The Mott-Hubbard metal insulator transition: a Dynamical Mean Field Theory Approach

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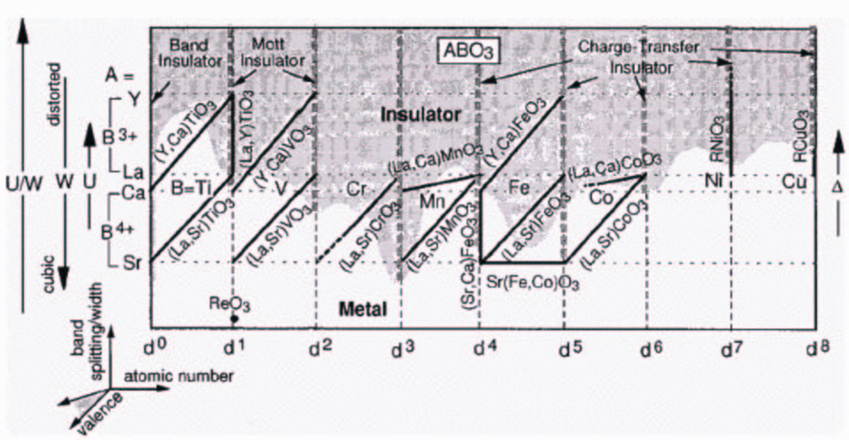
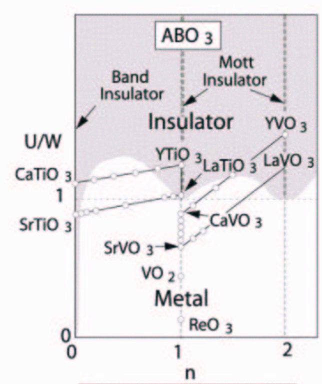
Outline

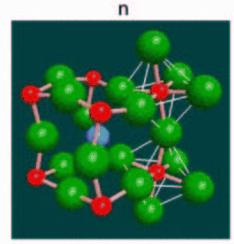
- Motivation: Why study the Mott metal insulator transition (MIT)?
- What is Dynamical Mean Field Theory (DMFT)?
- Hubbard model in DMFT
- Contact with experiments
- Future directions

Collaborators:
G. Kotliar (Rutgers University)
I. Inoue (AIST Japan)

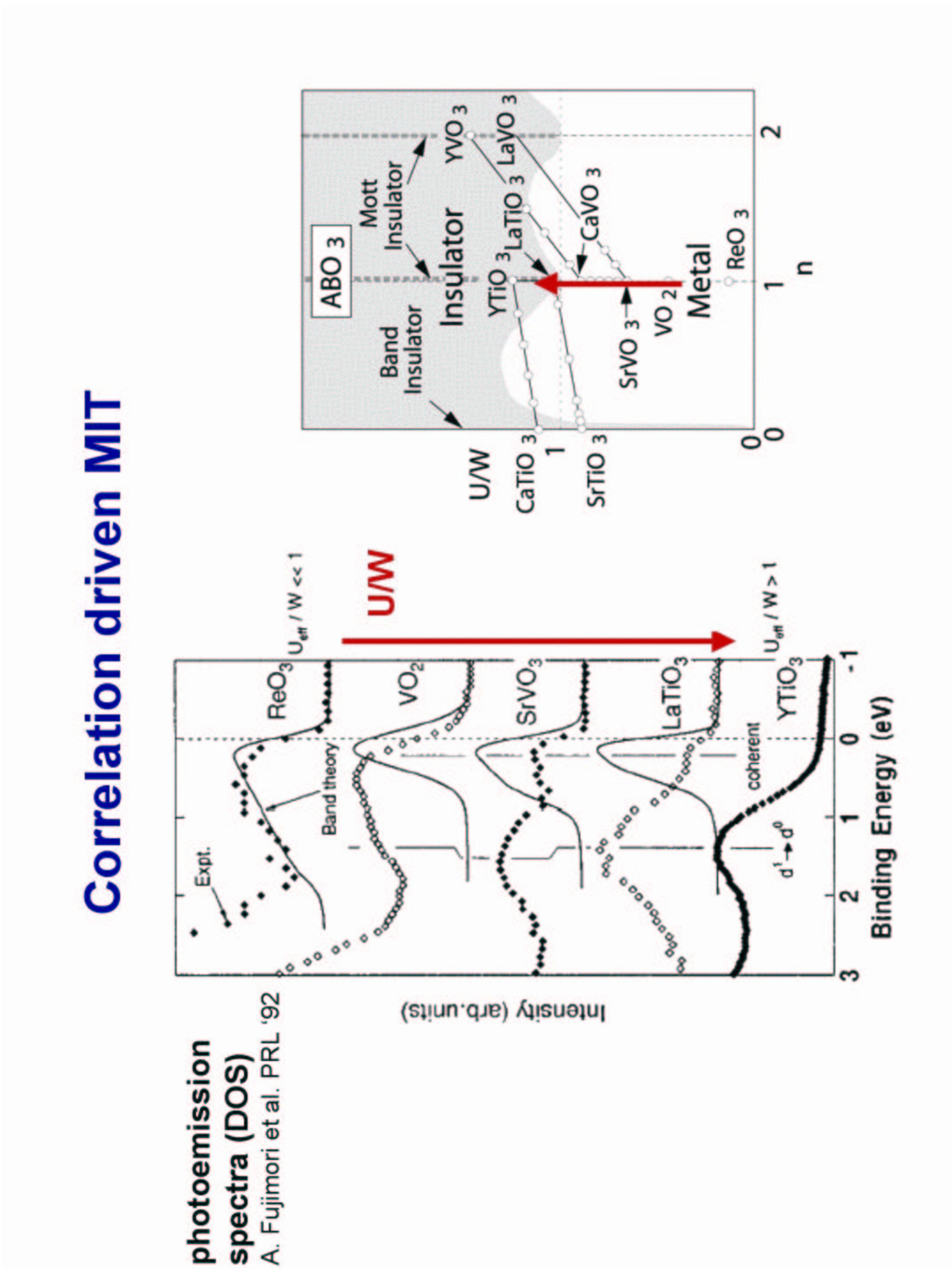
Map of the Transition Metal Oxides

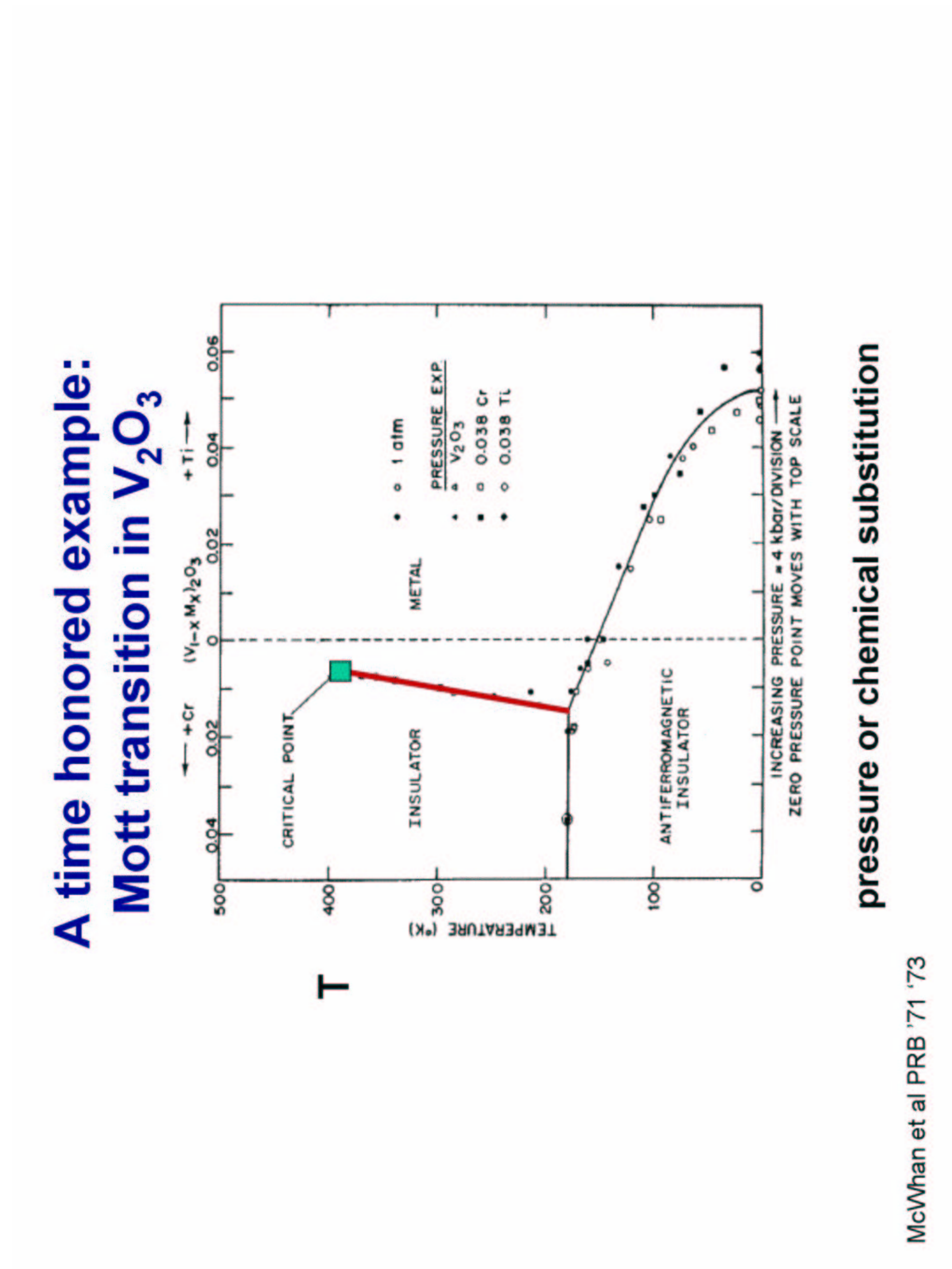






- metal
- oxygen
- rare earth

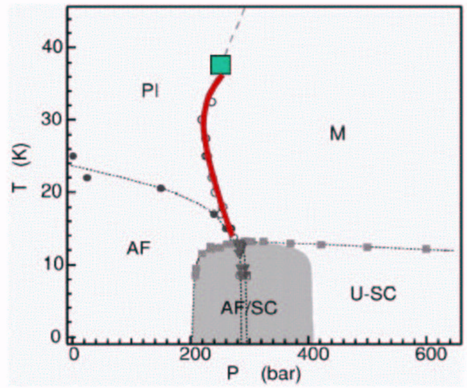

Correlation driven MIT
photoemission
spectra (DOS)
A. Fujimori et al. PRL '92
U/W
Intensity (arb.units)
Binding Energy (eV)
Expt.
Band theory
coherent
ReO3
VO2
SrVO3
LaTiO3
YTiO3
ABO 3
Band
Insulator
Mott
Insulator
Insulator
Metal
U/W
n
CaTiO 3
SrTiO 3
YVO 3
LaVO 3
CaVO 3
SrVO 3
VO 2
ReO 3
LaTiO 3
YTiO 3


A time honored example:
Mott transition in V2O3
T
TEMPERATURE (°K)
CRITICAL POINT
INSULATOR
METAL
ANTIFERROMAGNETIC
INSULATOR
INCREASING PRESSURE = 4 kbar/DIVISION
ZERO PRESSURE POINT MOVES WITH TOP SCALE
pressure or chemical substitution
McWhan et al PRB '71 '73

The “in between” regime is an ubiquitous central theme in strongly correlated systems

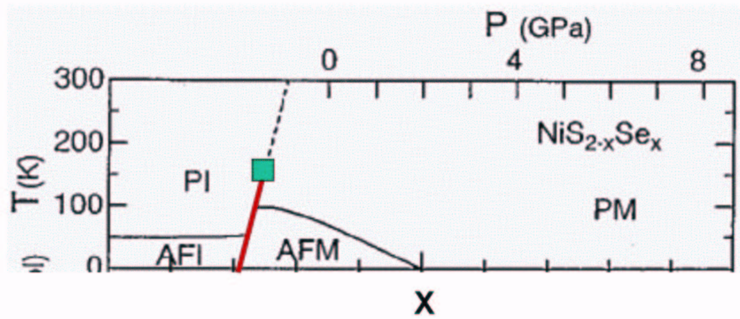
layered organic conductors

Lefebvre et al ‘00



pyrite $NiS_{2-x}Se_x$

Miyasaka et al PRL ‘97



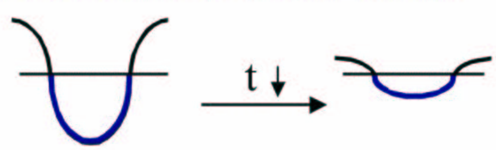
What is the Mott transition?

a correlation driven metal-insulator transition

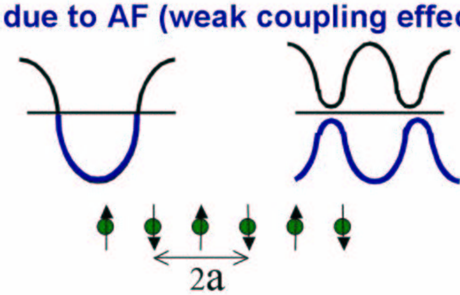
Mott ’49

$n \sim 1/a^3 \sim t$

cannot be obtained in band theory:



not due to AF (weak coupling effect):

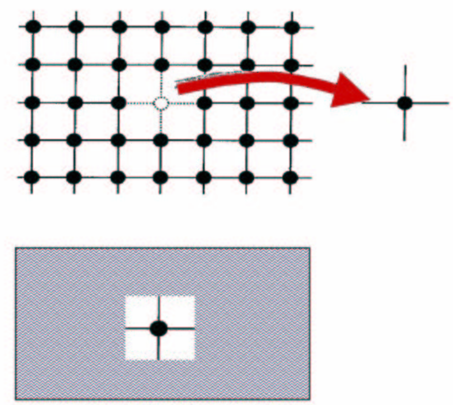


What is Dynamical Mean Field Theory?

A.Georges, G.Kotliar, W.Krauth and MR, Rev. Mod. Phys. '96

A natural generalization of the familiar MFT
to the problem of electrons in a lattice

Key idea: take one site out of a lattice and embed it in a self-consistent bath = mapping to an effective impurity problem



Mapping of the lattice model onto a single impurity in a self-consistent medium

Metzner & Vollhardt '90, Janis '91, Brandt & Mielsch '91, Georges & Kotliar '92, Ohkawa '91

$$Z = \int \prod_i Dc_{i\sigma}^{+} Dc_{i\sigma} e^{-S},$$

$$S = \int_o^\beta d\tau \Big(\sum_{i\sigma} c_{i\sigma}^{+} \partial_\tau c_{i\sigma} - \sum_{ij,\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^{+} c_i + U \sum_i n_{i\uparrow} n_{i\downarrow} \Big)$$

$$\frac{1}{Z_{\mathrm{eff}}} e^{-S_{\mathrm{eff}}[c_{o\sigma}^{+}, c_{o\sigma}]} \equiv \frac{1}{Z} \int \prod_{i \neq o, \sigma} Dc_{i\sigma}^{+} Dc_{i\sigma} e^{-S}$$

$$S_o = \int_0^\beta d\tau \Big(\sum_\sigma c_{o\sigma}^{+} (\partial_\tau - \mu) c_{o\sigma} + U n_{o\uparrow} n_{o\downarrow} \Big)$$

local site

$$\Delta S = -\int_0^\beta d\tau \sum_{i\sigma} t_{io} (c_{i\sigma}^{+} c_{o\sigma} + c_{o\sigma}^{+} c_{i\sigma}).$$

coupling to the environment
$\eta = t_{io} c_o$ is a "source term"

$$S_{\mathrm{eff}} = \sum_{n=1}^{\infty} \sum_{i_1 \cdots j_n} \int \eta_{i_1}^{+}(\tau_{i_1}) \cdots \eta_{i_n}^{+}(\tau_{i_n}) \eta_{j_1}(\tau_{j_1}) \times \cdots \eta_{j_n}(\tau_{j_n}) G_{i_1 \cdots j_n}^{(o)}(\tau_{i_1} \cdots \tau_{i_n}, \tau_{j_1} \cdots \tau_{j_n}) + S_o + \mathrm{const.}$$

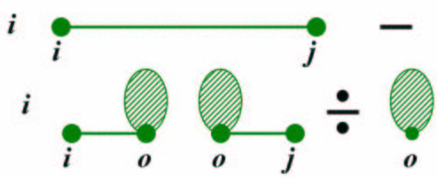
$G^{(o)}$ is the cavity GF

taking the limit d → infinity

$$S_{\mathrm{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^+_{o\sigma}(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_{o\sigma}(\tau') + U\int_0^\beta d\tau\, n_{o\uparrow}(\tau)n_{o\downarrow}(\tau)$$

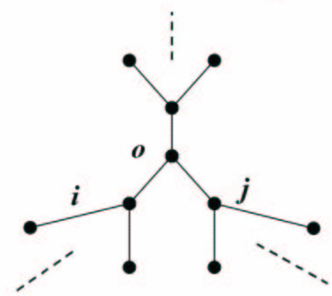
$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{oi}t_{oj}G^{(o)}_{ij}(i\omega_n)$$

$$G^{(o)}_{ij} = G_{ij} - \frac{G_{io}G_{oj}}{G_{oo}}$$



there is a simple geometrical relation between $G_{ij}^{(o)}$ and G_{ii}

in general $G_{ij}^{(o)} = F(G_{ii})$,
for the Bethe lattice $G_{ij}^{(o)} = G_{ii}\delta_{ij}$



DMFT equations

$$S_{\mathrm{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^+_{o\sigma}(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_{o\sigma}(\tau') + U\int_0^\beta d\tau\, n_{o\uparrow}(\tau)n_{o\downarrow}(\tau)$$

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G(i\omega_n)$$

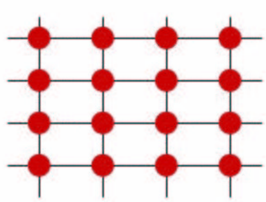
$$\Sigma(i\omega_n) = \mathscr{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n)$$ self energy

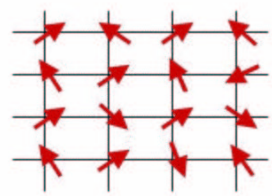
$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)}$$ lattice Green function

$$G(i\omega) = \sum_{\mathbf{k}} G(\mathbf{k}, i\omega) = \int \frac{\rho(\epsilon)d\epsilon}{i\omega + \mu - \epsilon - \Sigma_{imp}(i\omega)}$$

- suggests approximations via $\varepsilon_{\mathbf{k}}$ and $\rho(\varepsilon)$ (ie LDA+DMFT)
- map the lattice problem onto a SIAM with
  $$t^2 G(\omega) = \Delta(\omega)$$
- solve using QMC, NRG, IPT, ED, etc...

Analogy with conventional MFT





$$H = -\sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$S_{eff}[G_0] = -\int\int d\tau d\tau \; c^{+}_{0\sigma} \; \underline{G_0^{-1}} \; c_{0\sigma} + U \int d\tau' \; n_{0\uparrow} n_{0\downarrow}$$

$$\underline{G_0^{-1}} = i\omega_n + \mu - t^2 G(i\omega_n)$$

$$t_{ij} \sim 1/\sqrt{z}$$

$$H = \sum_{ij} J_{ij} S_i S_j$$

$$H_{eff} = (\sum_i J_{0i} S_i) S_0 = zJ\underline{m}S_0 = \underline{h_{eff}} S_0$$

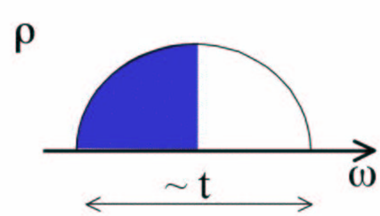
$$\underline{m} = \langle S_0 \rangle = tanh(\beta z J \underline{m})$$

$$J_{ij} \sim 1/z$$

The Hubbard model is a minimal model for the metal – insulator transition

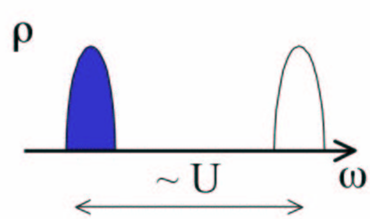
$$H = -\sum_{\langle ij \rangle,\sigma} t_{ij} (c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

U = 0



metal

t = 0

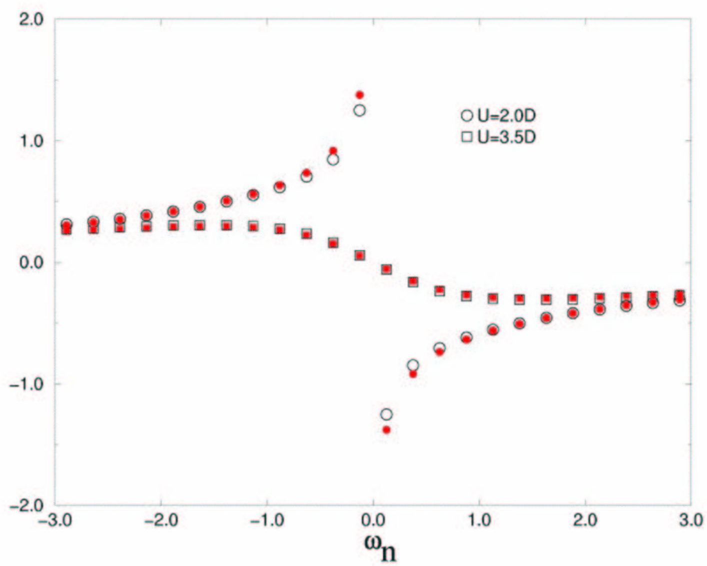


insulator

✓ in 1-d is always an insulator

Metal – Insulator transition in the Hubbard model in DMFT

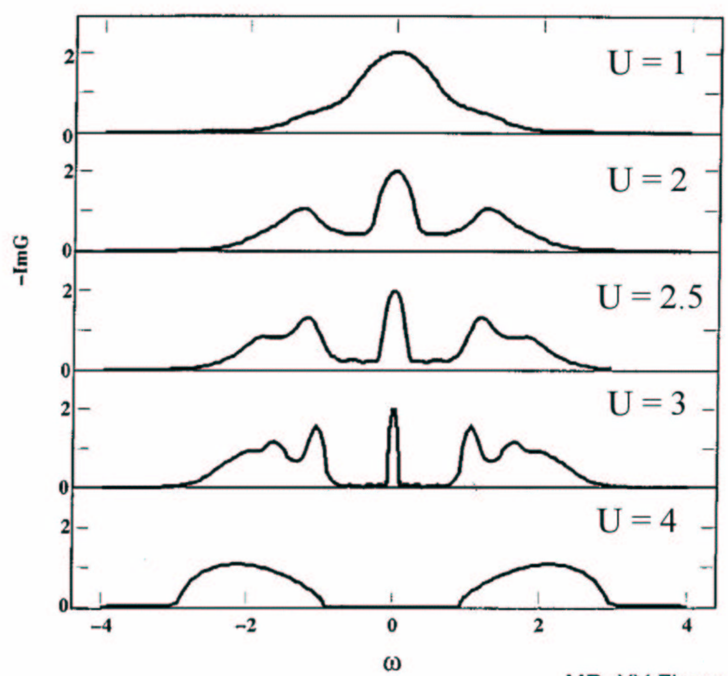
$\mathrm{Im}[G(i\omega_n)]$



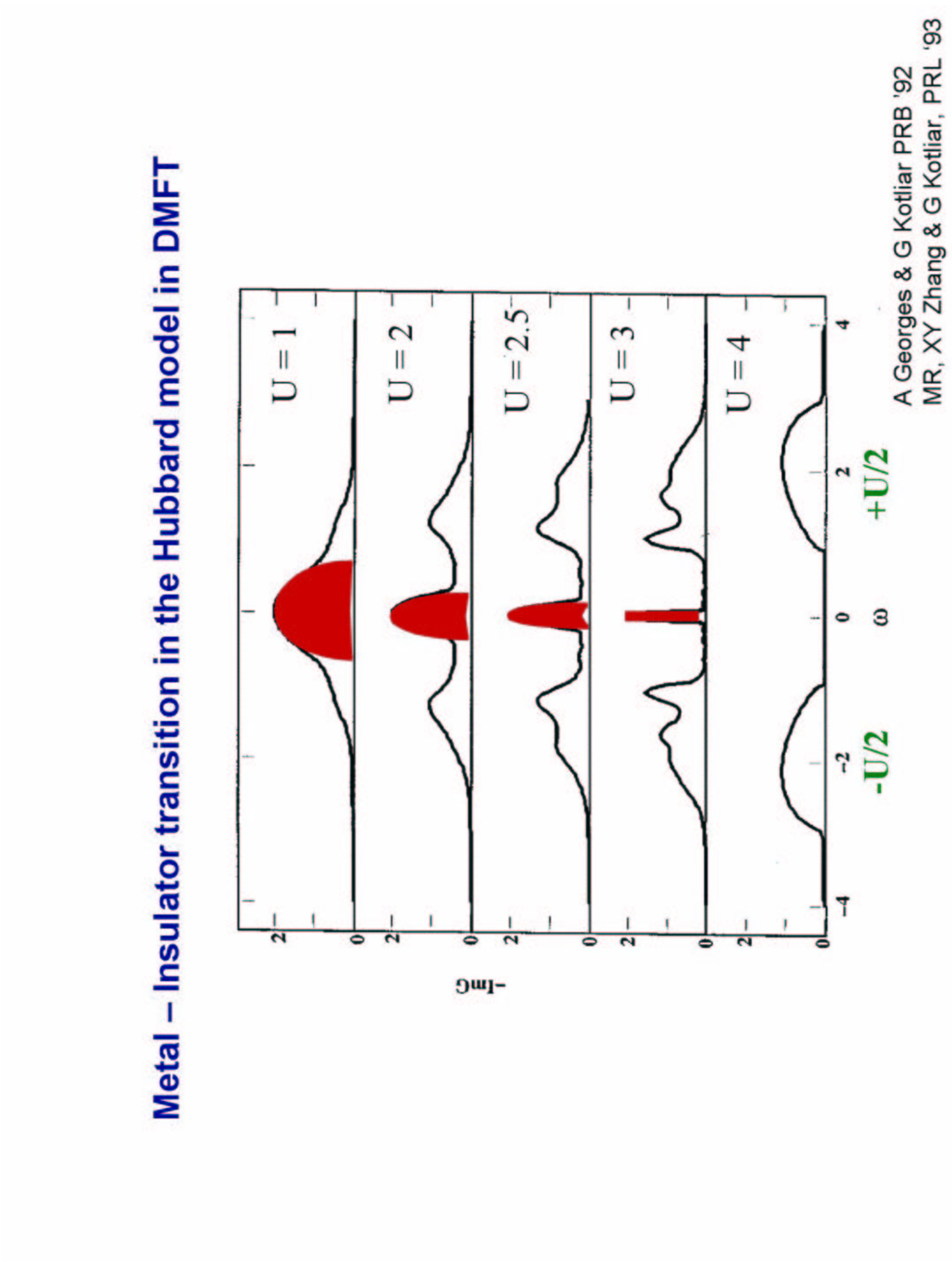
Iterated Perturbation Theory (IPT)

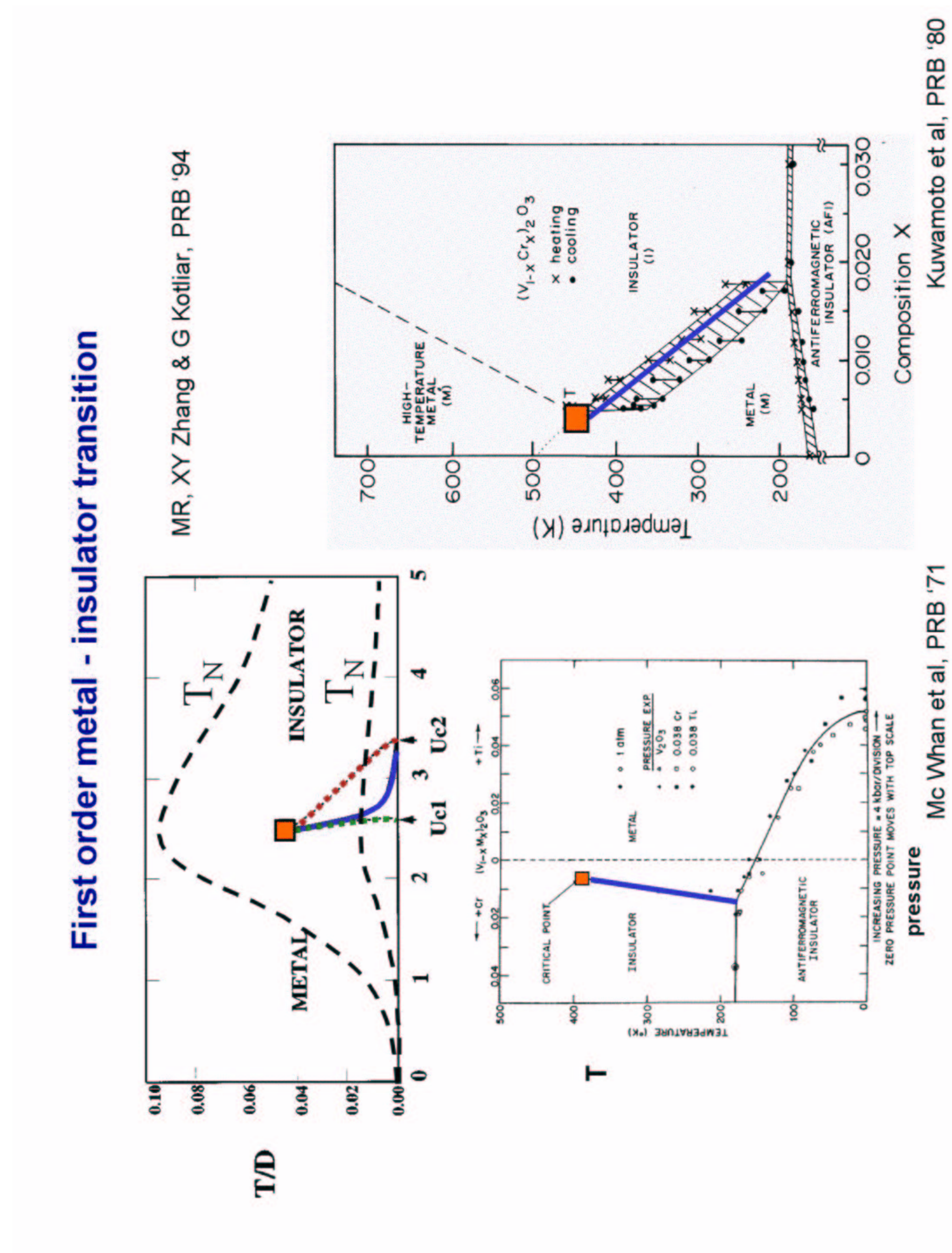
$\Sigma = U^2 G_0^3$

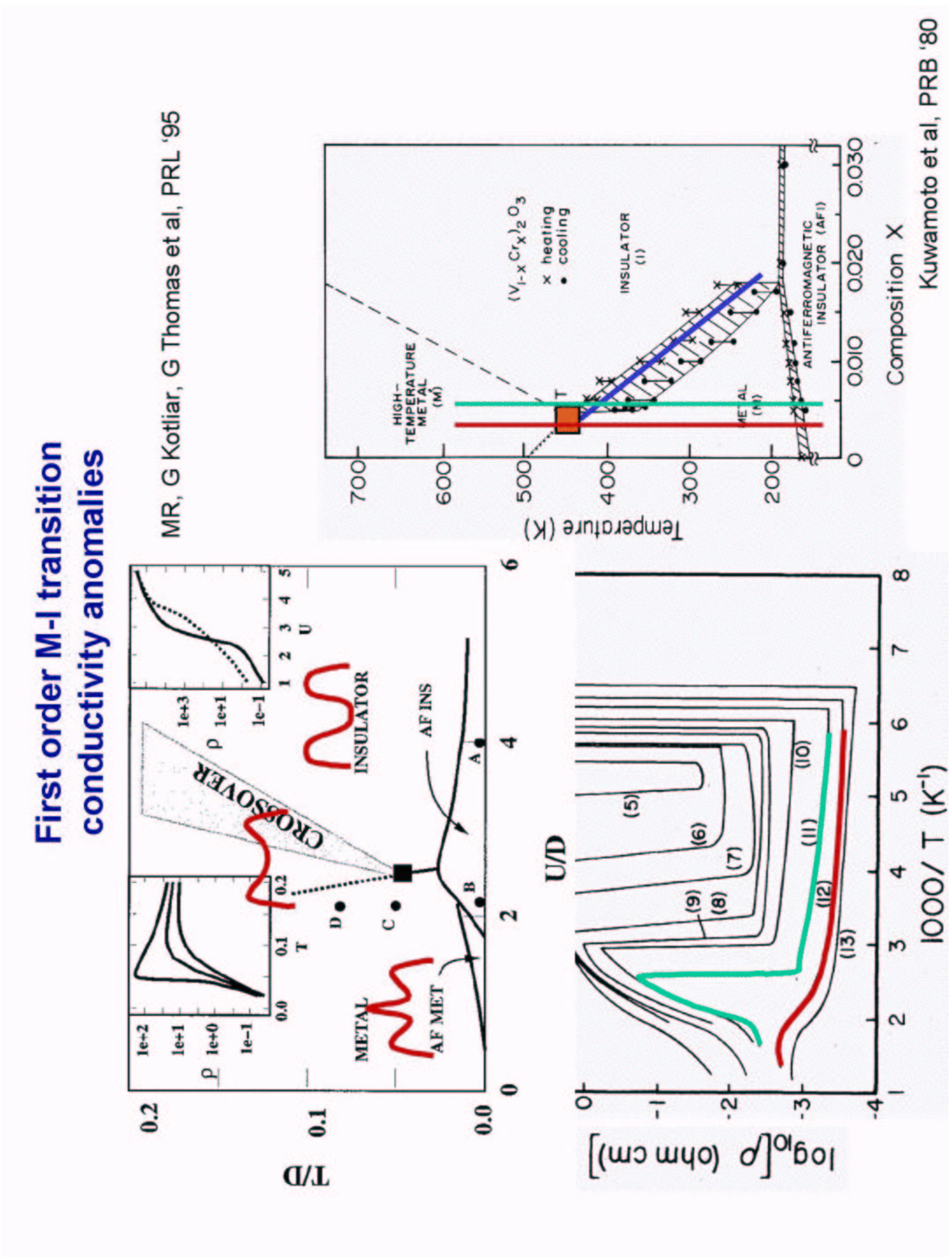
Metal – Insulator transition in the Hubbard model in DMFT

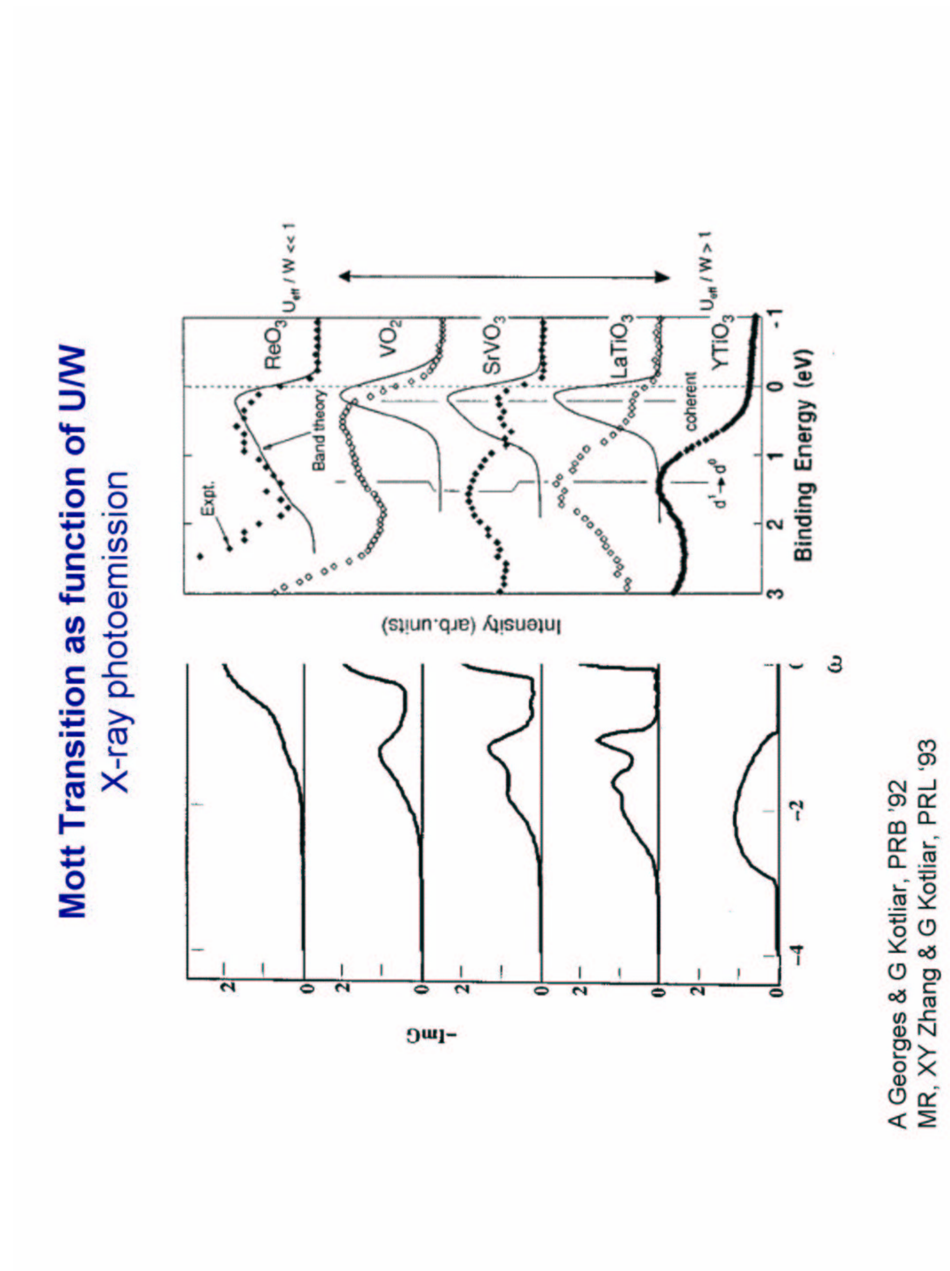


MR, XY Zhang & G Kotliar, PRL '93

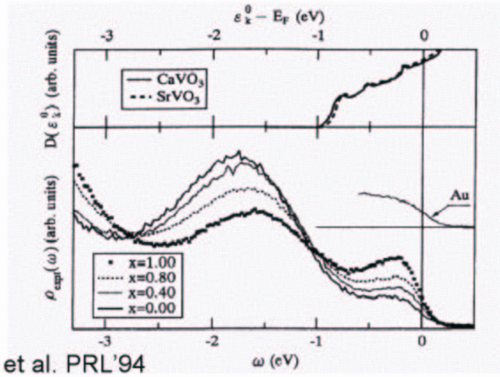

Metal – Insulator transition in the Hubbard model in DMFT
U = 1
U = 2
U = 2.5
U = 3
U = 4
-ImG
ω
-U/2
+U/2
A Georges & G Kotliar PRB '92
MR, XY Zhang & G Kotliar, PRL '93


First order metal - insulator transition
MR, XY Zhang & G Kotliar, PRB '94
T/D
METAL
INSULATOR
T_N
Uc1
Uc2
Temperature (K)
Composition X
HIGH-TEMPERATURE METAL (M)
INSULATOR (I)
METAL (M)
ANTIFERROMAGNETIC INSULATOR (AFI)
Kuwamoto et al, PRB '80
T
pressure
CRITICAL POINT
INSULATOR
METAL
ANTIFERROMAGNETIC INSULATOR
Mc Whan et al, PRB '71

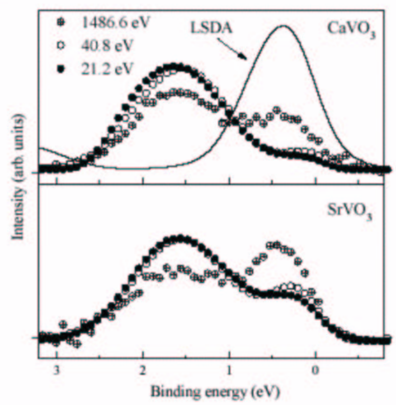

First order M-I transition
conductivity anomalies
MR, G Kotliar, G Thomas et al, PRL '95
Kuwamoto et al, PRB '80
T/D
U/D
CROSSOVER
INSULATOR
METAL
AF MET
AF INS
Temperature (K)
Composition X
HIGH-TEMPERATURE METAL (M)
INSULATOR (I)
ANTIFERROMAGNETIC INSULATOR (AFI)
$(V_{1-x}Cr_x)_2O_3$
× heating
• cooling
$\log_{10}[\rho$ (ohm cm)]
1000/ T (K^{-1})


Mott Transition as function of U/W
X-ray photoemission
ReO_3
VO_2
$SrVO_3$
$LaTiO_3$
$YTiO_3$
Expt.
Band theory
coherent
Intensity (arb.units)
Binding Energy (eV)
-ImG
ω
A Georges & G Kotliar, PRB '92
MR, XY Zhang & G Kotliar, PRL '93

$Sr_{1-x}Ca_xVO_3$ photoemission... small qp-peak?

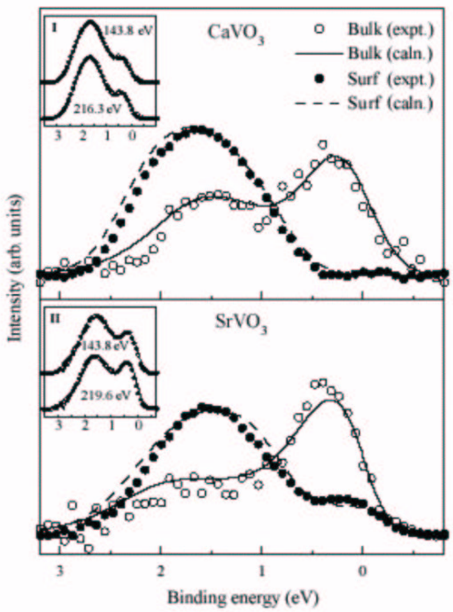


Inoue et al. PRL'94

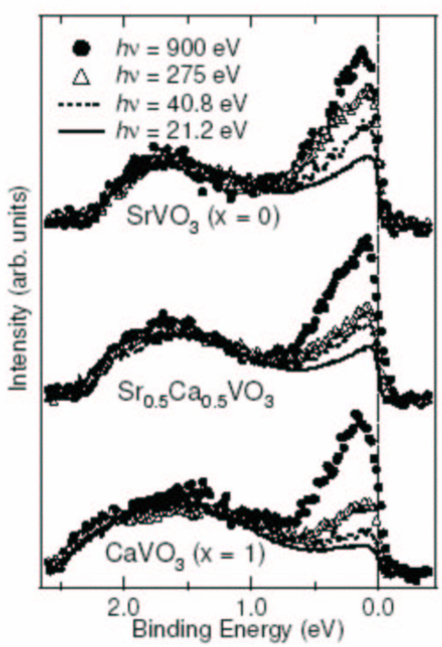


high ***hν*** **spectroscopy**

Maiti, Sarma, MR, Inoue et al. EPL'01

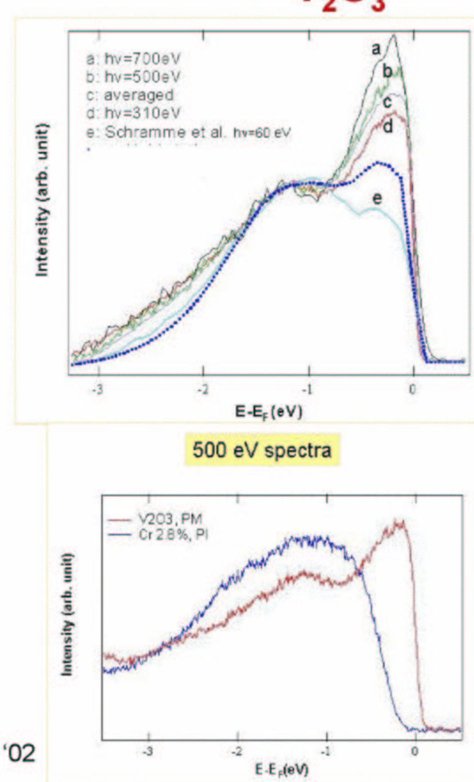


recent photoemission



Suga et al '02

V_2O_3

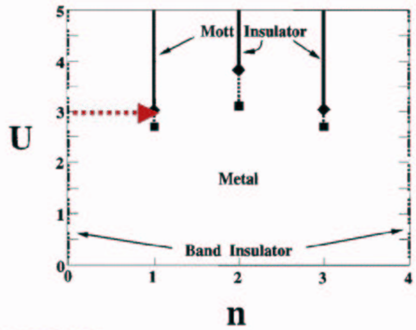


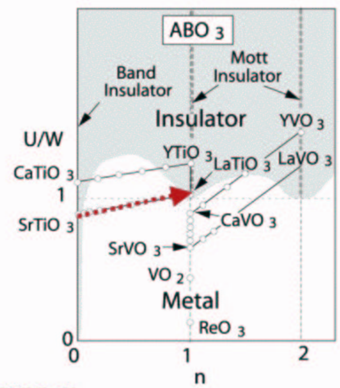
J.Allen et al '02

Mott transition as a function of doping

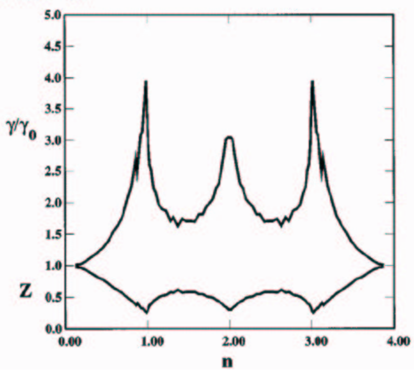
Divergence of the specific heat due to the divergence of m*

2-band degenerate Hubbard model

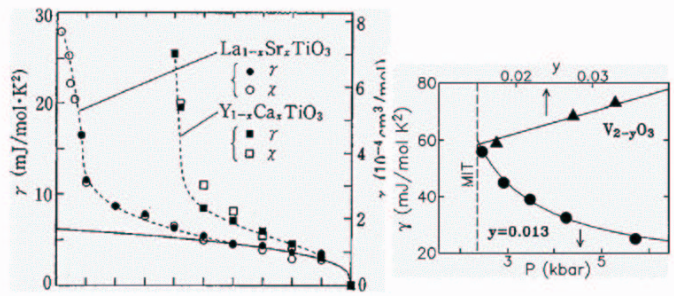




MR, PRB RC '97

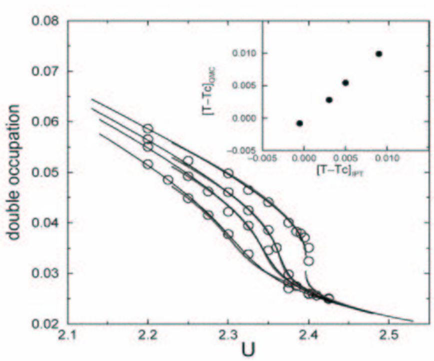


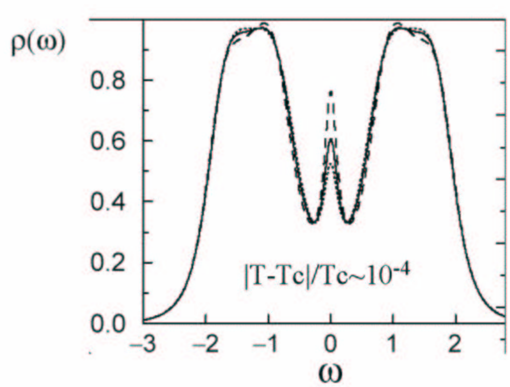
divergence of γ

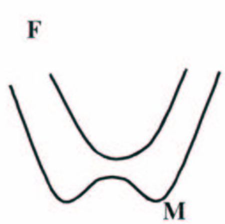


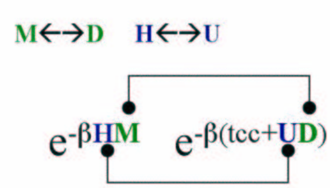
Ginzburg-Landau scenario of the MIT

G Kotliar, E Lange and MR, PRL'00

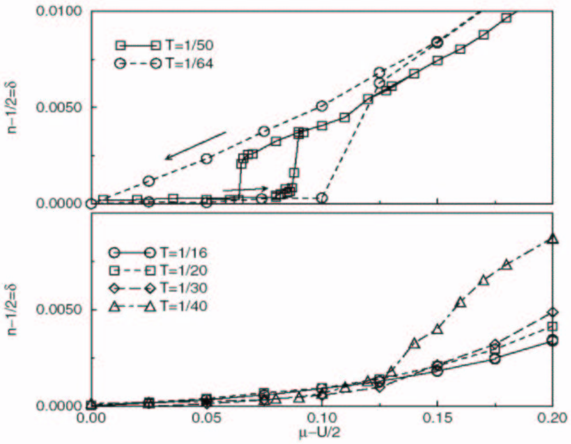








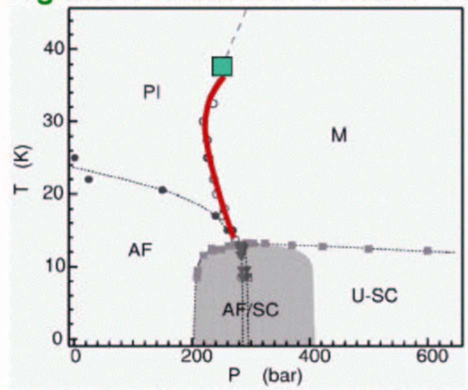
Compressibility divergence at the end of the 1st order line



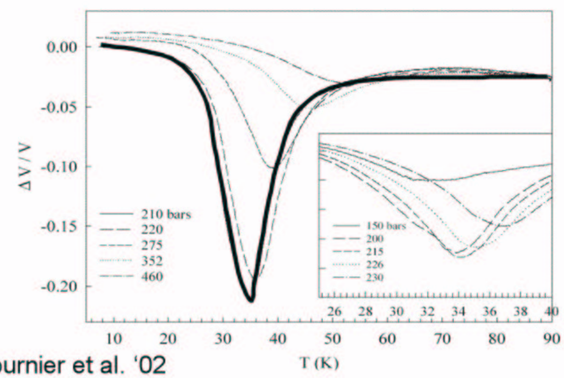
critical behavior of the compressibility $\kappa = \delta n/\delta\mu$

G Kotliar, S Murthy and MR, PRL'02

2-d organic conductors κ-BEDT-TTF



huge ultra sound anomaly @ MIT!!



D. Fournier et al. '02

Summary and Perspectives

- **Derivation of DMFT equations**
  - **Generalization of MFT to electrons on a lattice**
- **Application to the Mott Hubbard transition**
  - **Coexisting Hubbard bands and QP peak**
  - **Dynamically generated low energy scale**
- **Contact with experiments**
  - **Phase diagram of V_2O_3 (and others)**
  - **Photoemission trends in TMO series**
  - **Physics close to the MIT point (GL Theory)**

Towards a realistic theory of strongly correlated materials

- **DMFT + electronic structure calculations (DFT etc. - best of 2 worlds)**
  - **35% volume defect of δ–Pu (largest DFT failure!)**
  - S. Savrasov, G. Kotliar and E. Abrahams Nature '01
- **Extensions to clusters**
  - **E-DMFT, C-DMFT, DCA, etc.**
- **Further model hamiltonian investigations**
- **Strongly correlated electron materials design!**