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

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Workshop “Localization in Quantum Systems”
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MIT Quantum Criticality?

Can’t decide
(quantum critical region)

T

Insulator QCP Metal

Fermi energy
Mechanisms for Localization?

Friend or Foe???

Sir Neville Mott: interaction

Order parameters??

P. W. Anderson: disorder

E_{gap}
Experimental puzzles I: Mott limit and Mooij Correlation


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

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

Bad conductor: phonons+disorder???

Mooij (1973) correlation???

Breakdown of Mathiessen’s rule:

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

Good metal: phonons

FIG. 20. Resistivity as a function of temperature for LuRh4B4 at various damage levels. The numbers represent the α-particle dose in units of 10^4/cm². From Dynes, Rowell, and Schmidt (1981).
Experimental puzzles II: STM in GaMnAs

Visualizing Critical Correlations Near the Metal–Insulator Transition in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$


A $-100 \text{ mV}$  
B $-50 \text{ mV}$  
C $E_F$

D $+50 \text{ mV}$  
E $+100 \text{ mV}$  
F $+150 \text{ mV}$
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
Renormalization group, field theory

Metal-Insulator Transitions:

NO symmetry breaking!
Order parameter???
Huge spatial fluctuations
Many metastable states ("glass")

"...orthodox phase transition theory will be of little help to us for the time being, and thus the great body of literature in the field is simply irrelevant..."

III—Condensed Matter, 1979
Phillip W. Anderson
Dynamical Mean-Field Theory

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

Exact for "maximal frustration"

Suppress all (inter-site) spin correlations!

Local scattering processes

"Kondo physics" forms Fermi liquid

Gabri Kotliar

Paul Cezzane
Dynamical Mean-Field Theory (DMFT)

Heisenberg: \( p \) or \( x \)?

Dynamics: Golden Rule

\[ \Delta(\omega) = t^2 \rho_c(\omega) \sim 1/\tau \]

Escape rate (disorder: Anderson 1958)

Spectrum of the “cavity”

Matrix element
Quantum Critical Transport near the Mott Transition

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DMFT theory around crossover line

\[ T_c \sim 2\% T_F \]
Mott organics: **universal** high-T scaling


\[
\tilde{\rho} = \exp\left[\pm \left(\frac{T}{T_0}\right)^{-1/z_v}\right]
\]

“stretched exponential”

\(z_v = 0.60\) and \(c = 25.3\) for \(\kappa\)-Cu\(_2\)(CN)\(_3\)

\(z_v = 0.55\) and \(c = 65.8\) for \(\kappa\)-Cl

\(z_v = 0.65\) and \(c = 18.9\) for EtMe\(_3\)Sb-dmit

mirror symmetry!
Formalism: Hubbard model with disorder

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

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

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

\[ S_{\text{loc}} = \sum_i S_{\text{loc}}(i) \quad S_{\text{hop}} = \sum_{\langle ij \rangle} S_{\text{hop}}(i,j) \]

\[ S_{\text{loc}} = \sum_i \left[ \sum_{\alpha,s} \int_0^\beta d\tau \overline{c}_s^\alpha_i \left[ \partial_\tau + \varepsilon_i - \mu \right] c_s^\alpha_i \right] + U \sum_{\alpha} \int_0^\beta d\tau \overline{c}_{\uparrow, i}^\alpha c_{\uparrow, i}^\alpha \overline{c}_{\downarrow, i}^\alpha c_{\downarrow, i}^\alpha \]

\[ = \sum_{\langle ij \rangle} \left[ -t_{ij} \sum_{\alpha,s} \int_0^\beta d\tau \left[ \overline{c}_s^\alpha_i c_{s,j}^\alpha + \text{H.c.} \right] \right] \]
Integrate out $z-1$ branches:

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

Recursion relation (EXACT!!)

Functional of local fields only (all powers)
DMFT as the large $z$ limit

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

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

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

Depends on local site energy $\varepsilon_i$
Cavity field: self-consistency

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

\[ = t_{ij}^2 G_{j,s}(\omega_n) , \quad \text{self-averaged (many neighbors)} \]

\[ G_{j,s}(\omega_n) = \langle \bar{c}_{j,s}(\omega_n) c_{j,s}(\omega_n) \rangle_{S_{\text{eff}}(j)} \quad \text{site-dependent} \]

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

\[ \alpha \neq \alpha', \quad \langle \bar{c}^\alpha c^{\alpha'} \rangle = \langle \bar{c} \rangle \langle c \rangle = 0 \quad \text{(particle conservation)} \]

\( U=0 \) limit - “CPA” (no Anderson localization)
Local (DMFT) perspective?

\[ \Sigma_i(\omega) = \left(1 - \frac{1}{Z_i} \right) \omega - \varepsilon_i + \bar{\varepsilon}_i / Z_i \]

Bethe lattice simulation
Can local spectrum recognize Anderson localization?

\[ \rho_i(\omega) = \frac{1}{\pi} \text{Im} \frac{1}{\omega - \varepsilon_i - \Delta_i(\omega)} \]

\[ = \sum_n \delta(\omega - \omega_n) |\psi_n(i)|^2 \]

Yazdani, STM experiments GaMnAs (close to localization)

Bethe lattice simulation

\[ \text{NO DISORDER} \]

\[ \text{MODERATE DISORDER} \]

\[ -\text{Im}\Delta \rightarrow \]

\[ \text{STRONG DISORDER} \]
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

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)

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

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

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

Self-consistency: $G_o(\omega - \Sigma(\omega)) = G_{\text{typ}}(\omega)$
Excellent quantitative agreement with exact diagonalization in 3D
TMT-DMFT of Mott-Anderson transition

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

M. C. O. Aguiar, V. Dobrosavljević, E. Abrahams, and G. Kotliar

Figure: T=0 Slave-Boson solution and Disorder-driven (increasing W)

Only fraction of $Z_i$ vanish - two fluid behavior!
TMT-DMFT of Mott-Anderson transition: finite T - coexistence region + QC behavior?


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, 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.

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)
Disorder-Driven Metal-Insulator Transitions in Deformable Lattices

Domenico Di Sante, Simone Fratini, Vladimir Dobrosavljević, and Sergio Ciuchi

\[ H = H_{el} + H_{ph} + H_{e-ph} + H_{dis} \]

- Einstein phonons, frequency \( \omega_0 \)
- Tight-binding half bandwidth \( D \) half-filled band

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

\[ E_{pot} = g^2 / \omega_0 \quad \lambda = 2 E_P / D \]

Clean limit: polaron transition at (unphysically) strong coupling \( \sim O(1) \)
Anderson-Holstein Transition: Disorder-Induced Polarons

Qualitatively different critical behavior: mobility gap due to polarons

- Insulator (localized polarons)
- Metal
- Mott limit
- Polaron transition

**Figure 1.**

- Phase diagram showing the metal-insulator transition (MIT) at $\lambda_0 \neq 0$, identified by a transition from a metal to an Anderson insulator, decreasing as anticipated, the polarized polaron transition.
- Both quantities, calculated here in the classical phonon limit (Fig. 2(a)), are accessible experimentally through local spectroscopic probes.
- The inset shows the effect of increasing phonon quantum fluctuations.
- The behavior seen in transport (see text). The dashed line is a sketch of the expected behavior approaching the clean limit.

**Inset (c).**

- $w < w_c$: a transition from a metal to an Anderson insulator, decreasing.
- $w > w_c$: as anticipated, the polarized polaron transition.

**Inset (d).**

- CPA: coherent potential approximation, or CPA, can describe certain properties of the noninteracting limit is known as the coherent potential approximation.
- The theory identifies the mobility edge, and its value

**Inset (e).**

- The typical escape rate is therefore proportional to the TDOS, providing, respectively, the average DOS and the TDOS, and
- The correlation between the typical density of states (TDOS) is defined as the geometric average of the local DOS over sites with
- The quantities: the typical density of states (TDOS) is defined as the geometric average of the local DOS over sites with
- The solution of the TMT-DMFT equations. In the absence of the expected behavior approaching the clean limit. The inset, are accessible experimentally through local spectroscopic probes.

**Figure 2.**

- A mobility gap opens at $\lambda_0 = \lambda_c$, a transition from a metal to an Anderson insulator, decreasing.
Mott limit and Mooij Correlation

A15 - experiment (Dynes)

TMT-DMFT theory

\[ \rho = \rho_0 + AT \]

“Separatrix” = Mott Limit

\[ k_F \ell \sim O(1) \]
TMT vs. STM: GaMnAs

Visualizing Critical Correlations Near the Metal–Insulator Transition in Ga$_{1-x}$Mn$_x$As

Anthony Richardella$^1$$^2$$^*$, Pedram Roushan$^1$$^*$, Shawn Mack$^3$, Brian Zhou$^1$, David A. Huse$^1$, David D. Awschalom$^3$ and Ali Yazdani$^{1,1}$
Not your ordinary Anderson transition: **pseudogap**

STM: Gap opening at MIT?

Anderson: smooth DOS

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

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

Coulomb glass from Extended DMFT

EDMFT + replicas = **Parisi theory**

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

Universal Efros-Shklovskii gap

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

(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

A. -100 mV  
B. -50 mV  
C. $E_F$

D. +50 mV  
E. +100 mV  
F. +150 mV
Spatial Correlations: “Landau-Ginzburg” TMT

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

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

\[ \xi \sim \frac{1}{\sqrt{r(\omega)}} \sim \frac{1}{\omega} \]
To learn more:

http://badmetals.magnet.fsu.edu  
(just Google “Bad Metals”)

Book:

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