Metal - Insulator transitions: overview, classification, descriptions

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Collaboration:

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- Dieter Vollhardt - Augsburg University

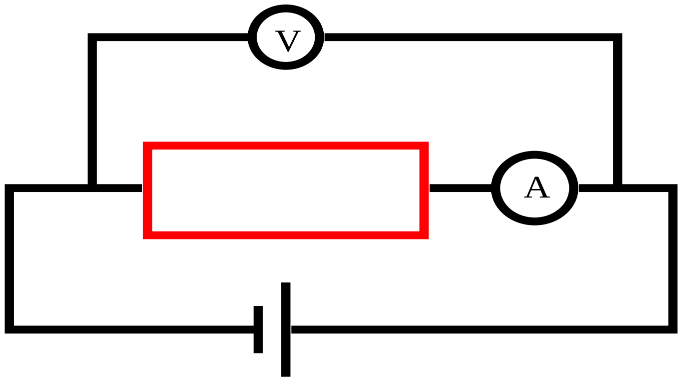
Plan of the talk:

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
5. Mott - Hubbard MIT at noninteger fillings
6. Mott - Anderson MIT at integer filling
7. 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

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

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

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

Definition:
Ideal conductor is a system where

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

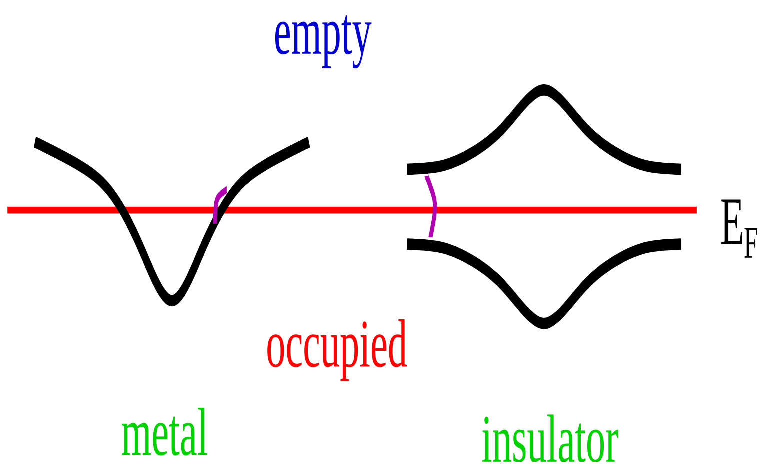
For a translationally invariant system $\tau^{-1} \rightarrow 0$

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: $\Delta(\lambda) = \left[\mu^{+}(\lambda) - \mu^{-}(\lambda)\right]_{\text{extended}}$

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

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

Insulator at finite T

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

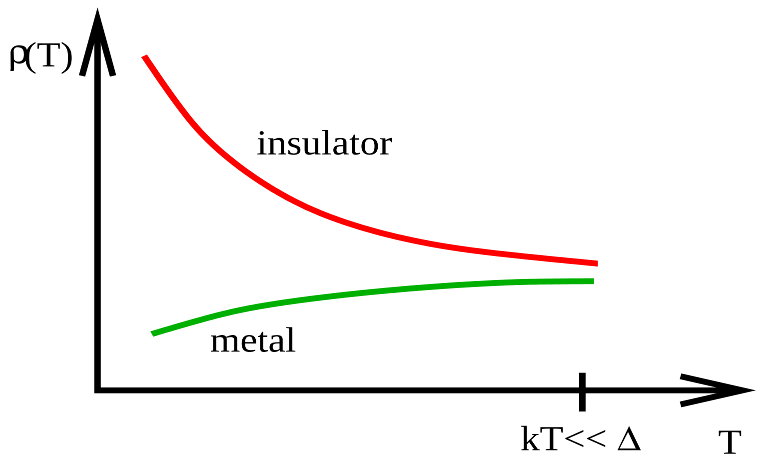
good – bad conductor – obscure meaning

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

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

activation energy $\Delta(\lambda)$:

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

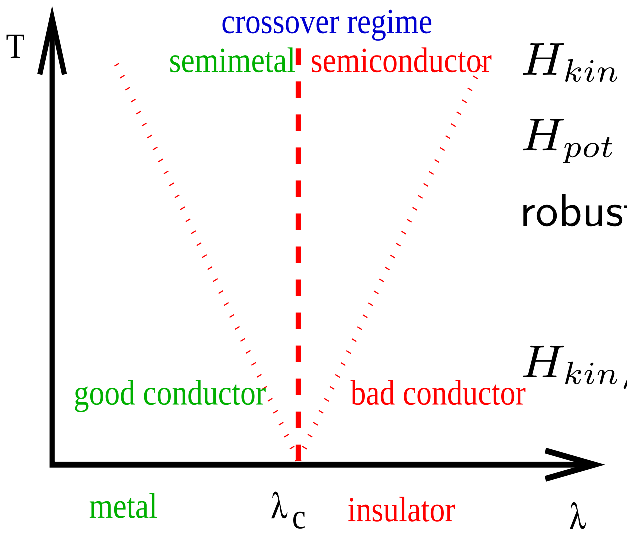


Gap at finite T

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

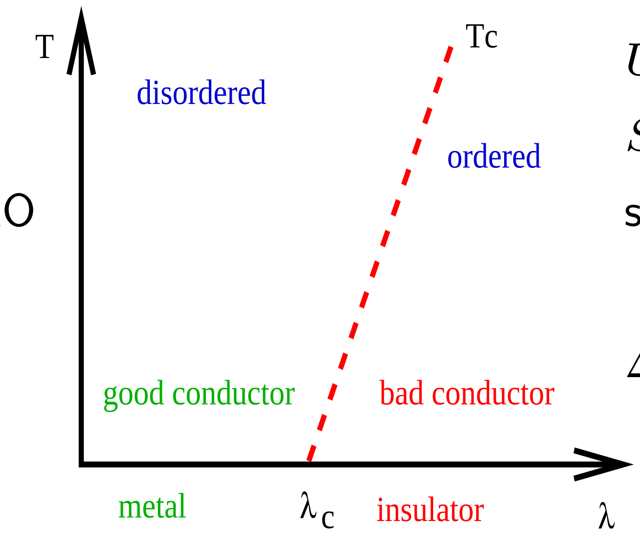


H_{kin} – delocalized

H_{pot} – localized

robust gap without LRO

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



U – ordered

S – disordered

soft gap with LRO

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

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

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

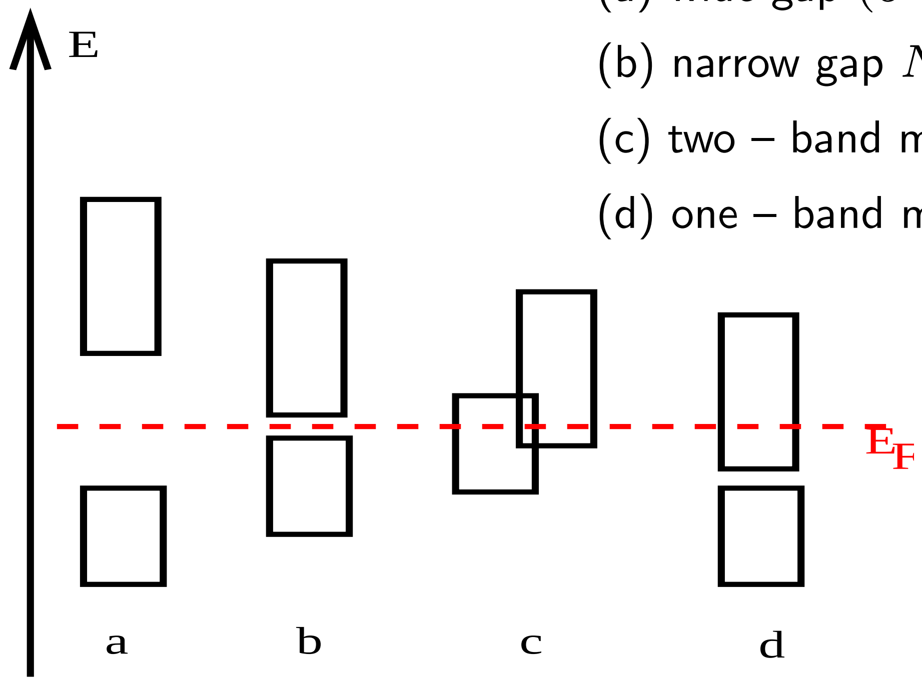
ideal lattice – $\Psi_{\mathbf{k},n}(\mathbf{r})$, $E_{\mathbf{k},n}$ – Bloch states, $2N$ states in a band, completely filled bands do not participate in transport, robust gap in a single – particle spectrum

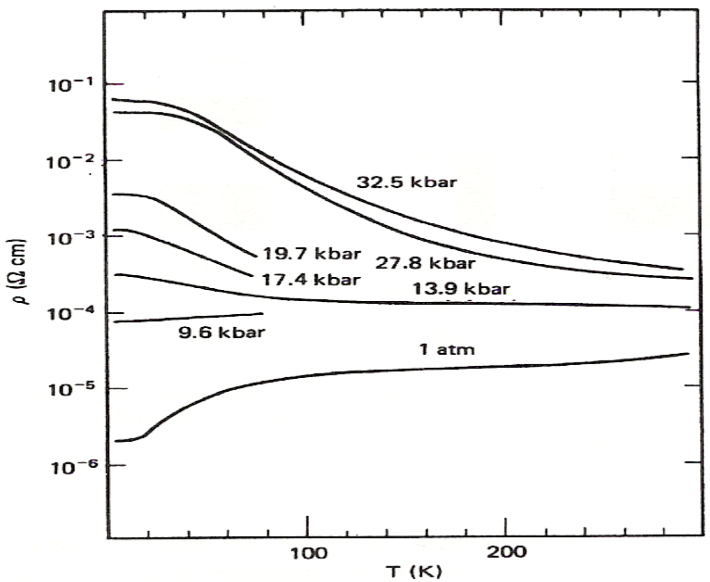
(a) wide gap $(5-10eV)$ insulator (diamond, noble atom crystals)

(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, ...)

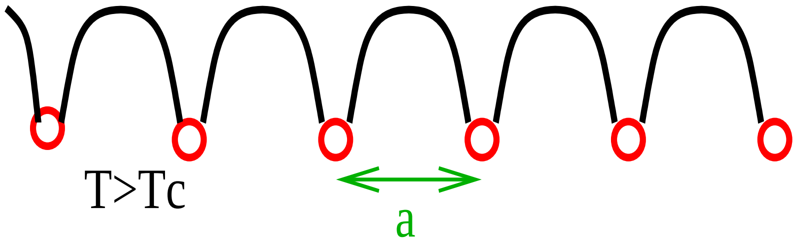




quantum MIT in Yb (iterb) at $p_c = 13kbar$

Peierls insulators

Coupling electron – phonon leads to formation of lattice deformation

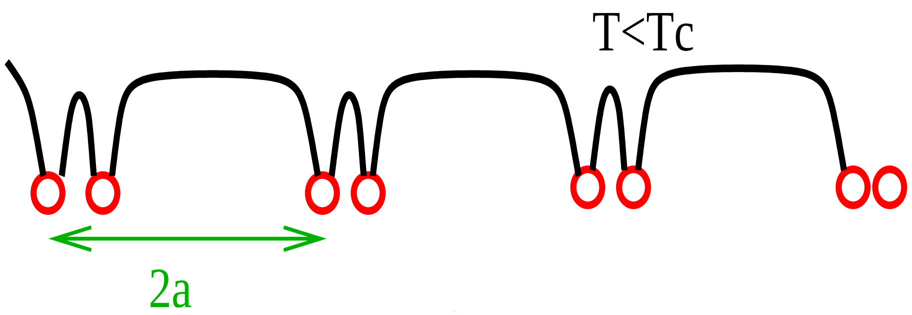


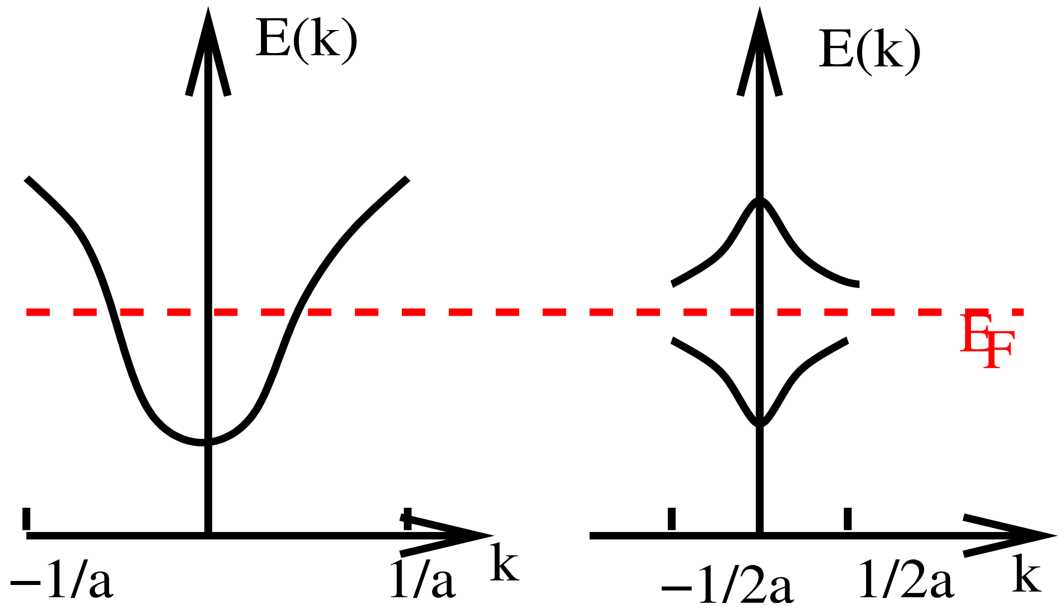
soft – gap in SSB at $T < T_c$

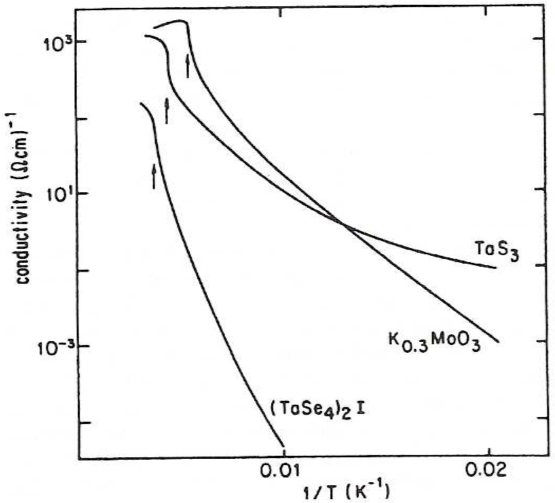
charge – density wave (CDW)

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

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



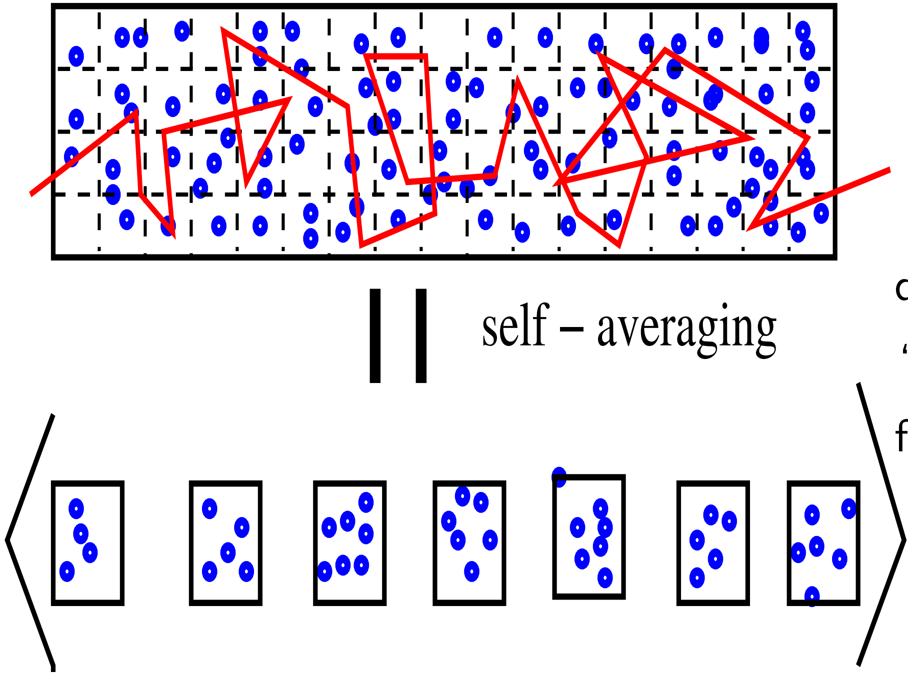




thermodynamic MITs

Waves in random system:

propagation of waves in a randomly inhomogeneous medium



random conservative linear wave equation

$$\frac{\partial^2 w}{\partial t^2} = c(x)^2 \frac{\partial^2 w}{\partial x^2}$$

$$i\frac{\partial w}{\partial t} = -\frac{\partial^2 w}{\partial x^2} + \nu(x) w$$

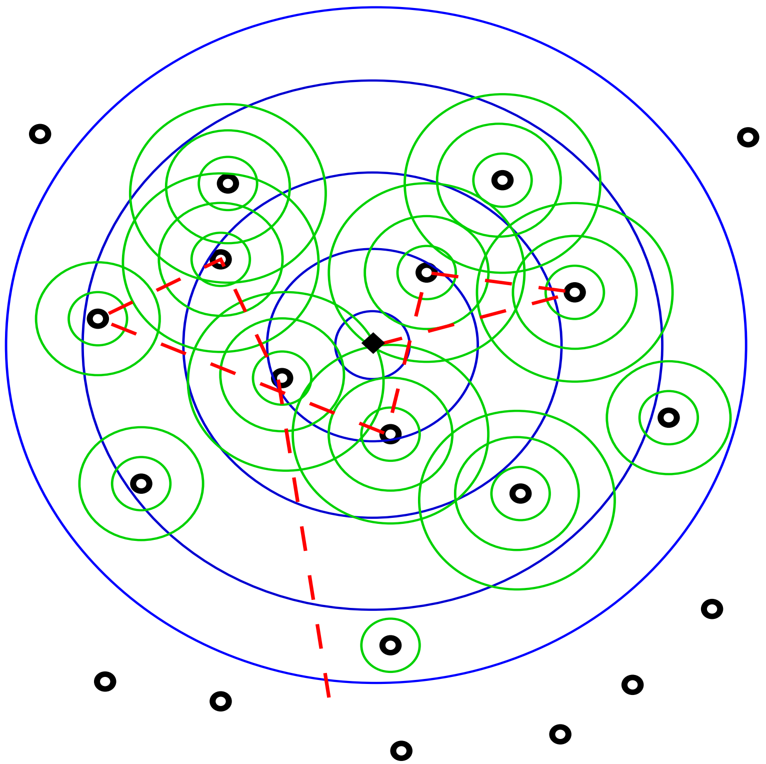
diffusive motion, memory of $\vec{V}(0)$ lost,

“random walk” over long distances,

friction imposed by averaging

Anderson localization:

propagation of waves in a randomly inhomogeneous medium



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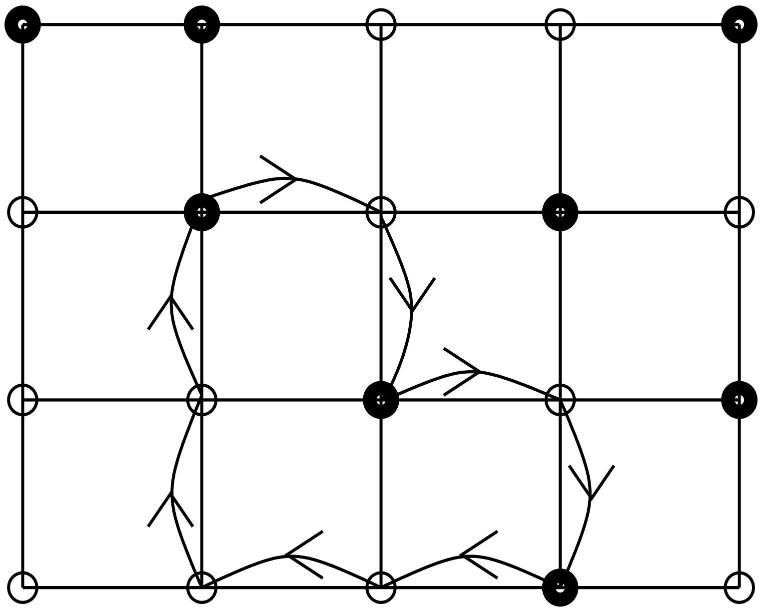
$$i\frac{\partial w}{\partial t} = -\frac{\partial^2 w}{\partial x^2} + \nu(x) w$$

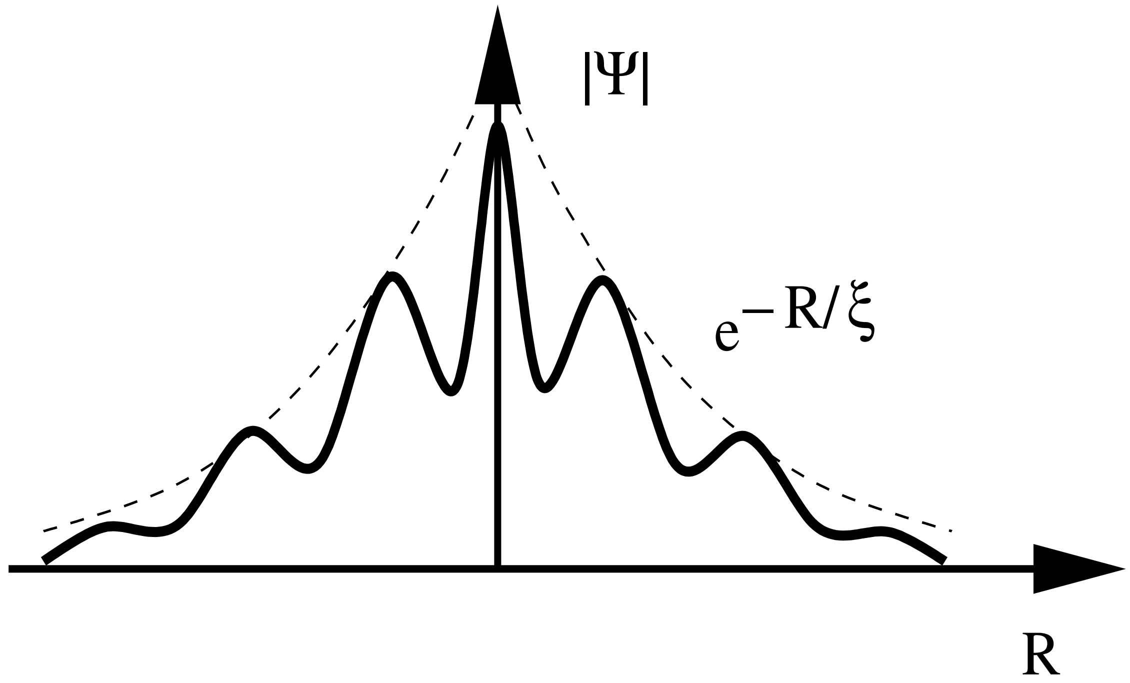
Anderson 1958: (no averaging) – strong scattering forms "standing" waves, sloshing back and forth in a bounded region of space

Localization is a destruction of coherent superposition of spatially separated states

Anderson MIT - cont.:

Returning probability $P_{j\to j}(t \to \infty; V \to \infty)$?





$P_{j\to j}(t \to \infty; V \to \infty) = 0$ for extended states

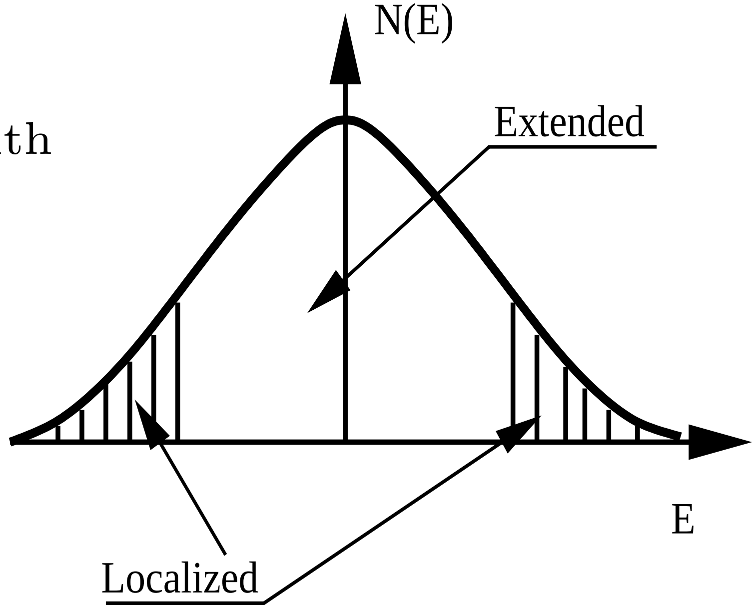
$P_{j\to j}(t \to \infty; V \to \infty) > 0$ for localized states

Anderson MIT - cont.:

According to one-parameter scaling theory $[g = g(L)]$ (noninteracting system)

- If dim$=1$ or 2 all states are localized
- If dim$=3$ there is a critical disorder above which the states are localized

$$\Delta_c \sim \mathrm{band-width}$$



Characterization of Anderson localization:

- Decaying of wavefunction $|\Psi_n(r_i)| \sim e^{-|r-r_i|/\xi(E_n)}$
  - metal $\xi \rightarrow \infty$
  - insulator $\xi < \infty$
- Inverse participation ratio P^{-1} [inverse number of sites that contribute to $\Psi_n(r_i)$]
  - metal $P^{-1} \sim 1/N$
  - insulator $P^{-1} \sim \mathrm{const}$
- Conductance G
  - metal $G > 0$
  - insulator $G = 0$
- Local Density of States (LDOS)

  $\rho_i(E) = \sum_{n=1}^{N} |\Psi_n(r_i)|^2 \delta(E - E_n)$

Local DOS

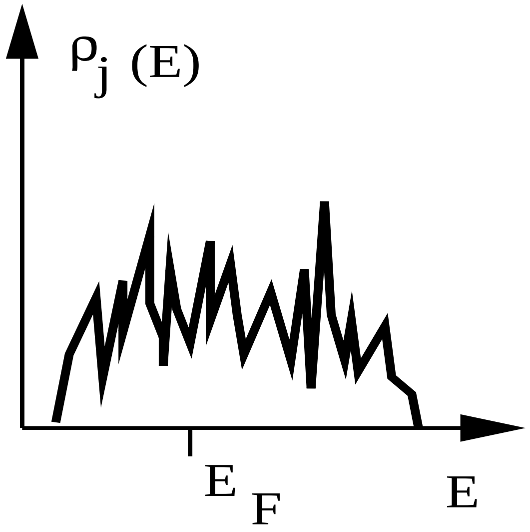
Heuristic arguments:

$$P_{j\to j}(t) = |G_j(t)|^2$$

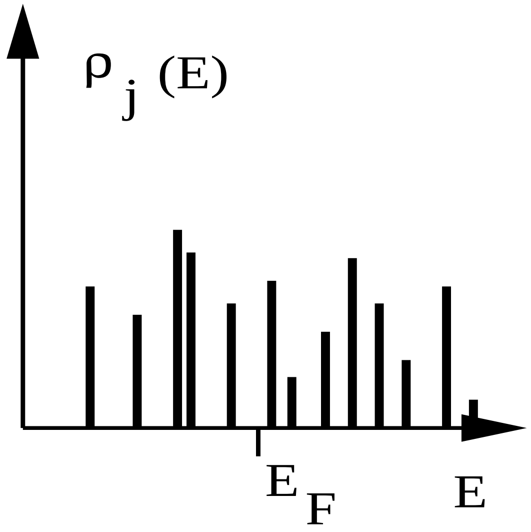
$$G_j(t) \sim e^{i(\epsilon_j+\Sigma'_j)t-|\Sigma''_j|t} \sim e^{-\frac{t}{\tau_{\rm esc}}}$$

Fermi Golden Rule

$$\frac{1}{\tau_{\rm esc}} \sim |t_{ji}|^2 \rho_j(E_F)$$



metal



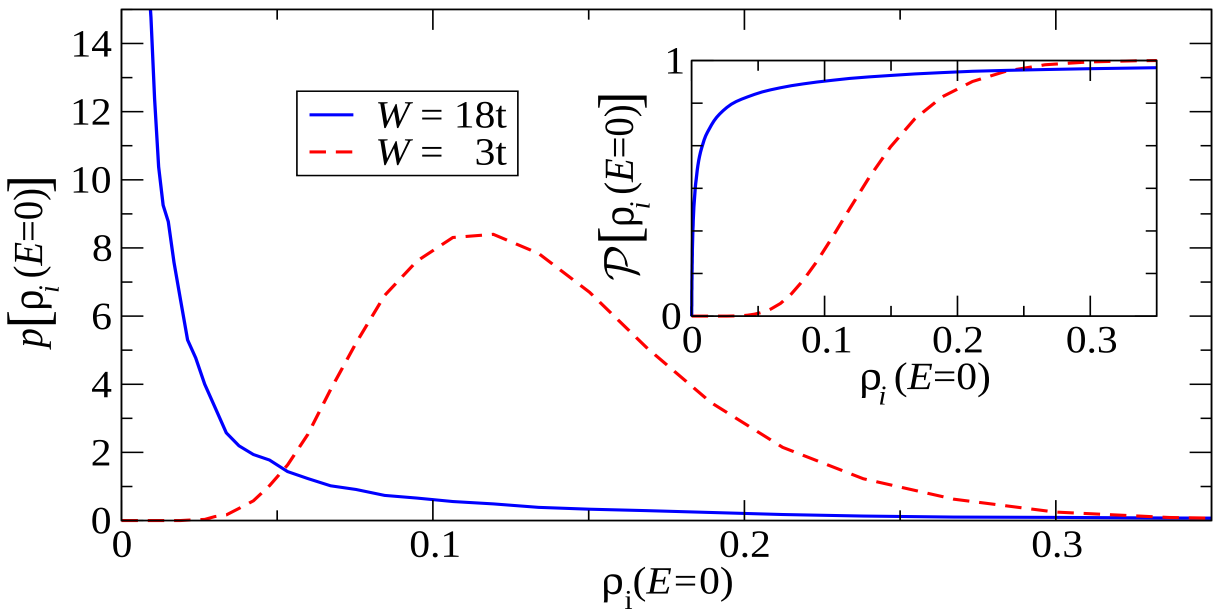
insulator

Statistics of LDOS:

$\rho_j(E)$ is different at different R_j!
Random quantity!

Statistical description $P[\rho_j(E)]$!

Exact diagonalization – Schubert et al. cond-mat/0309015



Broadly distributed $P[\rho_j(E_F)]$

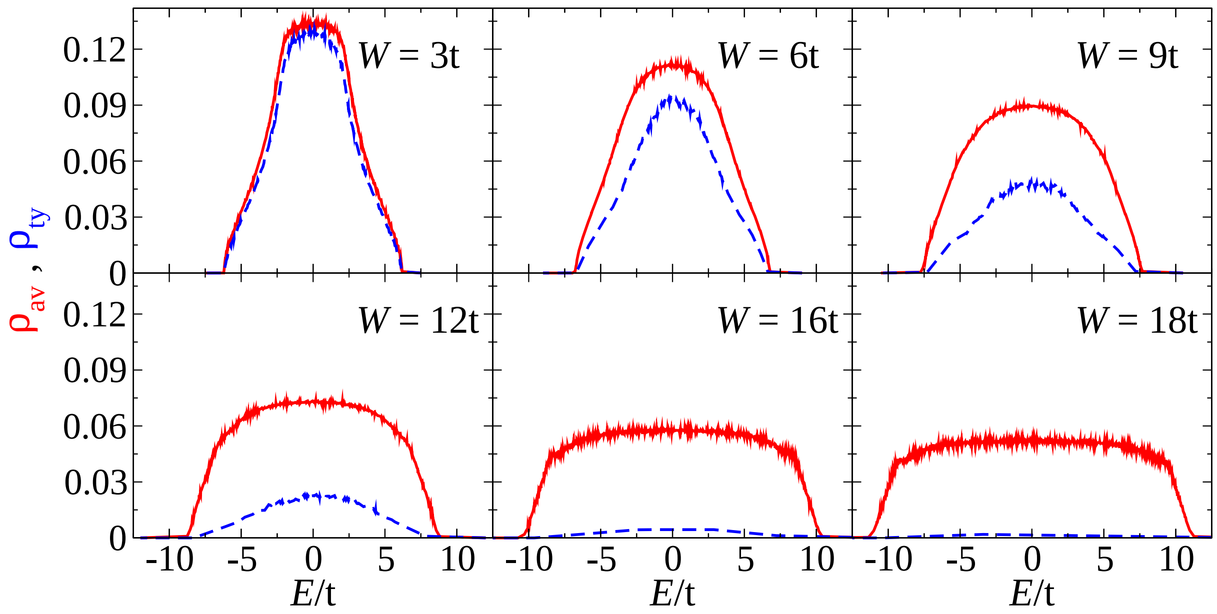
Multifractality - $\langle M^{(k)}\rangle \sim L^{-f(k)}$

Typical escape rate is determined by the typical LDOS

Anderson MIT - cont.:

Near Anderson localization typical LDOS is approximated by geometrical mean

$$\rho_{typ}(E) \approx \rho_{geom}(E) = e^{\langle \ln \rho_i(E) \rangle}$$



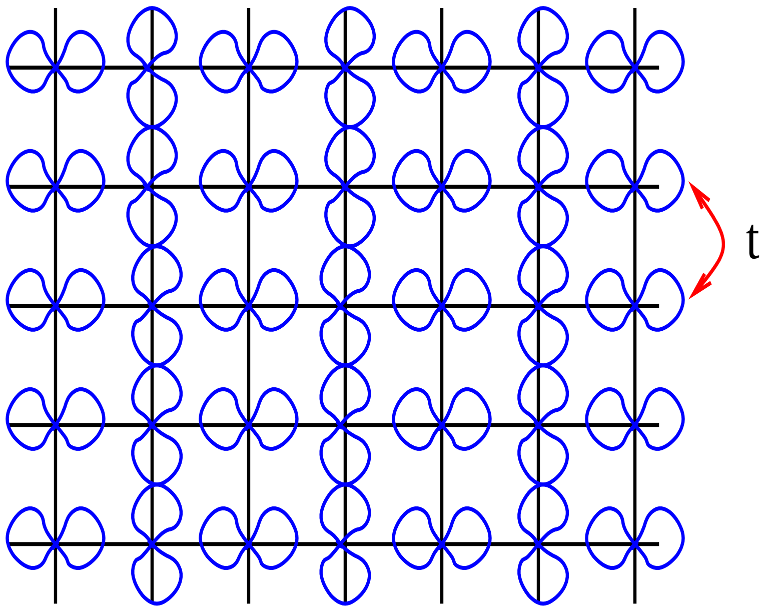
Schubert et al. cond-mat/0309015

Theorem (F.Wegner 1981):

$$\rho(E)_{av} = \langle \rho_i(E) \rangle > 0$$

within a band for any finite Δ

Many body insulators;
when interaction becomes important



Kinetic energy

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

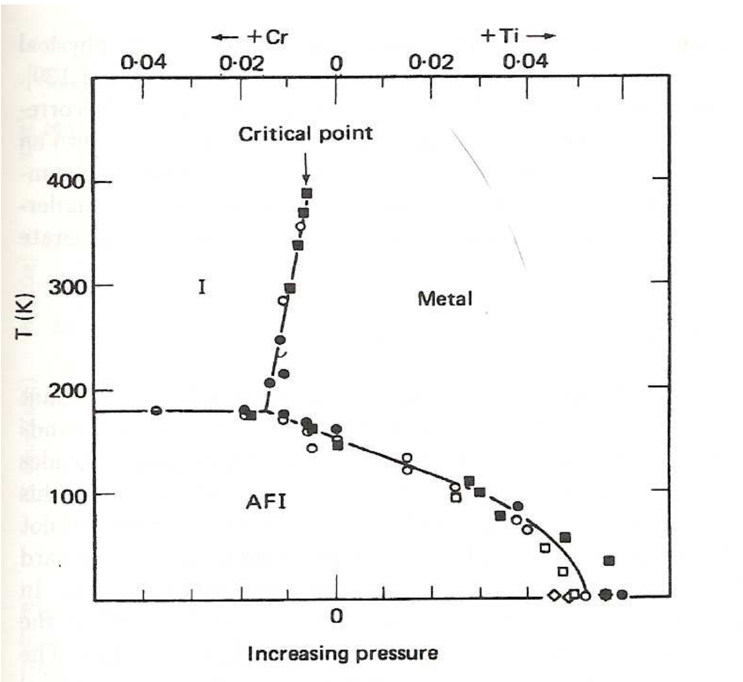
Interaction energy

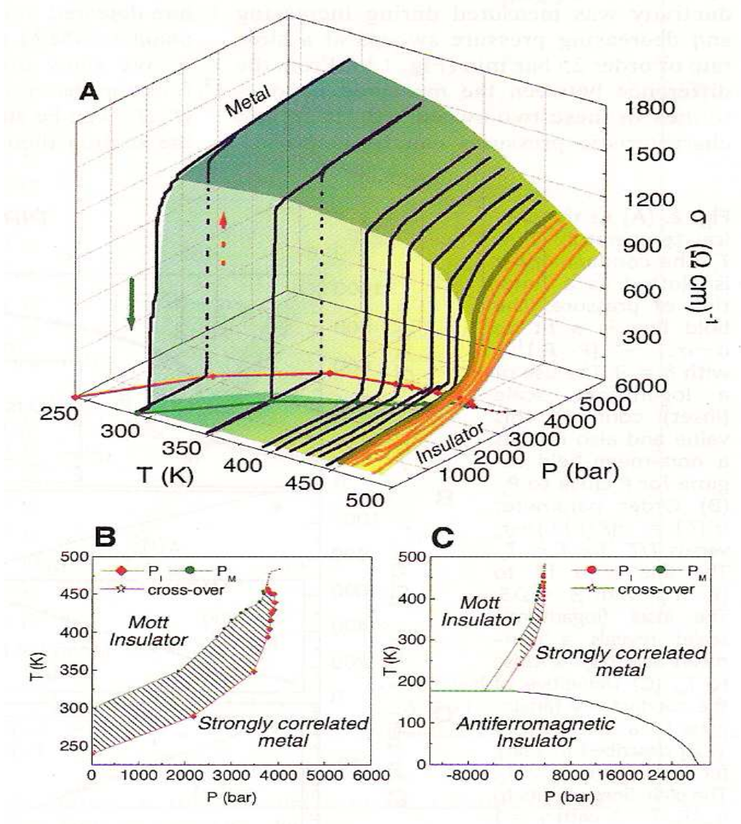
$$U = \int d_3r d_3r' \; \Phi_i^*(\mathbf{r}) \Phi_i^*(\mathbf{r}') \frac{e}{|\mathbf{r}-\mathbf{r}'|} \Phi_i(\mathbf{r}') \Phi_i(\mathbf{r})$$

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

Canonical example: V_2O_3

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





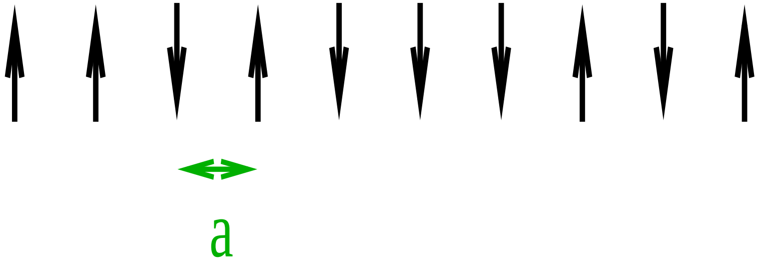
True Mott insulator

persists above T_N

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

Slater insulators

Weak coupling insulator due to LRO

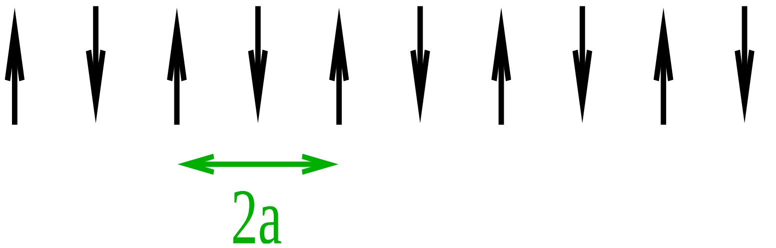


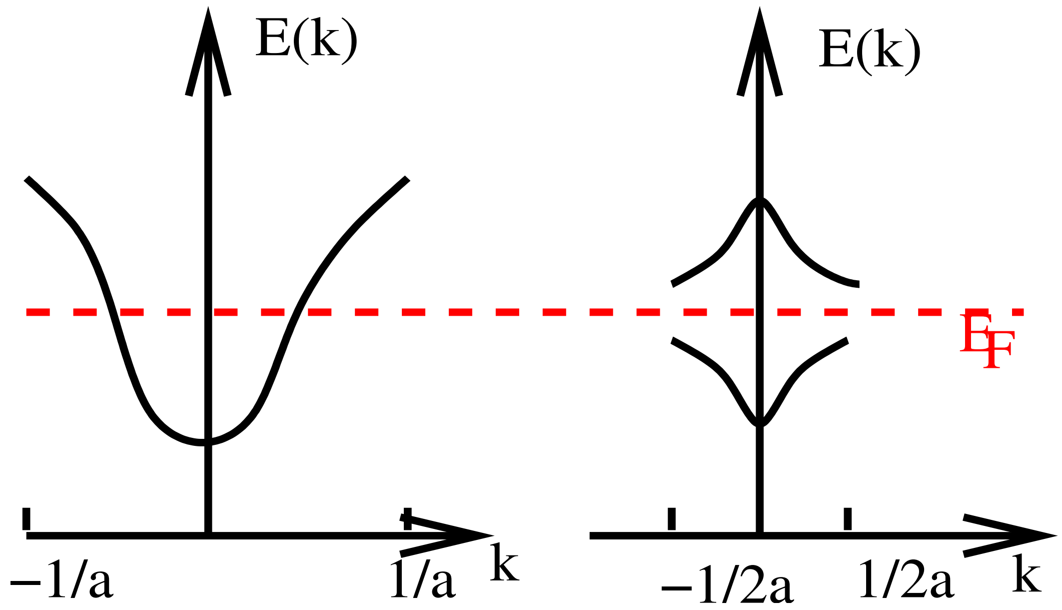
soft – gap in SSB at $T < T_c$

spin – density wave (SDW)

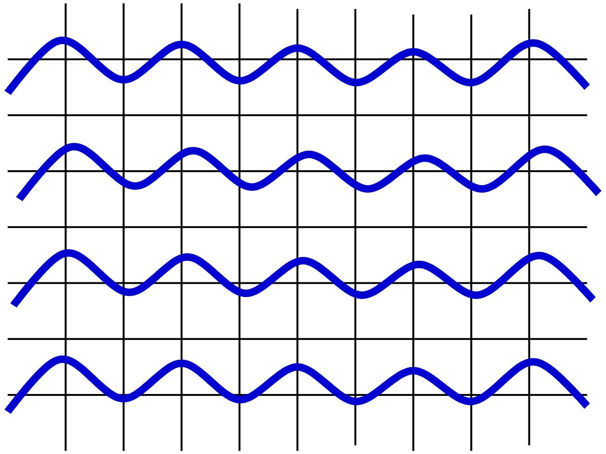
$\langle S^z(x) \rangle \sim \Delta \cos(2k_F x)$

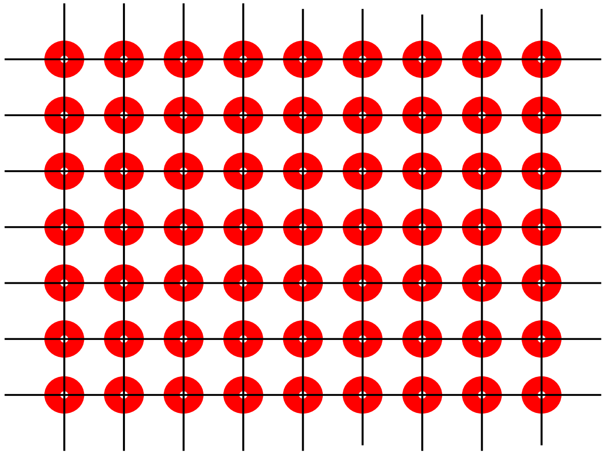
$E(k) = E_F \pm \sqrt{\epsilon_k^2 + \Delta^2},\ \Delta(T) \sim \sqrt{T_c - T}$





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

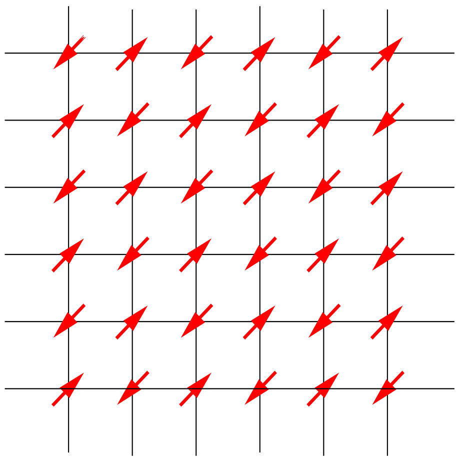




$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$

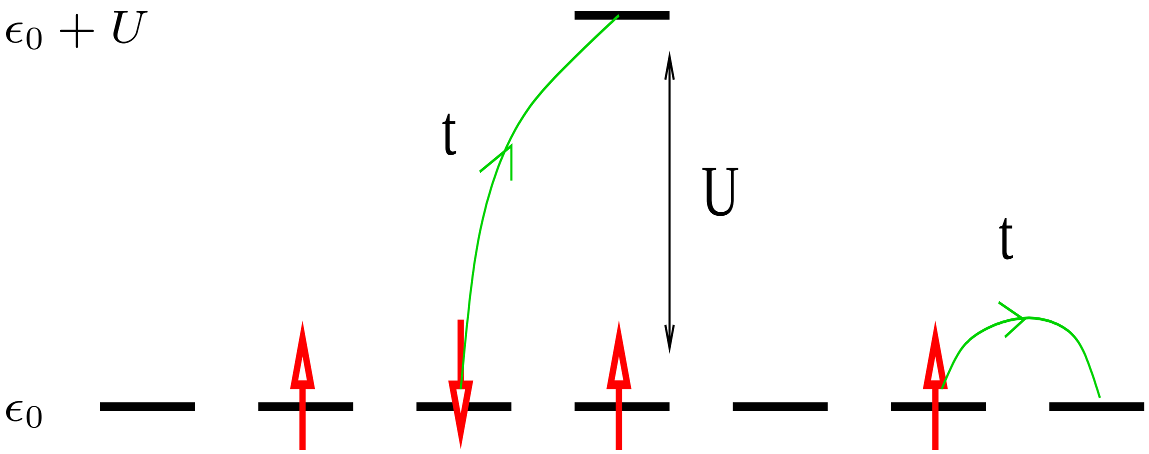
$U \gg |t_{ij}|$, $\Delta\mathbf{r} = 0$

Antiferromagnetic Mott insulator



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

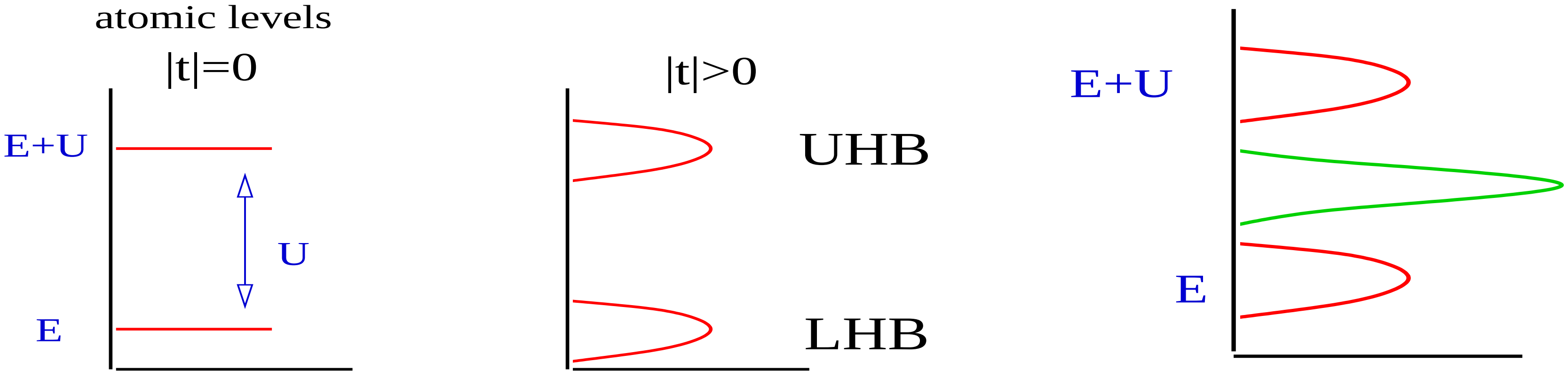
Hubbard model to capture right physics



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

- 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

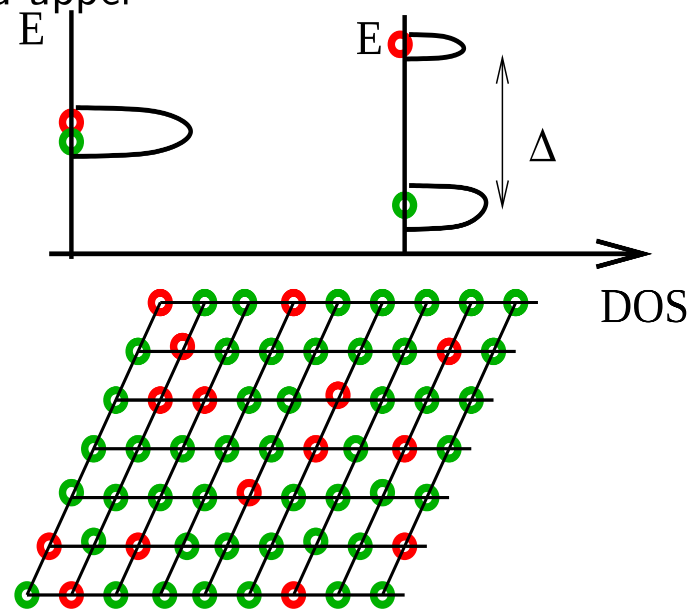
Mott MIT in binary alloy

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



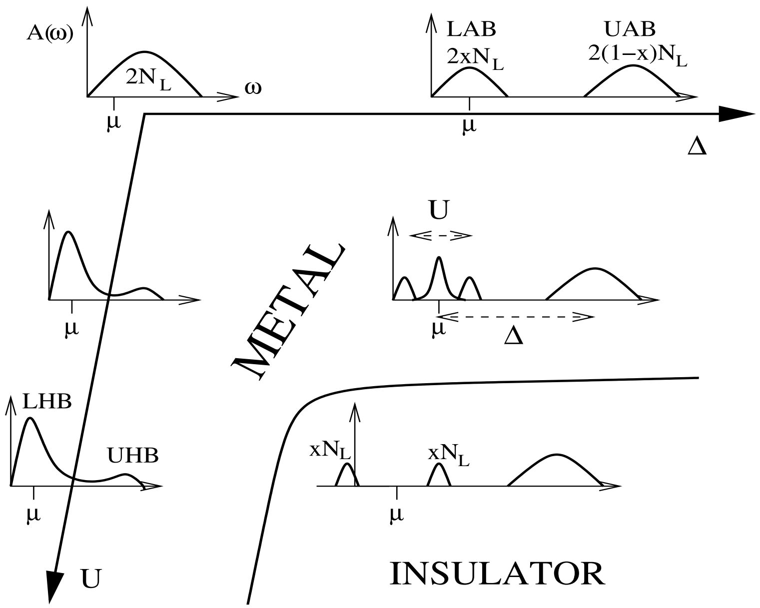
Is there Mott MIT at $n \neq 1$?

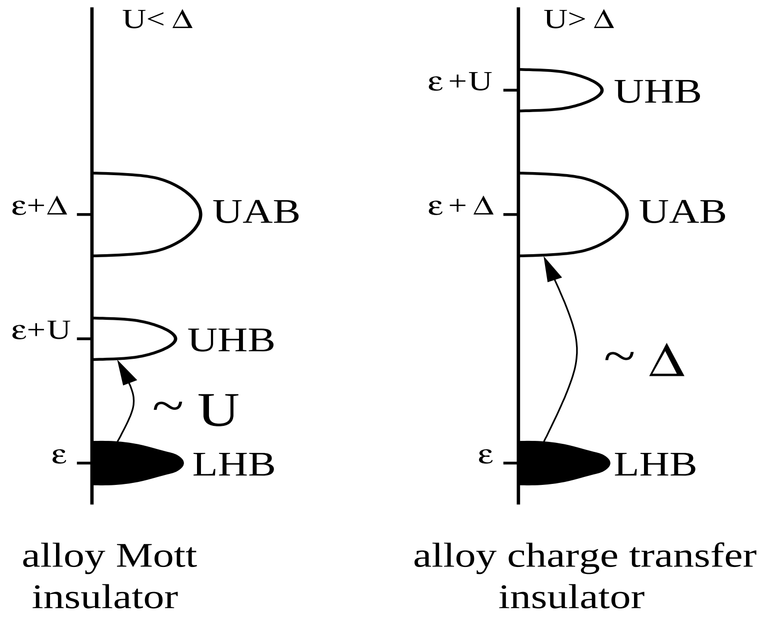
DMFT + $G(\omega) = \int d\epsilon_i \mathcal{P}(\epsilon_i) G(\omega, \epsilon_i)$

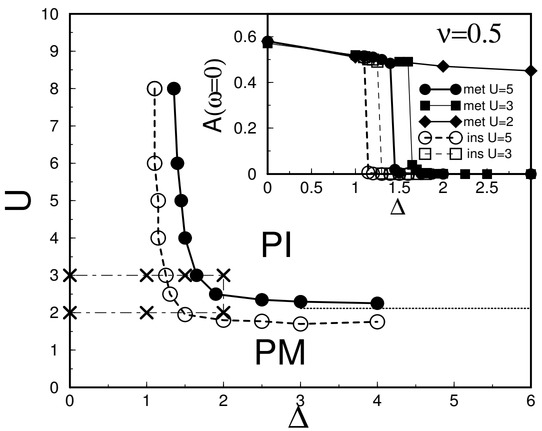
Mott MIT in binary alloy at $n \neq 1$

Byczuk et al., PRL03, PRB04

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







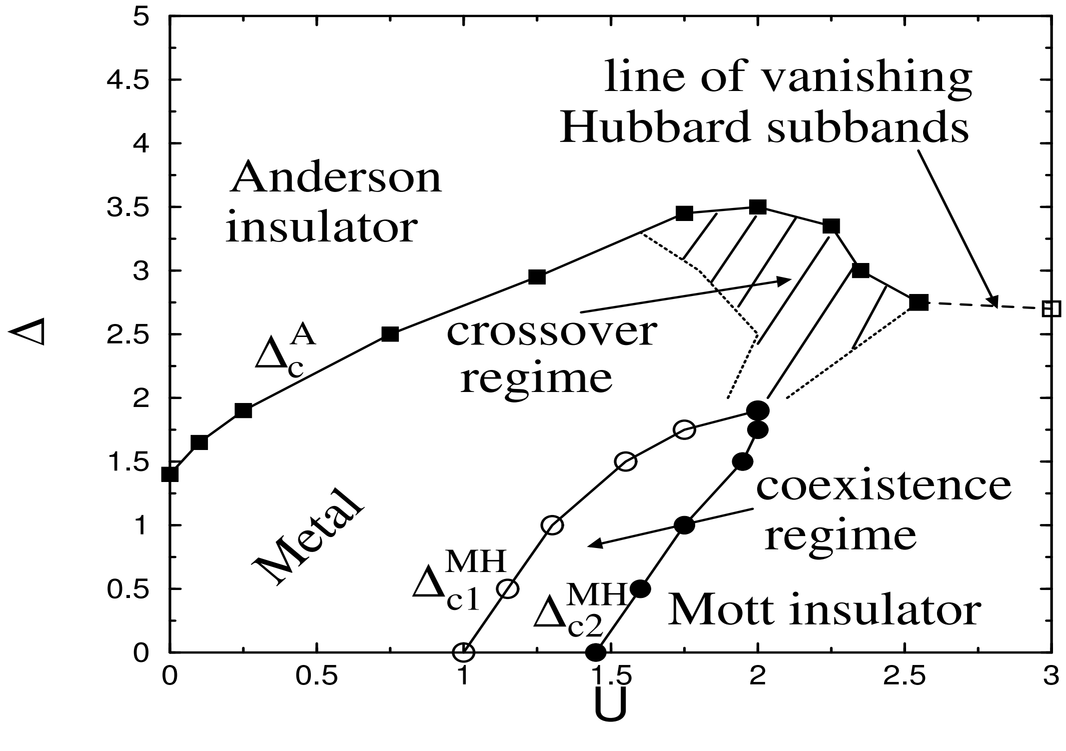
$$U_c^{\Delta\to\infty} = 6t^*\sqrt{x}$$

Anderson and Mott transitions:

Byczuk et al. PRL05, PhysicaB05

$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4}G(\omega)$$

$T = 0$, $n = 1$, $W = 2D = 1$, continous disorder, geometrical averaging



U - interaction, Δ - disorder

Summary

- Conductors and insulators, classification
- 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
- Anderson and Mott MIT at $n = 1$