Center for
Electronic Correlations and Magnetism
University of Augsburg

Theory of correlated fermionic condensed matter

3. Correlation-induced phenomena in electronic systems

b. Electronic correlations and disorder

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 8, 2009

Dieter Vollhardt

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Outline:

- Metal-Insulator transitions: Examples
- Disorder and averaging
- Mott-Hubbard transition vs. Anderson localization

In collaboration with:

Krzysztof Byczuk
Walter Hofstetter

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:

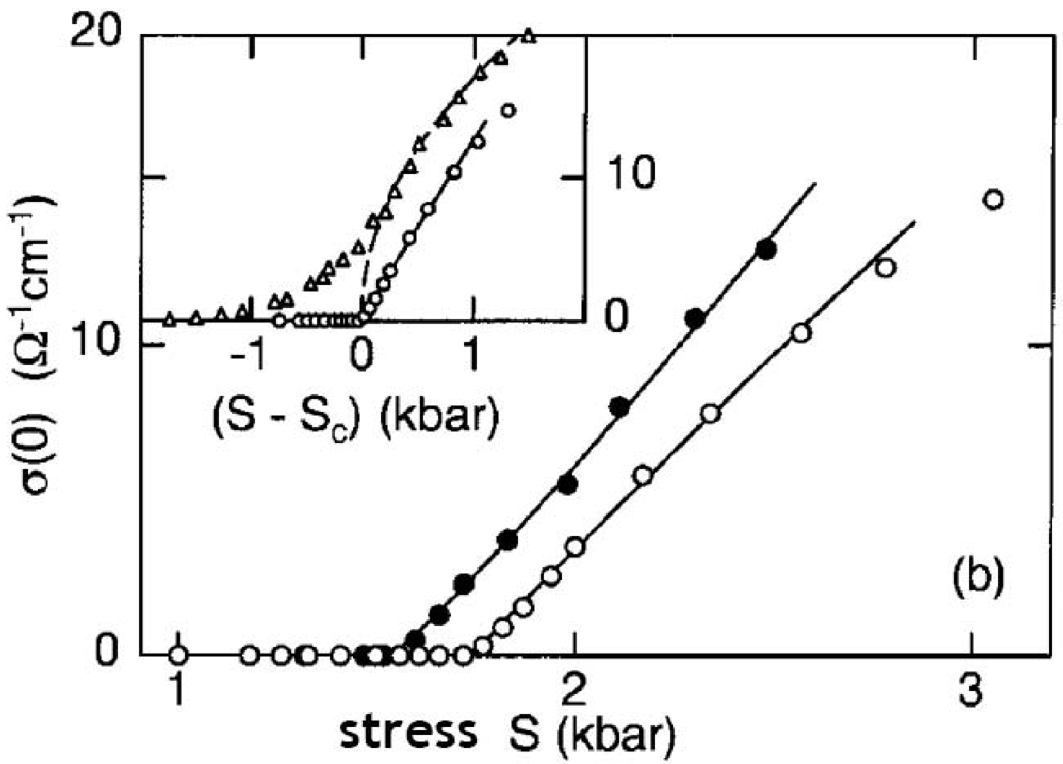
single-particle effects vs. many-particle effects

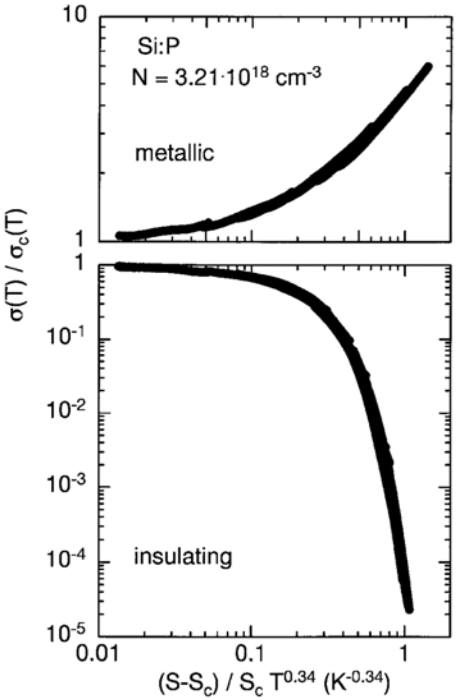
single-particle effects	many-particle effects
Band filling (Bloch-Wilson)	Electronic correlations (Mott-Hubbard)
Lattice deformations (e.g., Peierls)	Long-range order (Slater, Heisenberg,...)
Disorder/randomness (Anderson)	

Metal-Insulator Transitions in the Presence of Disorder: Examples

Anderson metal-insulator transition:
(disorder induced)

d=3

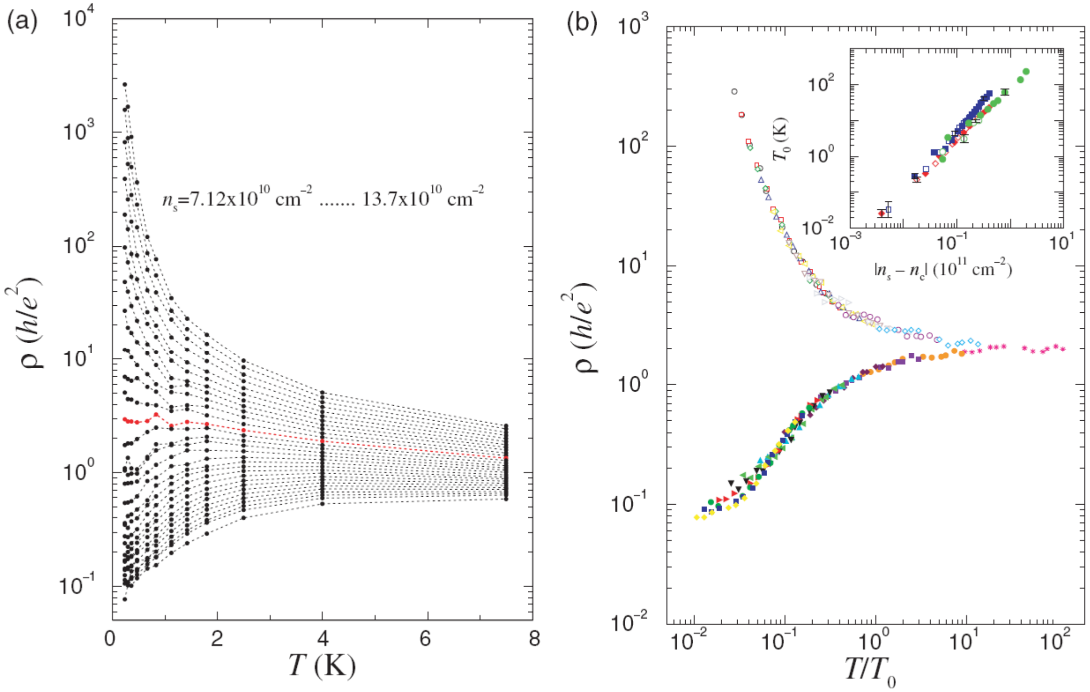




Waffenschmidt, Pfleiderer, v. Löhneysen (1999)

Metal-insulator transition in a dilute, low-disordered Si MOSFET

d=2



Kravchenko, Mason, Bowker, Furneaux, Pudalov, D'Iorio (1995)

Disorder
(quenched)

Anderson disorder model on the lattice

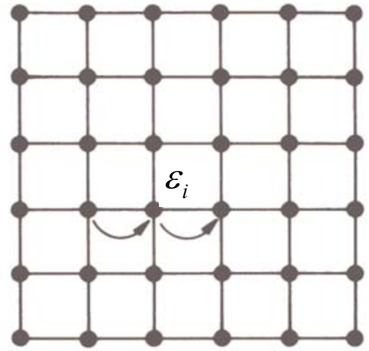
$$H = \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} t_{ij} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$

Random hopping (t_{ij}) — Random local potential (ε_i)

Anderson disorder model on the lattice

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$

Random local potential



Disorder → Scattering of a (quantum) particle

Scattering time τ →

$$\Sigma(\omega = 0) \propto \frac{1}{\tau}$$

Weak scattering (d=3)

$$\sigma(0) \equiv \sigma_0 = \frac{e^2 n}{m} \tau$$

Drude/Boltzmann conductivity

Anderson disorder model on the lattice

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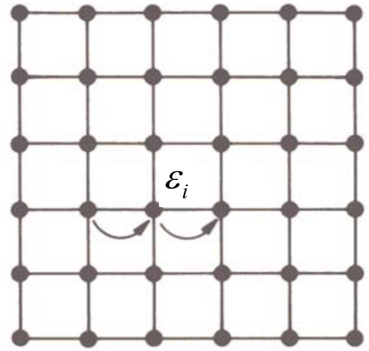
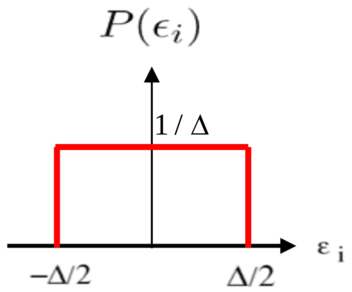
Random local potential



Disorder distributions, e.g.,:

Box disorder

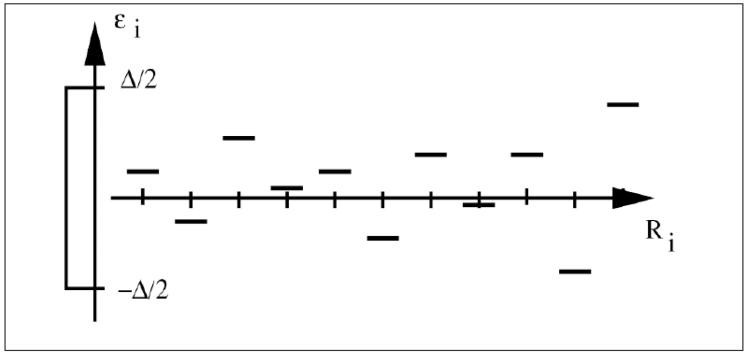
$$P(\epsilon_i) = \frac{\Theta(\frac{\Delta}{2} - |\epsilon_i|)}{\Delta}$$



Δ: disorder strength

$$\langle O_i \rangle_{\text{arith}} = \int d\varepsilon_i P(\varepsilon_i) O_i$$

e.g., local DOS $\langle \rho(\varepsilon_i) \rangle_{\text{arith}}$



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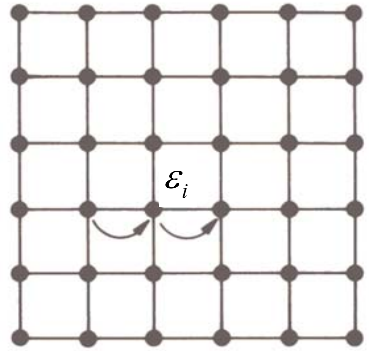
Random local potential



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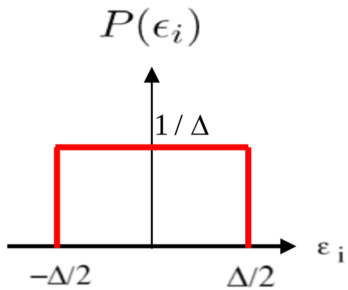

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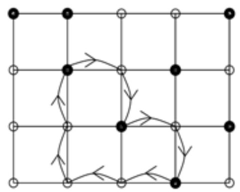
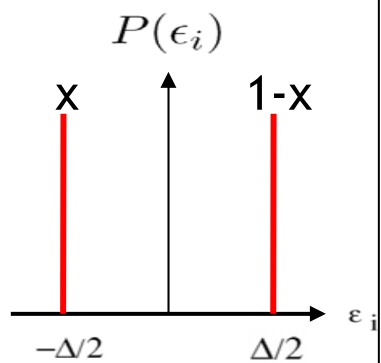
Binary alloy disorder (alloys $A_{1-x}B_x$, *e.g.*, $Fe_{1-x}Co_x$)

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





Disorder affects wave fct. $\psi(\mathbf{r}) = |\psi(\mathbf{r})| e^{i\phi(\mathbf{r})}$

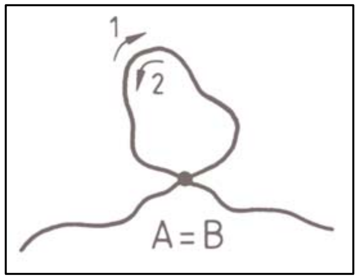
Localization of a particle, $\sigma(0) = 0$, due to, *e.g.*,

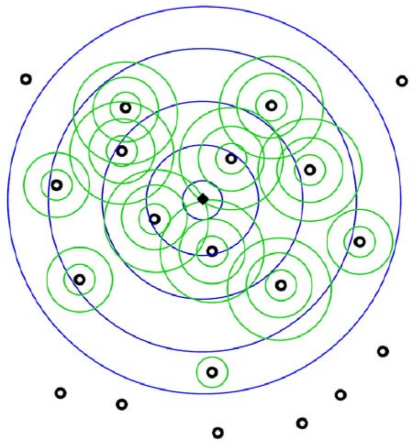
Anderson localization

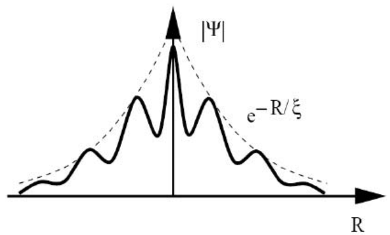
$\Delta \geq \Delta_c$: Anderson localization (1958)
due to coherent back scattering

$\Delta_c \begin{cases} = 0, & d=1,2 \\ > 0, & d=3 \end{cases}$

Strong scattering $\Rightarrow$ „standing" electronic waves







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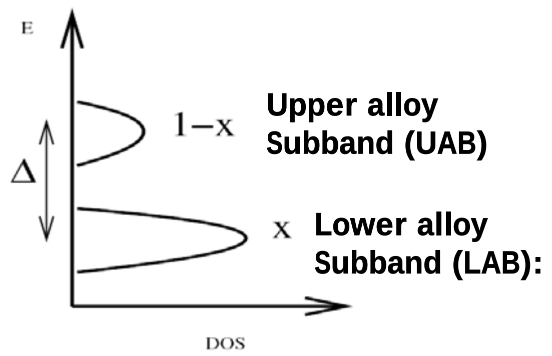
Alloy band splitting

Binary alloy disorder, bounded Hamiltonian

$\Delta > \Delta_c \gg \max(|t|, U), \text{ for } d \geq 1$



DMFT for disordered systems

Anderson disorder model on the lattice

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$

Coherent potential approximation (CPA)
("best single-site approximation")

Soven (1967)
Taylor (1967)

- robust results for $\langle \rho(\varepsilon_i) \rangle_{\text{arith}}$
- cannot describe Anderson localization

Example: CPA results for phonon DOS for disordered cubic crystal

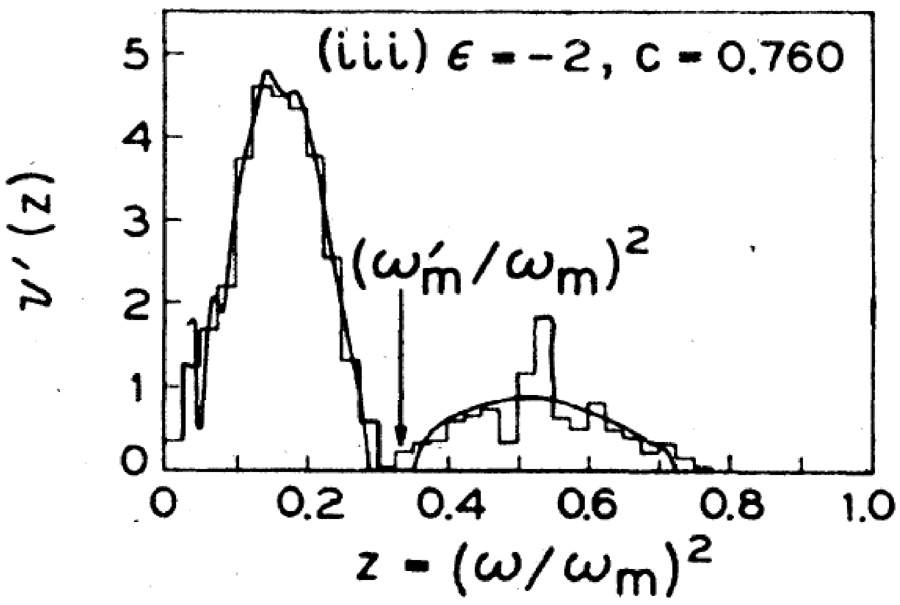


FIG. 20. The phonon density of states $\rho(\omega^2)$ versus $\omega^2/\omega_M{}^2$ for disordered simple cubic lattices with $M_B = 3M_A$ at four concentrations c of B atoms. A comparison between the CPA (solid line) and the machine calculations of Payton and Visscher (1967) [after Taylor (1967)].

Elliot, Krumhansl, Leath (RMP, 1974)

Coherent Potential Approximation and $d\to\infty$

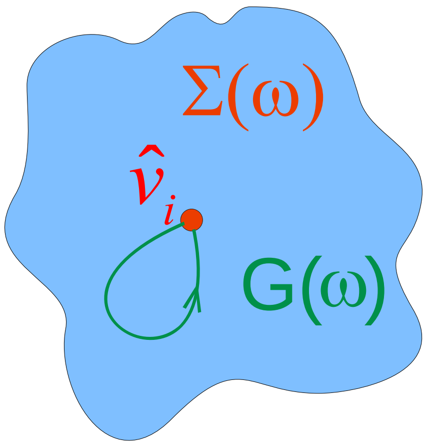
CPA = exact solution of the Anderson disorder model in $d\to\infty$

Vlaming, DV (1992)

More precisely: DMFT with $\langle\rho(\varepsilon_i)\rangle_{\text{arith}} \Leftrightarrow$ CPA

Generalization of DMFT to disordered and interacting lattice electrons

Janiš, DV (1992)



Local potential operator:

$$\hat{v}_{i\sigma}=\tfrac{1}{2}U\hat{n}_{i,-\sigma}+\epsilon_i-\mu_\sigma$$

Mott-Hubbard Transition
vs.
Anderson Localization

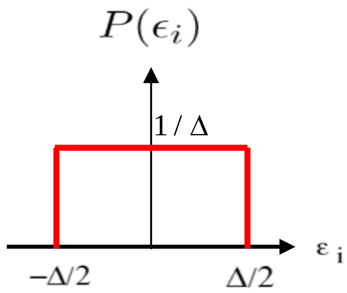
Anderson-Hubbard Hamiltonian

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

n=1

Box disorder

$$P(\epsilon_i) = \frac{\Theta(\frac{\Delta}{2} - |\epsilon_i|)}{\Delta}$$



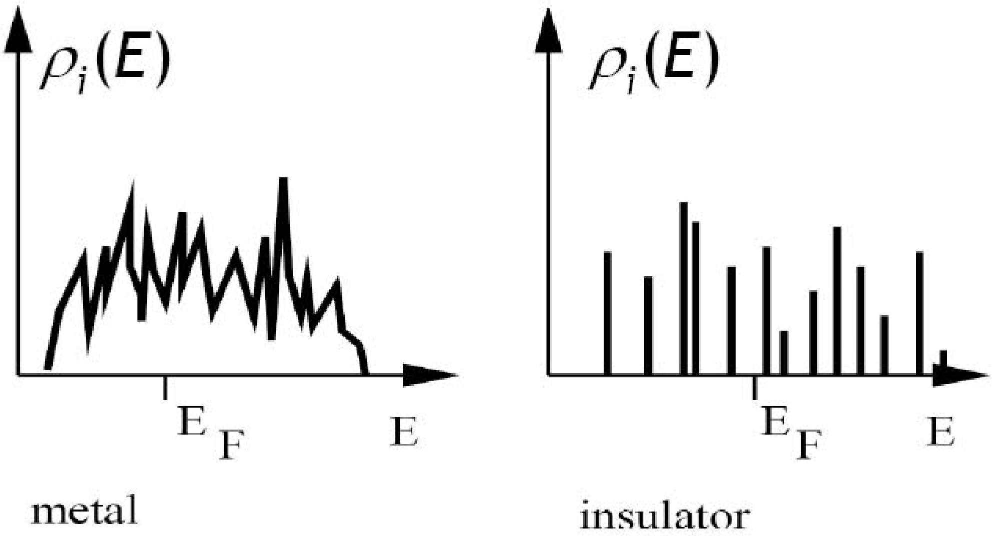
Δ: disorder strength

Δ=0: Mott-Hubbard metal-insulator transition for $U>U_c$
U=0: Anderson localization for $\Delta > \Delta_c > 0$ in d>2

1. Can both transitions be characterized by the average local DOS?
2. Further destabilization of correlated metallic phase by disorder?
3. Are the Mott insulator and Anderson insulator separated by another (metallic) phase?

Anderson localization characterized by

local density of states (LDOS) $\rho_i(E)$ Anderson (1958)



Search for „typical“ value of $\rho_i(E)$

= most probable value
= maximum of probability distribution function (PDF)

Usually unknown

Approximation of PDF: calculate averages + moments

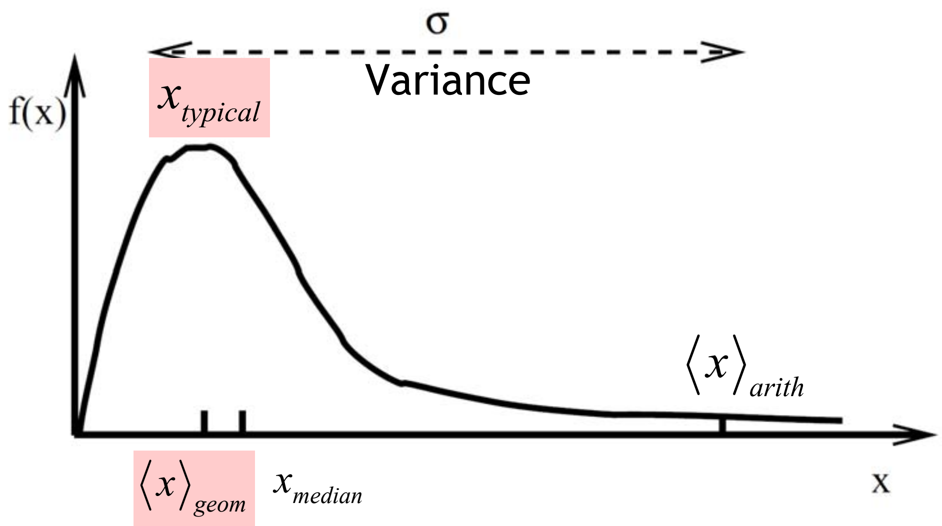
$\langle \rho_i(E) \rangle_{arith} > 0$ Wegner (1981)

→ cannot detect localization

Why? Because arithmetic average does not yield the max. of the PDF!

Which averages?

PDF of disordered systems: very broad/long tails



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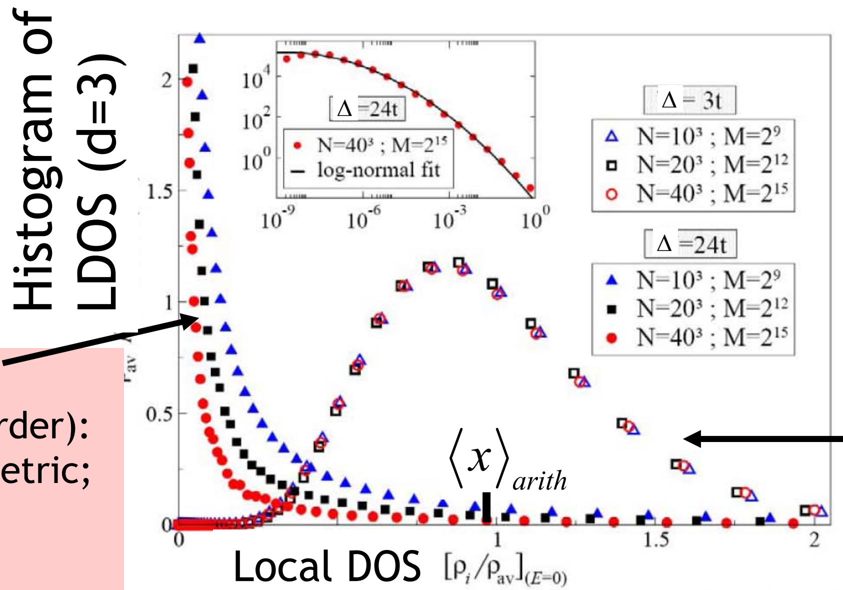
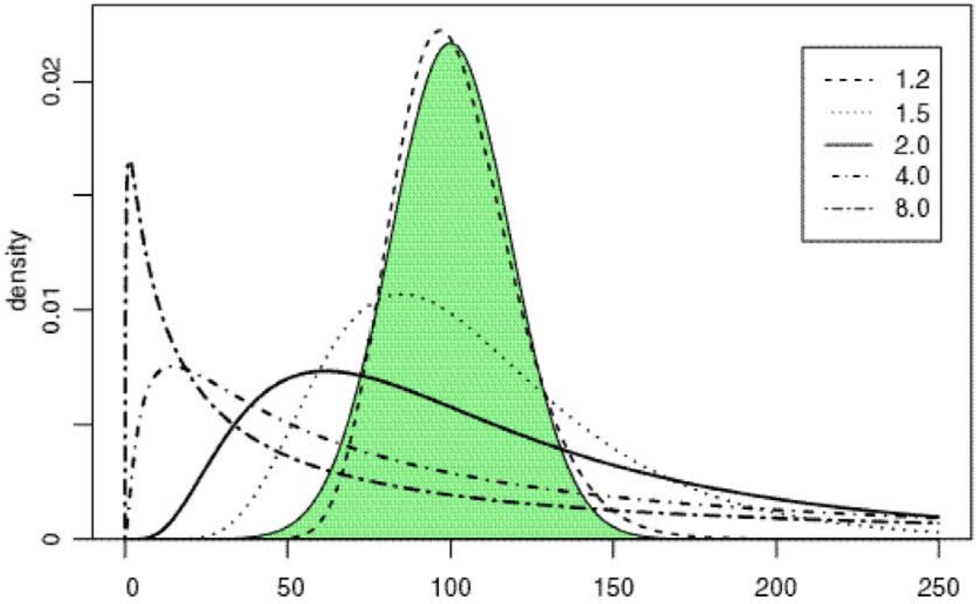


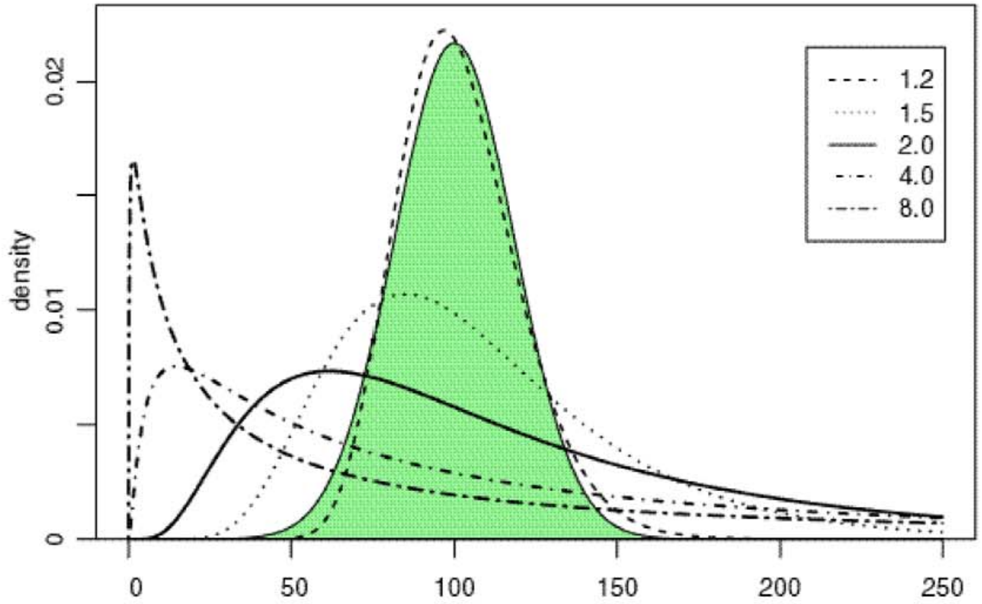
Localized (strong disorder): Very asymmetric; Long tails (Log-normal distribution)

Metallic (weak disorder): Rather symmetric; peak close to arithmetic mean

Schuberth, Weiße, Fehske (2003/2005)



Property	Normal distribution (Gaussian, or additive normal,distribution)		Log-normal distribution (Multiplicative normal distribution)
	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma^2}\right)^2}$		$\frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{x} e^{-\frac{1}{2}\left(\frac{\ln x-\mu}{\sigma^2}\right)^2}$
	x	$\longrightarrow$	ln x
Effects (central limit theorem)	Additive		Multiplicative
Shape of distribution	Symmetrical		Skewed
Mean	$\bar{x}$, Arithmetic		$\bar{x}$* Geometric



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	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma^2}\right)^2}$	$\frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{x} e^{-\frac{1}{2}\left(\frac{\ln x-\mu}{\sigma^2}\right)^2}$
	x →	ln x

Life is log-normal

Limpert, Stahel (2001)

Anderson localization: $\rho_i(E)\big|_{\text{typical}} = \left\langle \rho_i(E) \right\rangle_{\text{geometric}} = e^{\langle \ln \rho_i(E) \rangle}$

Anderson (1958)

DMFT for Anderson-Hubbard model

$$G(\omega, \epsilon_i) \to \rho_i(\omega) = -\frac{1}{\pi}\mathrm{ImG}(\omega, \epsilon_\mathrm{i})$$

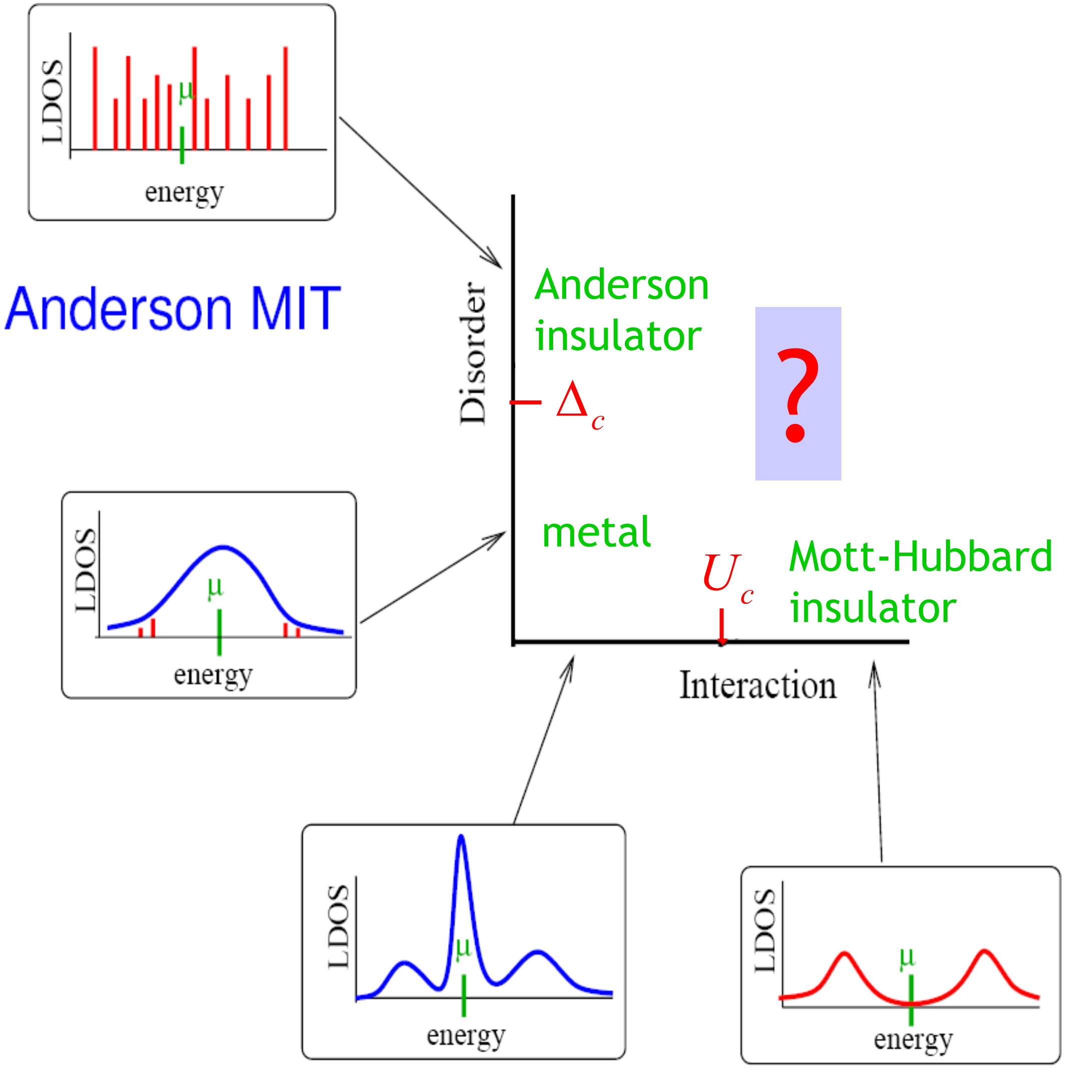
$$\rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'}$$

lattice Green function

Dobrosavljevic, Pastor, Nikolic (2003)

Mott-Hubbard Transition vs. Anderson Localization

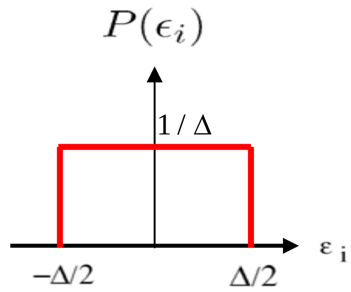
Disorder ↔ Anderson MIT



Interaction ↔ Mott-Hubbard MIT

Anderson-Hubbard Hamiltonian

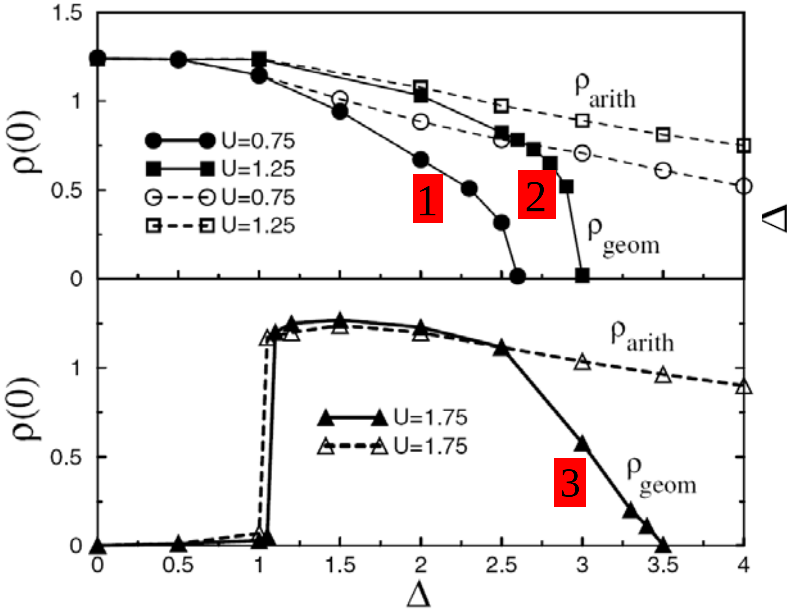
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$



Δ: disorder strength

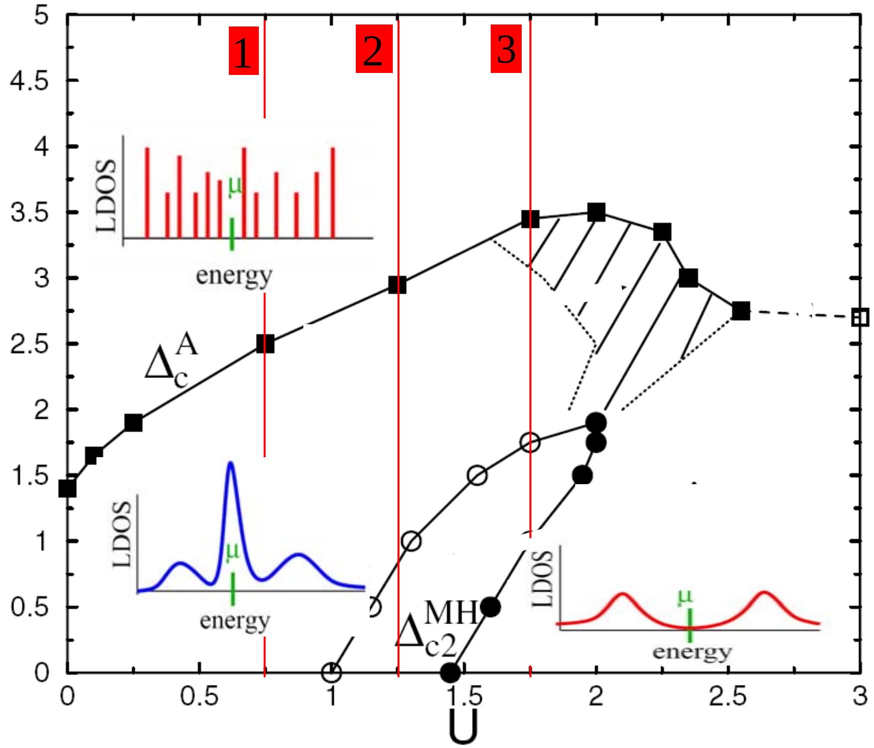
Solution by DMFT(NRG)

Local DOS



Critical behavior at localization transition

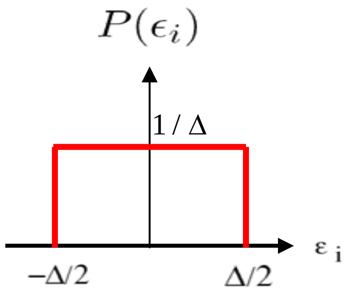
Non-magnetic phase diagram; n=1,T=0



Byczuk, Hofstetter, DV (2005)

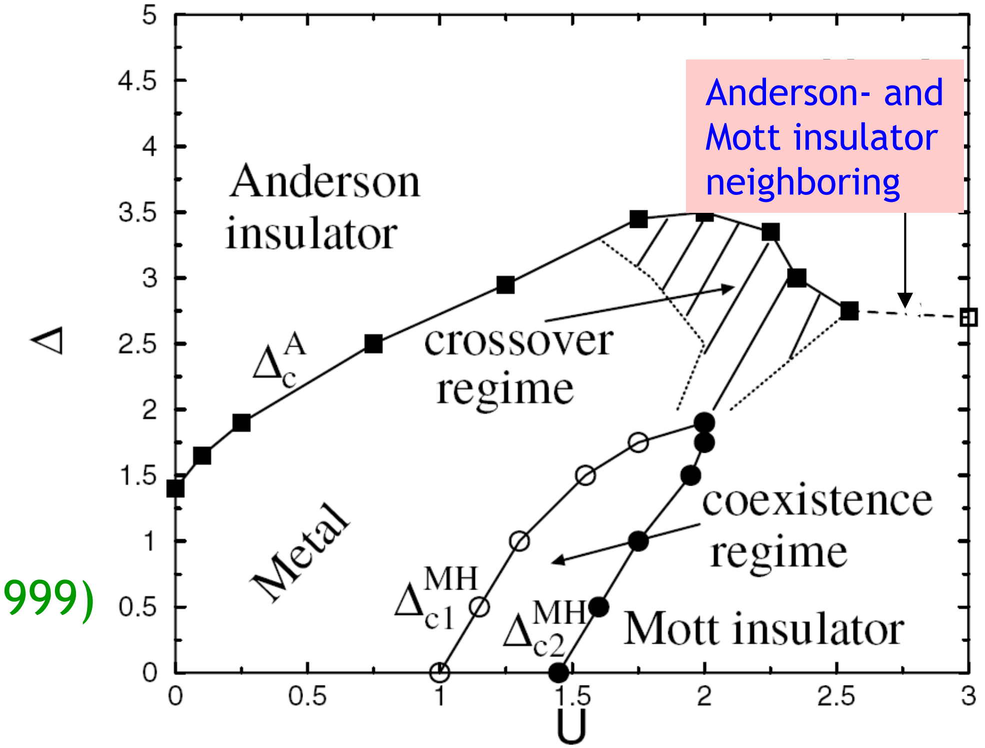
Anderson-Hubbard Hamiltonian

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



Δ: disorder strength

Non-magnetic phase diagram; n=1,T=0



Byczuk, Hofstetter, DV (2005)

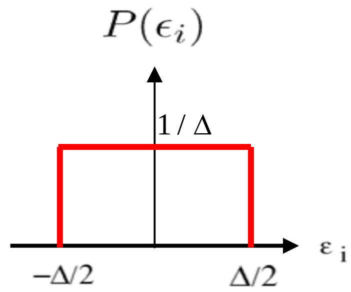
- Disorder increases U_c
- Interaction in/decreases Δ_c^A

→ Interactions may increase metallicity

d=2:
Denteneer, Scalettar, Trivedi (1999)

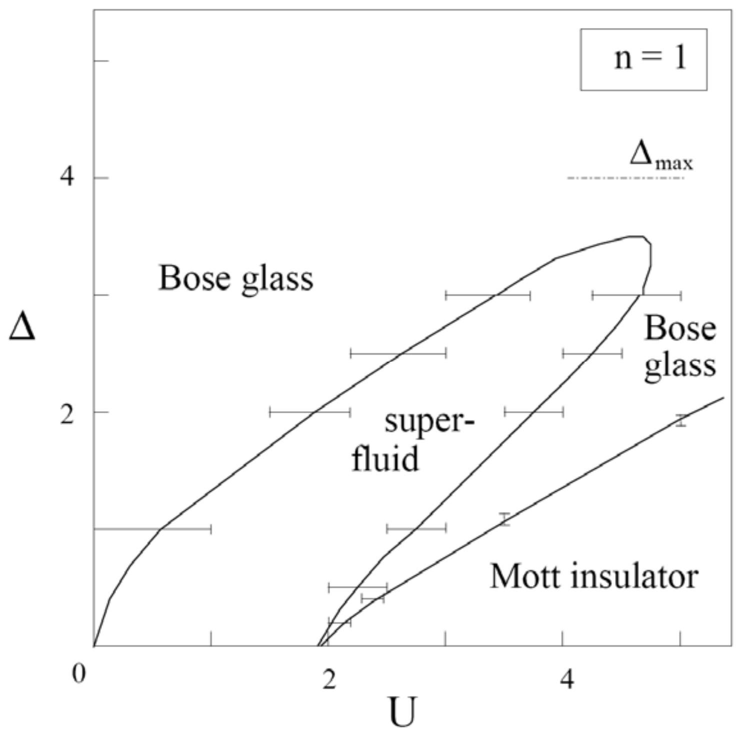
Anderson-Hubbard Hamiltonian

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



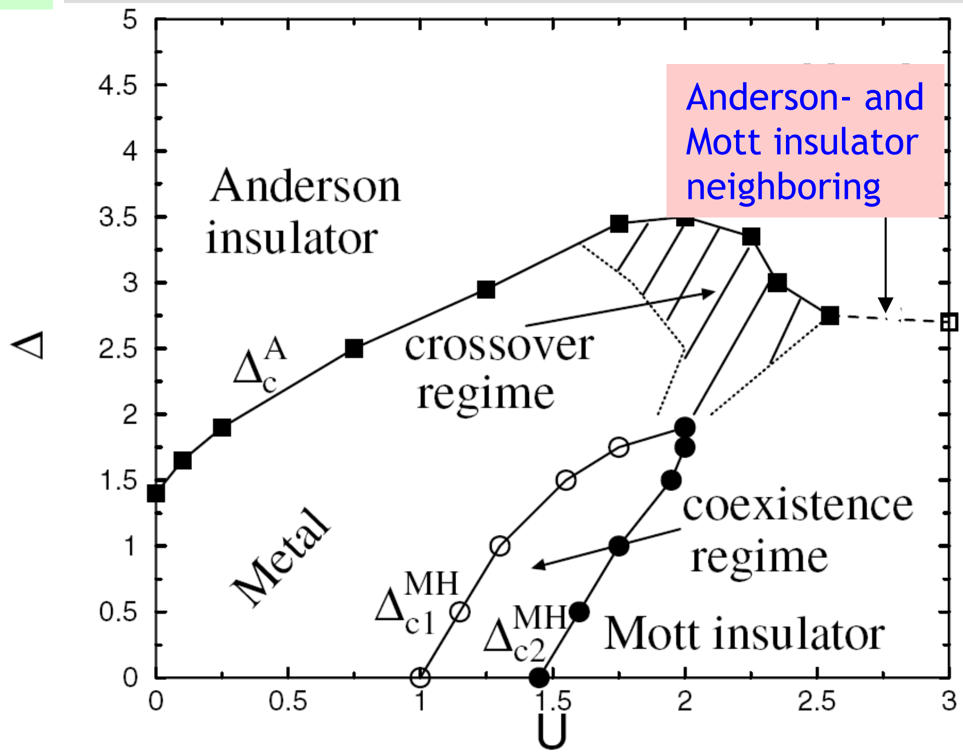
Δ: disorder strength

DMRG for disordered bosons in d=1



Rapsch, Schollwöck, Zwerger (1999)

Non-magnetic phase diagram; n=1,T=0



Byczuk, Hofstetter, DV (2005)

Antiferromagnetism
vs.
Anderson Localization

Anderson-Hubbard Hamiltonian

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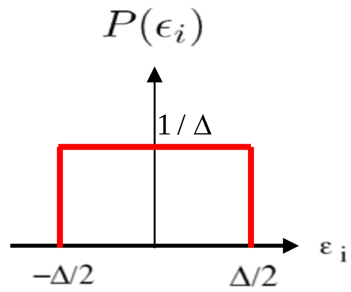
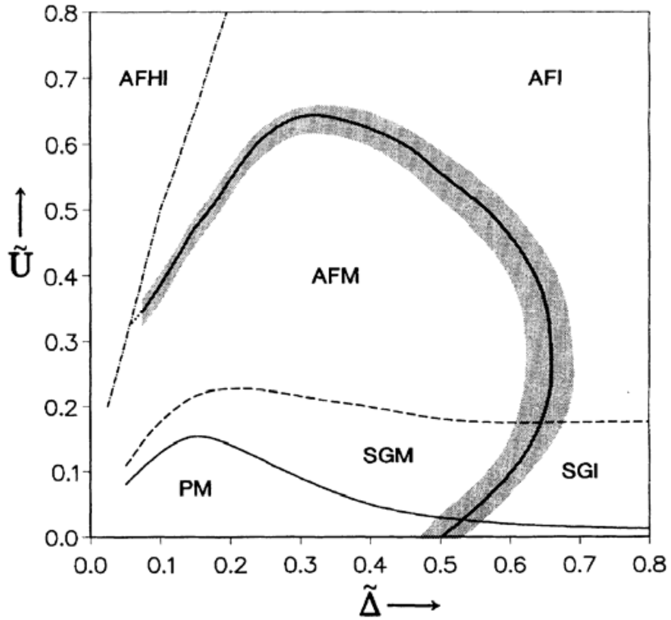


Δ: disorder strength

NN hopping, bipartite lattice, n=1:
Take into account antiferromagnetic order

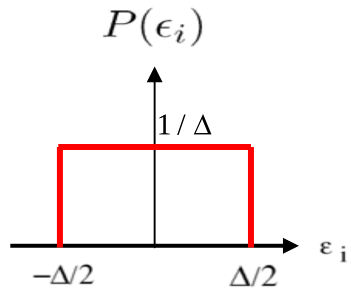
Unrestricted Hartree-Fock, d=3



Tusch, Logan (1993)

Anderson-Hubbard Hamiltonian

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



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NN hopping, bipartite lattice, n=1:
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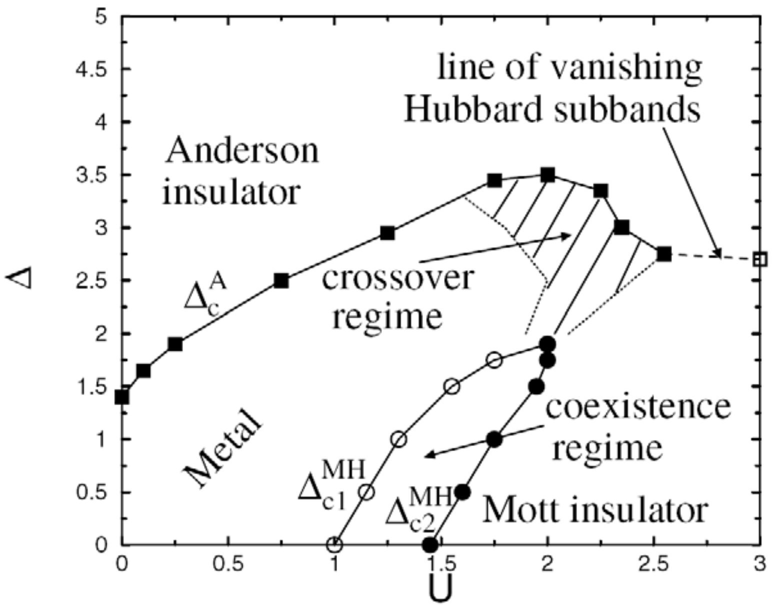
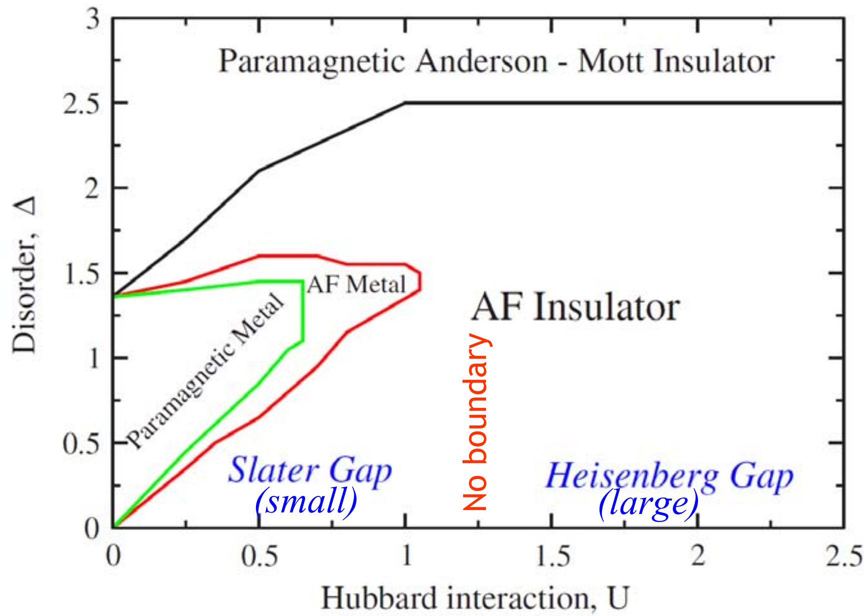
DMFT: Non-magnetic phase diagram



Magnetic phase diagram



Byczuk, Hofstetter, DV (2009)