Center for Electronic Correlations and Magnetism
University of Augsburg

Metal-insulator transitions of correlated lattice electrons in the presence of disorder

11th German-Japanese Symposium
New Quantum States and Phenomena in Condensed Matter

Hiroshima, Japan; September 15, 2010

Dieter Vollhardt

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Outline:

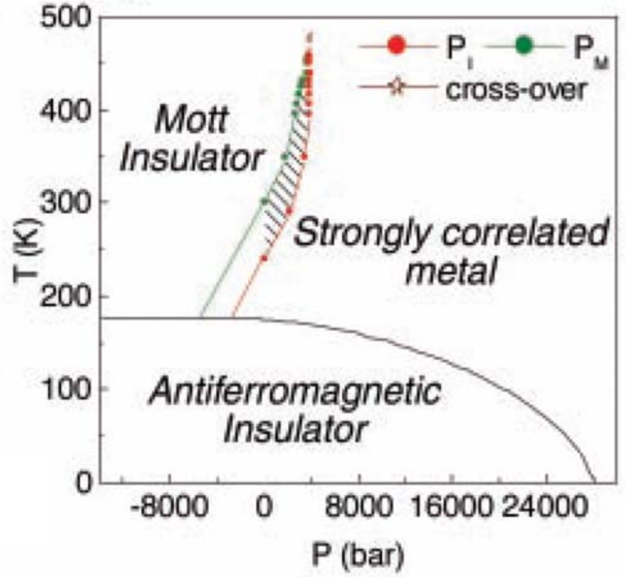
- Metal-Insulator transitions (MITs): Examples
- Anderson localization: local density of states and its probability distribution function
- Mott-Hubbard MIT vs. Anderson localization
- Universal critical conductivity at the MIT in d=2 ?

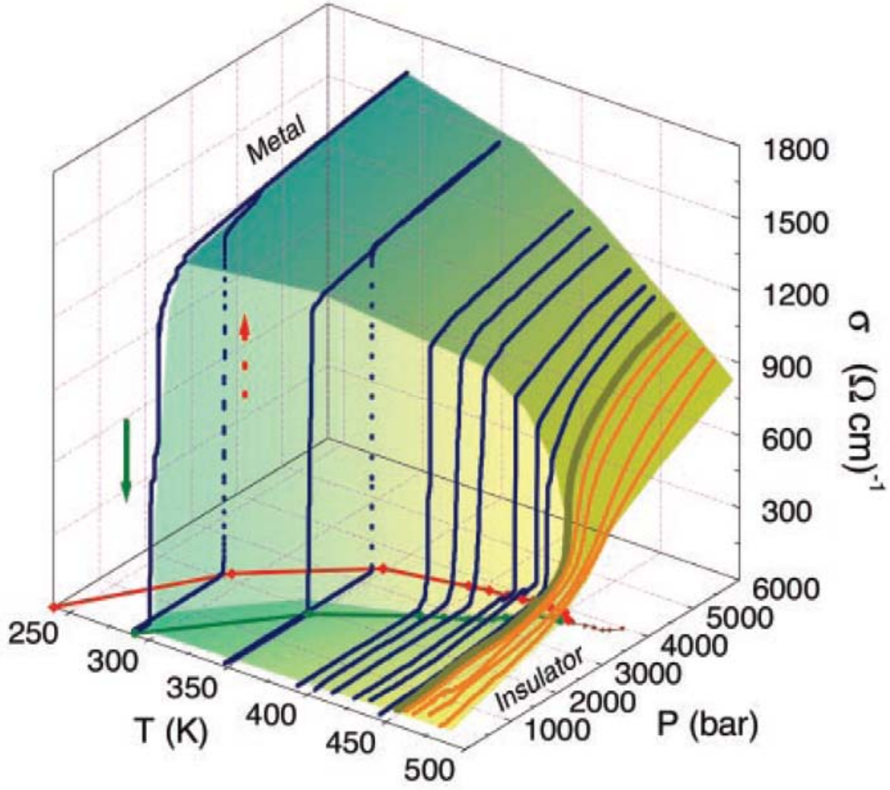
In collaboration with:

Krzysztof Byczuk (Augsburg, Warsaw)
Walter Hofstetter (Aachen, Frankfurt)

Prabuddha Chakraborty (Augsburg)

Mott-Hubbard MIT in V_2O_3 - driven by interactions d=3

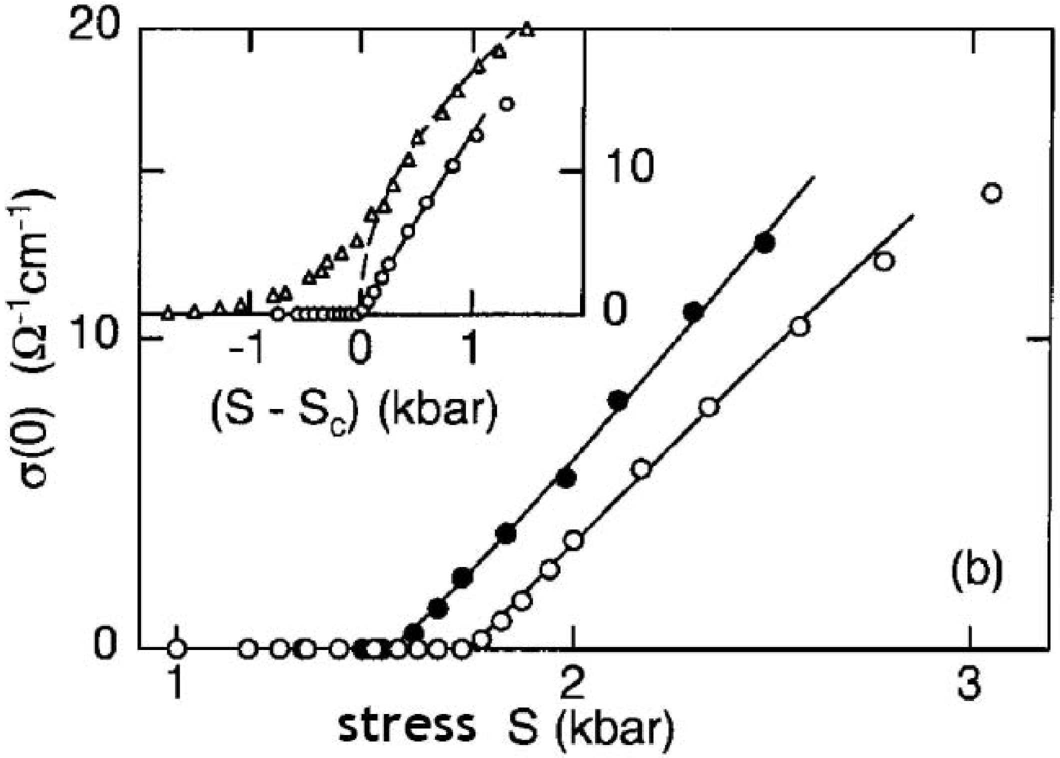


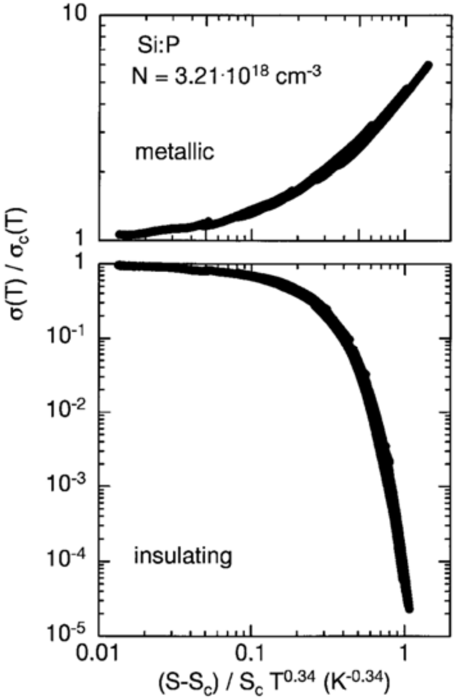


Limelette, Georges, Jérome, Wzietek, Metcalf, Honig (2003)

Anderson MIT in Si:P - driven by disorder

d=3

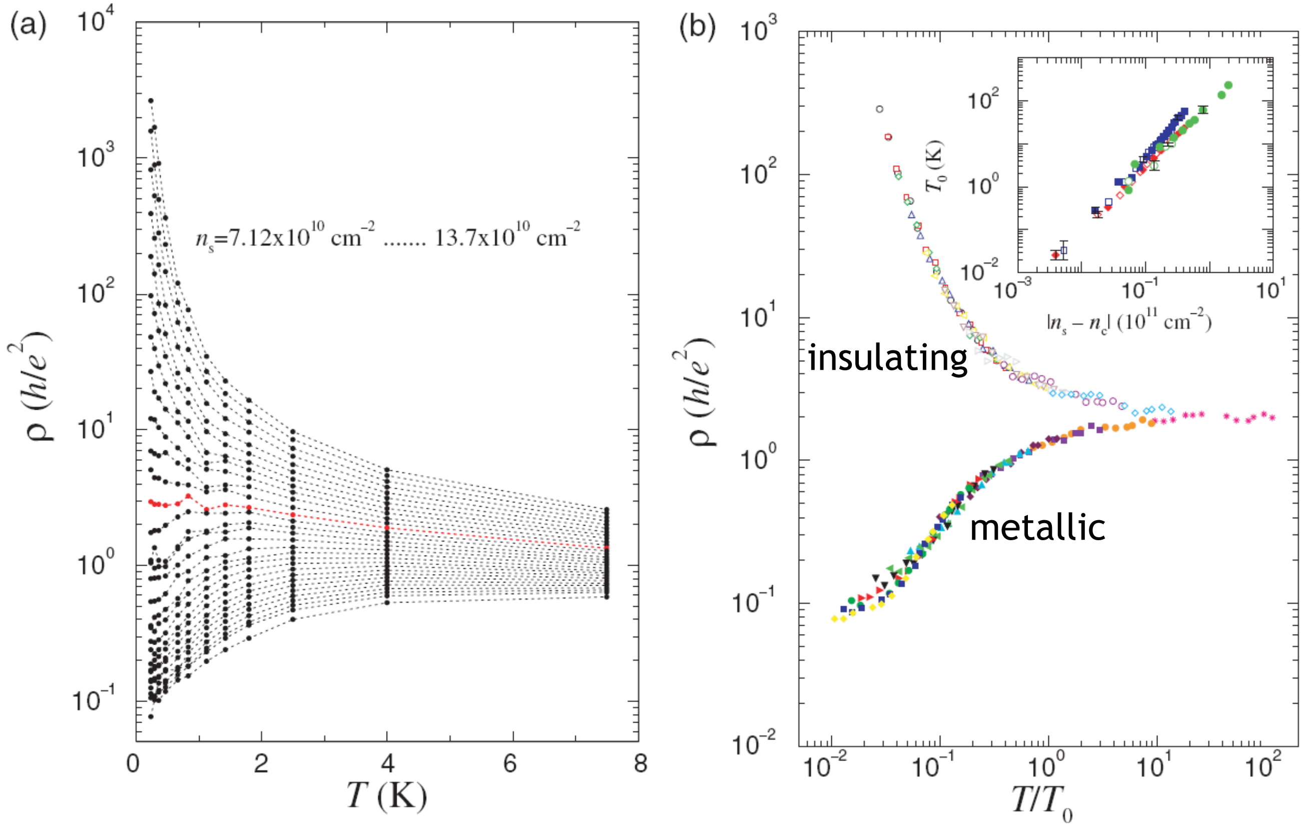




Waffenschmidt, Pfleiderer, v. Löhneysen (1999)

MIT in a dilute, low-disordered Si MOSFET - driven by interactions + disorder

d=2



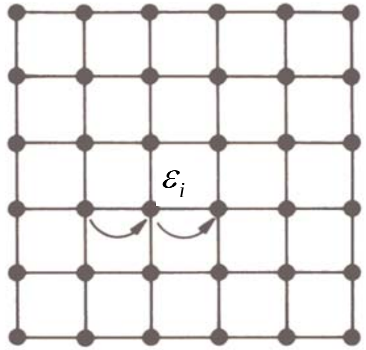
Kravchenko, Mason, Bowker, Furneaux, Pudalov, D’Iorio (1995)

Anderson Localization

Anderson disorder model on the lattice

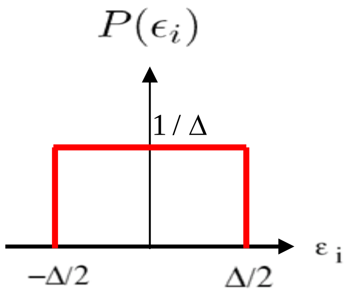
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$

Random local potential



Box disorder

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



Δ: disorder strength

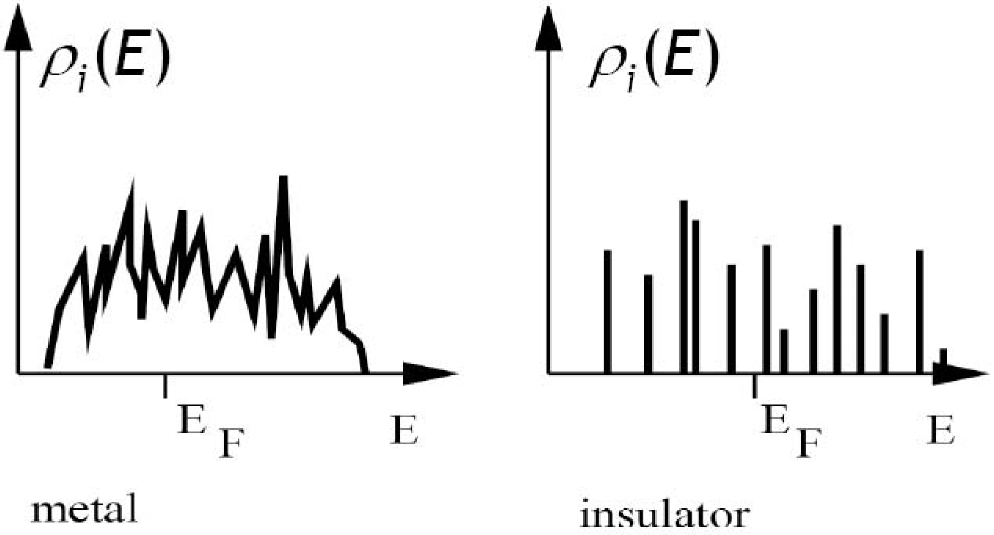
$$\langle O_i \rangle_{\text{arith}} = \int d\varepsilon_i P(\varepsilon_i) O_i$$

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

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

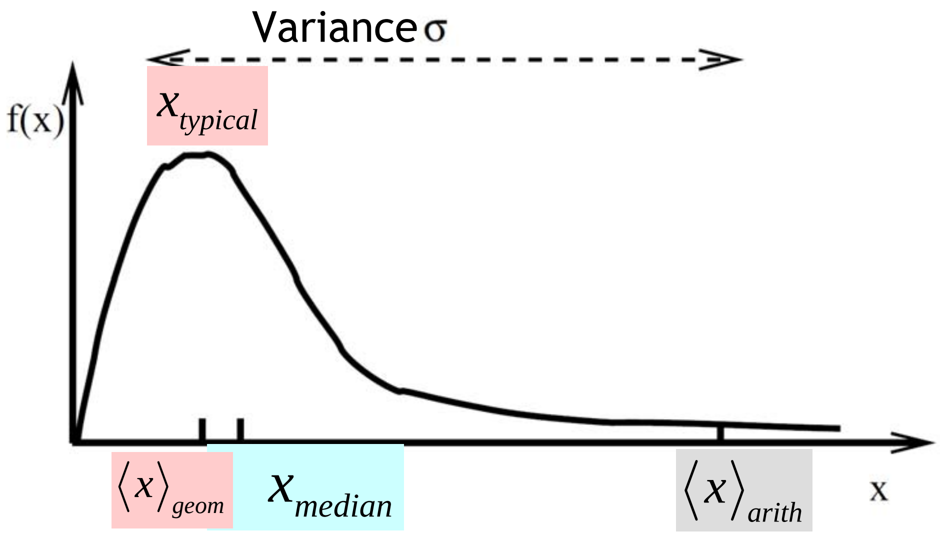
Why? Because arithmetic average does not yield the maximum of the PDF of the LDOS!

Which averages?

PDF of LDOS of disordered systems: very broad/long tails

“non-self-averaging“

Altshuler, Kravtsov, Lerner (1991)



Approximation of PDF: calculate averages + moments

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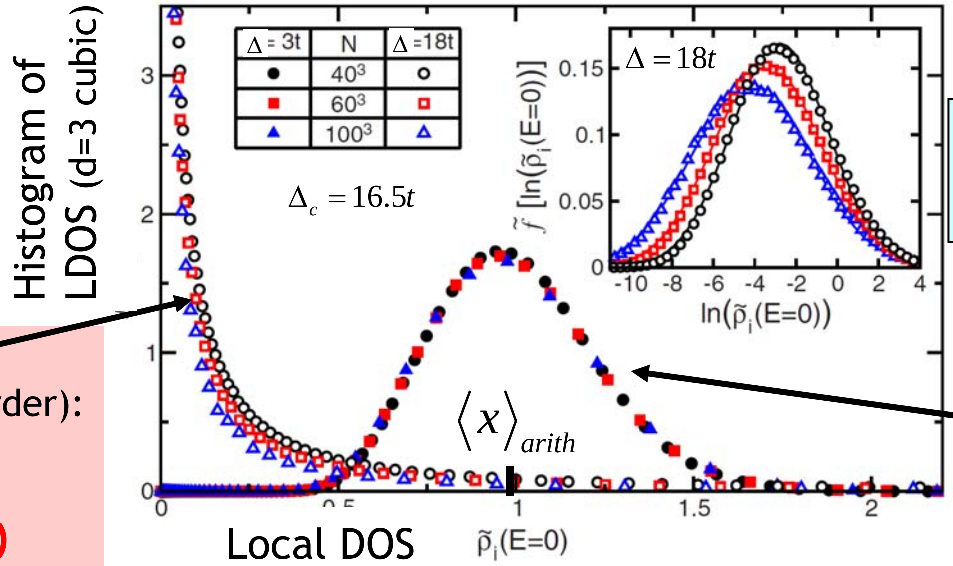


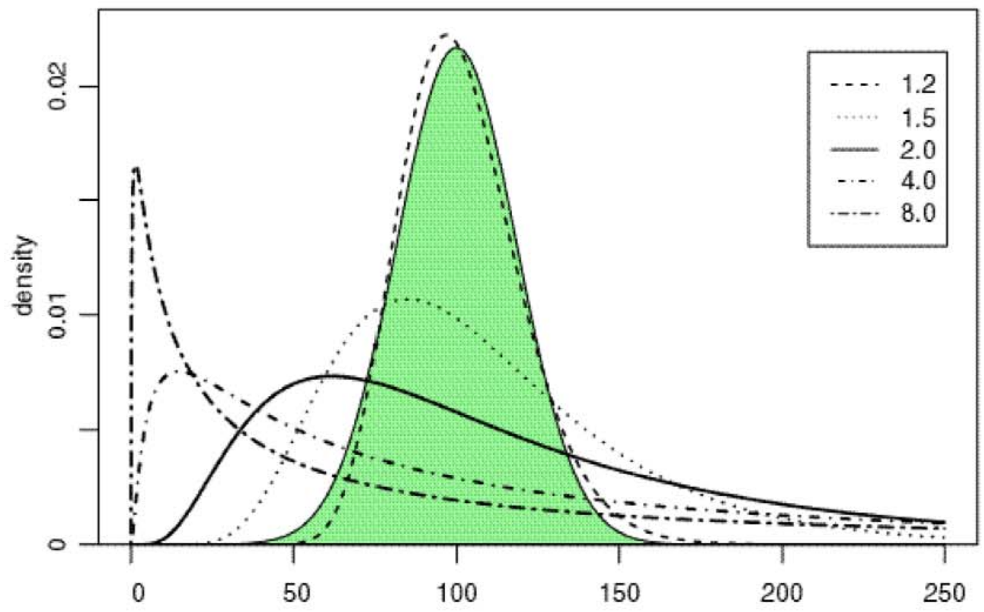
$\tilde{\rho}_i(E) = \rho_i(E) / \langle \rho_i(E) \rangle$

Schuberth, Schleede, Byczuk, Fehske, DV (2010)

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

Metallic (weak disorder):
~ Normal distribution; peak close to arithmetic mean

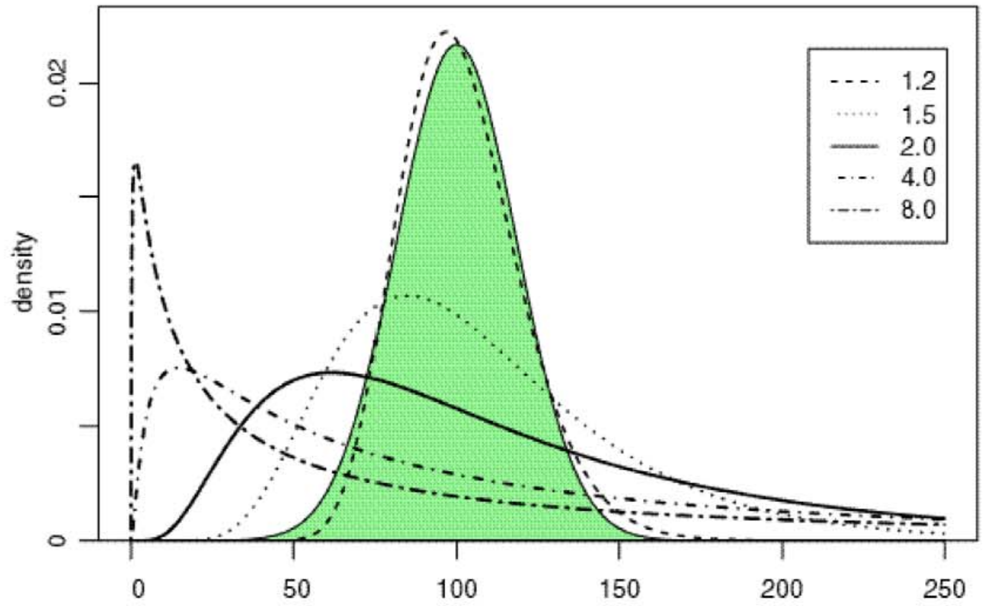
Similar PDF for conductance
Muttalib, Wölfle (1999)



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 →	ln x
Effects (central limit theorem)	Additive	Multiplicative
Mean	$\bar{x}$, Arithmetic	$\bar{x}^*$, Geometric

Life is log-normal

Limpert, Stahel (2001)



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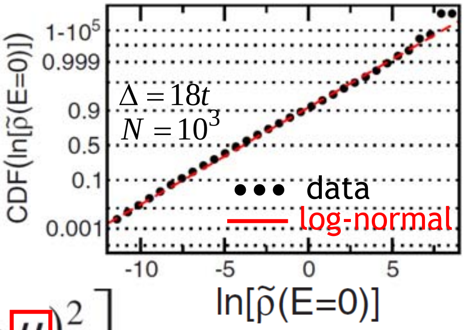
	x →	ln x
Effects (central limit theorem)	Additive	Multiplicative
Mean	$\bar{x}$, Arithmetic	$\bar{x}^*$, Geometric

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

Check log-normal distribution of LDOS



1. Normalized LDOS $\tilde{\rho}_i(E)=\rho_i(E)/\langle\rho_i(E)\rangle$

Log-normal distribution $\phi_0(\tilde{\rho}_i)=\frac{1}{\sqrt{2\pi\sigma_0^2}}\frac{1}{\tilde{\rho}_i}\exp\left[-\frac{(\ln\tilde{\rho}_i-\boxed{\mu})^2}{2\boxed{\sigma_0^2}}\right]$

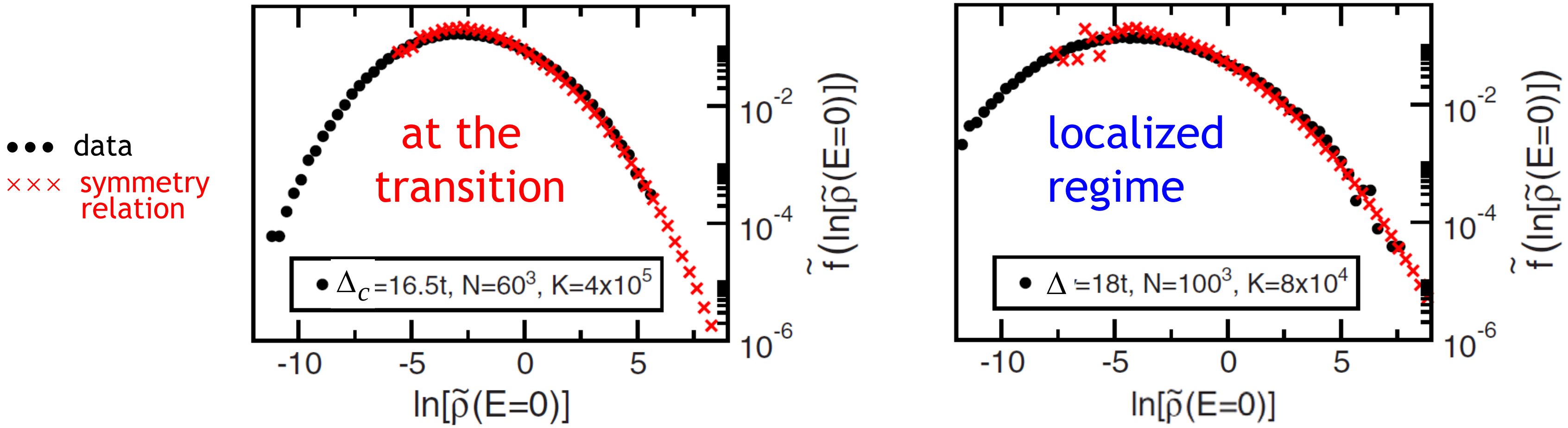
Schuberth, Schleede, Byczuk, Fehske, DV (2010)

2. Mean value and norm of distribution $f[\tilde{\rho}_i(E)]$ is unity

$\Rightarrow$ $2\mu=-\sigma_0^2$ $\Rightarrow$ symmetry relation $\boxed{\tilde{\rho}_i^3\,\phi_0(\tilde{\rho}_i)=\phi_0(\tilde{\rho}_i^{-1})}$

NLσ model (1D): Mirlin, Fyodorov (1994)

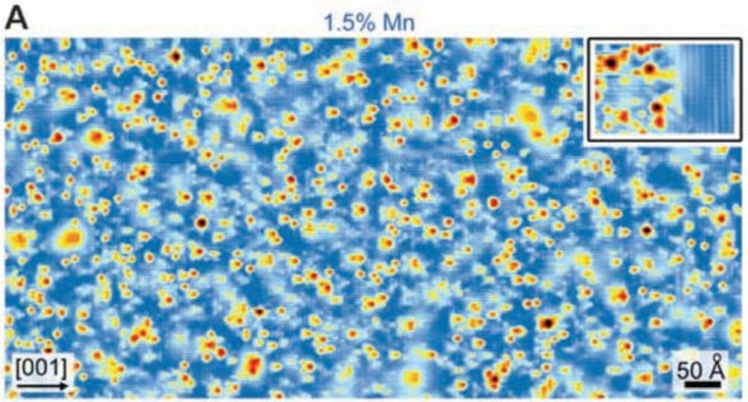
Check symmetry relation



Disorder + Interactions

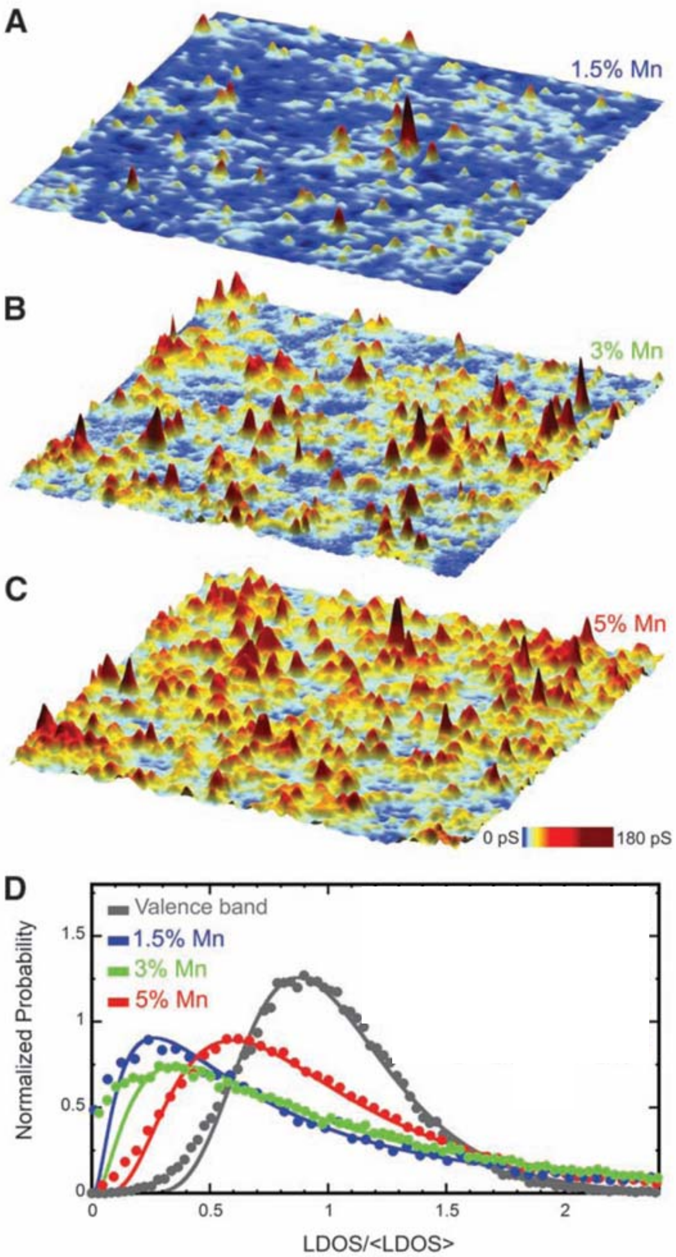
Visualizing Critical Correlations Near the Metal-Insulator Transition in $Ga_{1-x}Mn_xAs$

Anthony Richardella,[1,2]* Pedram Roushan,[1]* Shawn Mack,[3] Brian Zhou,[1] David A. Huse,[1] David D. Awschalom,[3] Ali Yazdani[1]† (2010)



STM topography of
the in-gap states of GaMnAs

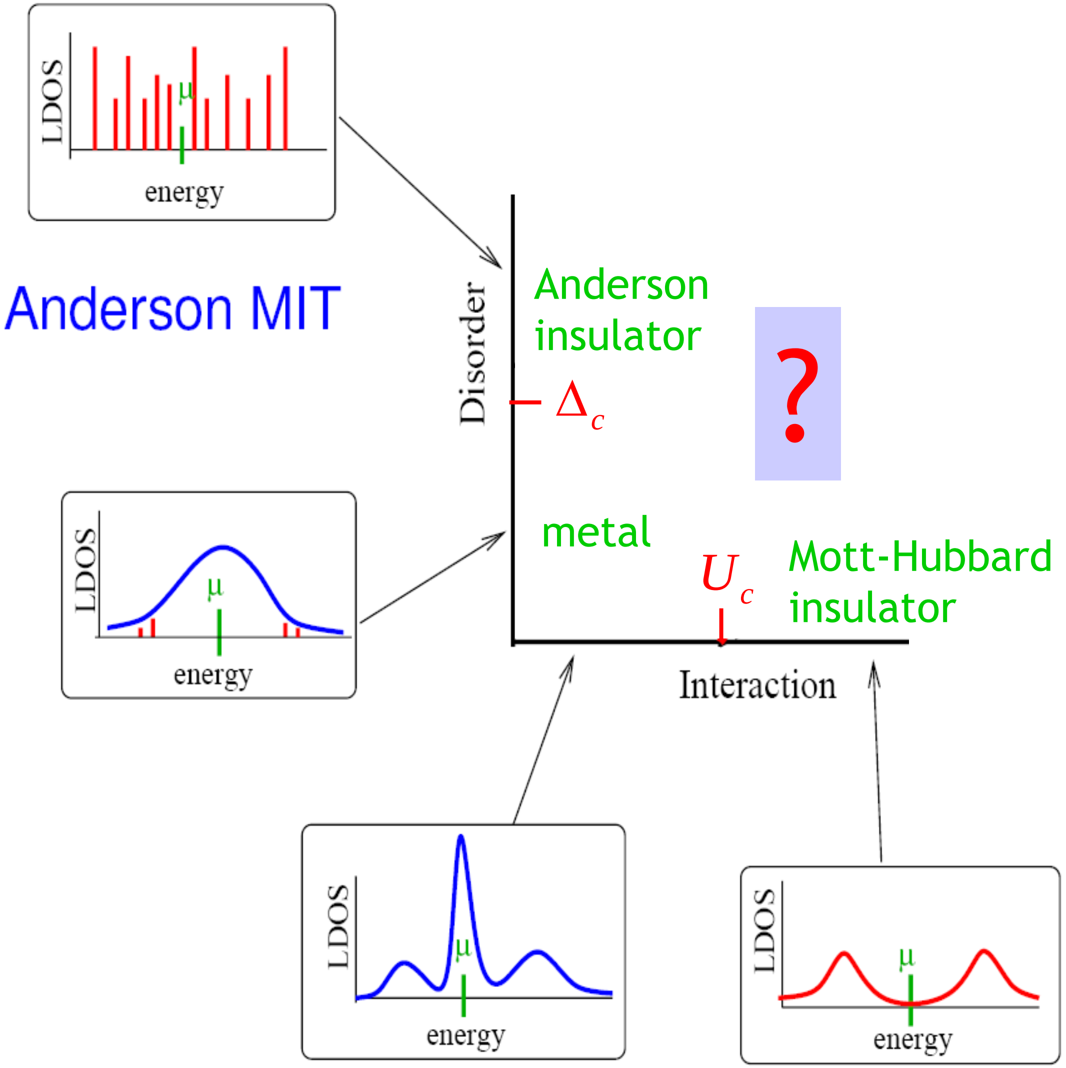
LDOS obeys log-normal distribution also in interacting, disordered systems
→ Geometric average required



The spatial variations of the
LDOS at the Fermi level

Anderson Localization
vs.
Mott-Hubbard Transition

Mott-Hubbard Transition vs. Anderson Localization



Disorder ↔ Anderson MIT

Interaction ↔ Mott-Hubbard MIT

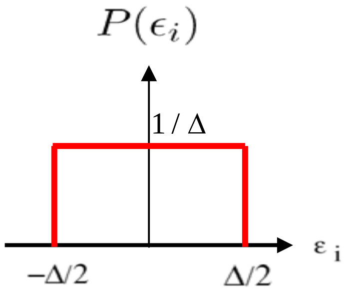
Anderson-Hubbard Hamiltonian

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

n=1

Box disorder

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



Δ: disorder strength

Δ=0: Mott insulator for U>U_c
U=0: Anderson insulator for $\Delta > \Delta_c > 0$ in d>2

1. Can both transitions be characterized by the average LDOS ?
2. Further destabilization of correlated metallic phase by disorder ?
3. Are the Mott insulator and Anderson insulator separated by some other phase?

Dynamical mean-field theory (DMFT) for the Anderson-Hubbard model

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

Vlaming, DV (1992)

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

Employ geometrically averaged LDOS:

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

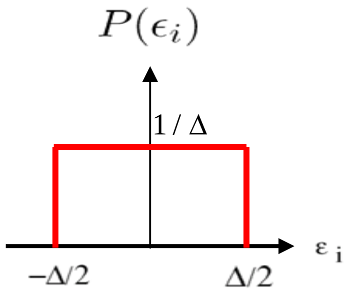
$$\rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'}$$

lattice Green function

Dobrosavljevic, Pastor, Nikolic (2003)

Anderson-Hubbard Hamiltonian

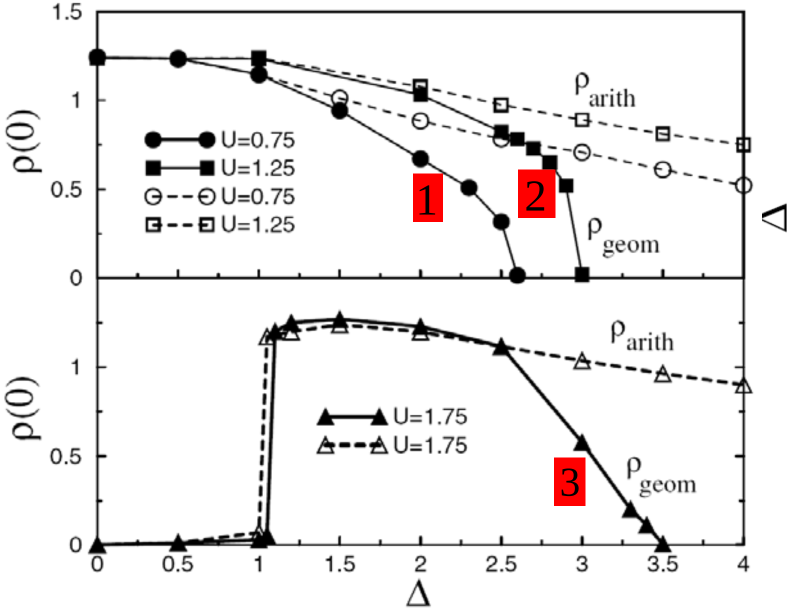
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + \sum_{\mathbf{i}\sigma} \varepsilon_i n_{\mathbf{i}\sigma}$$



Δ: disorder strength

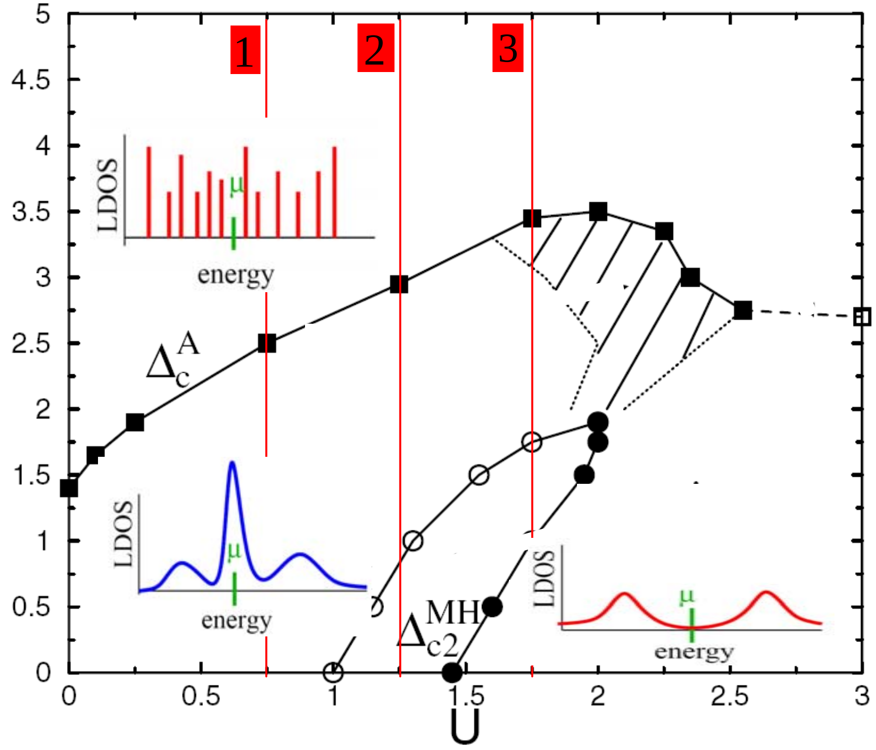
Solution by DMFT(NRG)

Local DOS



Critical behavior at localization transition

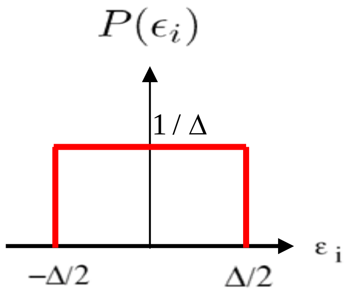
Non-magnetic phase diagram; n=1,T=0



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

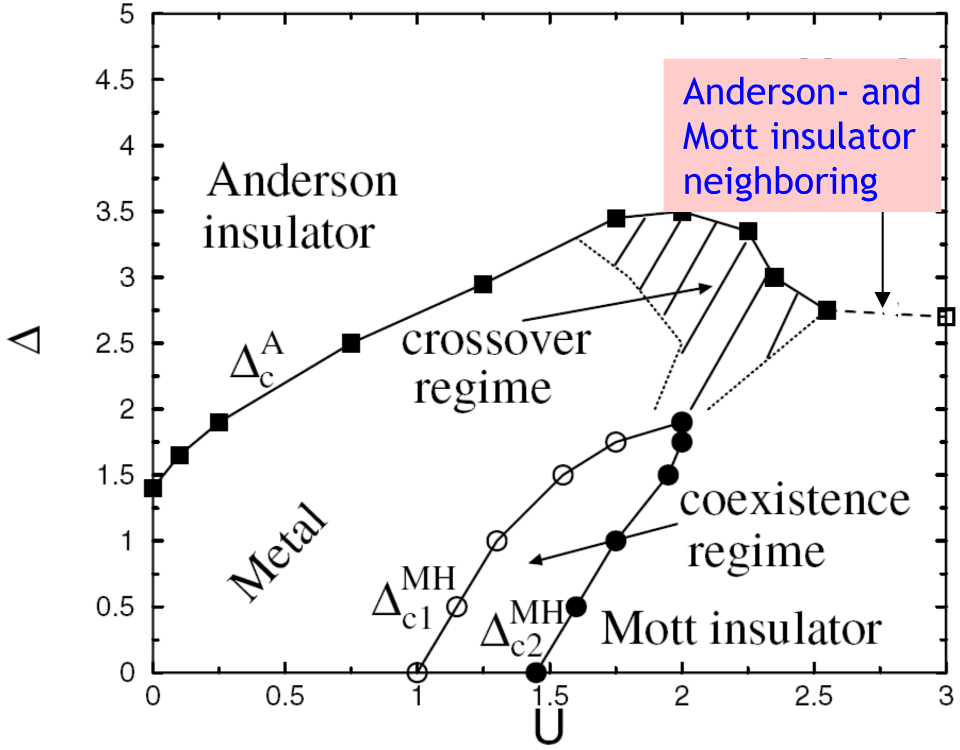
Solution by DMFT(NRG)

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

→ Interactions may increase metallicity

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

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



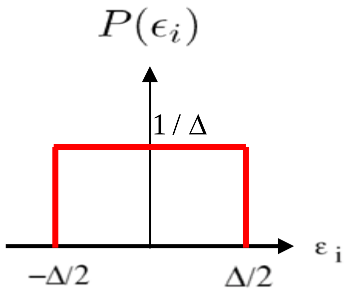
Anderson- and Mott insulator neighboring

Soft Hubbard gap:
Shinaoka, Imada (2009, 2010)

Byczuk, Hofstetter, DV (2005, 2010)

Anderson-Hubbard Hamiltonian

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

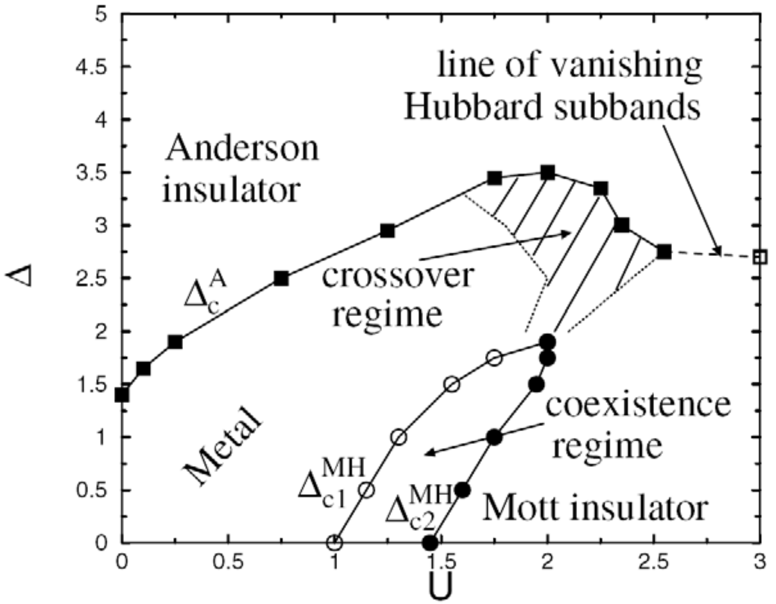


Δ: disorder strength

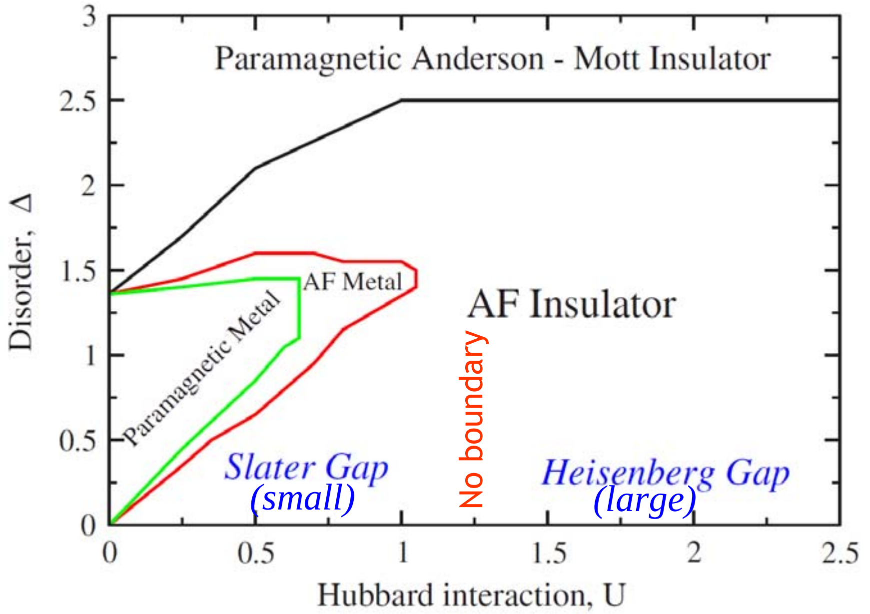
NN hopping, bipartite lattice, n=1:

Take into account antiferromagnetic order

DMFT: Non-magnetic phase diagram



Magnetic phase diagram



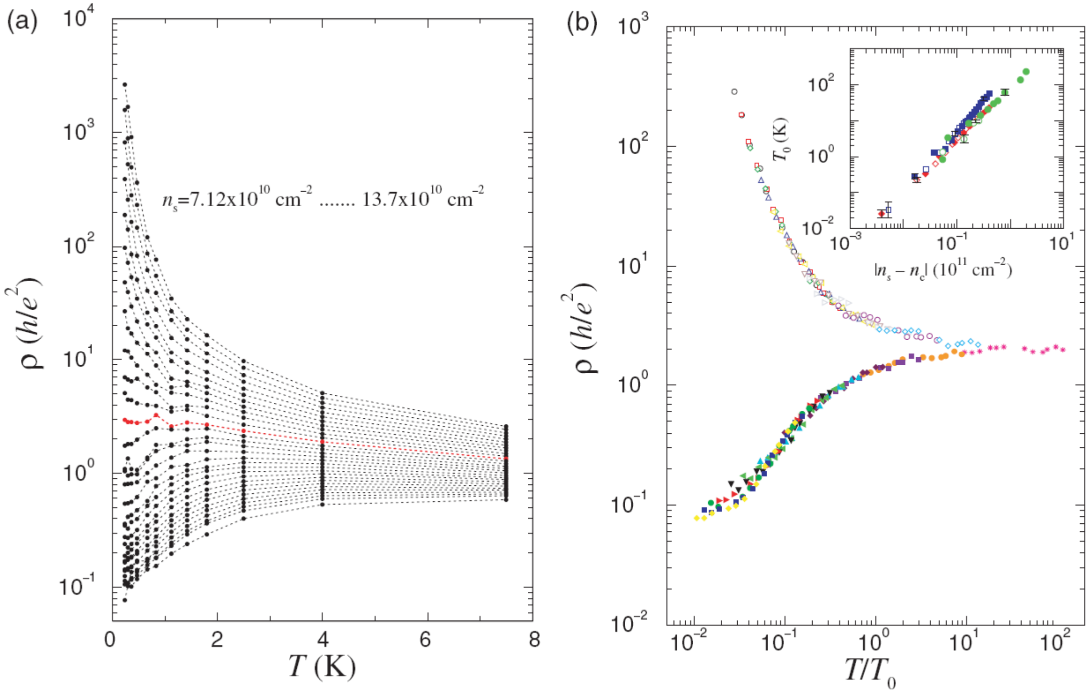
Byczuk, Hofstetter, DV (2009, 2010)

Universal critical conductivity at the MIT in d=2 ?

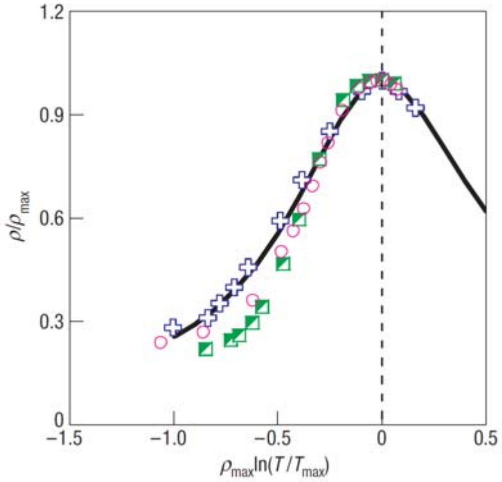
MIT in a dilute, low-disordered Si MOSFET

d=2

Interactions and disorder important



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



Quantum critical point?

NLσ model (two loop RG): Yes!

Punnoose, Finkel'stein (2005)
Anissimova, Kravchenko, Punnoose,
Finkel'stein, Klapwijk (2007)

Chakraborty, Byczuk, DV (2010, unpublished)

Current-current correlation function

$$\Lambda_{xx}(\vec{q},\tau) =< j_x(\vec{q},\tau) j_x(-\vec{q},\tau=0) >$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{e^{-\omega\tau}}{1-e^{-\beta\omega}} \mathrm{Im}\Lambda_{xx}(\vec{q},\omega)$$

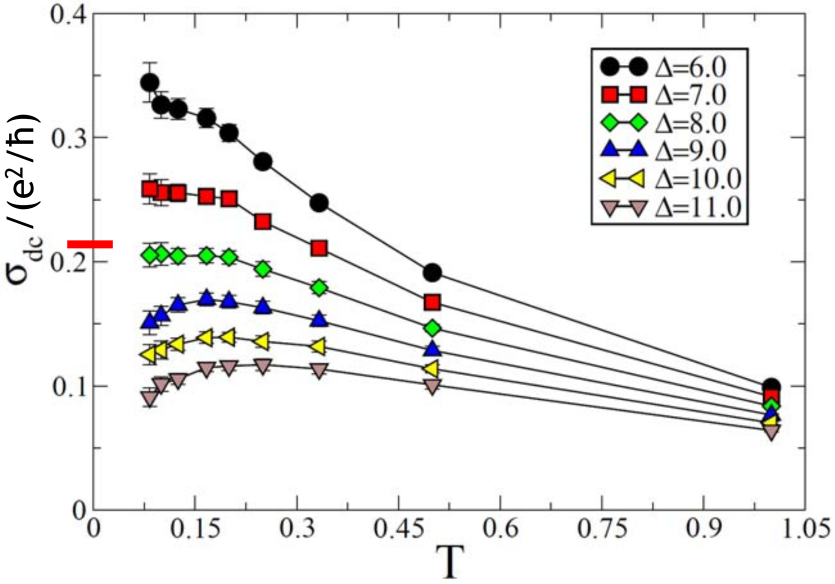
$$\Rightarrow \quad \sigma_{\mathrm{dc}} = \mathrm{lim}_{\omega\to 0} \frac{\mathrm{Im}\Lambda_{xx}(\vec{q}=0,\omega)}{\omega}$$

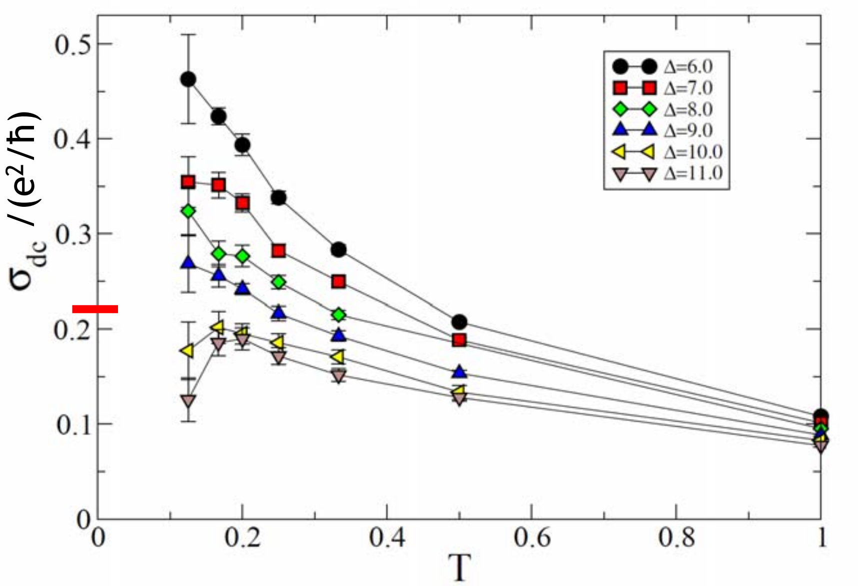
Low T $$= \frac{\beta^2}{\pi} \Lambda_{xx}\left(\vec{q}=0, \tau=\frac{\beta}{2}\right)$$

Evaluation with determinantal QMC in D=2 for box disorder

10x10 sites

Chakraborty, Byczuk, DV (2010, unpublished)





n=0.4, U=2: $\Delta_c = 8.0t$

n=0.5, U=4: $\Delta_c = 9.3t$

$$\boxed{\begin{aligned}\sigma_{dc,\,\text{crit}} &\simeq 0.2\ e^2/\hbar \\ &\simeq 1.3\ e^2/h\end{aligned}}$$

universal value (?)

Conclusion

MITs of correlated lattice electrons in the presence of disorder:

- Anderson insulator: LDOS follows log-normal distribution in D=2,3 over up to ten orders of magnitude
- DMFT with geometrically averaged LDOS → phase diagram incl. Mott-Hubbard and Anderson transition
- D=2: Numerical indications for a universal critical conductivity

$$\sigma_{dc,\,\mathrm{crit}} \simeq 1.3\ e^2 / h$$