Localization in Dynamical Mean Field Theory
Lecture 1: Effective Medium Approaches for Disorder within DMFT

Vladimir Dobrosavljevic
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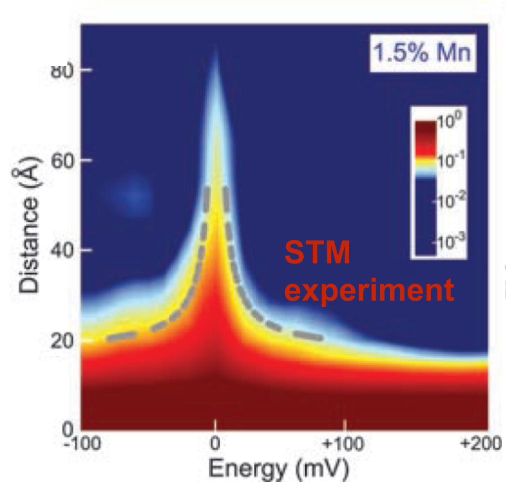
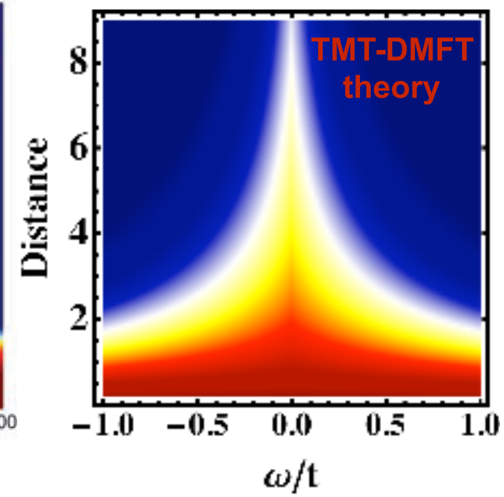
http://badmetals.magnet.fsu.edu





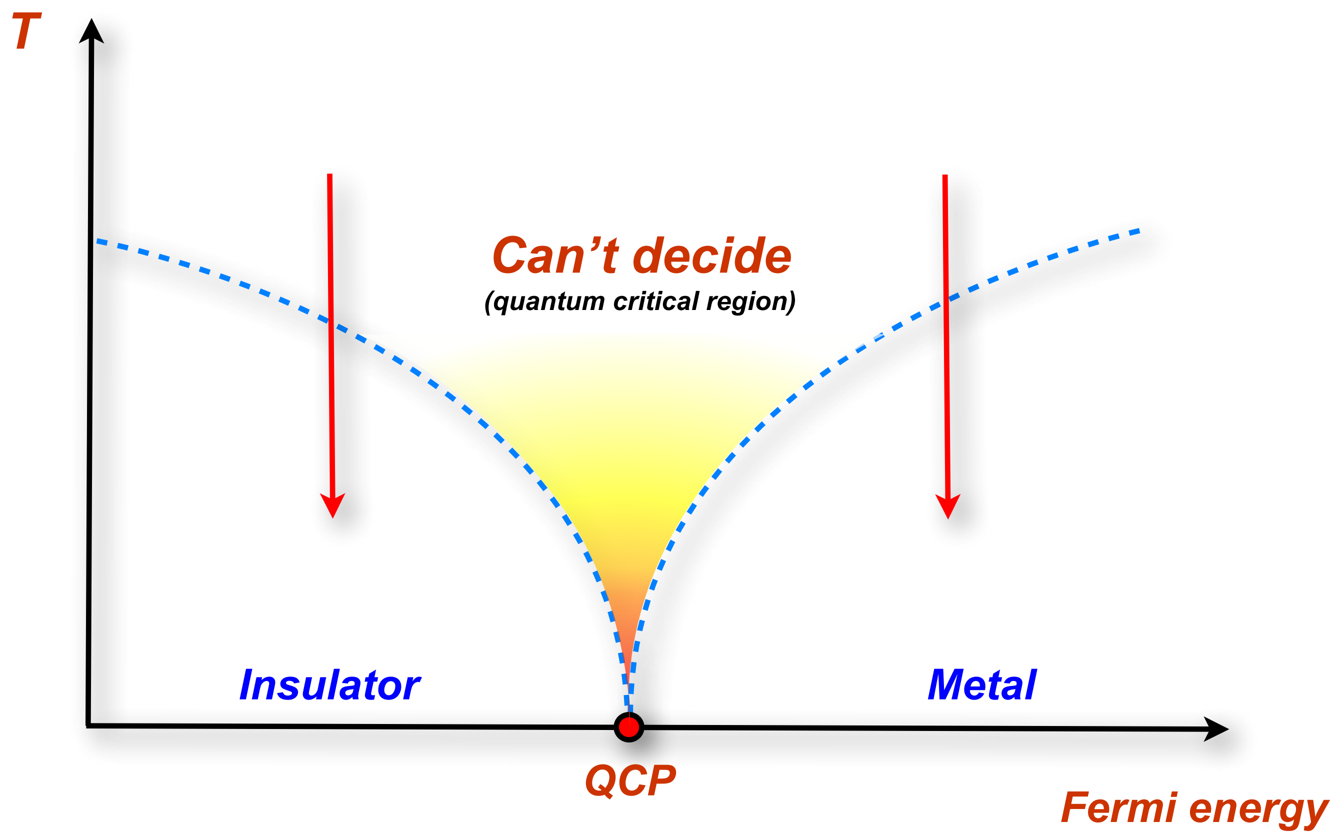
NATIONAL HIGH MAGNETIC FIELD LAB

Funding: ***NSF grants:***

DMR-9974311
DMR-0234215
DMR-0542026
DMR-1005751
DMR-1410132

Workshop "Localization in Quantum Systems"
Jun. 1-2, 2017, King's College London

MIT Quantum Criticality?

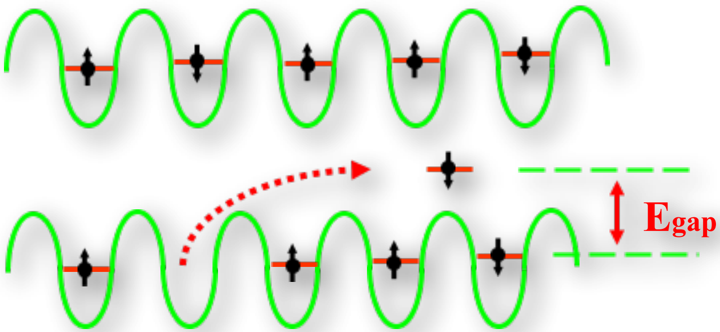


Mechanisms for Localization?

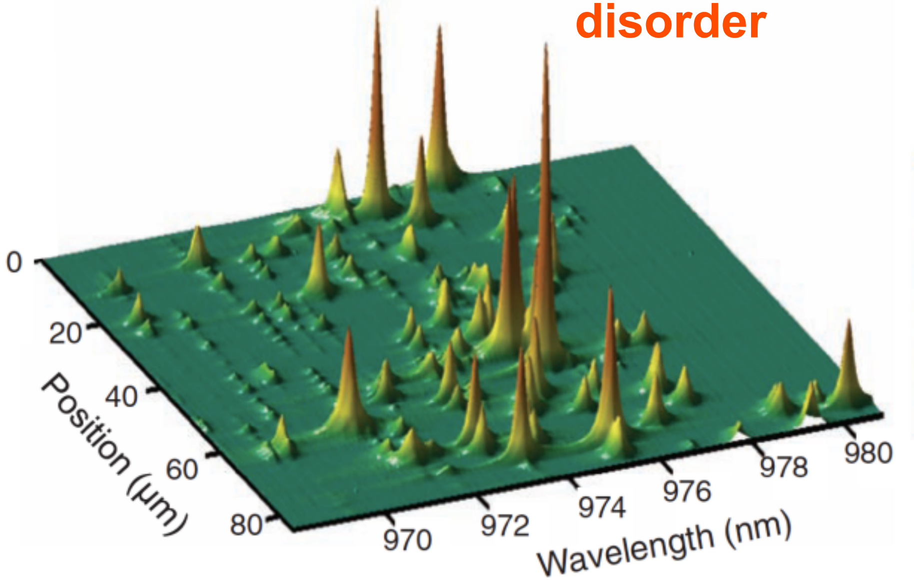
Sir Neville Mott:
interaction

Friend or Foe???

P. W. Anderson:
disorder



Order parameters??



Experimental puzzles I: Mott limit and Mooij Correlation

Lee and Ramakrishnan: Disordered electronic systems (Rev. Mod. Phys., Vol. 57, No. 2, April 1985

VII. REMARKS AND OPEN PROBLEMS
A. High-temperature anomalies

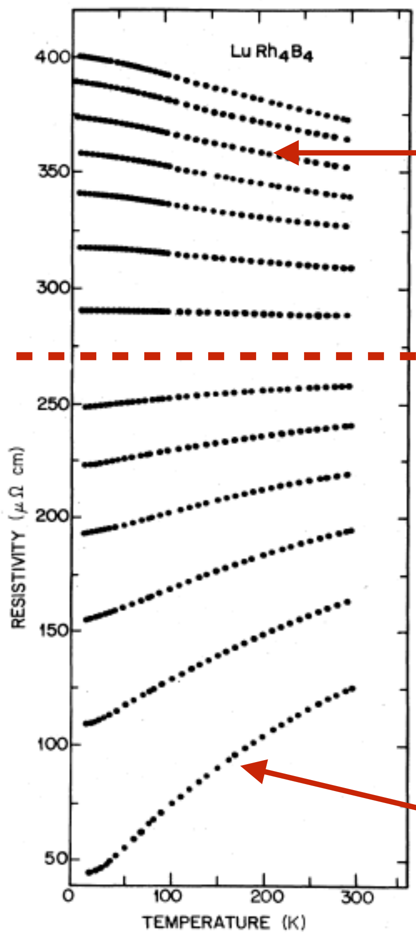


FIG. 20. Resistivity as a function of temperature for $LuRh_4B_4$ at various damage levels. The numbers represent the α-particle dose in units of $10^{16}/cm^2$. From Dynes, Rowell, and Schmidt (1981).

A15 compounds: Effect of disorder by ion radiation (Dynes et al., 1981)

Bad conductor: phonons+disorder???

ρ_0^c "Mott limit" $k_F\ell \sim O(1)$

Mooij (1973) correlation???

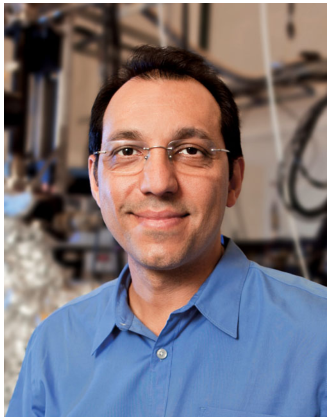
$$\boxed{\rho(T)=\rho_0+(\rho_0^c-\rho_0)AT}$$

Breakdown of Mathiessen's rule:

$$\rho_{\rm ideal}(T)=\rho_0+\rho_{\rm ph}(T)$$

Good metal: phonons

Experimental puzzles II: STM in GaMnAs



Science 5 February 2010:
Vol. 327 no. 5966 pp. 665-669
DOI: 10.1126/science.1183640

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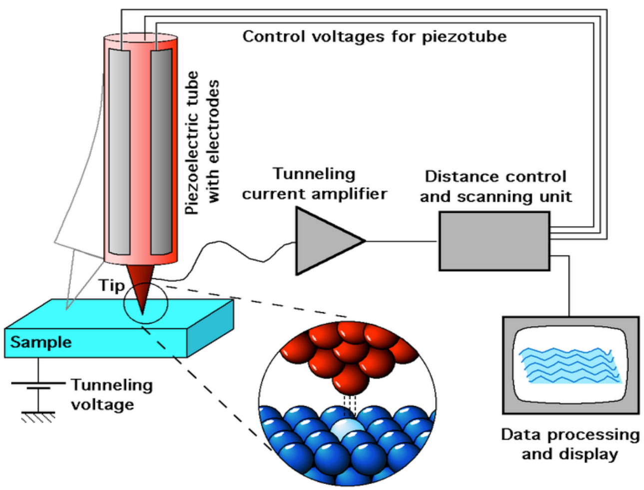
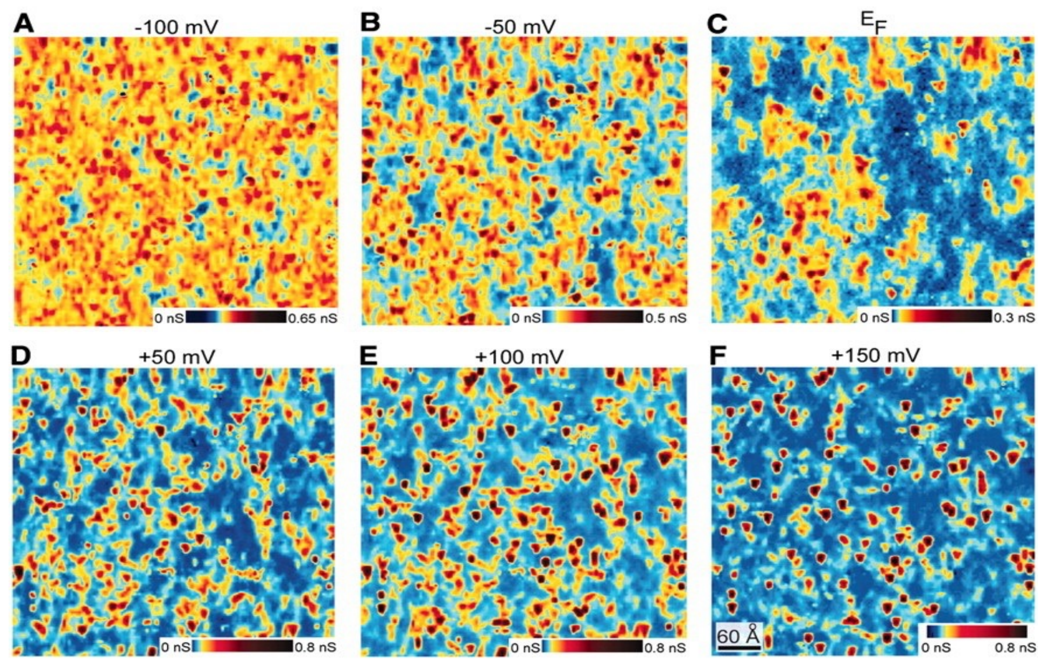
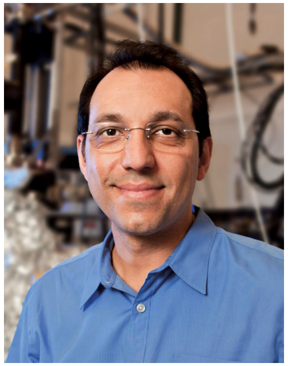
REPORT

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] and Ali Yazdani[1,†]

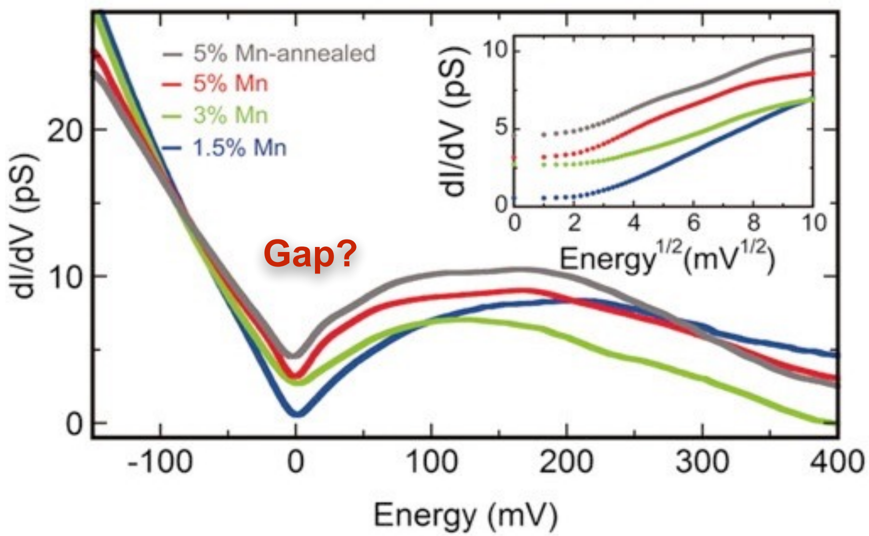




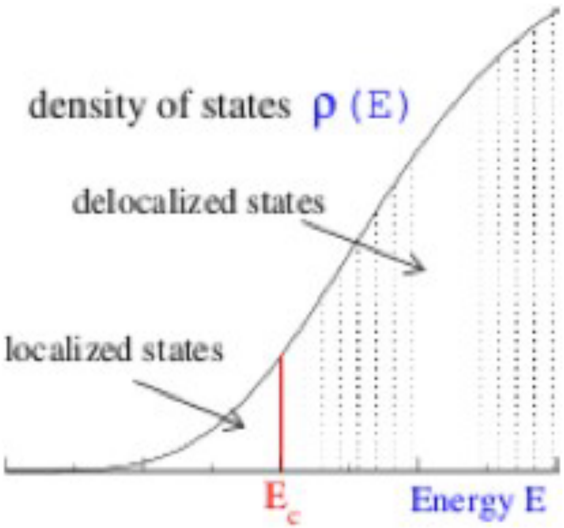


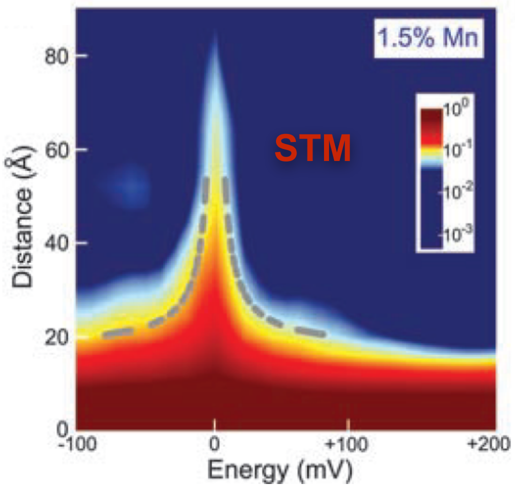
Not your ordinary Anderson transition: pseudogap

STM: Gap opening at MIT?



Anderson:
smooth DOS





Delocalization above and below Fermi energy

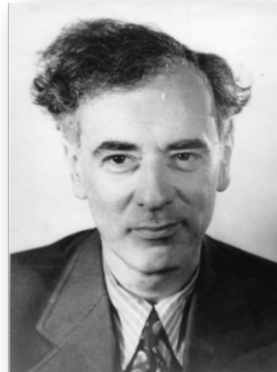
Strong interactions: DMFT approach

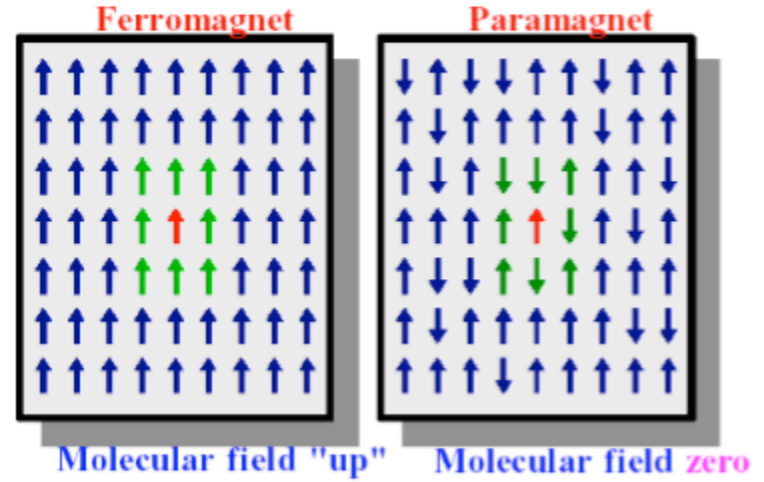
Standard critical points:

Spontaneous symmetry breaking

Order parameter, Landau-Ginzburg

Renromalization group, field theory





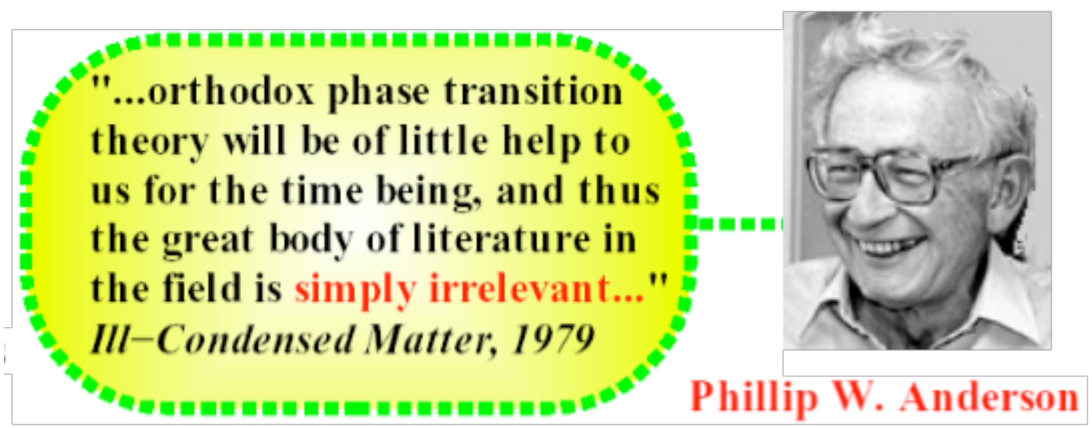
Metal-Insulator Transitions:

NO symmetry breaking!

Order parameter???

Huge spatial fluctuations

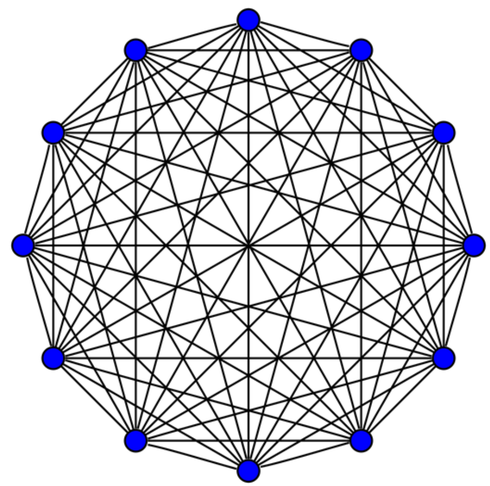
Many metastable states (“glass”)



Dynamical Mean-Field Theory

$$H = -t \sum_{\langle i,j \rangle,\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$$

Gabi Kotliar



Exact for "maximal frustration"

Suppress all (inter-site) spin correlations!

Local scattering processes

"Kondo physics" forms Fermi liquid

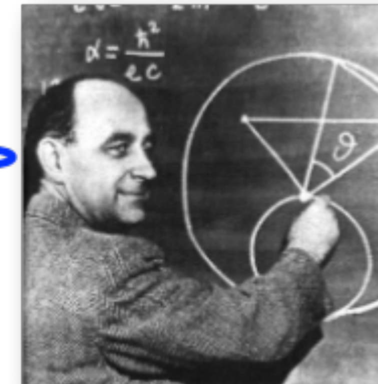
Paul Cezzane

Dynamical Mean-Field Theory (DMFT)

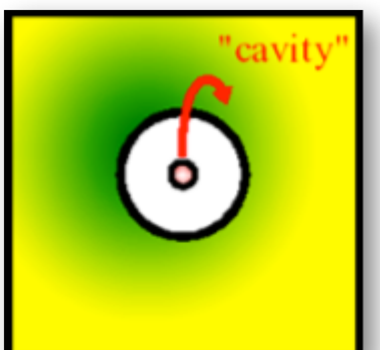
Heisenberg:

p or **x**??

Dynamics:
Golden Rule



Fermi



$$\boxed{\Delta(\omega) = t^2 \rho_c(\omega) \sim 1/\tau}$$

Escape rate
(disorder: Anderson 1958)

Spectrum of the "cavity"

Matrix element

PRL 107, 026401 (2011) PHYSICAL REVIEW LETTERS week ending 8 JULY 2011

Quantum Critical Transport near the Mott Transition

H. Terletska,[1] J. Vučičević,[2] D. Tanasković,[2] and V. Dobrosavljević[1]

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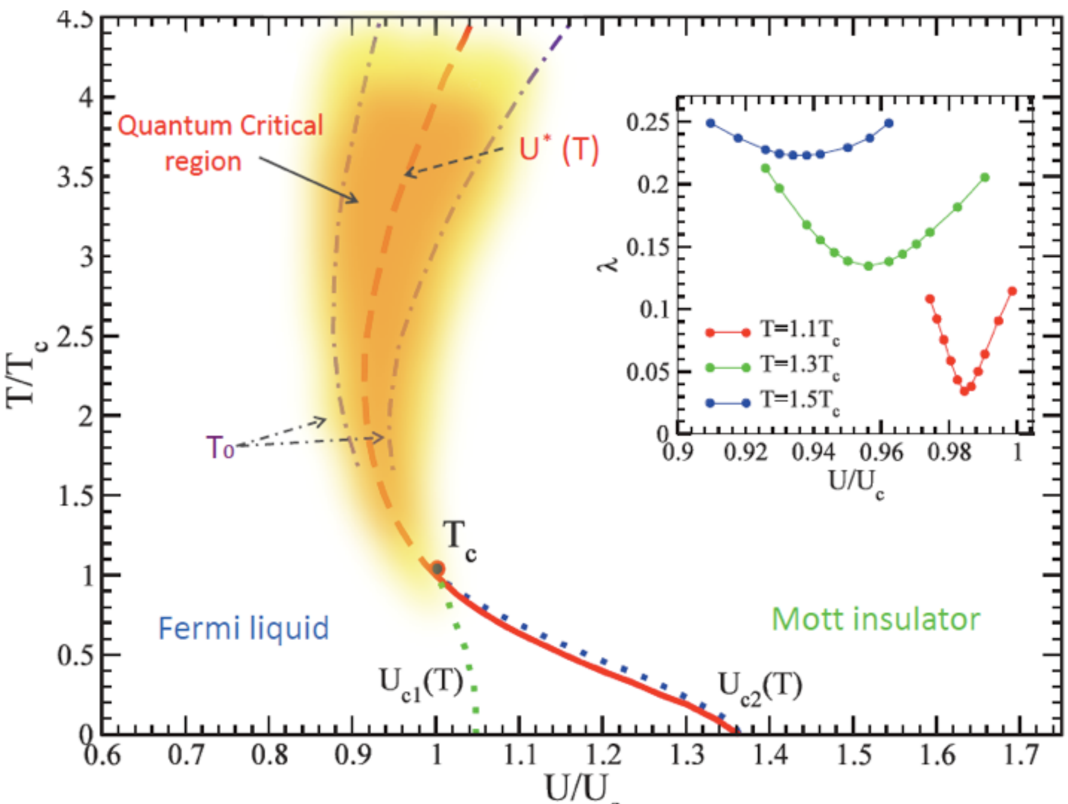
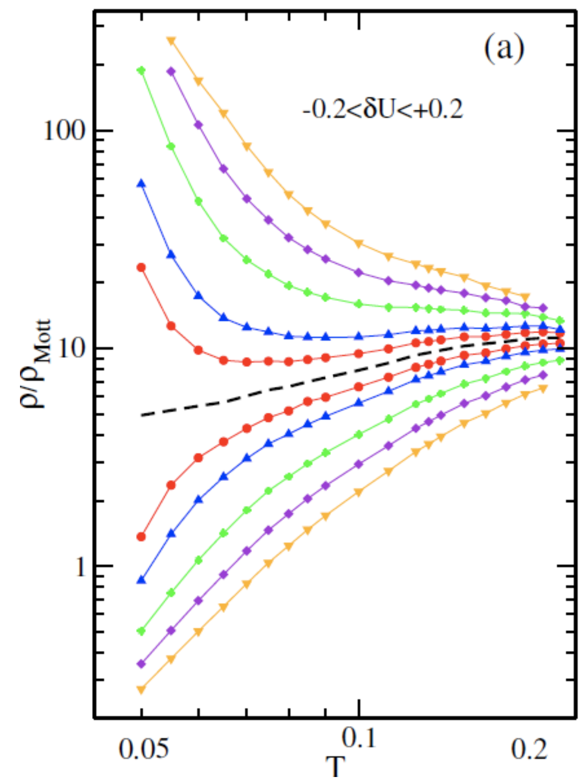
(Received 26 January 2011; published 5 July 2011)

DMFT theory



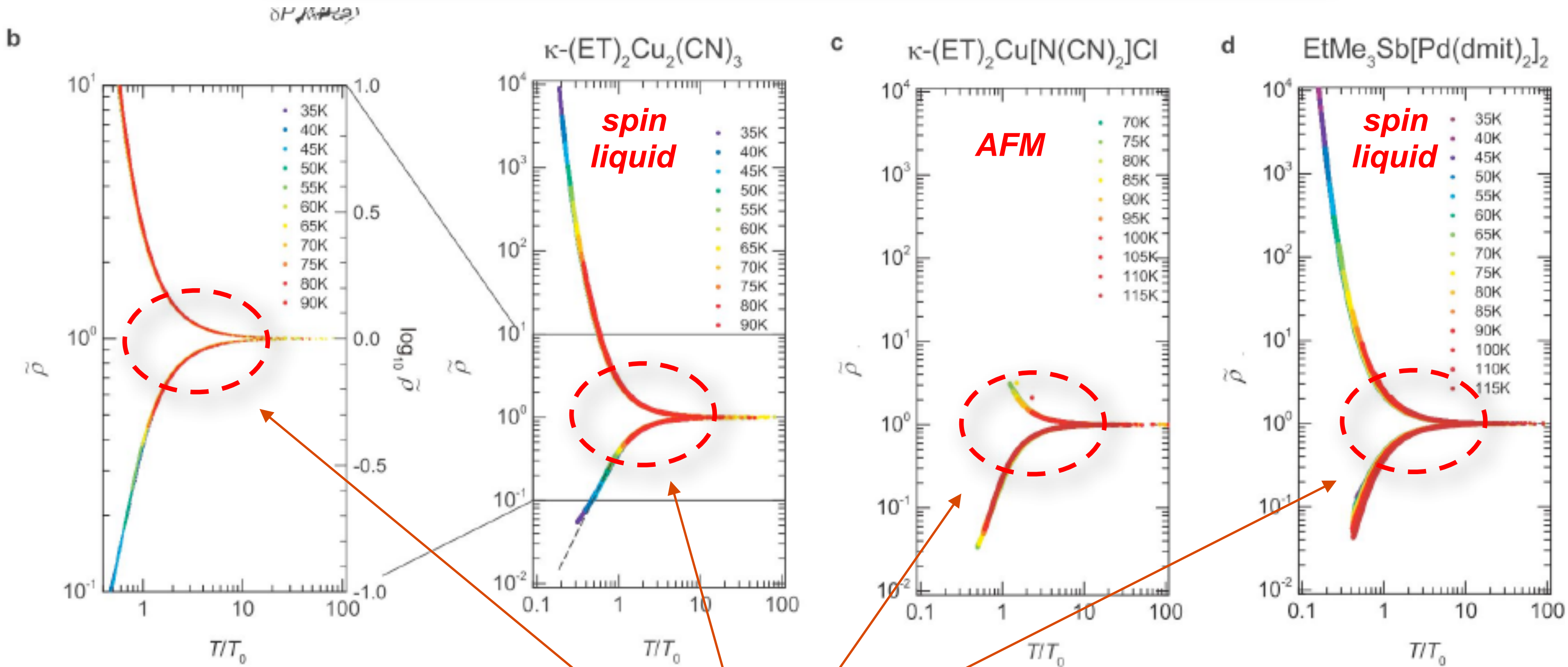
$T_C \sim 2\% T_F$

around crossover line



Mott organics: **universal** high-T scaling

K. Kanoda et al., Nature Physics (2015)



zv = 0.60 and c = 25.3 for κ-Cu$_2$(CN)$_3$

zv = 0.55 and c = 65.8 for κ-Cl

zv = 0.65 and c = 18.9 for EtMe$_3$Sb-dmit

mirror symmetry!

$$\tilde{\rho} = \exp[\pm(T/T_0)^{-1/z_\nu}]$$

"stretched exponential"

Formalism: Hubbard model with disorder

$$H=\sum_{ij}\sum_{\sigma}[-t_{ij}+\varepsilon_i\delta_{ij}]c_{i,\sigma}^{\dagger}c_{j,\sigma}+U\sum_{i}c_{i,\uparrow}^{\dagger}c_{i,\uparrow}c_{i,\downarrow}^{\dagger}c_{i,\downarrow}$$

Replicated functional-integral formulation: $\alpha=1,\ldots,n$

$$\overline{Z}^n=\int D\varepsilon_i P_S[\varepsilon_i]Dt_{ij}P_H[t_{ij}]\int D\bar{c}_i Dc_i\exp\{-S\}$$

$$S_{\rm loc}=\sum_i S_{\rm loc}(i)$$

$$=\sum_i\left[\sum_{\alpha,s}\int_0^{\beta}d\tau\,\bar{c}_{s,i}^{\alpha}[\partial_\tau+\varepsilon_i-\mu]c_{s,i}^{\alpha}+U\sum_{\alpha}\int_0^{\beta}d\tau\,\bar{c}_{\uparrow,i}^{\alpha}c_{\uparrow,i}^{\alpha}\bar{c}_{\downarrow,i}^{\alpha}c_{\downarrow,i}^{\alpha}\right]$$

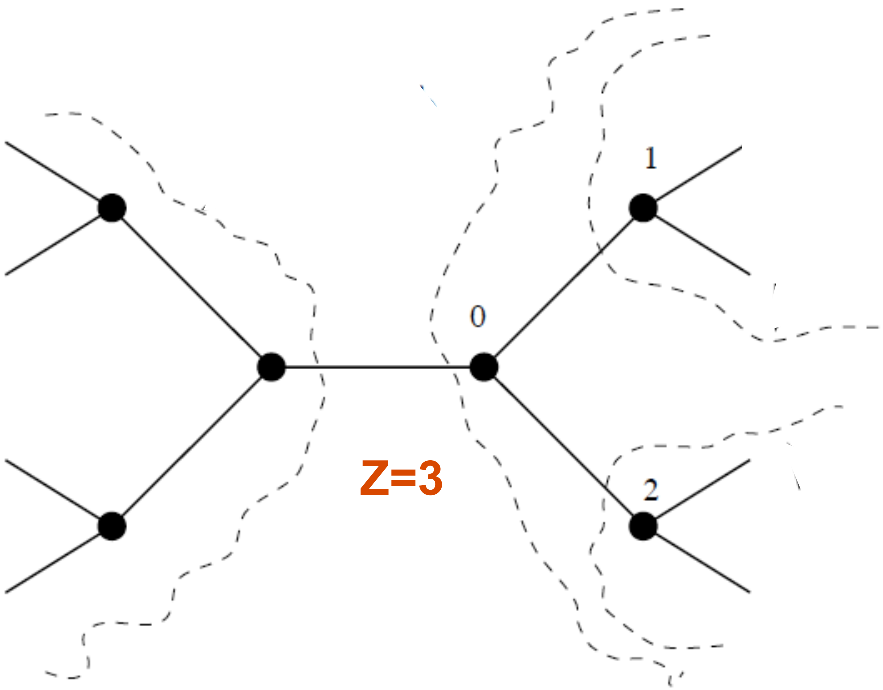
$$S_{\rm hop}=\sum_{\langle ij\rangle}S_{\rm hop}(i,j)$$

$$=\sum_{\langle ij\rangle}\left[-t_{ij}\sum_{\alpha,s}\int_0^{\beta}d\tau[\bar{c}_{s,i}^{\alpha}c_{s,j}^{\alpha}+\mathrm{H.c.}]\right]$$

Bethe Lattice - integral equation

Integrate out z-1 branches:

$$\Xi[i]=\left[\int D\bar{c}_j Dc_j D\varepsilon_j P_S(\varepsilon_j) Dt_{ij} P_H(t_{ij}) \times \exp\{-S_{\text{hop}}(i,j)-S_{\text{loc}}(j)\}\Xi[j]\right]^{z-1}$$



Recursion relation
(EXACT!!)

Functional of local fields only
(all powers)

DMFT as the large z limit

$$m = z - 1$$

To get finite result for $m \to \infty$ rescale: $t_{ij} \to t_{ij}/\sqrt{m}$

Expand in powers of $S_{\text{hop}} \sim 1/\sqrt{m}$

Local effective action: Anderson impurity model

"cavity field"

$$S_{\text{eff}}(i) = S_{\text{loc}}(i) - \ln \Xi(i)$$

$$= \sum_s \int_0^\beta d\tau \int_0^\beta d\tau' \, \bar{c}_{i,s}(\tau)[\delta(\tau-\tau')(\partial_\tau + \varepsilon_i - \mu) + \boxed{\Delta_{i,s}(\tau,\tau')}] c_{i,s}(\tau')$$

$$+ U \int_0^\beta d\tau \, \bar{c}_{i,\uparrow}(\tau) c_{i,\uparrow}(\tau) \bar{c}_{i,\downarrow}(\tau) c_{i,\downarrow}(\tau) \, .$$

Depends on local site energy ε_i

Cavity field: self-consistency

$$\Delta_{i,s}(\omega_n) = \int d\varepsilon_j P_S(\varepsilon_j) \int dt_{ij} P_H(t_{ij}) t_{ij}^2 G_{j,s}(\omega_n)$$

$$= \overline{t_{ij}^2 G_{j,s}(\omega_n)} \,,$$

self-averaged (many neighbors)

$$G_{j,s}(\omega_n) = \langle \bar{c}_{j,s}(\omega_n) c_{j,s}(\omega_n) \rangle_{S_{\text{eff}}(j)} \longleftarrow$$

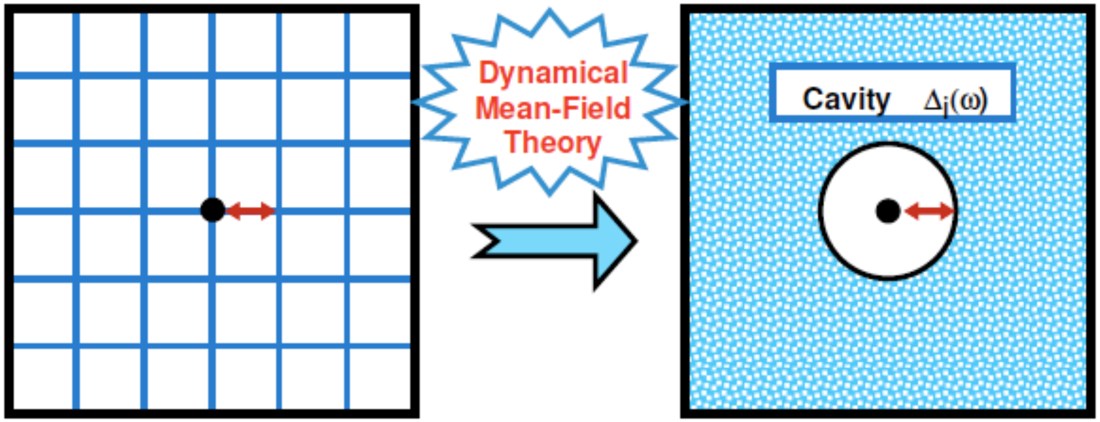
site-dependent

Note: *W* is diagonal in replicas (drop)

$$\alpha \neq \alpha', \; \overline{\langle \bar{c}^{\alpha} c^{\alpha'} \rangle} = \overline{\langle \bar{c} \rangle \langle c \rangle} = 0 \text{ (particle conservation)}$$

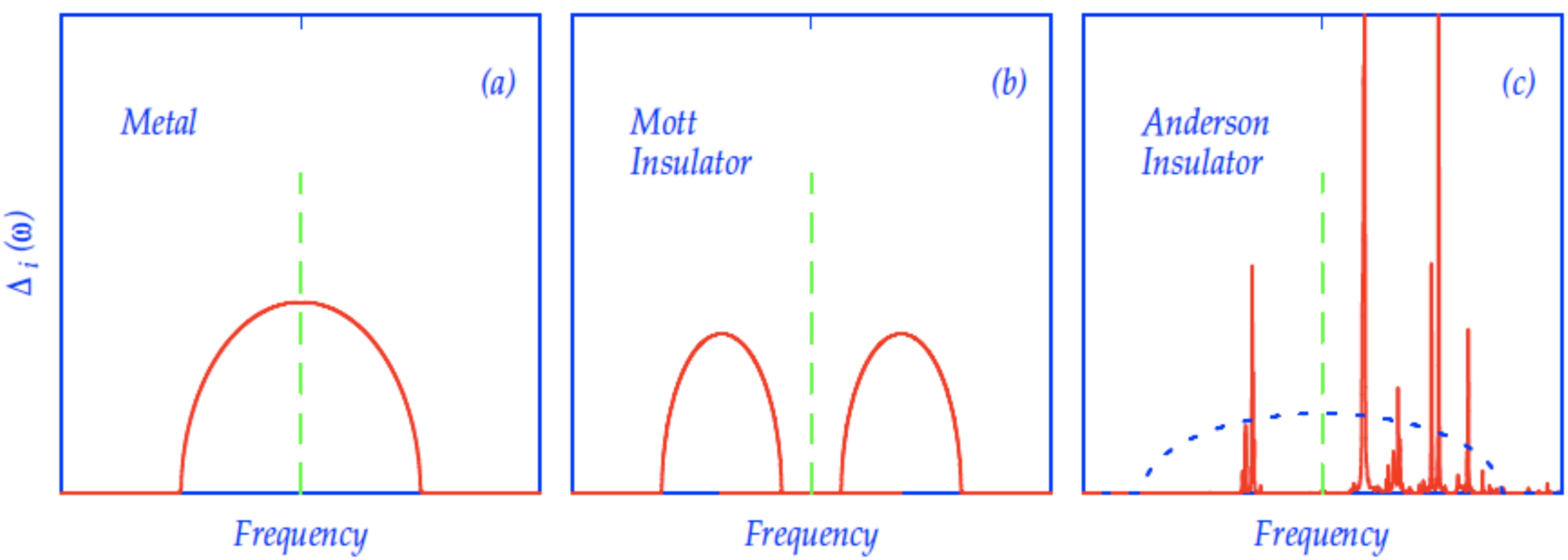
***U*=0 limit - "CPA" (no Anderson localization)**

Local (DMFT) perspective?
Fluctuating cavity field



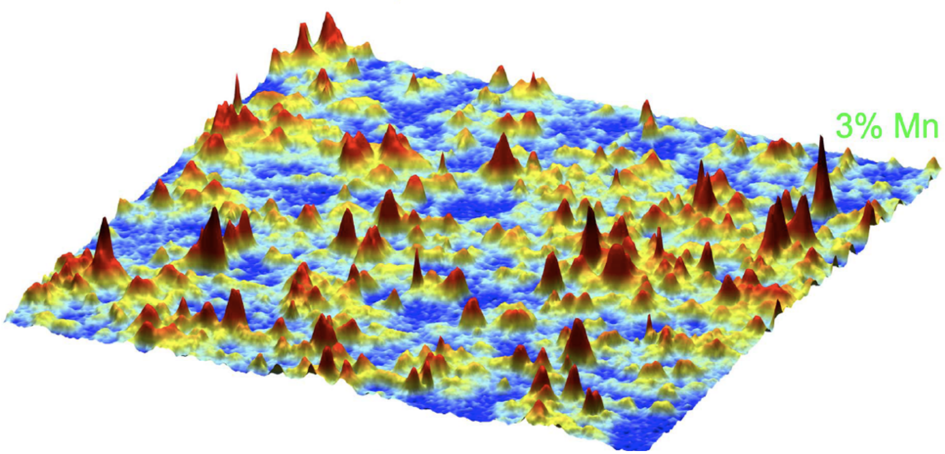
$$\Sigma_i(\omega) = \left(1 - Z_i^{-1}\right)\omega - \varepsilon_i + \bar{\varepsilon}_i / Z_i$$

Bethe lattice simulation



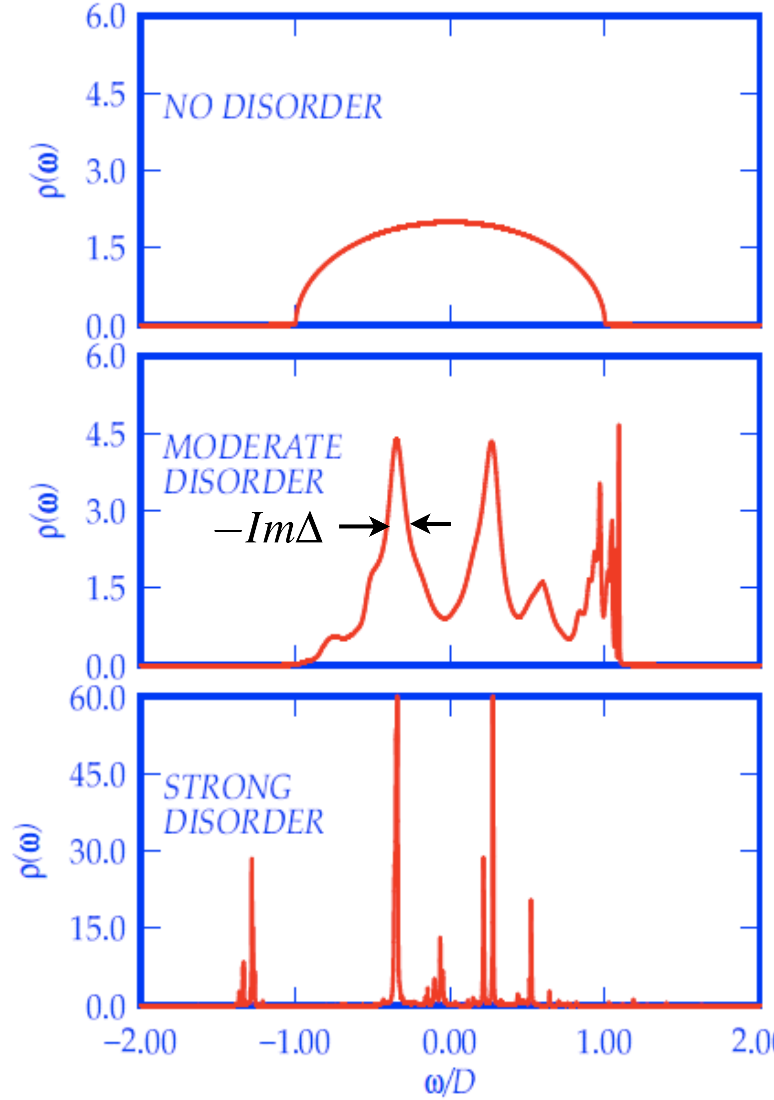
Can local spectrum recognize Anderson localization?

$$\rho_i(\omega) = \frac{1}{\pi} Im \frac{1}{\omega - \varepsilon_i - \Delta_i(\omega)}$$
$$= \sum_n \delta(\omega - \omega_n) |\psi_n(i)|^2$$

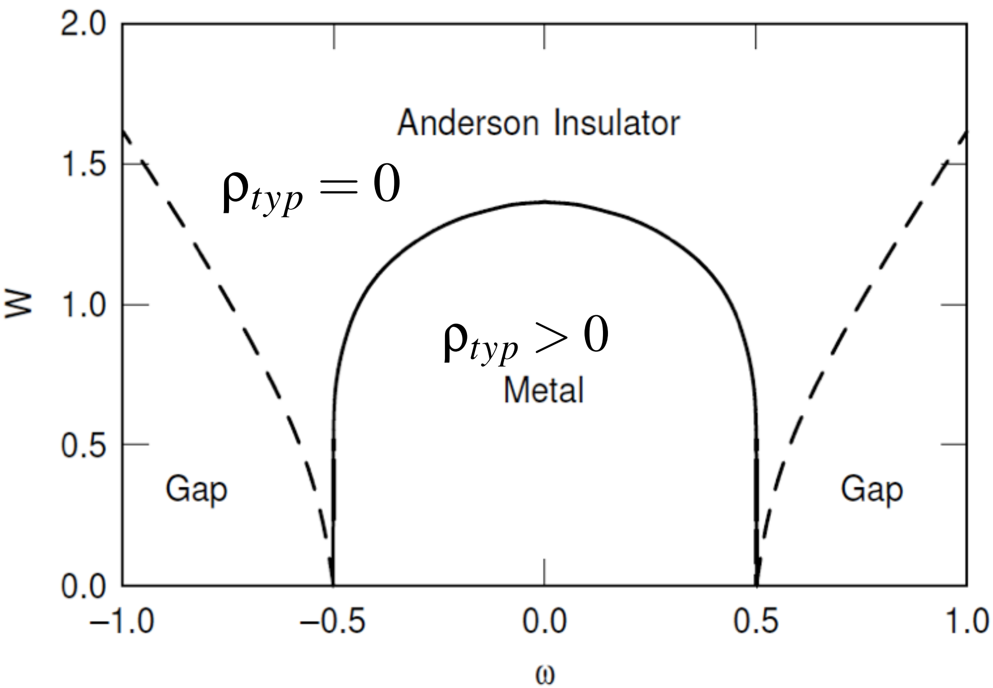


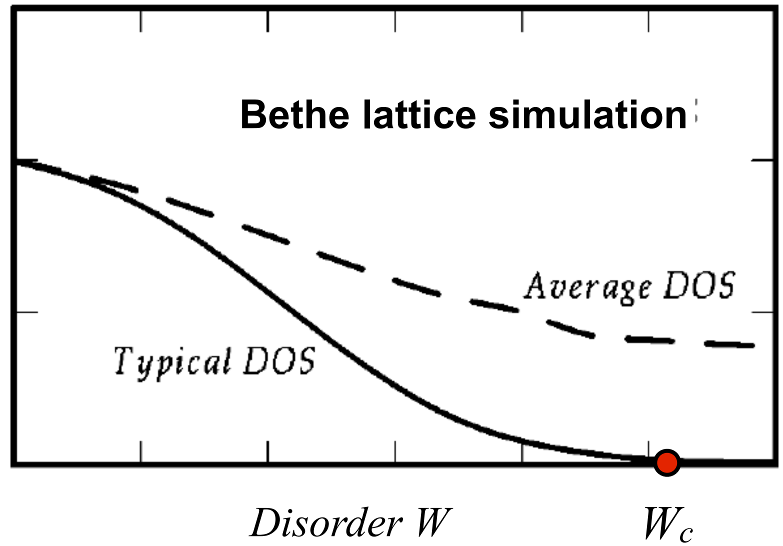
Yazdani, STM experiments GaMnAs
(close to localization)

Bethe lattice simulation



Typical DOS as order parameter for Anderson localization

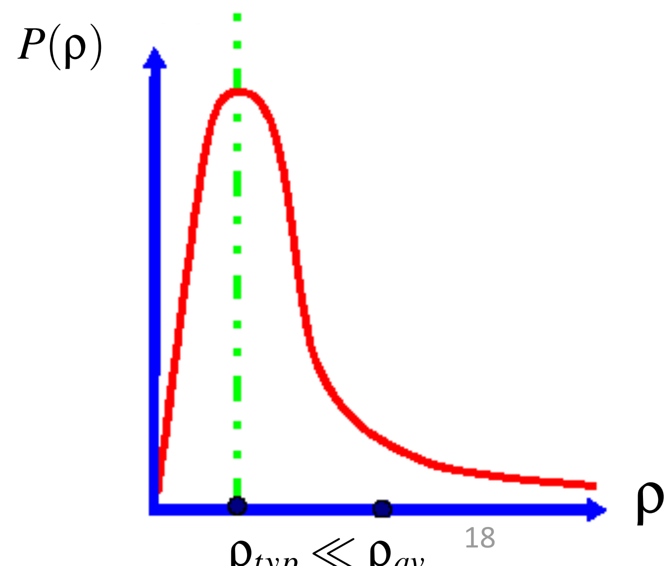




$$\rho_{av} = < \rho_i > \sim 1/W^2 \quad \text{(remains finite)}$$

$$\rho_{typ} = \exp\{< \ln \rho_i >\} \sim (W_c - W)^{\beta}$$

LOCAL order parameter



Typical Medium Theory for Anderson localization

V. Dobrosavljević, A. Pastor, and B. K. Nikolić, *Europhys. Lett.* **62**, 76–82, (2003)

Idea: **Localization: cavity function $\Delta_i(\omega)$ fluctuates**

DMFT (CPA) replaces it by average value (wrong)

TMT-DMFT: replace it by typical value (order parameter)

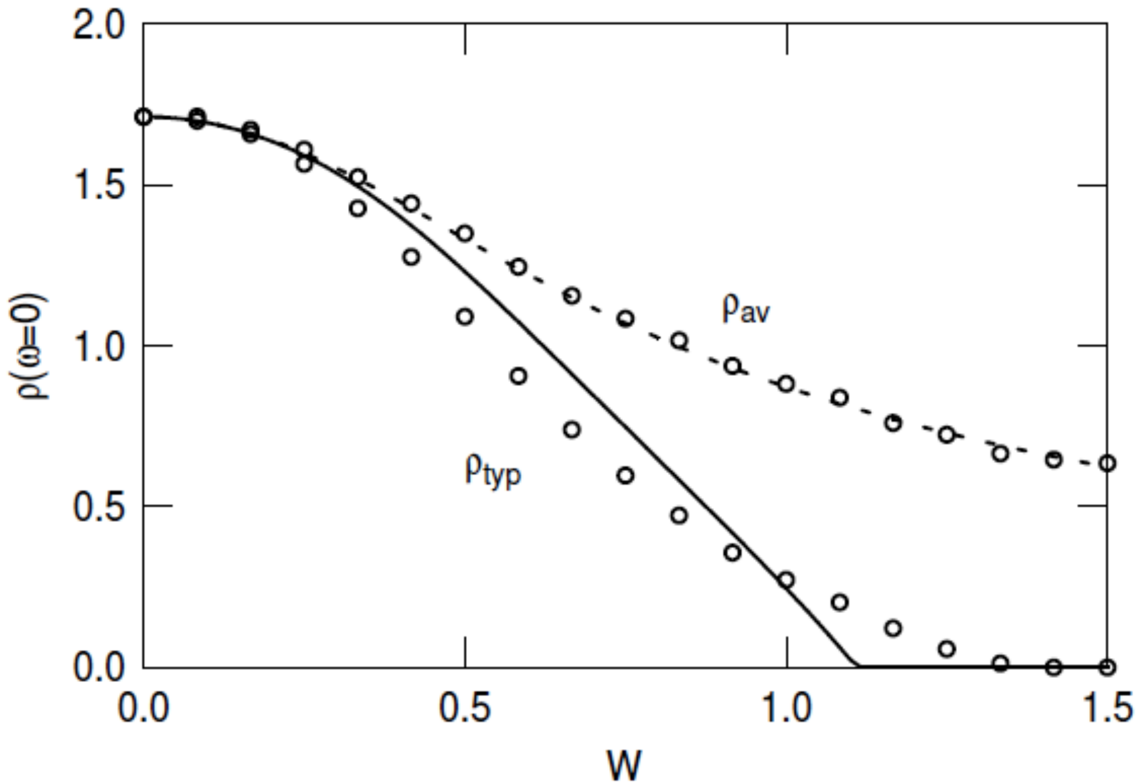
$$G(\omega,\varepsilon_i) = [\omega - \varepsilon_i - \Delta(\omega)]^{-1} \qquad \Delta(\omega) = \Delta_o(\omega - \Sigma(\omega))$$

$$\Delta_o(\omega) = \omega - 1/G_o(\omega) \qquad G_o(\omega) = \int_{-\infty}^{+\infty} d\omega' \, \frac{\rho_0(\omega')}{\omega - \omega'}$$

$$\boxed{\rho_{\rm typ}(\omega) = \exp\left\{\int d\varepsilon_i \; P(\varepsilon_i) \; \ln \rho(\omega,\varepsilon_i)\right\}} \qquad G_{\rm typ}(\omega) = \int_{-\infty}^{+\infty} d\omega' \, \frac{\rho_{\rm typ}(\omega')}{\omega - \omega'}$$

Self-consistency: $G_o(\omega - \Sigma(\omega)) = G_{\rm typ}(\omega)$

TMT vs. exact 3D behavior



Excellent quantitative agreement with exact diagonalization in 3D

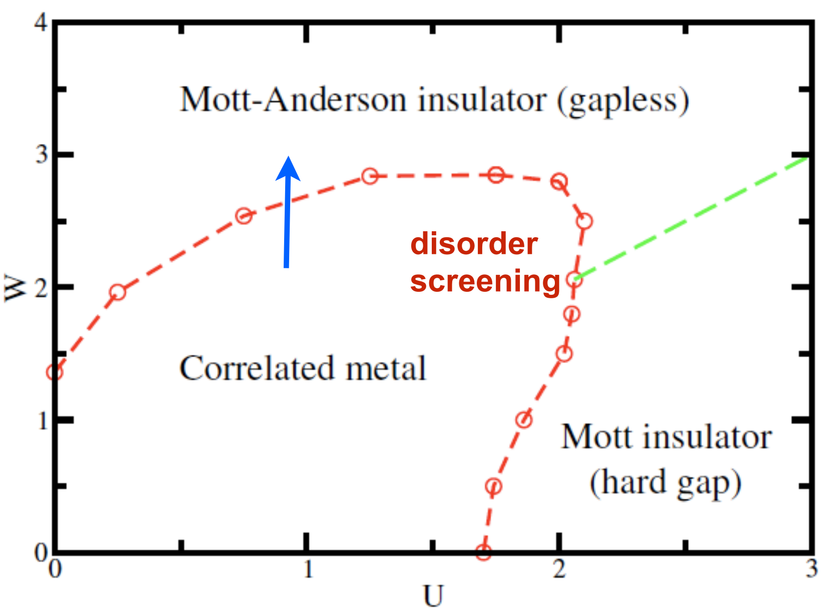
TMT-DMFT of Mott-Anderson transition

PRL 102, 156402 (2009) PHYSICAL REVIEW LETTERS week ending 17 APRIL 2009

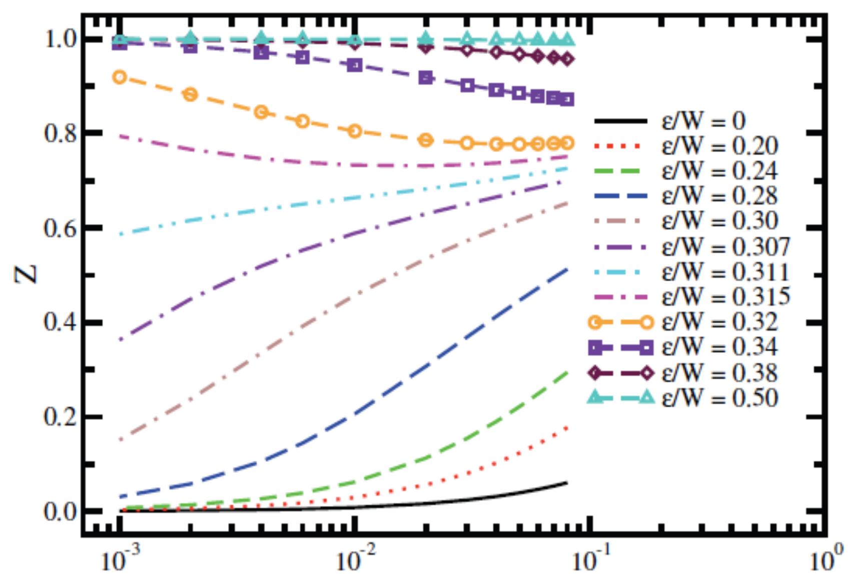
Critical Behavior at the Mott-Anderson Transition: A Typical-Medium Theory Perspective

M. C. O. Aguiar,[1] V. Dobrosavljević,[2] E. Abrahams,[3] and G. Kotliar[3]

T=0 Slave-Boson solution



Disorder-driven (increasing W)

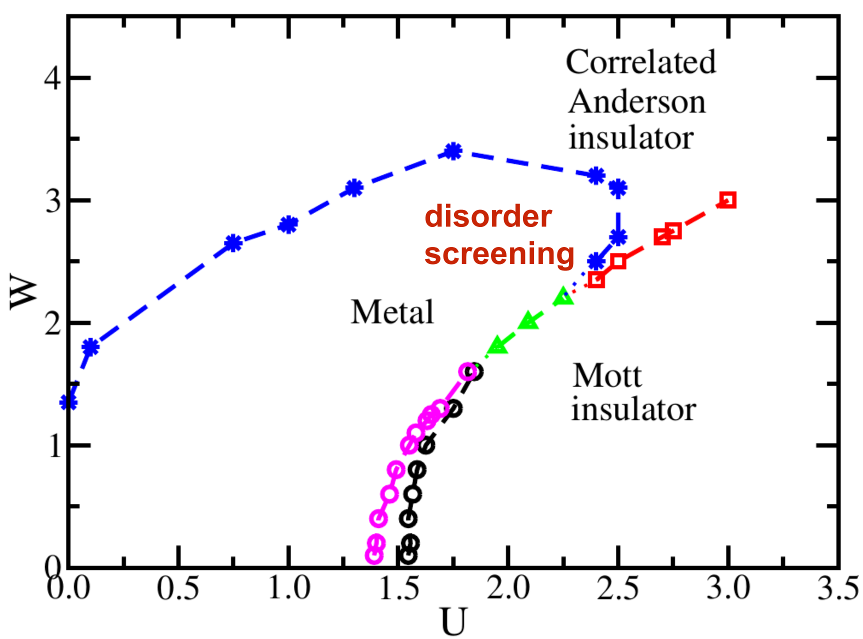


distance to transition

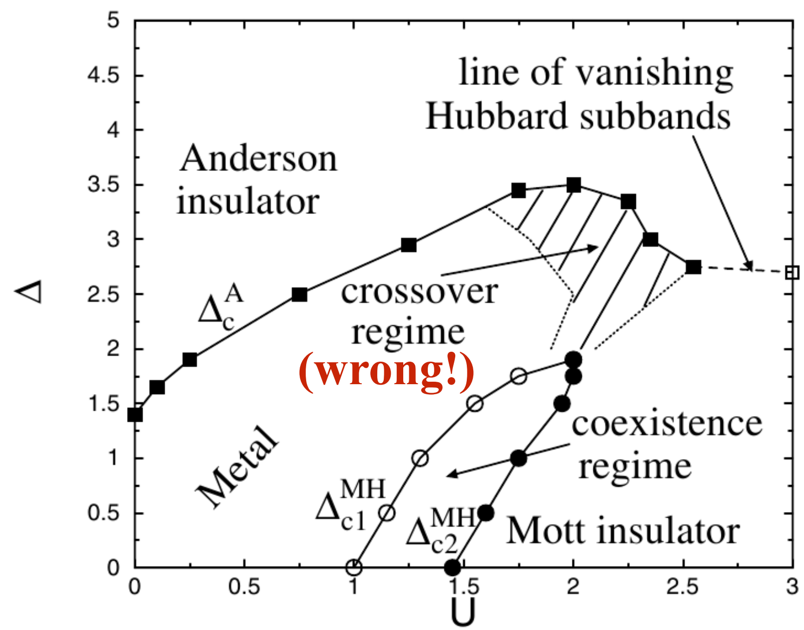
Only fraction of Z_i vanish - two fluid behavior!

TMT-DMFT of Mott-Anderson transition: finite T - coexistence region + QC behavior?

H. Bragança, M. C. O. Aguiar, J. Vučičević, D. Tanasković, V.D. (PRB 2015)



$T = 0.008$: this work



$T = 0$: Byczuk *et al.*, PRL **94**, 056404 (2005)

Current exp. work: K. Kanoda disorder in Mott organics

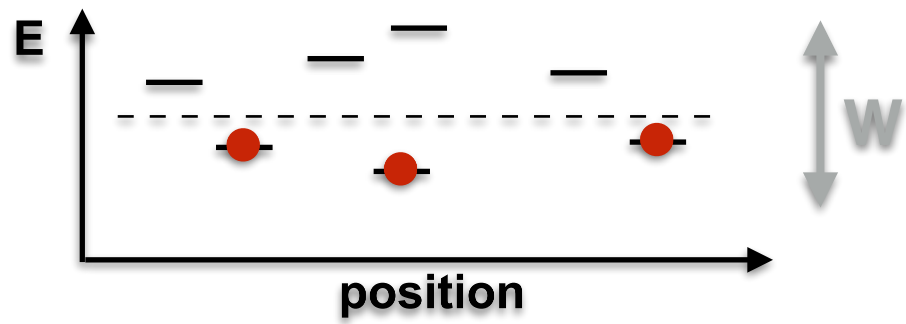
Anderson Localization in Deformable Lattices

Early ideas: Anderson, Nature 1972

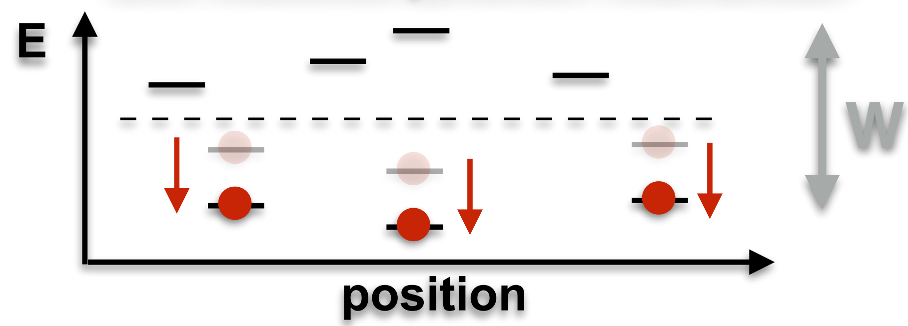
Effect of Franck–Condon Displacements on the Mobility Edge and the Energy Gap in Disordered Materials

IT has long been known that deep impurity centres in insulators, such as fluorescence centres, exhibit large Franck–Condon effects, involving energies of a few eV and many phonons, because the lattice nearby displaces considerably when the centre is occupied by an electron. This contrasts with the typical phonon self energy in a metal which is, by Migdal's theorem[1], confined to energies $\lesssim \hbar\omega_D$ and results entirely from virtual displacements. It has not, as far as I know, been realized previously that there is both a quantitative and qualitative difference between these two cases. An electron in a shallow donor state is shifted in energy by a finite displacement —but not very much—so qualitatively it resembles the deep state but quantitatively it is nearly free. The qualitative change from virtual to real atom displacements arises when the wave function becomes localized, because that is when recoil-free phonon emission is possible.

noninteracting



with electron-phonon interaction



Electron in bound state with impurities leads to polaronic self-trapping

Creates a gap in disordered insulators; anti-screening!

Metal-Insulator Transition?? (no theory before TMT)

TMT + Polaron DMFT: Anderson-Holstein Model

PRL 118, 036602 (2017) PHYSICAL REVIEW LETTERS week ending 20 JANUARY 2017

Disorder-Driven Metal-Insulator Transitions in Deformable Lattices

Domenico Di Sante,[1,2] Simone Fratini,[3] Vladimir Dobrosavljević,[4] and Sergio Ciuchi[5,6]

$$H = H_{el} + H_{ph} + \boxed{H_{e-ph}} + \boxed{H_{dis}}$$

Einstein phonons, frequency $\boldsymbol{\omega_0}$

tight-binding half bandwidth **D** half-filled band

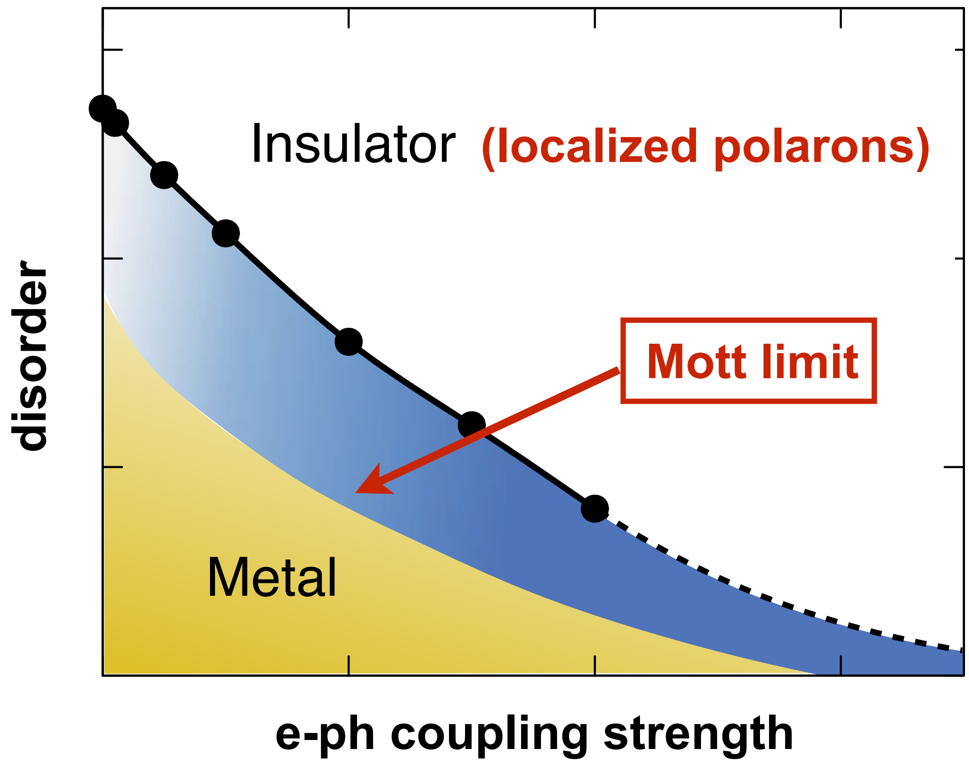
$$H_{e-ph} = g\sum_i c_i^\dagger c_i (a_i + a_i^\dagger) \longleftarrow$$

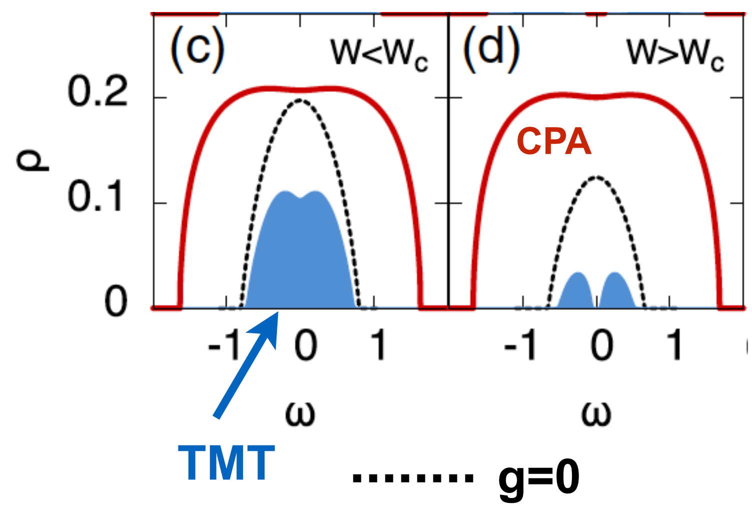
$\mathbf{E_{pot}=g^2/\omega_0}$ $\quad \lambda = 2E_P/D$

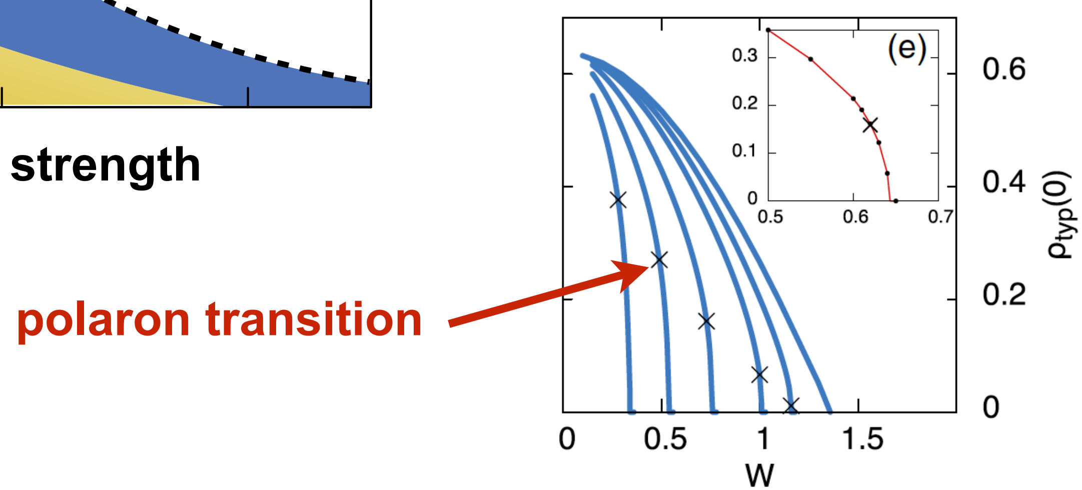
Clean limit: polaron transition at (unphysically) strong coupling ~ O(1)

Anderson-Holstein Transition: Disorder-Induced Polarons

Qualitatively different critical behavior: mobility gap due to polarons







Mott limit and Mooij Correlation

A15 - experiment (Dynes)

Mott
limit

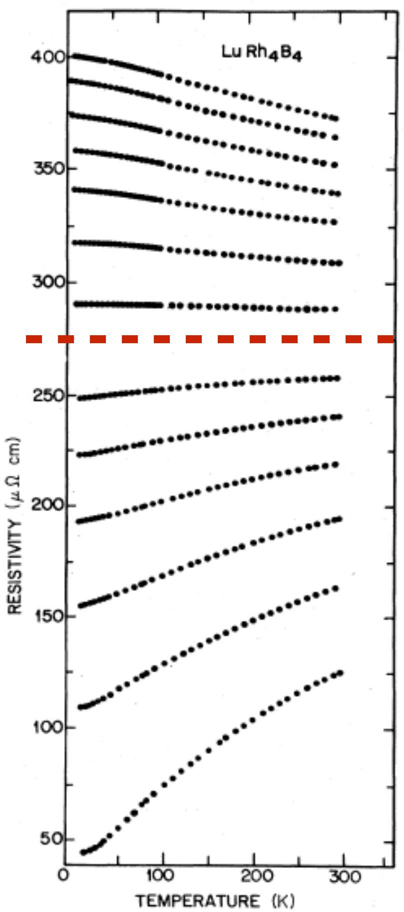
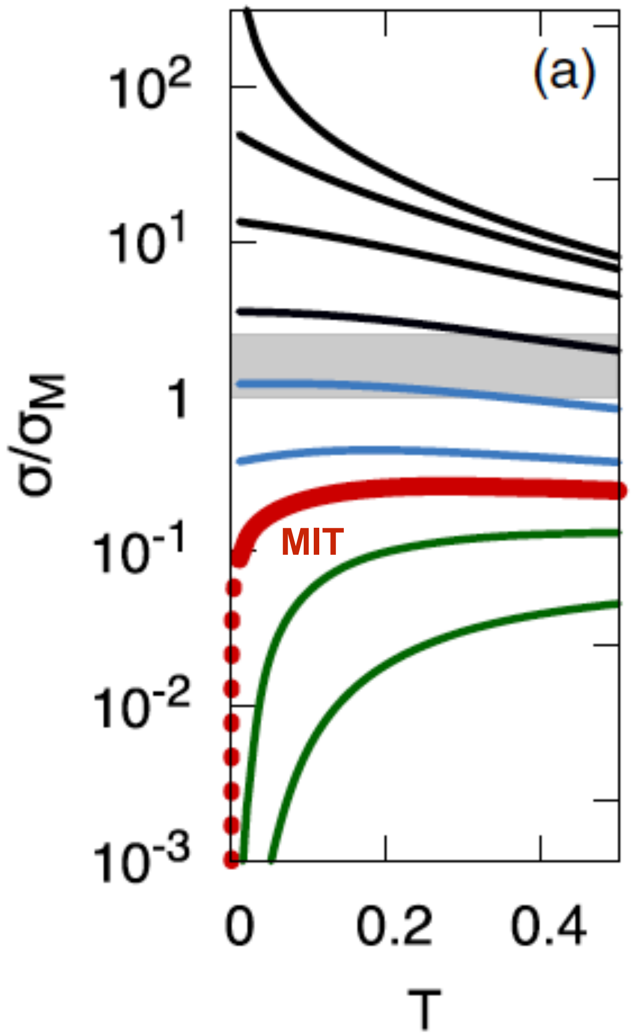
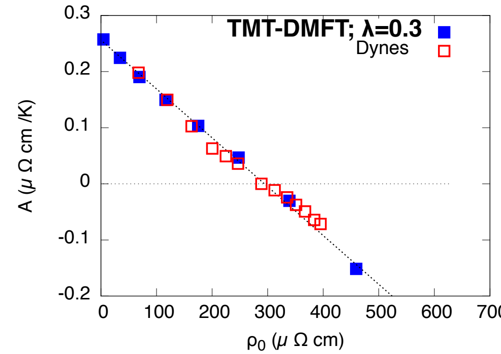


FIG. 20. Resistivity as a function of temperature for $LuRh_4B_4$ at various damage levels. The numbers represent the α-particle dose in units of $10^{16}/cm^2$. From Dynes, Rowell, and Schmidt (1981).

TMT-DMFT theory



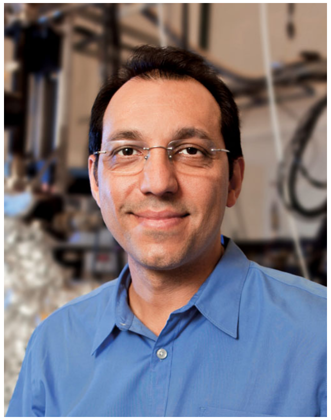


$$\rho = \rho_0 + AT$$

"Separatrix"= Mott Limit

$k_F\ell \sim O(1)$

TMT vs. STM: GaMnAs



Science 5 February 2010:
Vol. 327 no. 5966 pp. 665–669
DOI: 10.1126/science.1183640

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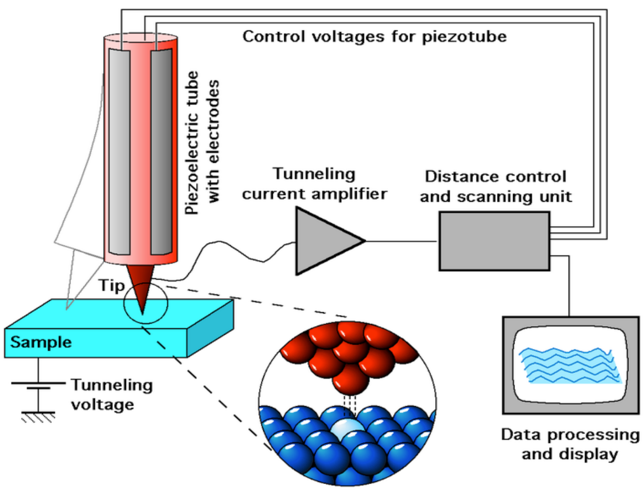
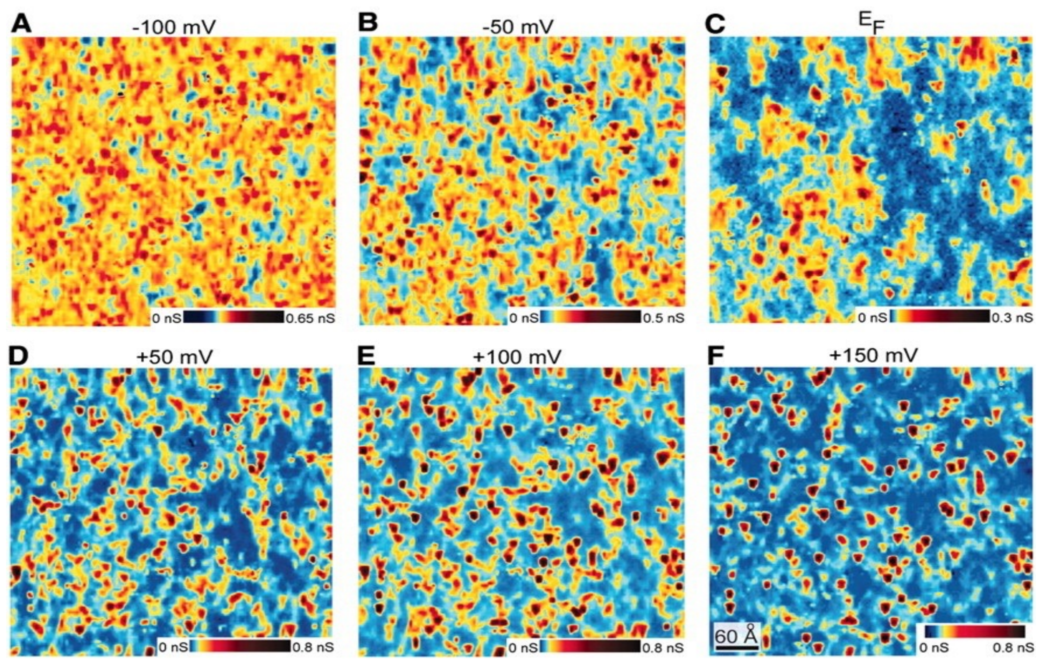
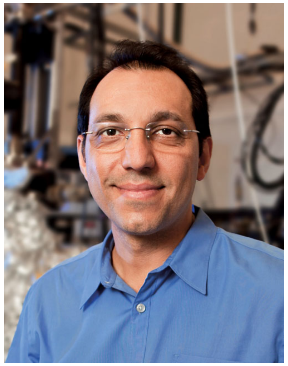
REPORT

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] and Ali Yazdani[1,†]

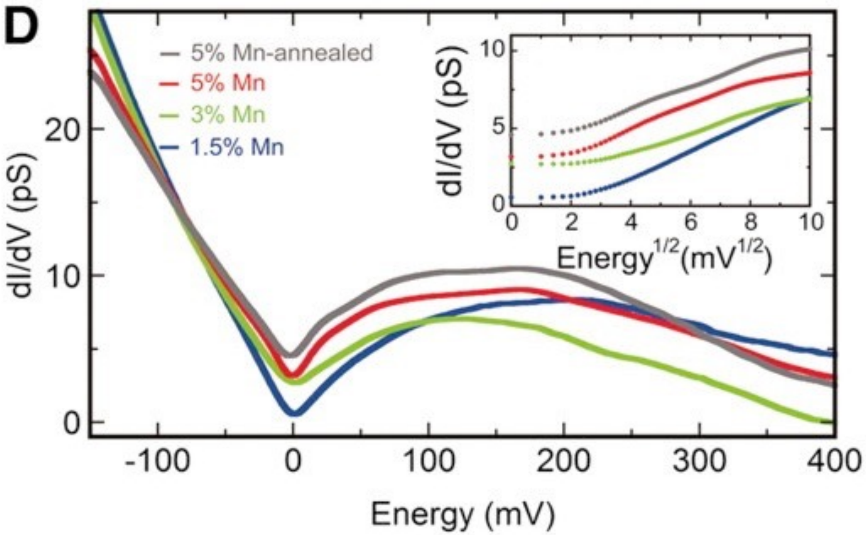




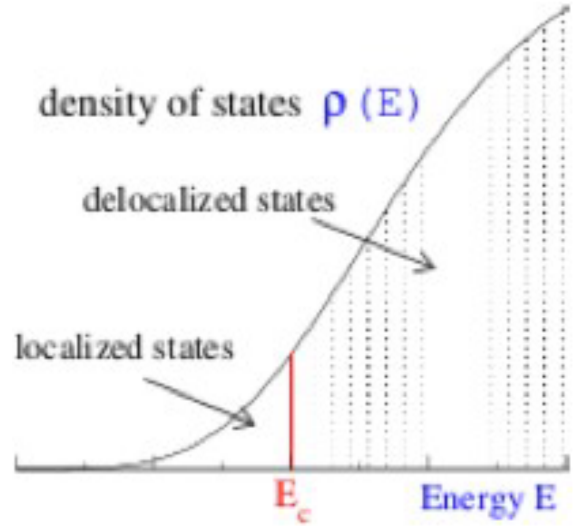


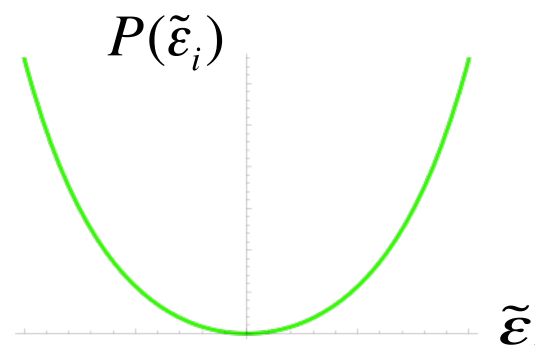
Not your ordinary Anderson transition: pseudogap

STM: Gap opening at MIT?



Anderson: smooth DOS





Modified disorder

Efros-Shklovskii “Coulomb Gap” (long-range!)

$$\tilde{\varepsilon}_i = \varepsilon_i + \sum_j \frac{n_i}{R_{ij}}$$

Amini, Kravtsov, Mueller, New J. Phys. 16 (2014)

Coulomb glass from Extended DMFT

PRL **94,** 046402 (2005) PHYSICAL REVIEW LETTERS week ending 4 FEBRUARY 2005

Nonlinear Screening Theory of the Coulomb Glass

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(Received 26 June 2004; published 2 February 2005)

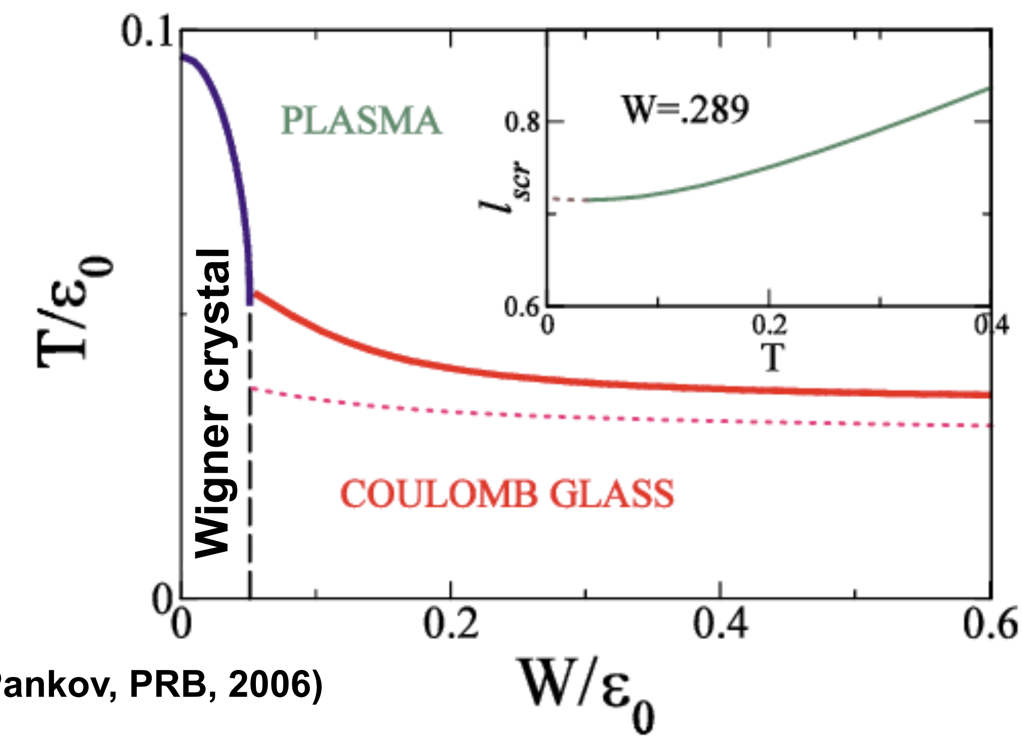
EDMFT + replicas = Parisi theory

Replica symmetry breaking
Marginal stability (replicon mode)
Self-organized criticality

Universal Efros-Shklovskii gap

$$\boxed{\rho(\varepsilon) \sim \varepsilon^{(d-\alpha)/\alpha}}$$

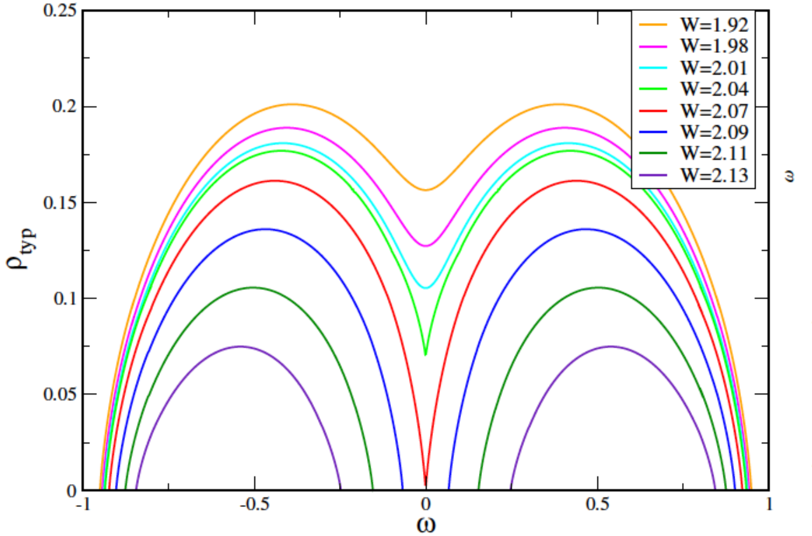
(Also: Mueller and Pankov, PRB, 2006)

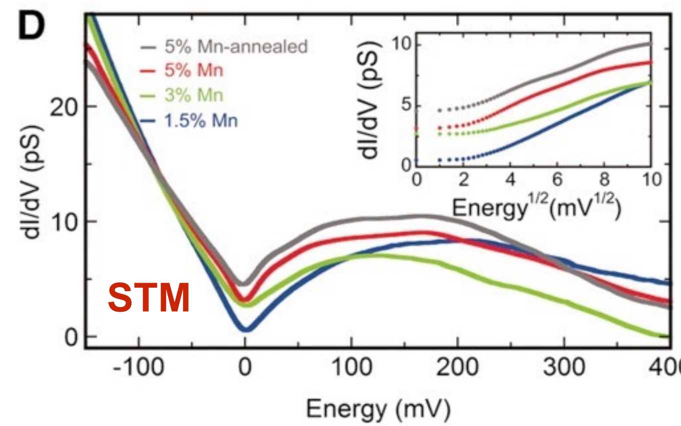


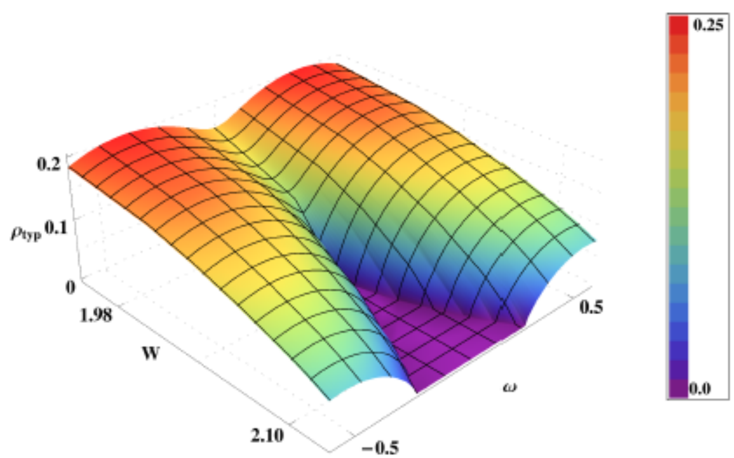
TMT vs. STM: Results

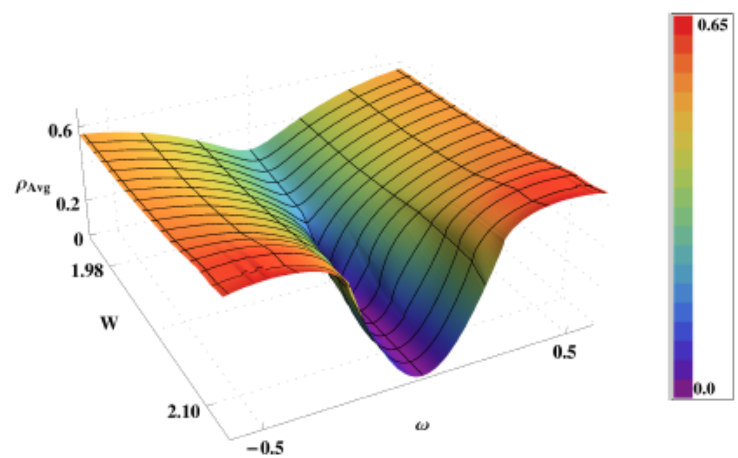
S. Mahmoudian, Shao Tang, V. D., (PRB 2015)

Typical DOS: hard gap





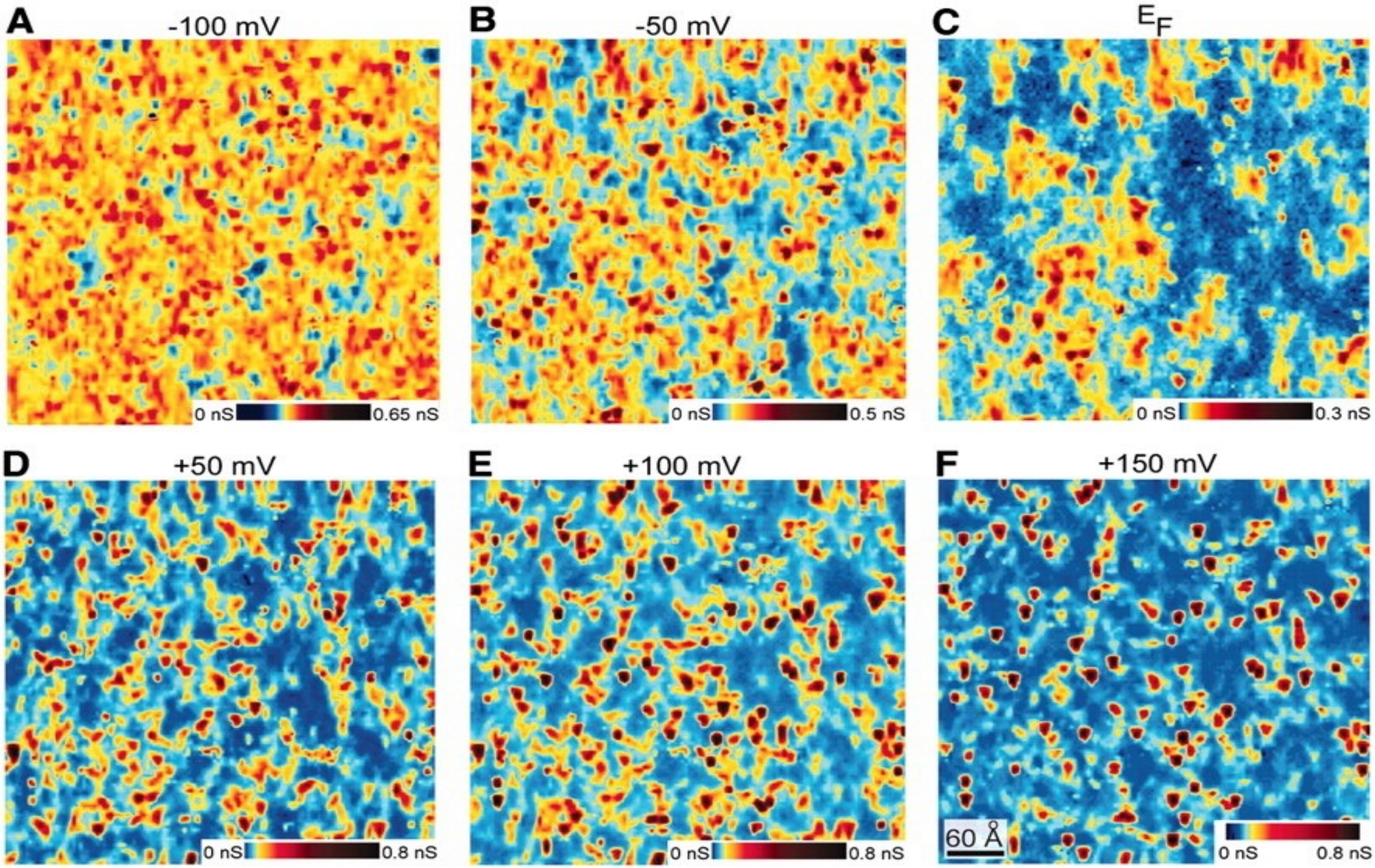




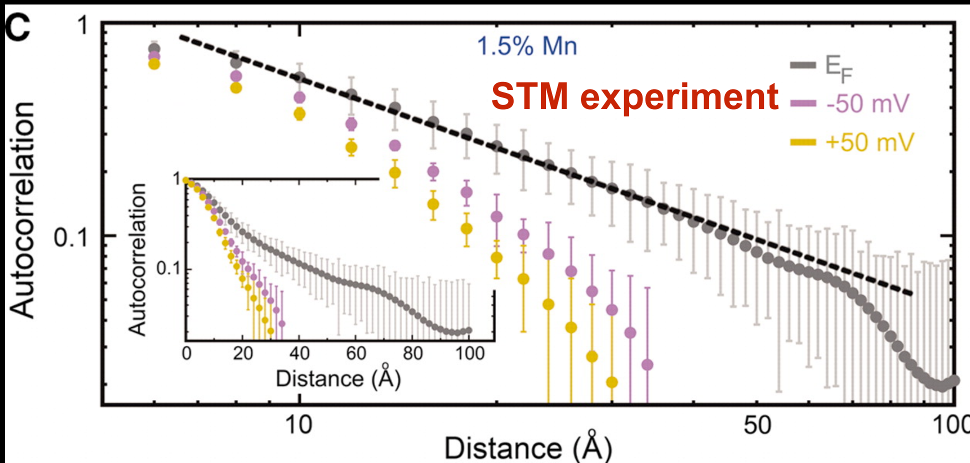
Typical DOS: hard gap

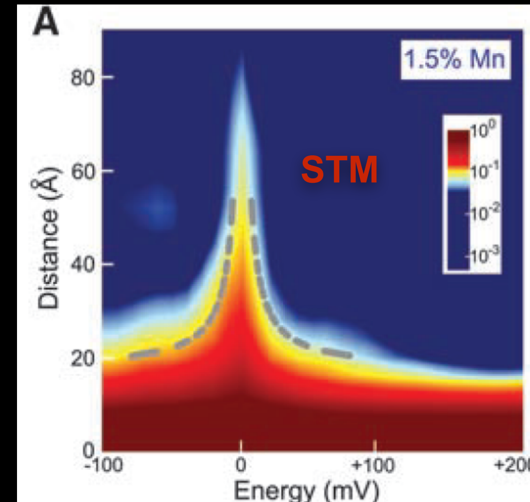
Average DOS: ES pseudogap

TMT vs. STM: GaMnAs

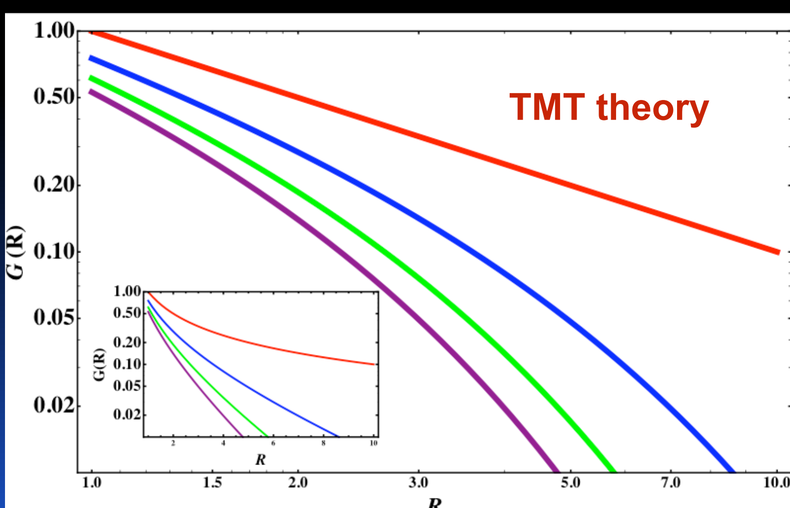


Spatial Correlations: “Landau-Ginzburg” TMT



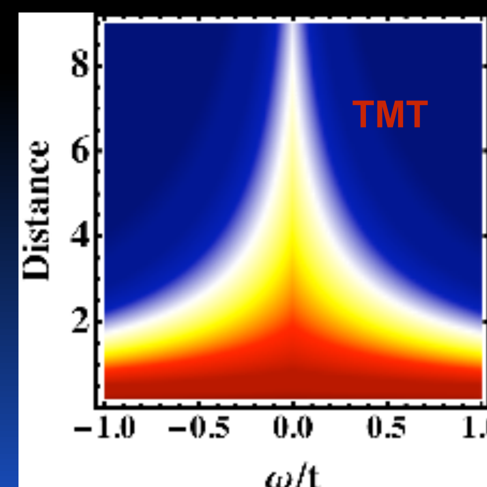


$$\chi(E,r)=\frac{1}{2\pi}\int d\theta\int d^2r'[g(E,r')-g_0(E)]\times[g(E,r+r')-g_0(E)]$$

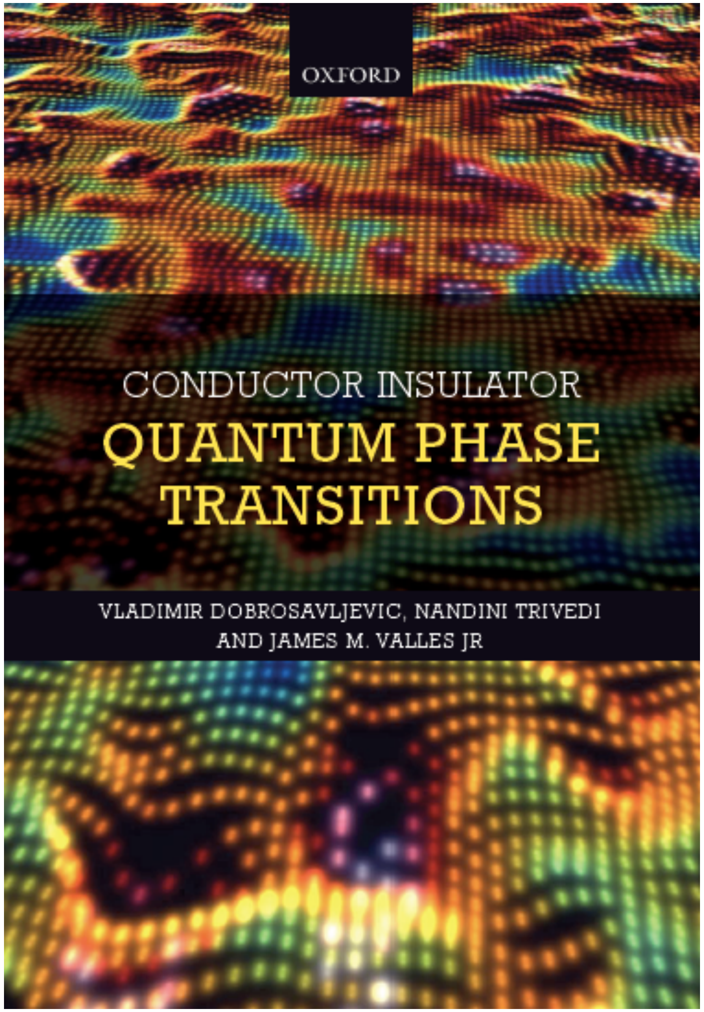


$$\delta\rho\propto G(R)\sim\frac{1}{R}e^{\left(\frac{-R}{\xi}\right)}$$

$$\xi\sim\frac{1}{\sqrt{r(\omega)}}\sim\frac{1}{\omega}$$



To learn more:



http://badmetals.magnet.fsu.edu

(just Google "Bad Metals")

Book:

Oxford University Press, June 2012

Already listed on Amazon.com

ISBN 9780199592593