

Landau Theory for Disorder-Driven Metal-Insulator Transitions in Deformable “Media”

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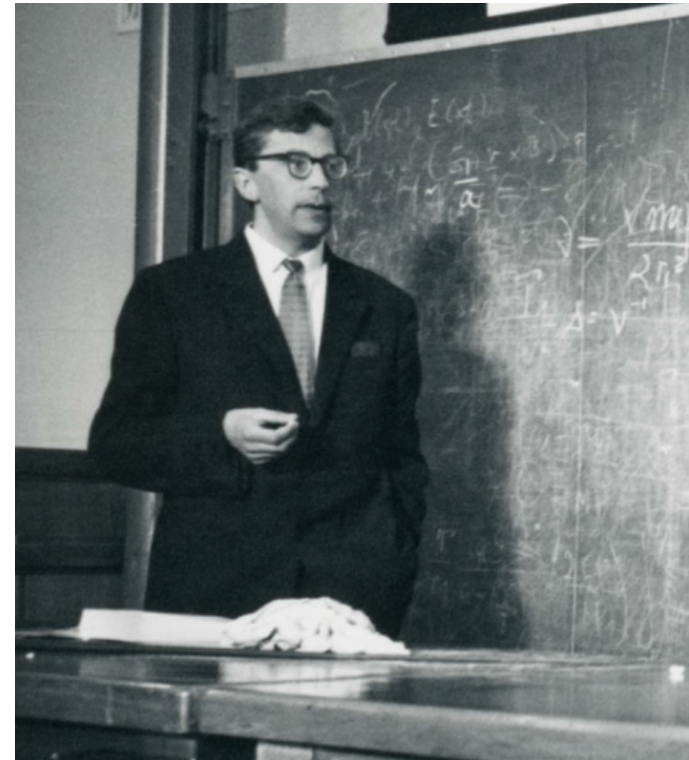
Collaborators:

Simone Fratini (Grenoble)

Sergio Ciuchi (Rome)

Domenico Di Sante (Würzburg)

Modern Trends in Condensed Matter Physics
(**Lev Gor'kov** Memorial Conference)
June, 24-27, 2019 L. D. Landau Institute



Funding:

NSF grants:

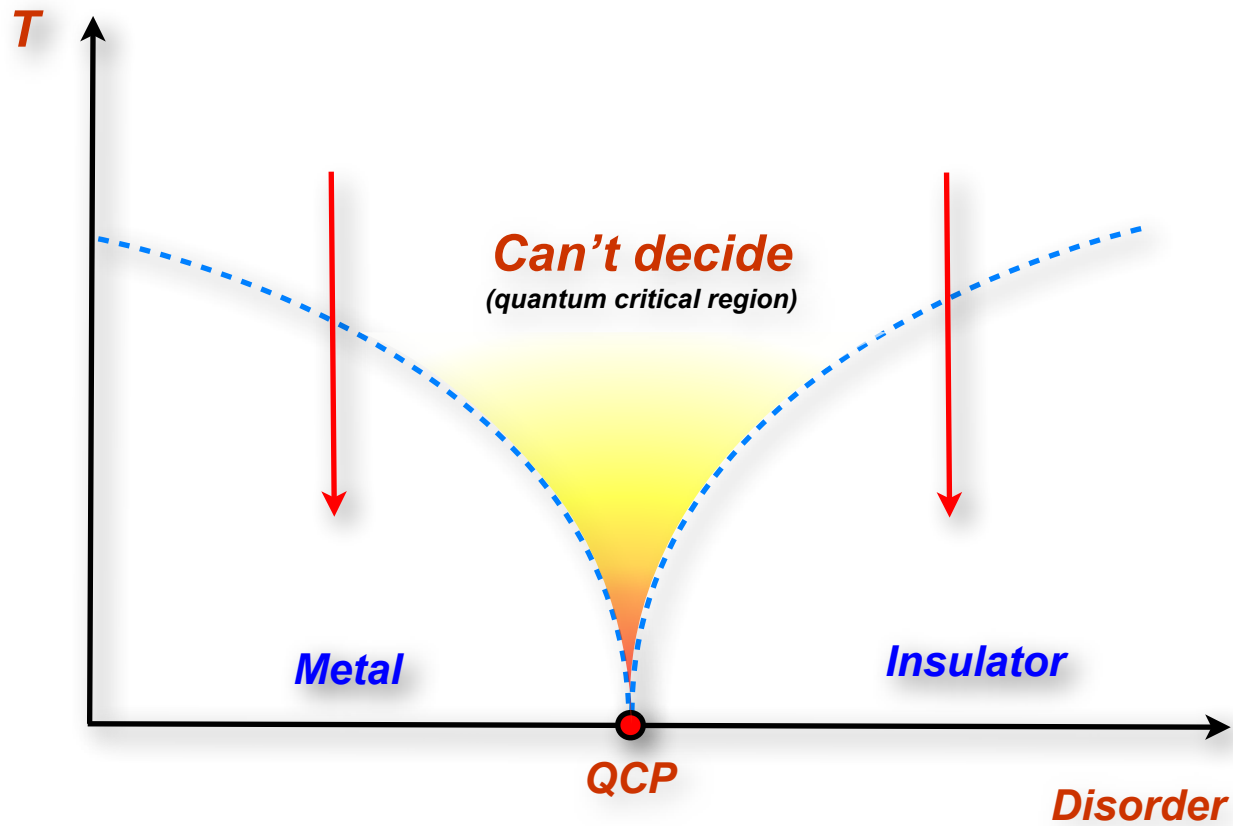
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...



MIT Quantum Criticality?



Mechanisms for Localization?

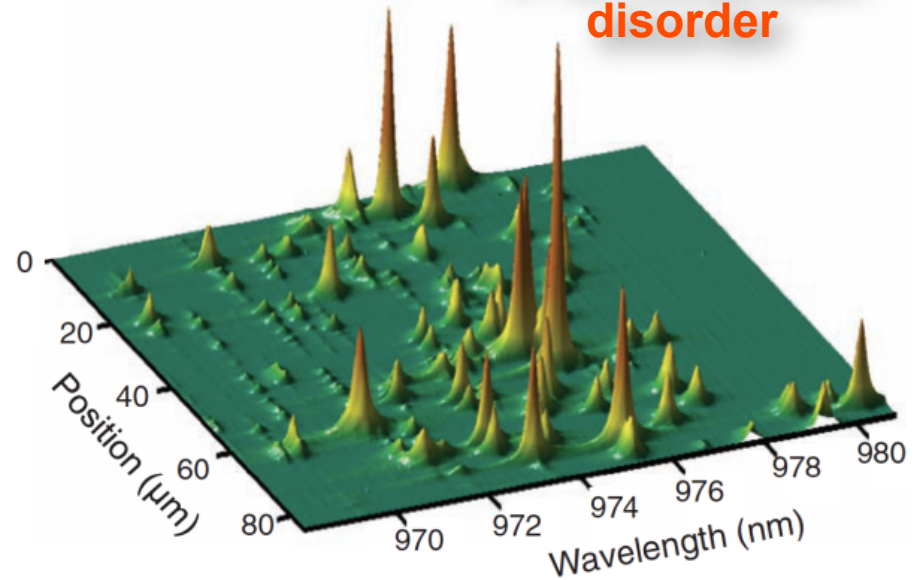
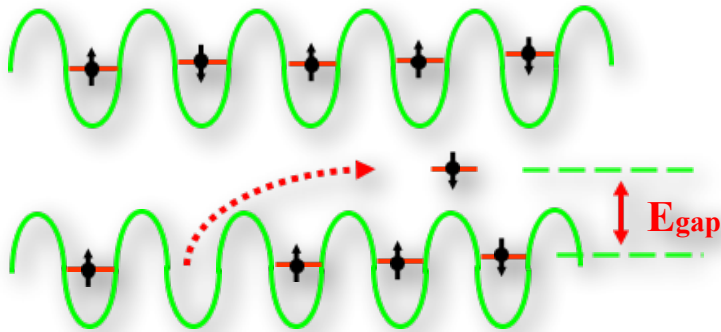


Sir Neville Mott:
(whatever) **interaction**

Friend or Foe???



P. W. Anderson:
disorder



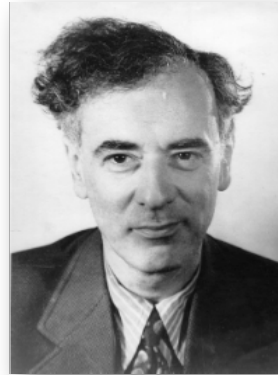
Theoretical Approaches

Standard critical points:

Spontaneous symmetry breaking

Order parameter, Landau-Ginzburg

Renormalization group, field theory



Metal-Insulator Transitions:

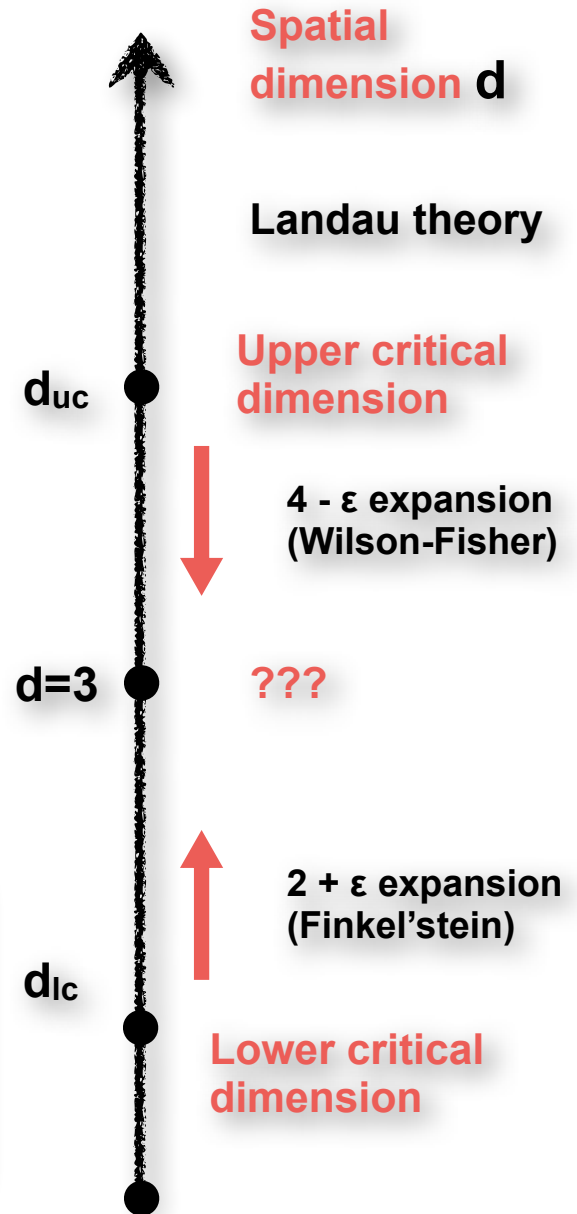
NO symmetry breaking!

Landau theory, upper critical dimension ???

“Forced” to use $2 + \epsilon$ expansion

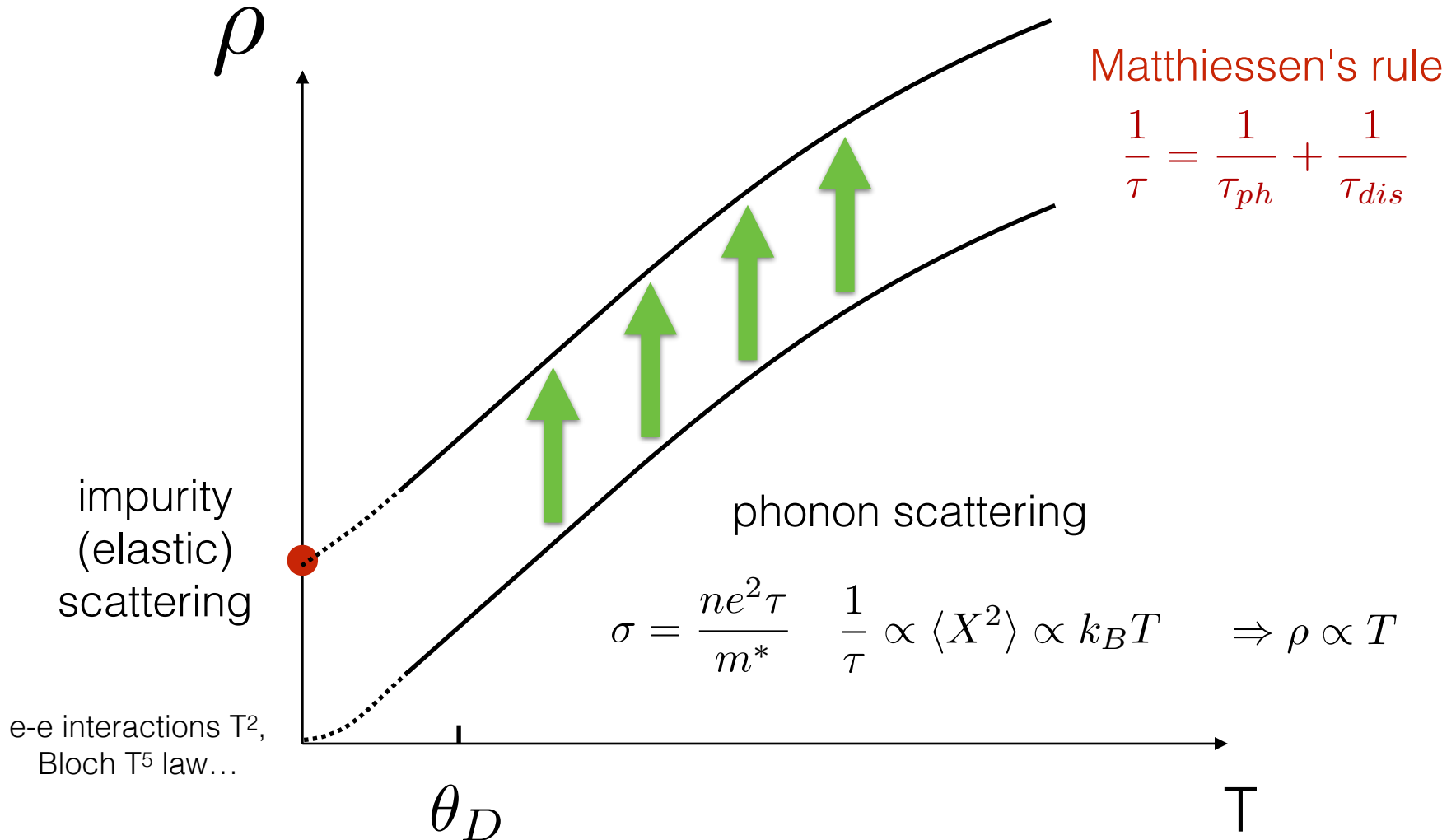
Problems:

weak-coupling, convergence in ϵ (Murthy)



$\rho(T)$ vs disorder in metals

What I remember from college:



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

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

Bad conductor: disorder+phonons???

“Mott-Ioffe-Regge (MIR) limit”
($k_{Fl} \sim O(1)$)

Breakdown of **Mathiessen’s rule:**

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

Good metal: phonons

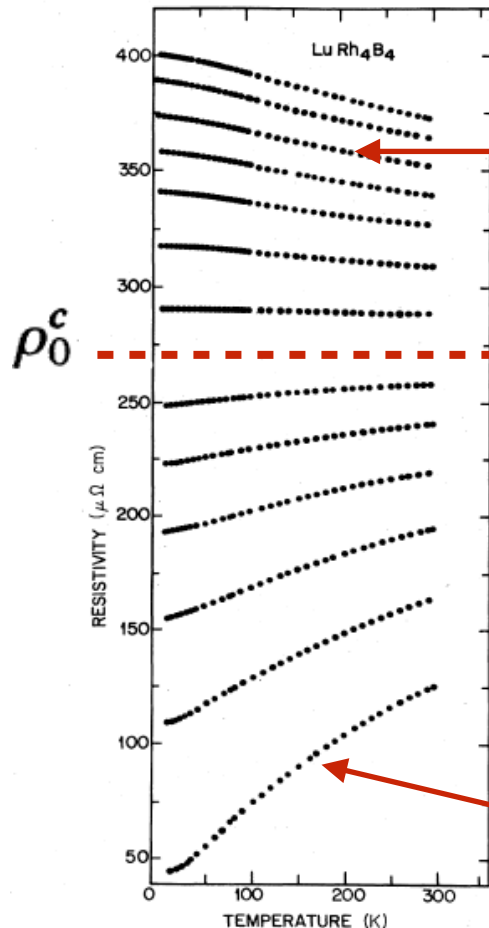
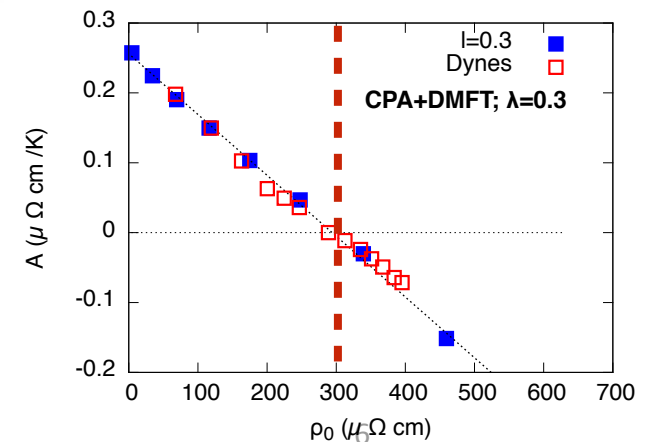


FIG. 20. Resistivity as a function of temperature for LuRh_4B_4 at various damage levels. The numbers represent the α -particle dose in units of $10^{16}/\text{cm}^2$. From Dynes, Rowell, and Schmidt (1981).

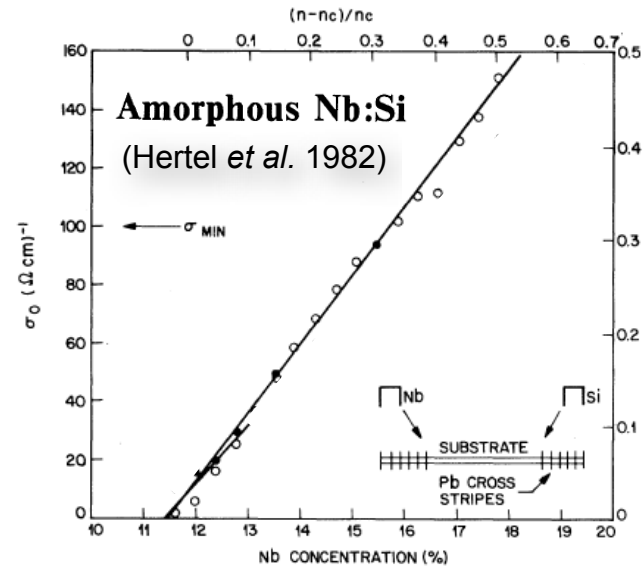
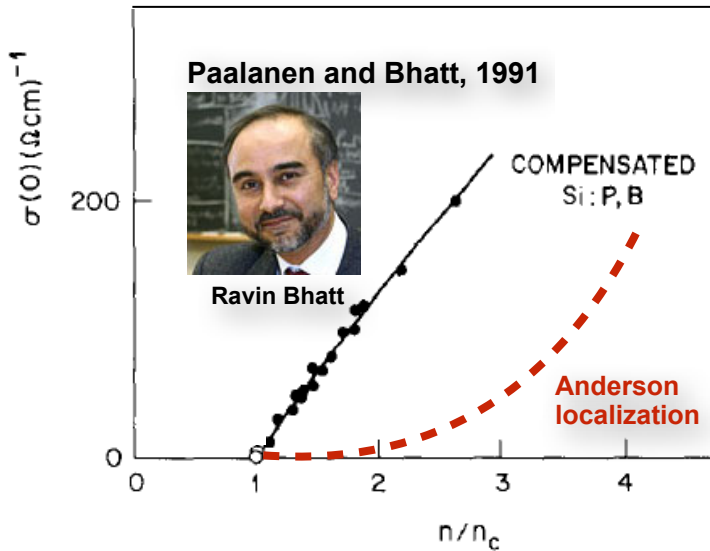
Mooij (1973) correlation???

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

(all cross at $T = 1/A$)



Experimental puzzles II: Robust Low-T Transport



Landau-like (?) critical behavior: $\sigma \sim (n-n_c)^\mu$

$$\mu = 1$$

Huge range of parameters: $(n-n_c)/n_c \sim O(1)$

~~Anderson localization: $\mu = 1.6 \gg 1$~~

~~Percolation: $\mu = 2 \gg 1$~~

Experimental puzzles III: Pseudogap at criticality (STM)



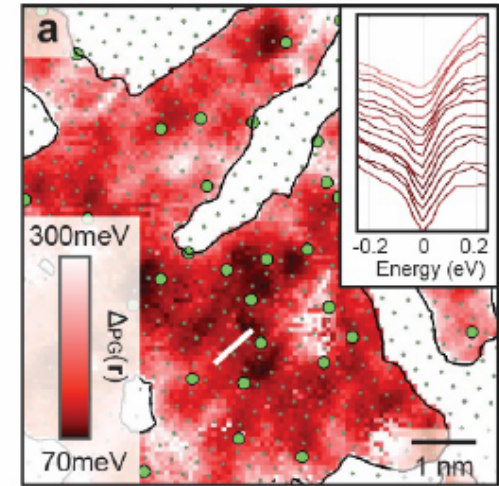
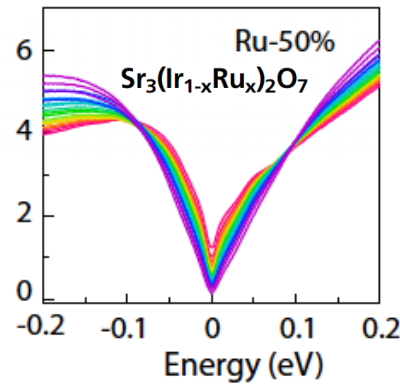
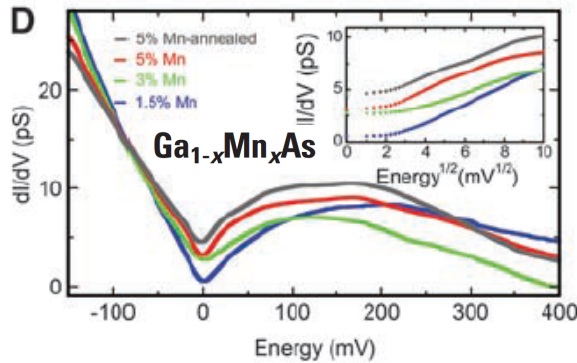
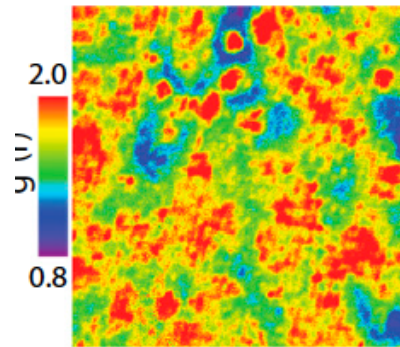
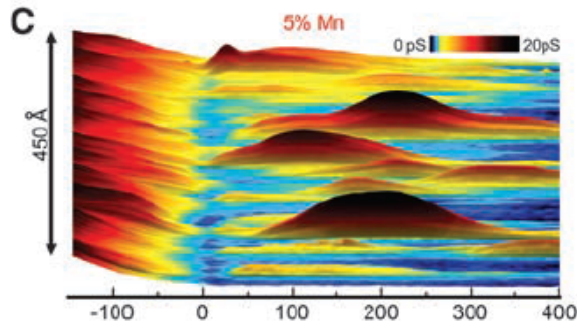
Ali Yazdani
SCIENCE, 2010



Vidya Madhavan
PNAS, 2018



Milan Allen
Nat. Phys. 2016



$(\text{Sr}_{1-x}\text{La}_x)_2\text{IrO}_4$

STM: LDOS statistics and spatial correlations at criticality?



Strong disorder in a Deformable “Medium”

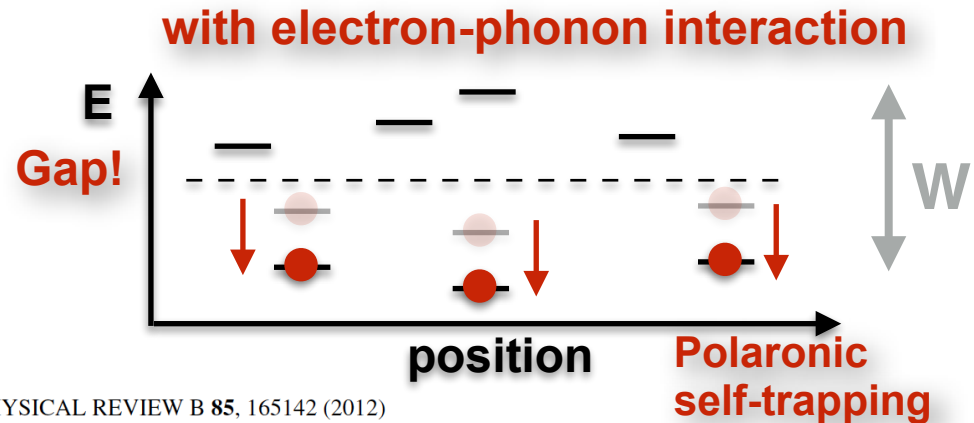
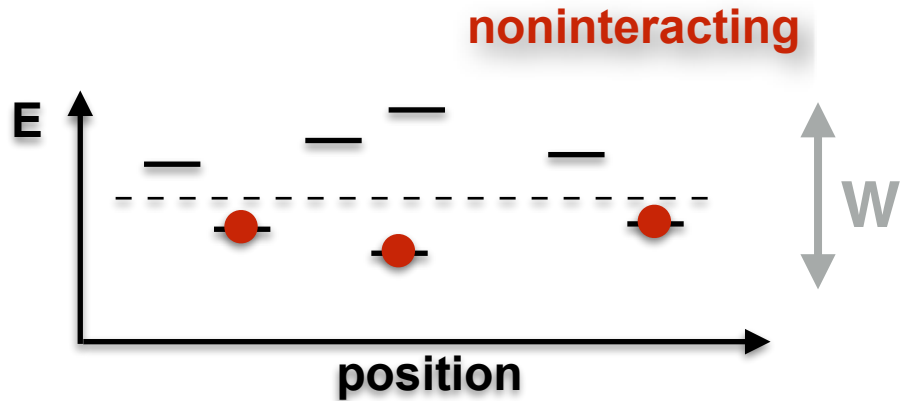
Early ideas: Anderson, Nature 1972

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 theorem¹, 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.



Strong electron-lattice coupling as the mechanism behind charge density wave transformations in transition-metal dichalcogenides



PHYSICAL REVIEW B 85, 165142 (2012)

Lev P. Gor'kov*

National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA

Similar also for: (1) Magnetic polarons, (2) Electronic polarons (Efros-Shklovskii),...??

Toy Model: 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}

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

Einstein phonons, frequency ω_0

tight-binding half bandwidth D half-filled band

$$H_{e-ph} = g \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) \quad \leftarrow \quad E_{\text{pot}} = g^2/\omega_0 \quad \lambda = 2E_P/D$$

boson (any?)

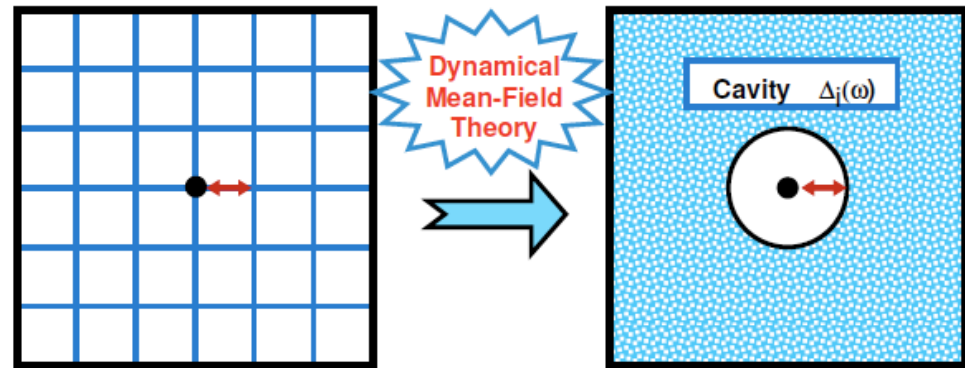
Clean limit: **polaron effects** at (un-physically) strong coupling $\sim O(1)$



Local Perspective: Dynamical Mean-Field Theory



Gabi Kotliar



Non-perturbative treatment of **interactions** and disorder
(Anderson-Yu, 1984)

Small polaron formation at strong disorder (*Millis et al.*)

TWO VERSIONS:

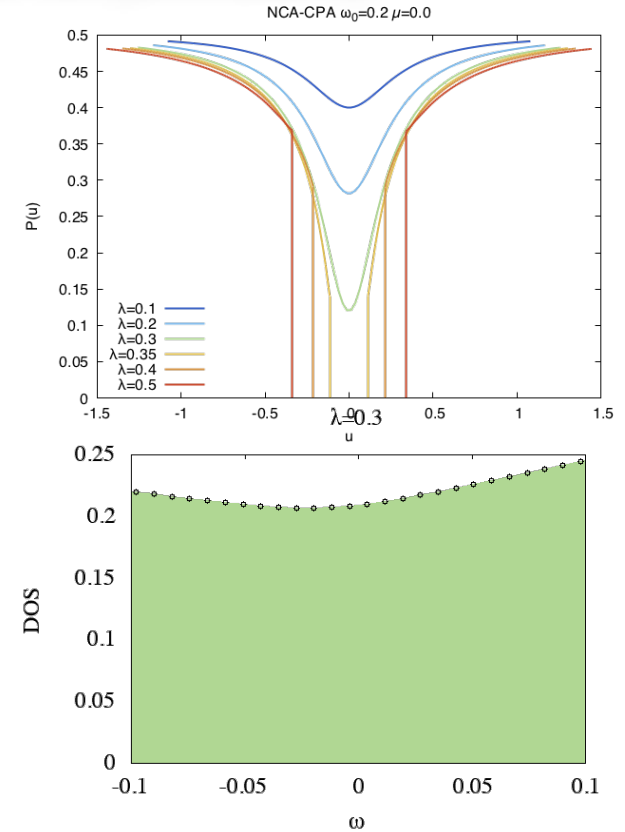
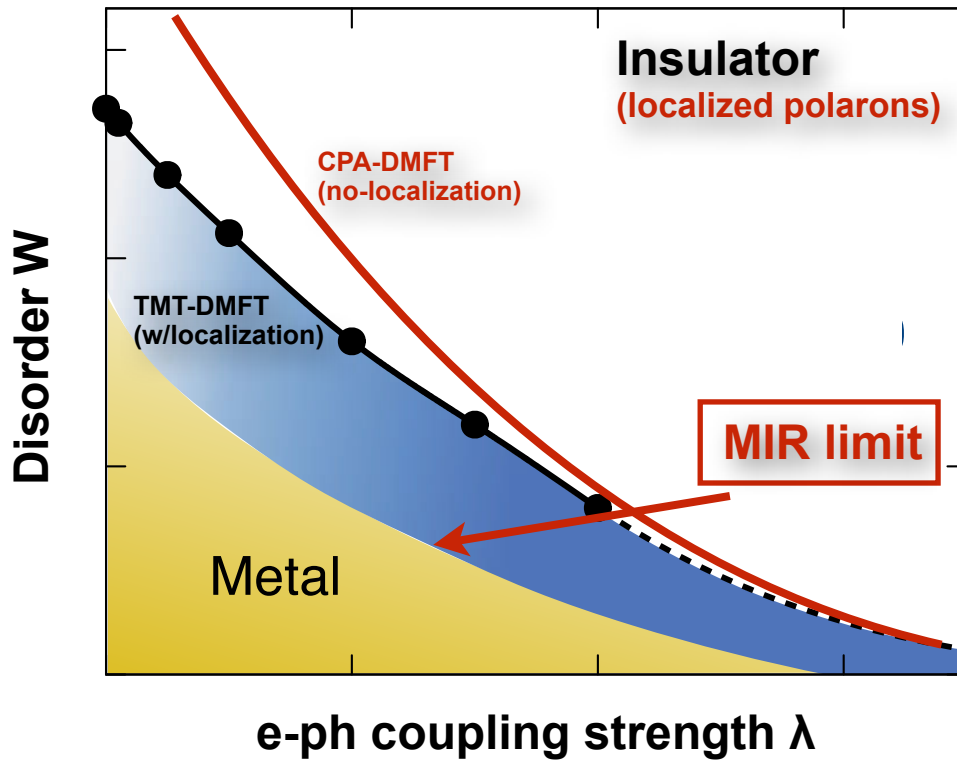
1. **TMT-DMFT** (with Anderson localization)
2. **CPA-DMFT** (no Anderson localization)

Exact in $d=\infty$, **new saddle-point** for field theory

Anderson-Holstein Transition: Disorder-Induced Polarons

Qualitatively different critical behavior: **gap opening at Fermi energy**

Mechanism “survives” **removing localization** in $d=\infty$. (CPA-DMFT)



Pseudogap opens in **disorder distribution**

$$\rho_c(\omega) \sim \omega^{1/3}$$

$$\sigma(T=0) \sim (W_c - W)$$

Universal behavior at arbitrary band-filling, finite compressibility

$$\mu = 1$$

ARTICLE OPEN

The origin of Mooij correlations in disordered metals

Sergio Ciuchi^{1,2}, Domenico Di Sante³, Vladimir Dobrosavljević⁴ and Simone Fratini⁵

A15 - experiment (Dynes)

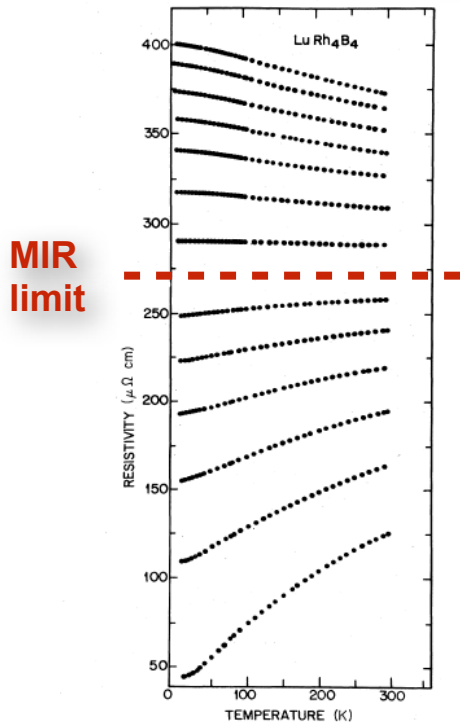
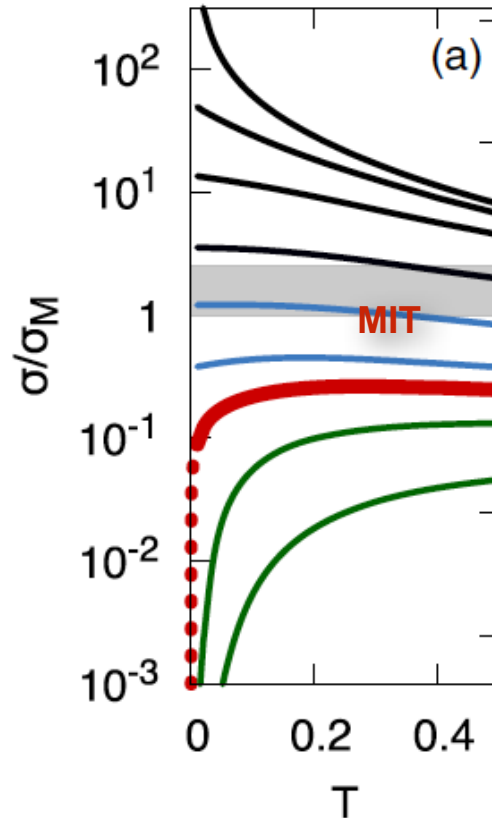


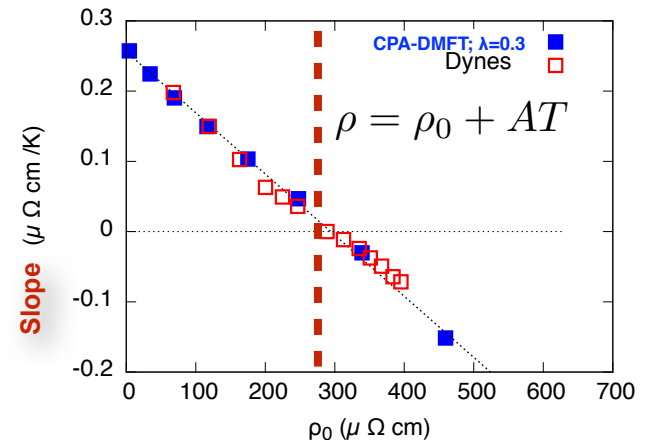
FIG. 20. Resistivity as a function of temperature for LuRh₄B₄ at various damage levels. The numbers represent the α -particle dose in units of $10^{16}/\text{cm}^2$. From Dynes, Rowell, and Schmidt (1981).

CPA-DMFT theory



Breakdown of Mathiessen's rule:

$$\Sigma = \Sigma_{el} + G_{el}^{-1} \left\langle \hat{G}_{el}^{\xi} \hat{\Sigma}_{in}^{\xi} \hat{G}_{el}^{\xi} \right\rangle G_{el}^{-1}$$



“Separatrix”= MIR Limit
 $k_{Fl} \sim O(1)$

Beyond DMFT: Field Theory Formulation

$$Z = \int \prod_i D\Psi_i^* D\Psi_i D x_i D\varepsilon_i P(\varepsilon_i) D t_{ij} P(t_{ij}), e^{-S[\Psi_i^*, \Psi_i, X_i]}$$

Wegner's "gauge invariant" model of disorder: $\langle t_{ij}^2 \rangle = t^2/z$

$$S_o[\Psi_i^*, \Psi_i, \varepsilon_i] = \sum_{\alpha=1}^n \sum_{ij} \int_0^\beta d\tau \Psi_{i,\alpha}^*(\tau) [(\partial_\tau - \varepsilon_i \mu) \delta_{ij} - t_{ij}] \Psi_{j,\alpha}(\tau),$$

$$S_{int}[\Psi_i^*, \Psi_i, X_i] = g \sum_i \sum_{\alpha} \int_0^\nu d\tau \Psi_{i,\alpha}^*(\tau) \Psi_{i,\alpha}(\tau) X_{i,\alpha}(\tau).$$

$$S_{hop} = \frac{1}{2z} t^2 \sum_{\alpha,\beta} \sum_{ij} \int_0^\beta d\tau \int_0^\beta d\tau' \Psi_{i,\alpha}^*(\tau) \Psi_{i,\beta}(\tau') \Psi_{j,\beta}^*(\tau') \Psi_{j,\alpha}(\tau)$$

Introduce Q-fields: $Q_i^{\alpha\beta}(\omega_1, \omega_2) = \frac{1}{z} \sum_i f_{ij} \Psi_{j,\alpha}^*(\omega_1) \Psi_{j,\beta}(\omega_2)$

$$S_{hop}[Q] = -\frac{t^2}{2} \sum_{\alpha\beta} \sum_{ii} \sum_{\omega_1\omega_2} K_{ij} Q_i^{\alpha\beta}(\omega_1, \omega_2) Q_j^{\alpha\beta}(\omega_1, \omega_2)$$

$$S_{loc}[Q] = -\sum_i \ln \int d\varepsilon_i P(\varepsilon_i) D\Psi_i^* D\Psi_i D X_i \exp\{-S_{eff}[\Psi_i^*, \Psi_i, \varepsilon_i, Q_i, X_i]\}$$

$$S_{eff}[\Psi_i^*, \Psi_i, \varepsilon_i, Q_i, X_i] = -\sum_{\alpha\beta} \sum_{ij} \sum_{\omega_1\omega_2} \Psi_{i,\alpha}^*(\omega_1) [(i\omega_1 + \mu - \varepsilon_i) \delta_{\alpha\beta} \delta_{\omega_1\omega_2} - t^2 Q_i^{\alpha\beta}(\omega_1, \omega_2)] \Psi_{i,\beta}(\omega_2) + S_{int}[\Psi_i^*, \Psi_i, X_i] + S_{ph}[X_i]$$

local effective action (DMFT)

(fluctuating) cavity field

DMFT as Saddle-Point

CPA- DMFT as **saddle-point**: (exact in $d \rightarrow \infty$):

$$\frac{\delta S[Q]}{\delta Q_i^{\alpha\beta}(\omega_1, \omega_2)} = 0 \quad [Q_i^{\alpha\beta}(\omega, \omega')]_{SP} = \delta_{\alpha\beta} \delta_{\omega\omega'} Q_{SP}(\omega)$$

$$Q_{SP}(\omega) = \bar{G}(\omega) = \int d\varepsilon_i P(\varepsilon_i) G_i(\omega) \quad G_i(\omega) = \langle \Psi_{i,\alpha}^*(\omega) \Psi_{i,\alpha}(\omega) \rangle_{S_{eff}[\Psi_i^*, \Psi_i, \varepsilon_i, Q_{SP}, X_i]}$$

Local density of states as **order-parameter**

Fluctuations about saddle-point: LG functional:

$$S[G] = \int dR \sum_{\omega_n} \left[-i\omega_n G(R, \omega_n) + \frac{1}{2} G(R, \omega_n) (r - \nabla^2) G(R, \omega_n) + \frac{1}{4} u G^4(R, \omega_n) + \dots \right]$$

Spatial correlations: $\chi(R, \omega) = \langle \rho_\omega(0) \rho_\omega(R) \rangle \sim \frac{1}{R^{d-2}} \exp\{-R/\xi(\omega)\}$

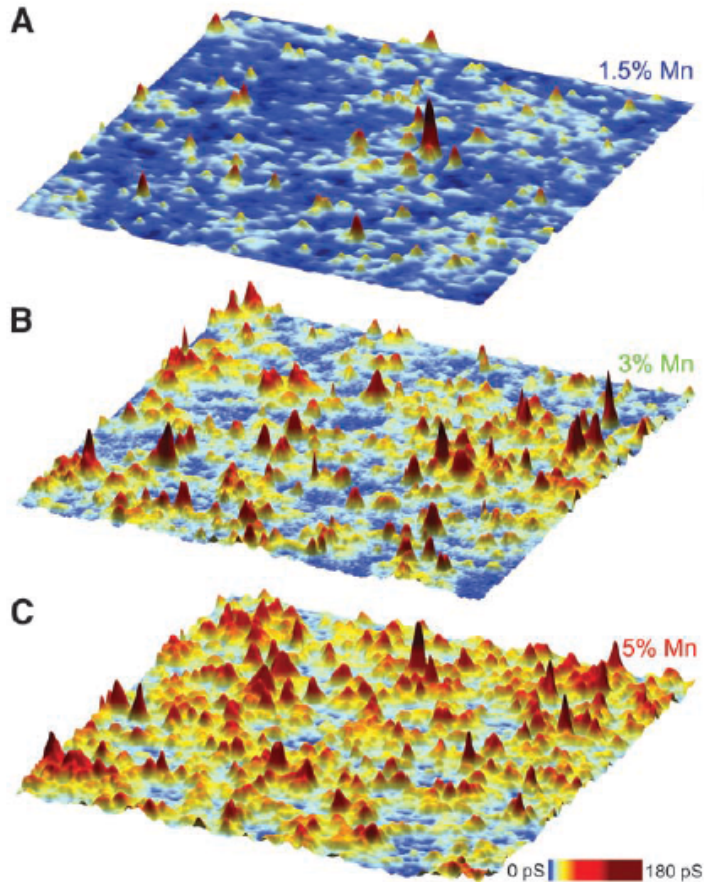
$$\xi \sim |r|^{-1/2} \text{ at } \omega = 0.$$

$$\xi \sim \omega^{-1/3} \text{ at } \bar{r} = 0$$

LDOS Spatial Fluctuations/Correlations

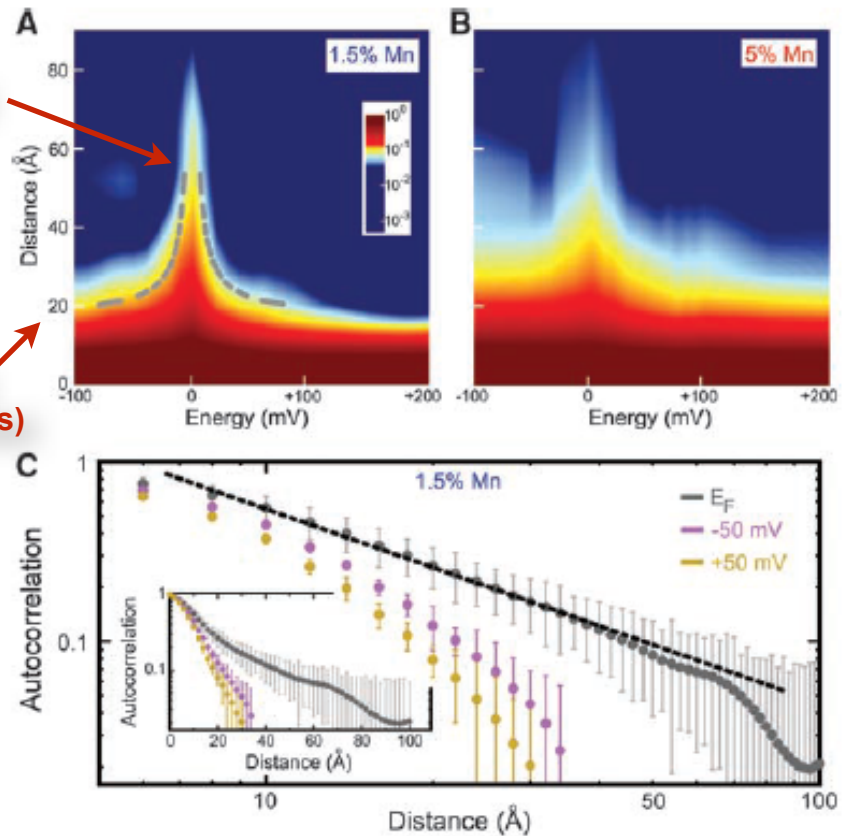


Ali Yazdani
SCIENCE, 2010



$\zeta_{\max} \sim 3a$

$\zeta_{\min} \sim a$
(Mg radius)



Agreement with LG theory:

$$\chi(R, \omega) = \langle \rho_\omega(0) \rho_\omega(R) \rangle \sim 1/R \quad (d=3)$$

Probing only “modest” length scales $a < \zeta < 3a$ - Landau theory (mean-field) regime!

Perspectives and challenges

- Dominant disorder **modification** due to correlations (CPA+DMFT)
- Quantitative description **Mooij correlation at MIR limit**
- Robust low-T critical transport of **Landau-like** critical behavior!
- Landau-Ginzburg MIT theory explains **pseudogap** at criticality (STM)
- Other interaction effect: magnetic polarons, “electronic polarons”,...?
- Long-distance processes: “weak localization”, “interaction-localization”?
- Metastability and glassy behavior?
- Beyond Landau: ϵ - expansion

