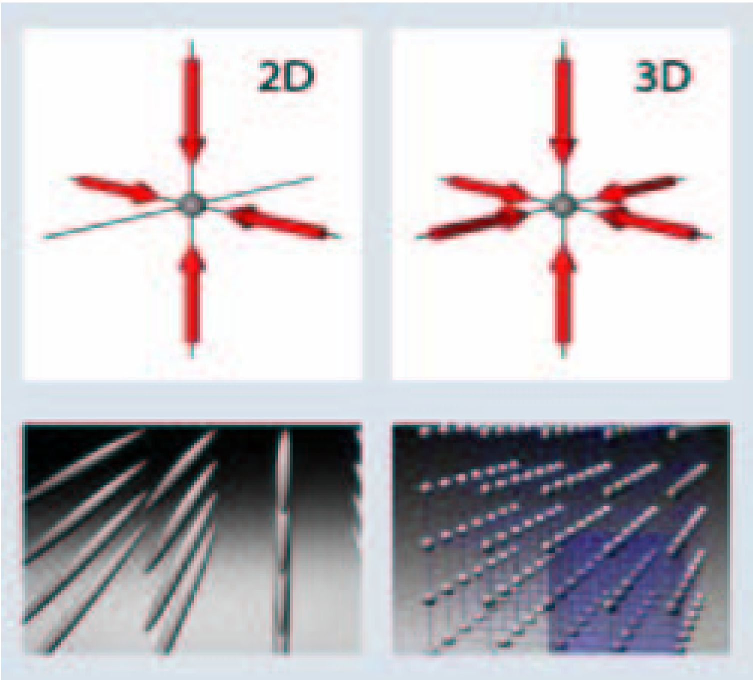


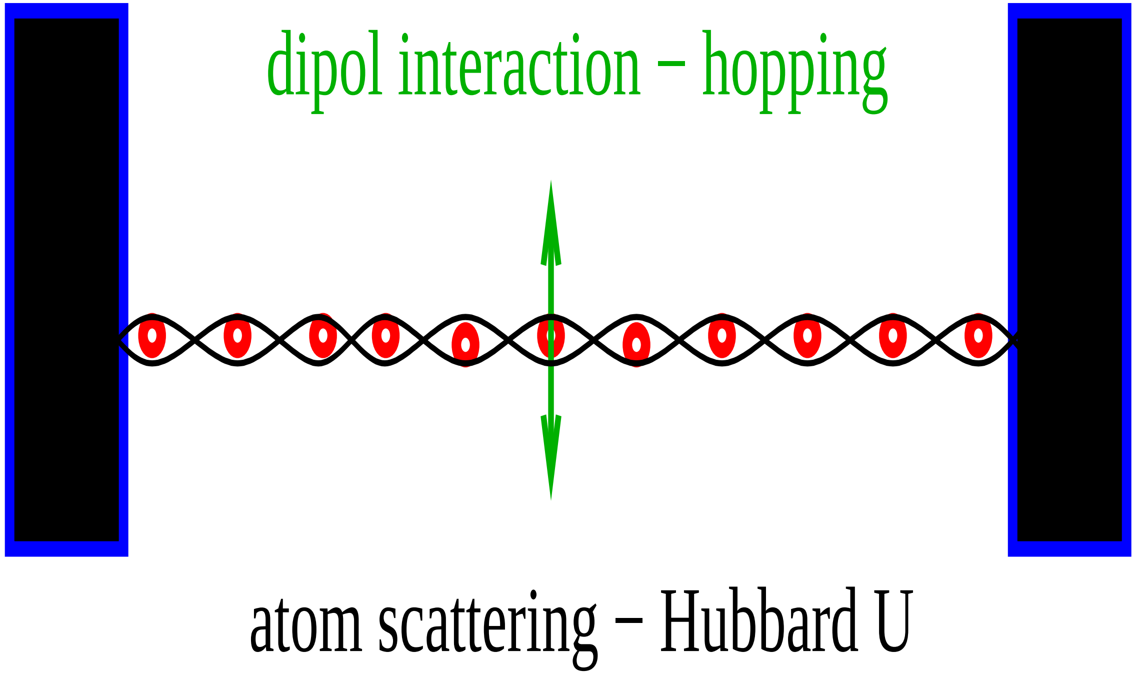


Mott transition in a Bose system

Greiner et al. 02

Using an atomic trap and standing waves of light one can create an optical lattice filled with bosonic (fermionic, not yet) atoms

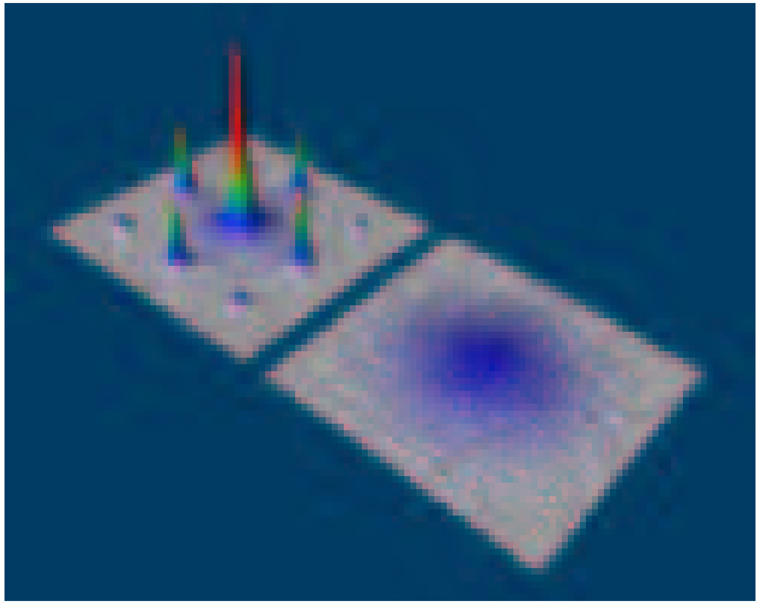




Two possible ground states

- **Bose-Einstein condensate if** $U \ll |t_{ij}|$
- **Mott insulator if** $U \gg |t_{ij}|$

Tuning t_{ij} **or** U **a superfluid - Mott - insulator transition observed**



Summary

- **Conductors and insulators**
- **Transitions between conductors and insulators**
- **Mott – Hubbard MIT at** $n = 1$
- **Mott – Hubbard MIT at** $n \neq 1$
  - **alloy band splitting**
  - **Mott – Hubbard MIT in alloy subband**
  - **Optical lattices possible realization**