Dynamical Mean Field Theory and the Mott Transition

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Strong correlations, where do they come from?

Solids have many particles. How do we deal with that?

$$H\Psi = E\Psi$$

$$H = P_x^2 + V(x) \longrightarrow \Psi(x)$$

$$H = h(x) + h(y) + h(z) \longrightarrow \Psi(x,y,z) = \phi(x)\,\phi(y)\,\phi(z)$$

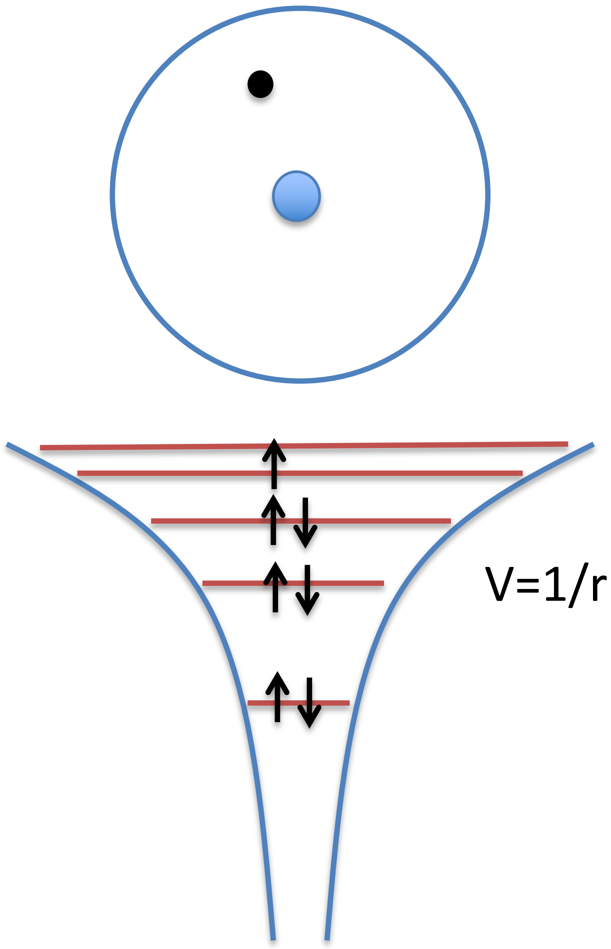
$$h(x)\,\phi(x) = E_x\,\phi(x) \qquad E = E_x + E_y + E_z$$

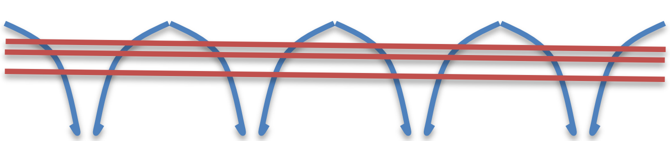
$$H = h(r_1) + h(r_2) + h(r_3) + \ldots \qquad \Psi(r_1, r_2, r_3, \ldots) = \phi(r_1)\,\phi(r_2)\,\phi(r_3)\ldots$$

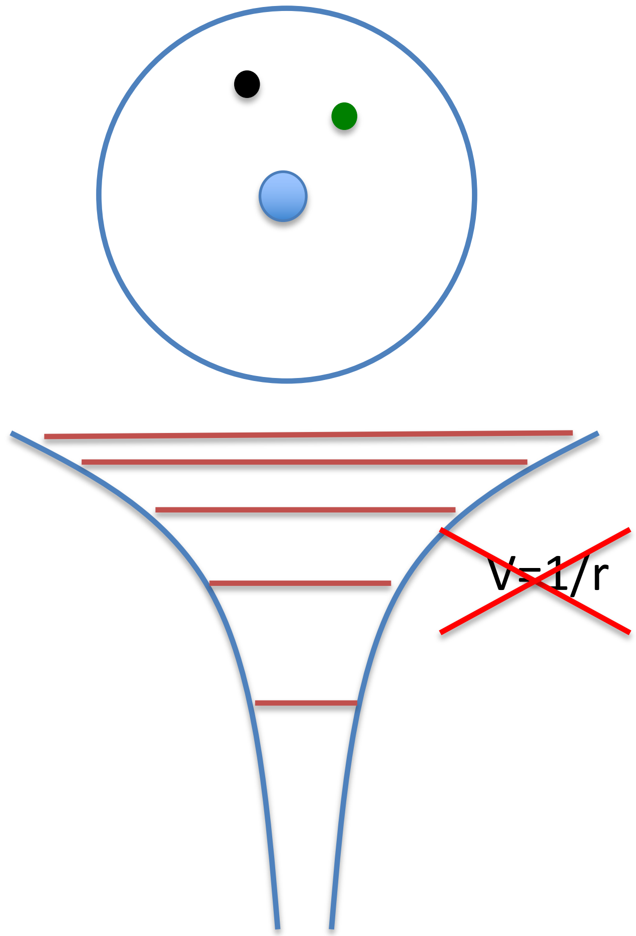
$$h(r_i)\,\phi(r_i) = E_i\,\phi(r_i)$$

one body, single e, independent e

One atom

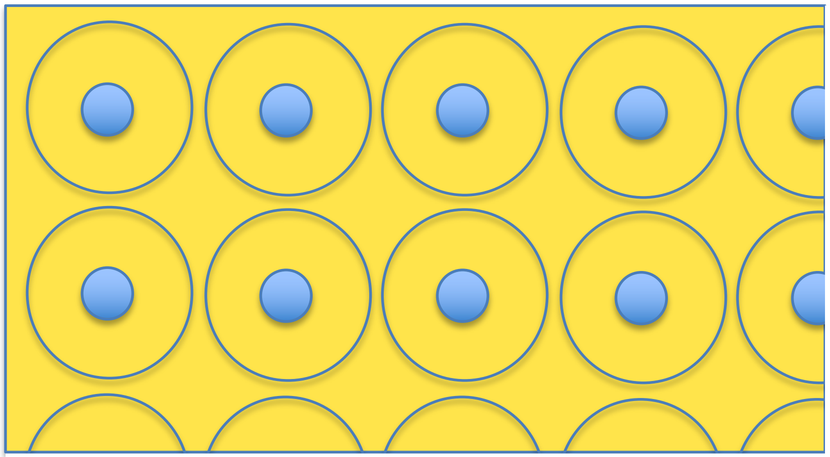






Even a 2 electron system is correlated

Strong correlations, where are them?
The TOE (in condensed matter)



$$H = \sum_i^N \frac{\vec{P}_i^2}{2M} + \sum_j \frac{\vec{p}_i^{\,2}}{2m} + \frac{(Ze)^2}{2} \sum_{i,i'} \frac{1}{|\vec{R}_i - \vec{R}_{i'}|} + \frac{e^2}{2} \sum_{j,j'} \frac{1}{|\vec{r}_j - \vec{r}_{j'}|} - \frac{Ze^2}{2} \sum_{i,j} \frac{1}{|\vec{R}_i - \vec{r}_j|}$$

K_{nuclei} $K_{electrons}$ V_{nuclei} $V_{electrons}$ $V_{elect\text{-}nuclei}$

$$H = \sum_i^N \frac{\vec{P}_i^2}{2M} + \sum_{j=cond} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i,i'} V_{i-i}(|\vec{R}_i - \vec{R}_{i'}|) + \frac{e^2}{2} \sum_{j,j'=cond} \frac{1}{|\vec{r}_j - \vec{r}_{j'}|} + \sum_{i,j} V_{e-i}(|\vec{R}_i - \vec{r}_j|) + E_{cores}$$

$$H = T_i + T_e + V_{i-i} + V_{e-e} + V_{e-i} + E_{cores}$$

separation of variables

$$H\psi = E\psi \qquad \psi(\vec{r}, \vec{R}) = \sum_n \Phi_n(\vec{R})\ \psi_{e_n}(\vec{r}, \vec{R})$$

Φ_n: ions; ψ_{e_n}: electrons

$$(T_i + V_{i-i} + E_{cores})\psi + \sum_n \Phi_n \underbrace{(T_e + V_{e-e} + V_{e-i})\psi_{e_n}(\vec{r}, \vec{R})}_{\text{constant x } \psi_{e_n}(\vec{r}, \vec{R})} = E\psi$$

1

$$\sum_n (T_i + V_{i-i} + E_{cores}) + E_{e_n} - E)\Phi_n\ \psi_{e_n} = 0$$

2

$$\underbrace{(T_e + V_{e-e} + V_{e-i})}_{= H}\psi_{e_n}(\vec{r}, \vec{R}) = E_{e_n}\psi_{e_n}(\vec{r}, \vec{R})$$

Let's consider an orbital basis $\{\phi_\nu(\mathbf{r})\}$ and evaluate $<H>$

$$\langle H \rangle = \sum_\nu \int d\vec{r}\, [-\frac{\hbar}{2m}|\nabla\phi_\nu|^2 + \phi^*_\nu(\vec{r})V_{ion}(\vec{r})\phi_\nu(\vec{r})] \quad + V_{\text{e-e}}$$

$$\langle H \rangle = \sum_\nu \int d\vec{r}\, [-\frac{\hbar}{2m}|\nabla\phi_\nu|^2 + V_{ion}(\vec{r})|\phi_\nu(\vec{r})|^2] \quad +$$

$$\sim \phi_\nu(\mathbf{r}_1)\, \phi_\lambda(\mathbf{r}_2) - \phi_\nu(\mathbf{r}_2)\, \phi_\lambda(\mathbf{r}_1)$$

$$+ \frac{1}{2}\sum_{\nu,\lambda}\int d\vec{r}_1 d\vec{r}_2\; |\phi_\nu(\vec{r}_1)|^2 \frac{e^2}{|\vec{r}_1-\vec{r}_2|}|\phi_\lambda(\vec{r}_2)|^2 - \frac{1}{2}\sum_{\nu,\lambda}\int d\vec{r}_1 d\vec{r}_2\; \phi^*_\nu(\vec{r}_1)\phi_\nu(\vec{r}_2)\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\phi^*_\lambda(\vec{r}_2)\phi_\lambda(\vec{r}_1)$$

$$+ \sum_\nu \int d\vec{r}_1\, [\frac{1}{2}\sum_\lambda \int d\vec{r}_2\, \frac{e^2}{|\vec{r}_1-\vec{r}_2|}|\phi_\lambda(\vec{r}_2)|^2]\; |\phi_\nu(\vec{r}_1)|^2$$

exchange term

mean field effect

$$[-\frac{\hbar}{2m}\vec{\nabla}^2 + V_{ion}(\vec{r}) + \sum_\lambda \int d\vec{r}_1\, n_\lambda(\vec{r}_1)\frac{e^2}{|\vec{r}_1-\vec{r}|}\,]\,\phi_\nu(\vec{r}) - \sum_\lambda [\int d\vec{r}_1\, \phi^*_\lambda(\vec{r}_1)\phi_\nu(\vec{r}_1)\frac{e^2}{|\vec{r}_1-\vec{r}|}\,]\,\phi_\lambda(\vec{r}) \;=\; \epsilon_\nu\, \phi_\nu(\vec{r})$$

Self-consistent solution of an almost S. E.

$$[-\frac{\hbar}{2m}\vec{\nabla}^2 + V_{ion}(\vec{r}) + \sum_\lambda \int d\vec{r}_1\, n_\lambda(\vec{r}_1)\frac{e^2}{|\vec{r}_1 - \vec{r}|}\,]\,\phi_\nu(\vec{r}) - \sum_\lambda [\int d\vec{r}_1\, \phi^*_\lambda(\vec{r}_1)\phi_\nu(\vec{r}_1)\frac{e^2}{|\vec{r}_1 - \vec{r}|}\,]\,\phi_\lambda(\vec{r}) \;=\; \epsilon_\nu\, \phi_\nu(\vec{r})$$

approximations go here
« ab initio » methods

$$|\psi_k\rangle_n(\vec{r}) = e^{ikr}\;\; u_{k,n}(\vec{r})$$

Bloch states

$$|\phi_i\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-ikR}\;|\psi_k\rangle$$

Wannier orbitals

Second quantization

$$|\psi_k\rangle \rightarrow c_k^+$$

$$|\phi_i\rangle \rightarrow c_i^+$$

$$H = \sum_{i,j,\sigma} t_{ij}\; c^{+}_{i,\sigma} c_{j,\sigma} \;+\; h.c. \;+\; \frac{1}{2} \sum_{i,j,i',j',\sigma,\sigma'} U_{iji'j'}\; c^{+}_{i,\sigma} c^{+}_{j,\sigma'} c_{j',\sigma'} c_{i',\sigma}$$

$$t_{ij} = \tfrac{1}{N} \sum_{k} \epsilon_k \; e^{ik(\vec{R}_i - \vec{R}_j)}$$

$$U_{iji'j'} = \int d\vec{r}_1 d\vec{r}_2 \;\; \phi^{*}_{i,\sigma}(\vec{r}_1)\phi_{j,\sigma'}(\vec{r}_2)\; V(\vec{r}_1 - \vec{r}_2)\; \phi_{i'\sigma}(\vec{r}_1)\phi_{j'\sigma}(\vec{r}_2)$$

$$t_{ij} = t$$

$$U_{iji'j'} = U\delta_{ij}\delta_{i'j'}\delta_{ii'}$$

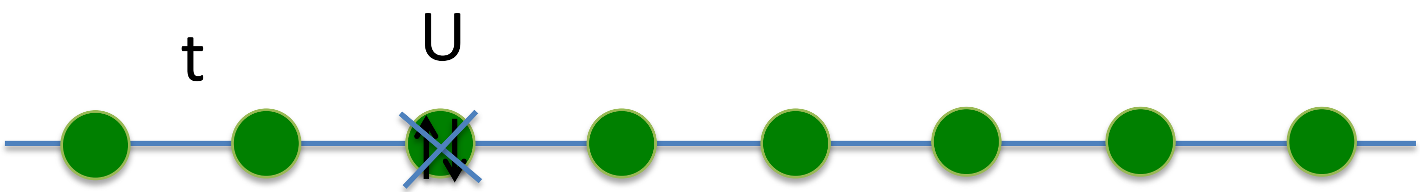
Hubbard model

$$H = t \sum_{\langle i,j\rangle,\sigma} [c^{+}_{i,\sigma} c_{j,\sigma} \;+\; h.c.] \;+\; U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

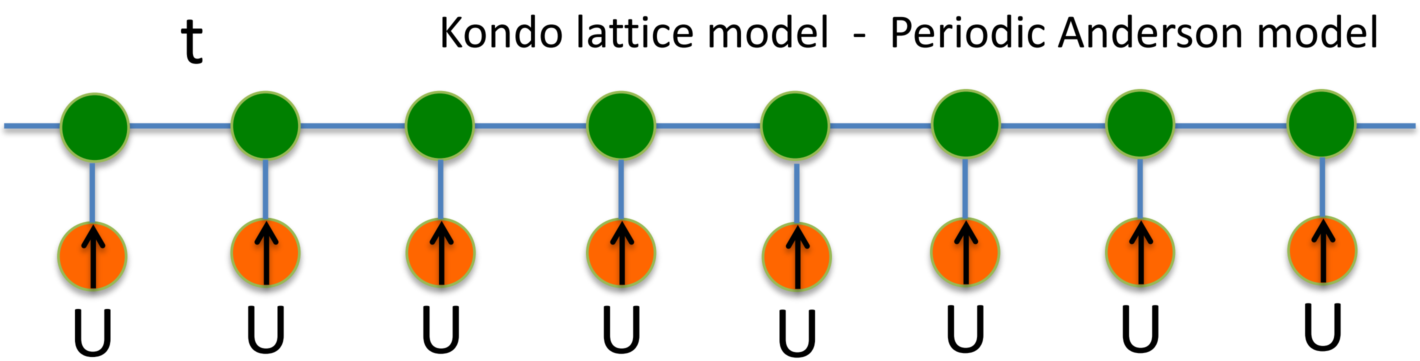
Main models of SCES

Hubbard model

$$H = t \sum_{\langle i,j \rangle, \sigma} [c^{+}_{i,\sigma} c_{j,\sigma} \; + \; h.c.] \; + \; U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

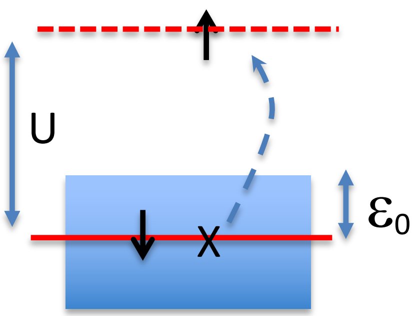


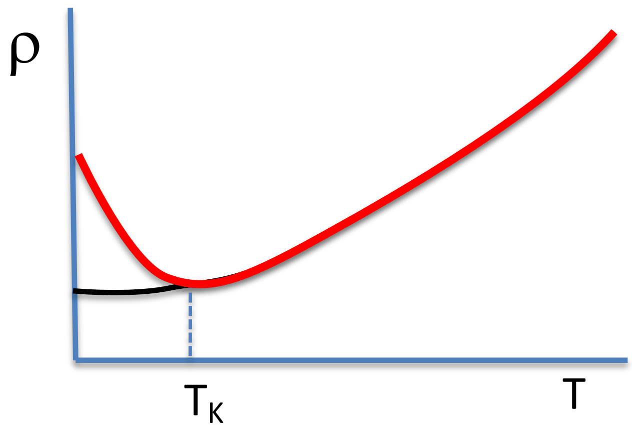
Kondo lattice model - Periodic Anderson model

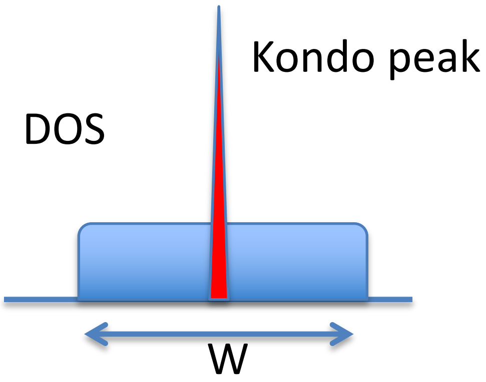


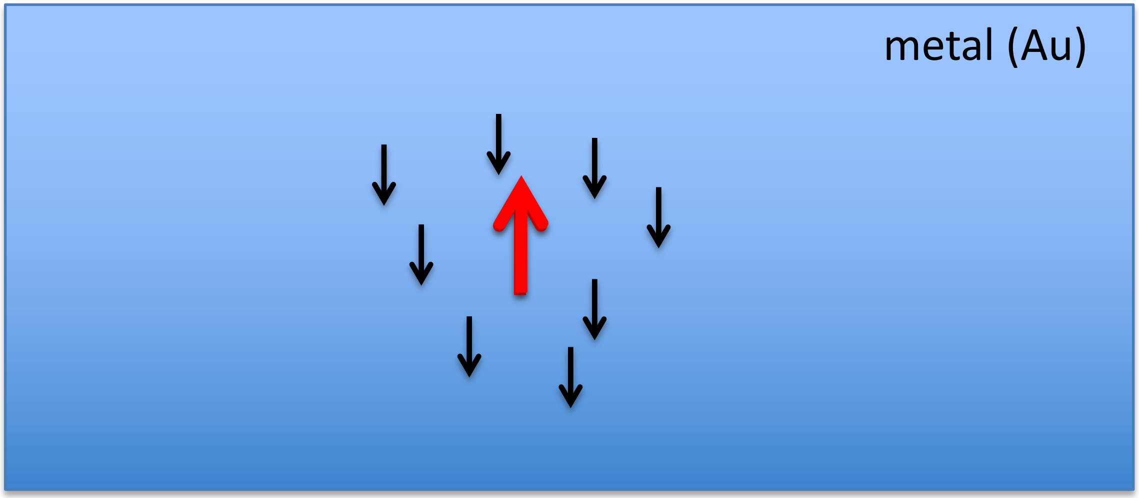
Kondo effect

Do magnetic moments survive in a metal?





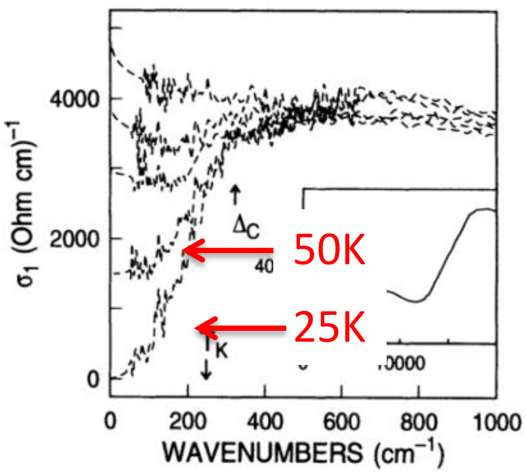




Strong correlations, how do we notice them?

Optical conductivity

$Ce_3Bi_4Pt_3$

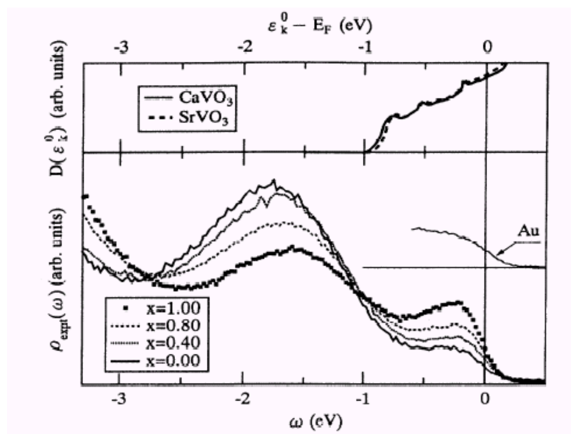


T = 25K, 50K, 75K, 100K, 300K
Δ_C = 400K

Bucher et al. PRL' 94

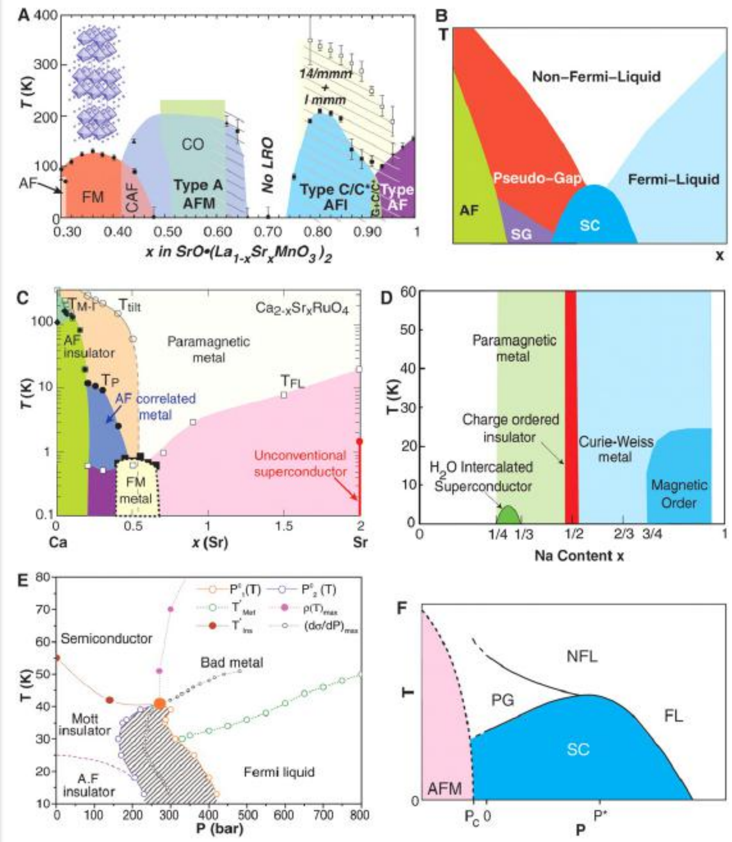
Electronic photemission

$Sr_{1-x}Ca_xVO_3$



Inoue et al. PRL' 94

Complex electronic phase diagrams

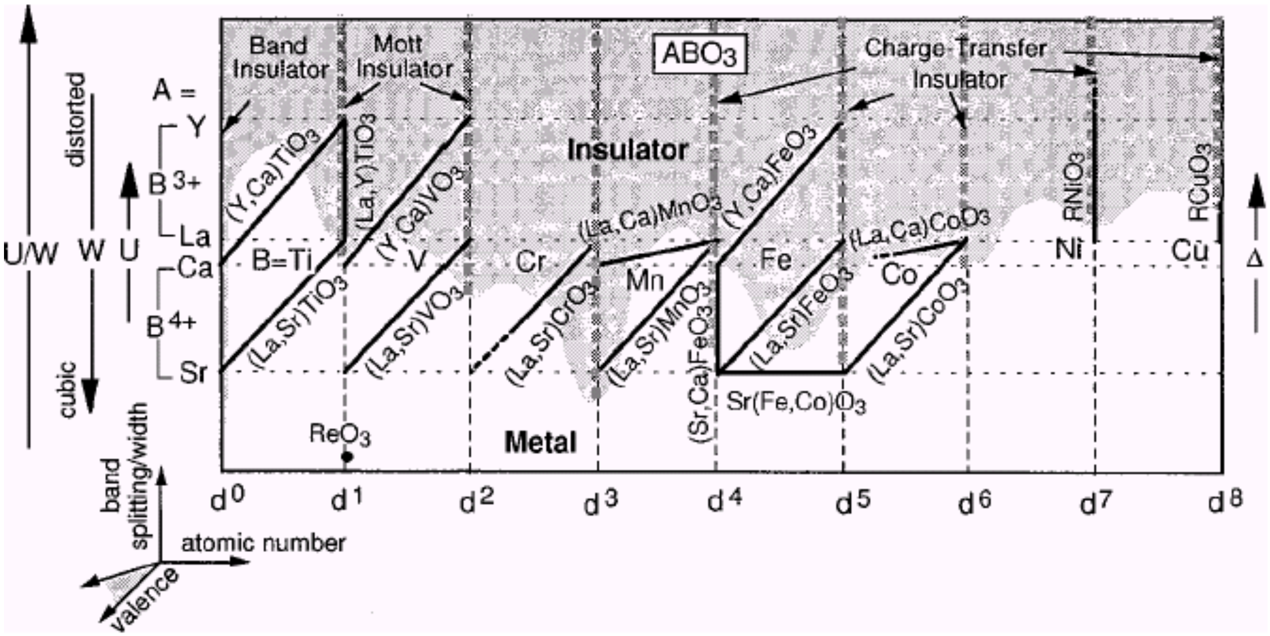


Dagotto

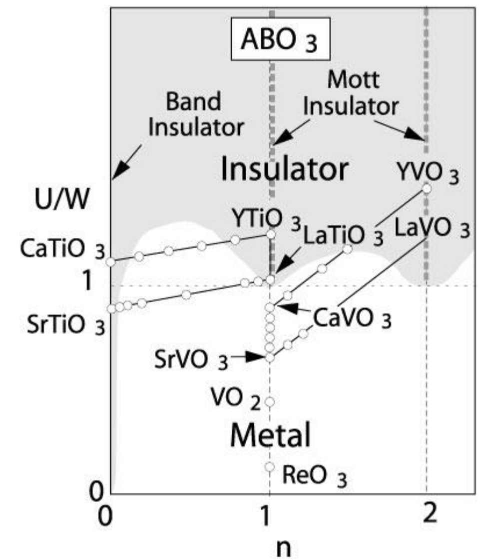
Strong correlations in oxides

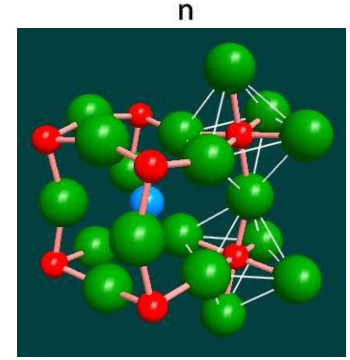
The Metal-Insulator transition and the Hubbard model in DMFT

Map of the Transition Metal Oxides



Fujimori



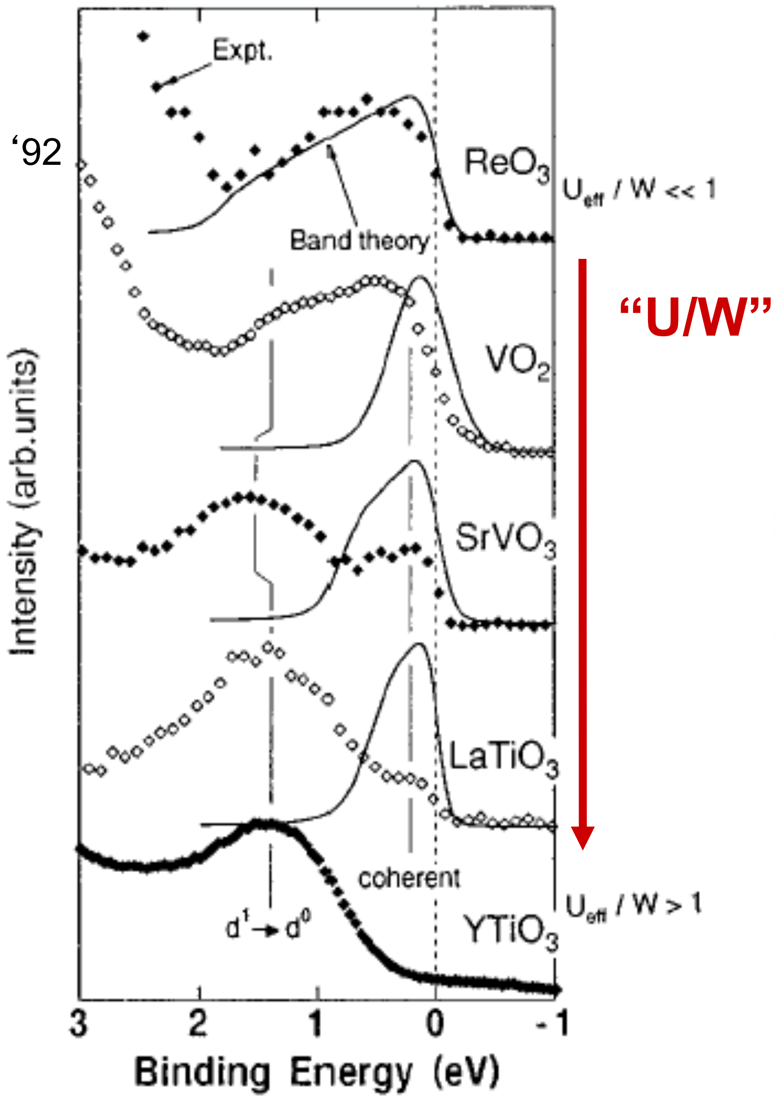


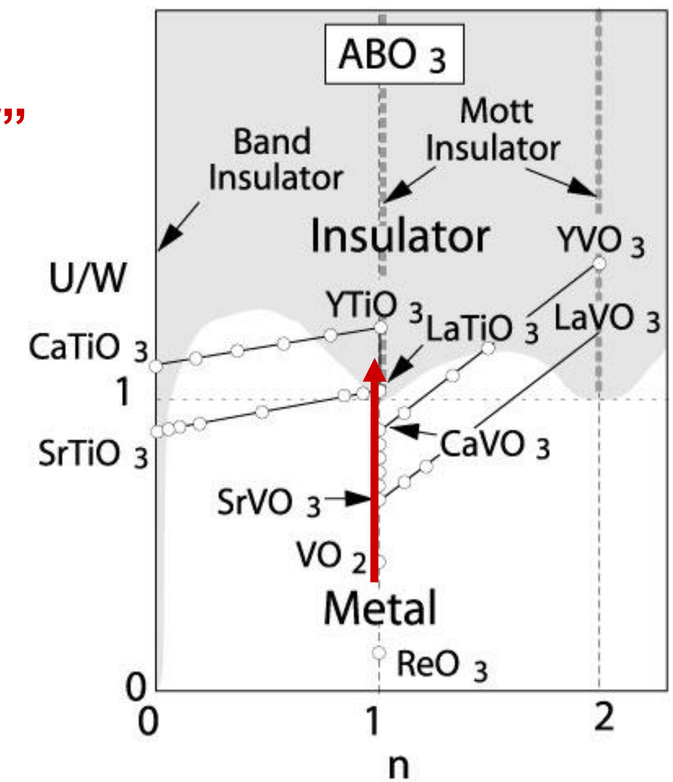
- metal
- oxygen
- rare earth

Correlation driven Metal-Insulator Transition

photoemission spectra (DOS)

A. Fujimori et al. PRL ‘92





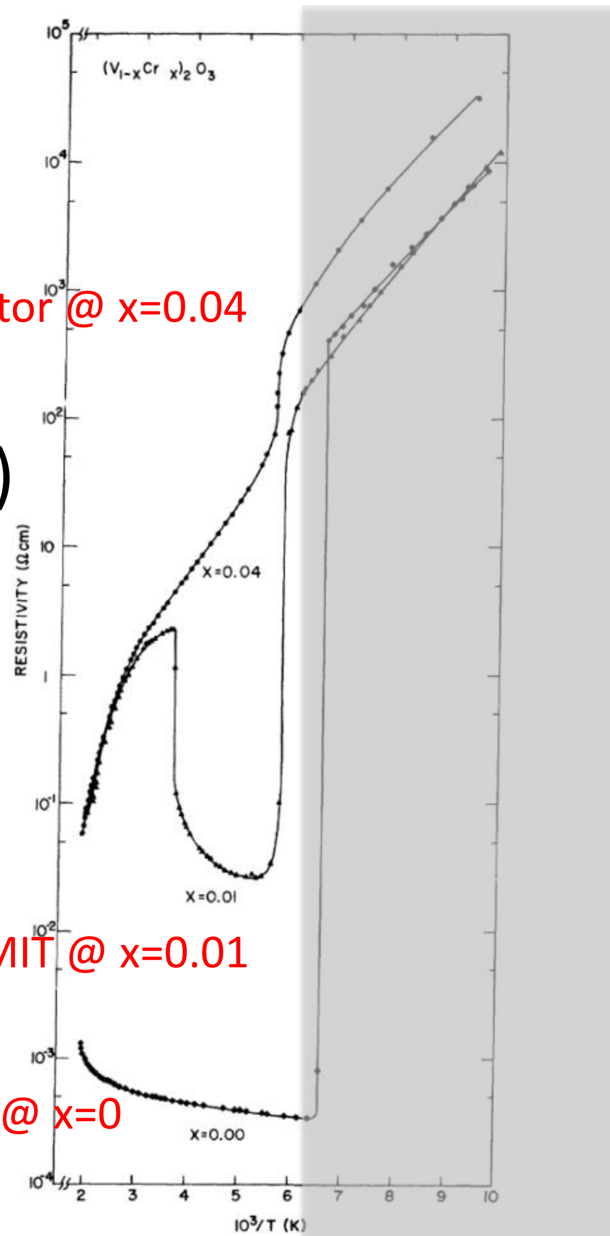
The classic example: Mott transition in V_2O_3

$\rho(1/T)$

insulator @ x=0.04

MIT @ x=0.01

metal @ x=0



Metal-Insulator Transition in $(V_{1-x}Cr_x)_2O_3$

D. B. McWhan and J. P. Remeika

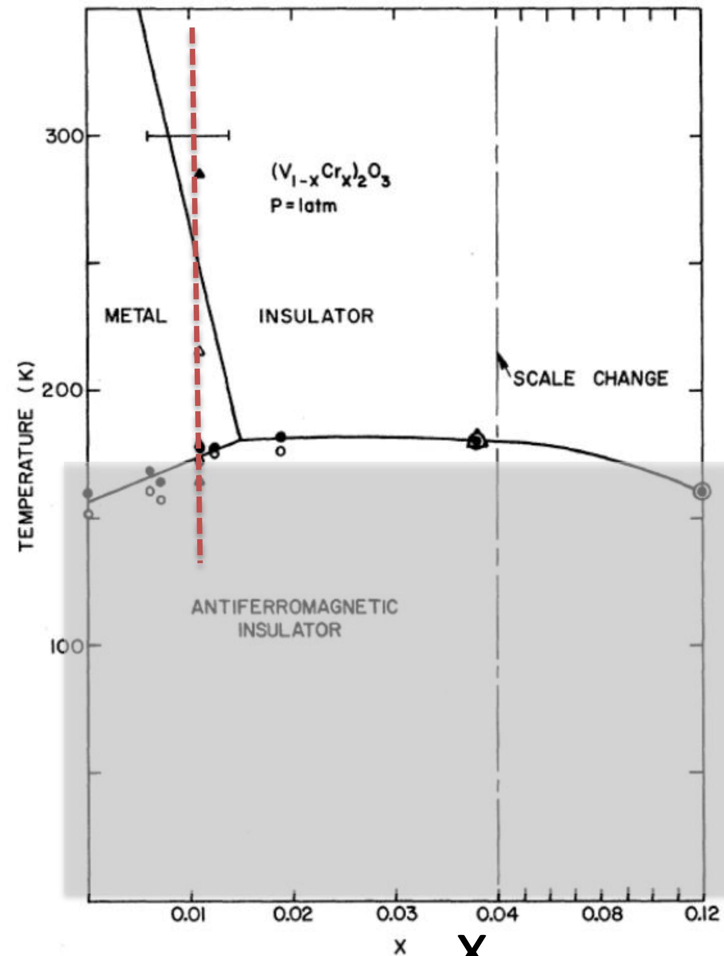
Bell Telephone Laboratories, Murray Hill, New Jersey 07974

(Received 24 April 1970)

PRL '69

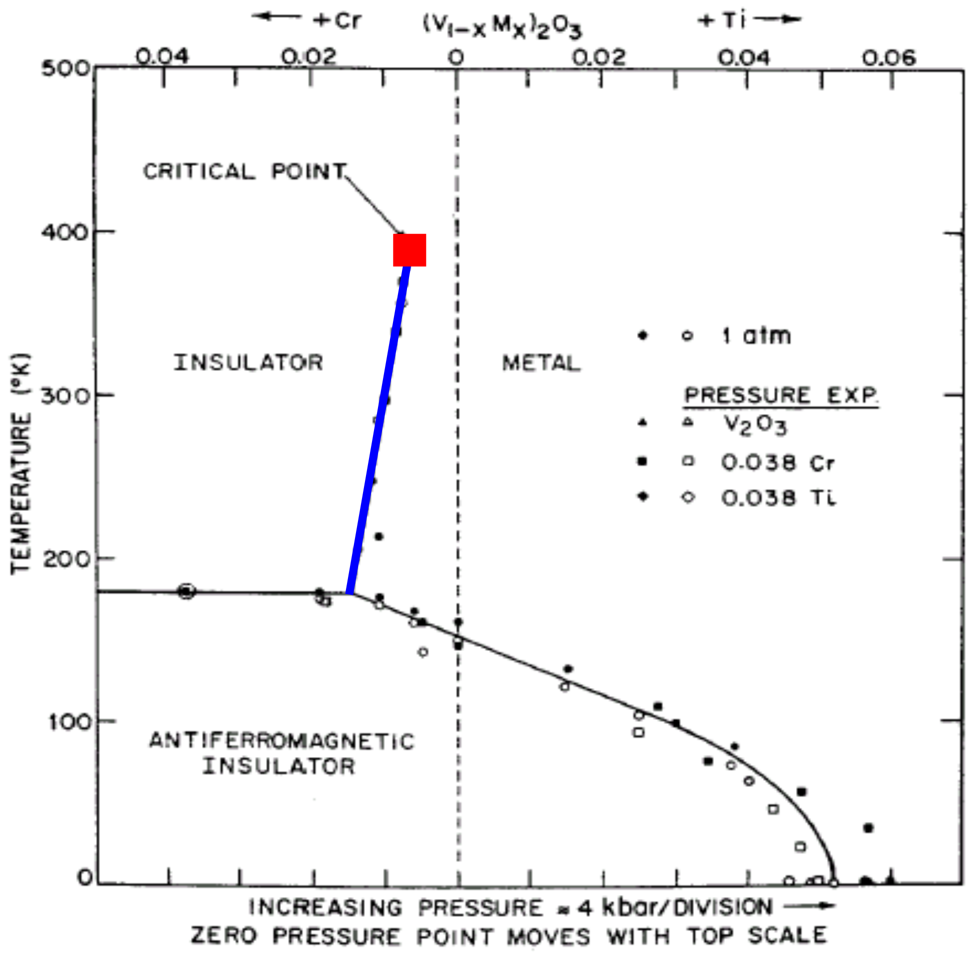
PRB '70

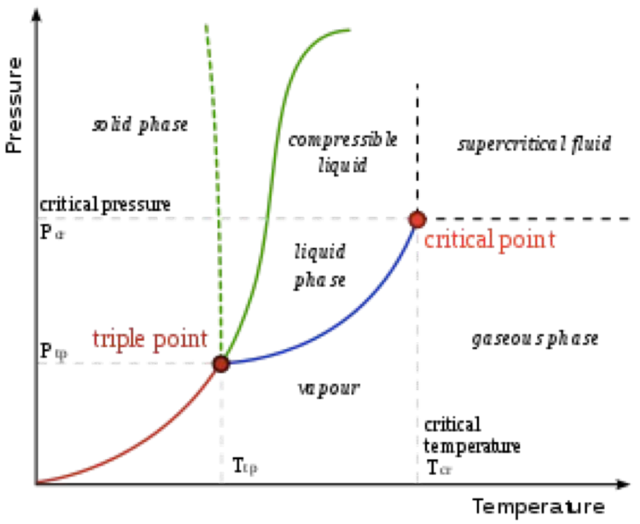
T



X

Phase diagram of V_2O_3



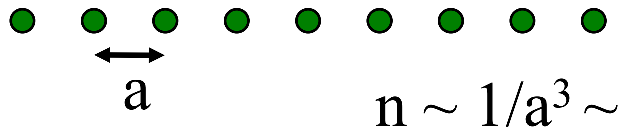


McWhan et al PRB '71 '73

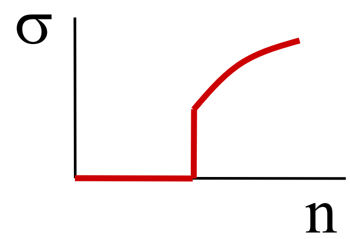
What is the Mott transition?

a correlation driven metal-insulator transition

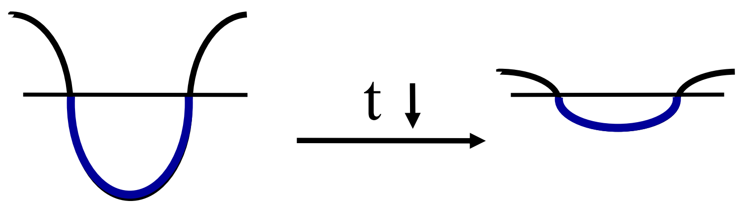
Mott ’49



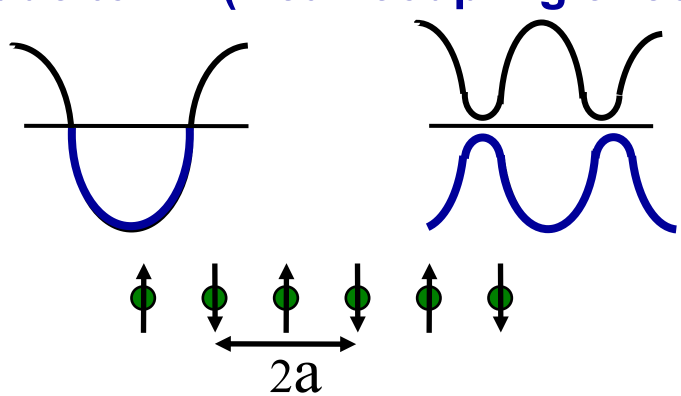
$n \sim 1/a^3 \sim t$



cannot be obtained in band theory:



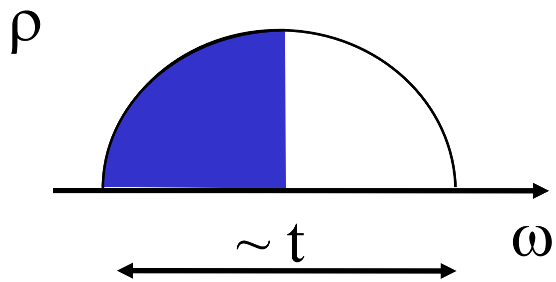
not due to AF (weak coupling effect):



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

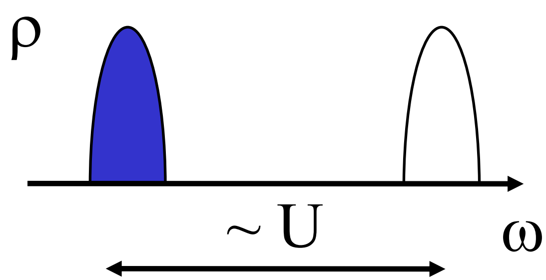
$$H = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$U = 0$



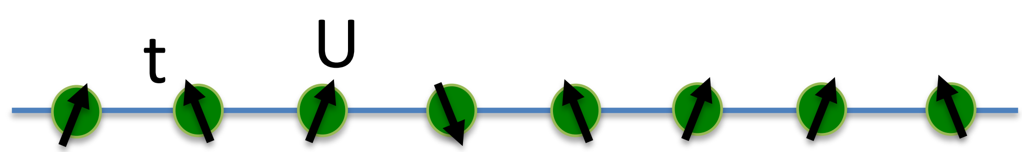
metal

$t = 0$



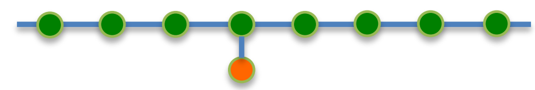
insulator

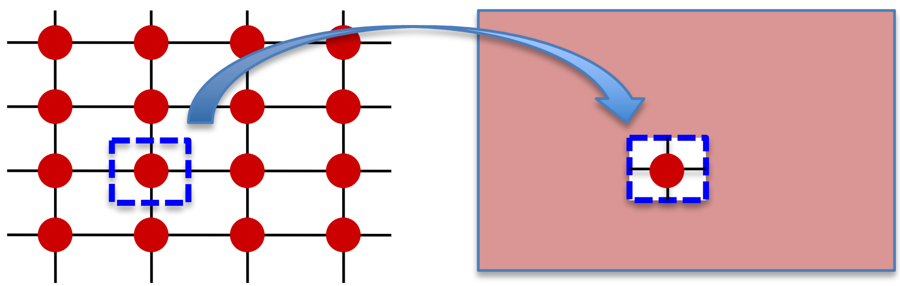
✓ in 1-d is always an insulator



Dynamical Mean Field Theory a cartoon

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



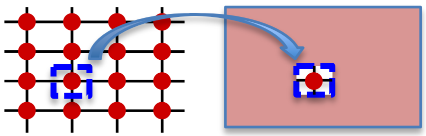


1) Take one site of the original lattice
2) Embed it in a medium (quantum impurity problem)
3) Determine the medium self-consistently

$$G(k,\omega) = \frac{1}{\omega - \epsilon_k + i\eta} \qquad A(k,\omega) = -\tfrac{1}{\pi}\mathrm{Im}[G(k,\omega)]$$

$$H = H_0 + U\sum_i n_{i\uparrow}n_{i\downarrow}\ ;\ H_0 = -t\sum_{\langle i,j\rangle\sigma} c^+_{i\sigma}c_{j\sigma}$$

$$S = \int_0^\beta d\tau\Big(\sum_{i\sigma} c^+_{i\sigma}\partial_\tau c_{i\sigma} - t\sum_{\langle i,j\rangle\sigma} c^+_{i\sigma}c_{j\sigma} - \mu\sum_{i\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}\Big)$$



$$S = S_0 + \Delta S + S^{(0)}$$

$$S_0 = \int_0^\beta d\tau\big(c^+_{0\sigma}(\partial_\tau - \mu)c_{0\sigma} + Un_{0\uparrow}n_{0\downarrow}\big)$$

$$\Delta S = \int_0^\beta d\tau\Big(-t\sum_{<i0>\sigma} c^+_{i\sigma}c_{0\sigma} + c^+_{0\sigma}c_{i\sigma}\Big)$$

← focus on 0 site

$$S_{eff} = \int_0^\beta d\tau\Big(c^+_{0\sigma}(\partial_\tau - \mu)c_{0\sigma} - \sum_{ij\sigma} t_{0i}t_{j0}G^{(0)}_{ij} + \ldots + U\sum_i n_{i\uparrow}n_{i\downarrow}\Big)$$

← still exact

$$S_{QIP} = \sum_{n\sigma} c^+_{0\sigma}\mathcal{G}_0^{-1}(i\omega_n)c_{0\sigma} + \beta U n_{0\uparrow}n_{0\downarrow}$$

← infinite D

$$\mathcal{G}_0^{-1} = i\omega_n + \mu - t^2\sum_{(ij)} G^{(0)}_{ij}(i\omega_n) \qquad G^{(0)}_{ij} = G_{loc}\delta_{ij}$$

← Bethe lattice

$$t \rightarrow t/\sqrt{z}. \qquad \mathcal{G}_0^{-1} = i\omega_n + \mu - t^2 G_{loc}(i\omega_n)$$

← self-consistency

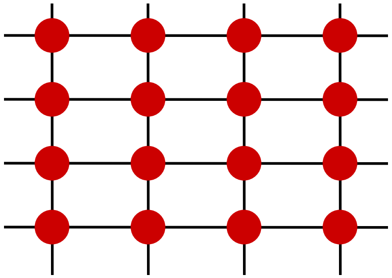
$$\mathcal{G}_0^{-1}(i\omega_n) - \Sigma(i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n)} = G_{loc}(i\omega_n)$$

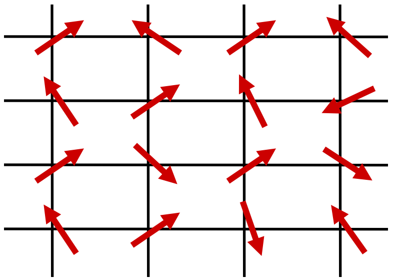
← general case

$$G(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \Sigma(i\omega_n)}$$

← solution

Analogy with conventional MFT





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

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

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

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

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

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

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

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

Quantum Impurity Solvers

$$\mathcal{G}_0^{-1}(i\omega_n) \approx i\omega_n$$ ← seed

$$S_{QIP} = \sum_{n\sigma} c_{0\sigma}^{+} \mathcal{G}_0^{-1}(i\omega_n) c_{0\sigma} + \beta U n_{0\uparrow} n_{0\downarrow}$$ ← 1-site many-body problem **QMC, NRG, DMRG, PT**, etc

$$G_{loc}(i\omega_n) \qquad \Sigma(i\omega_n)$$ ← solution of many-body problem

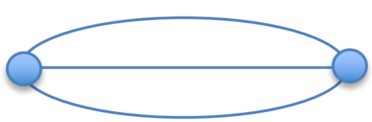
$$\mathcal{G}_0^{-1}(i\omega_n) = G_{loc}(i\omega_n) + \Sigma(i\omega_n)$$ ← solution of many-body problem

Simplest of all QIS

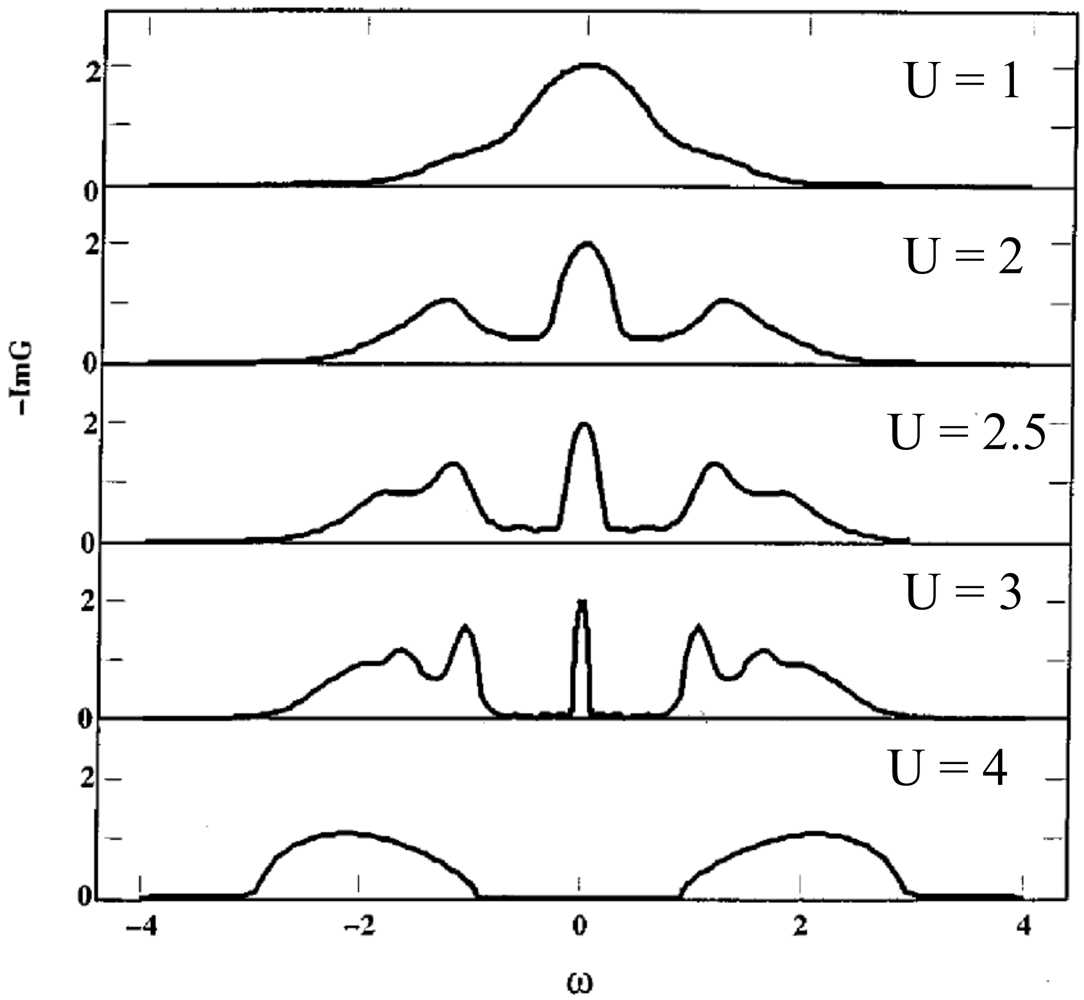
$$\Sigma^{(2)}(\tau) = U^2[\mathcal{G}_0(\tau)]^3$$

Just multiply U^2 times $\mathcal{G}_0{}^3$

Feynmann diagram



Metal – Insulator transition in the Hubbard model in DMFT



MR, XY Zhang & G Kotliar, PRL ‘93

k-resolved A(ω)   (=-1/π Im[G])

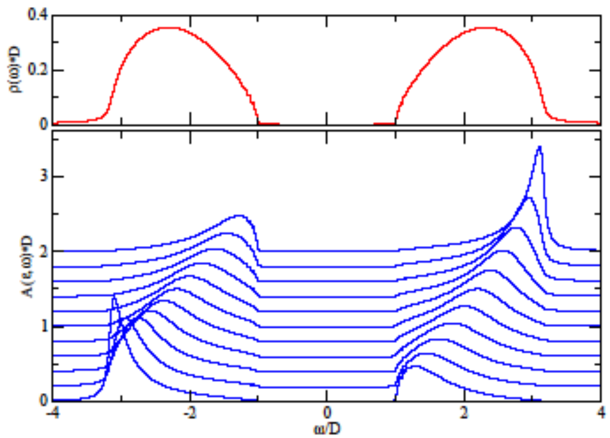
$$\Sigma^{(2)}(\tau) = U^2[\mathcal{G}_0(\tau)]^3$$

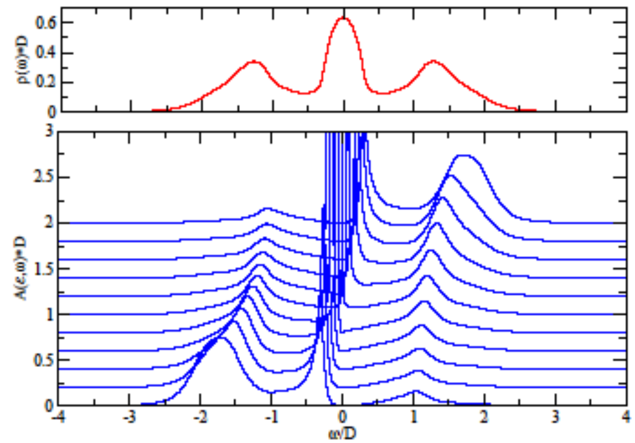
$$G(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \Sigma(i\omega_n)}$$

insulator

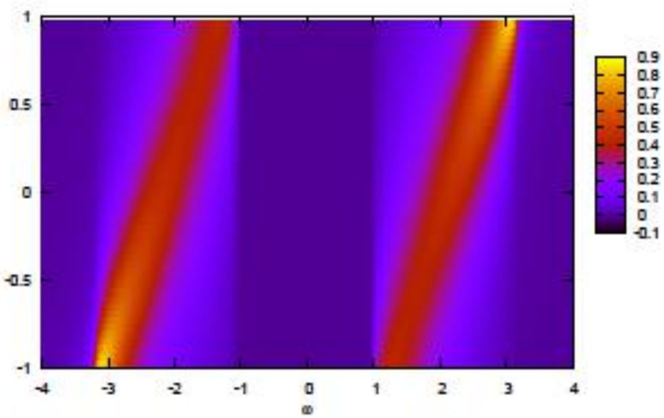
metal

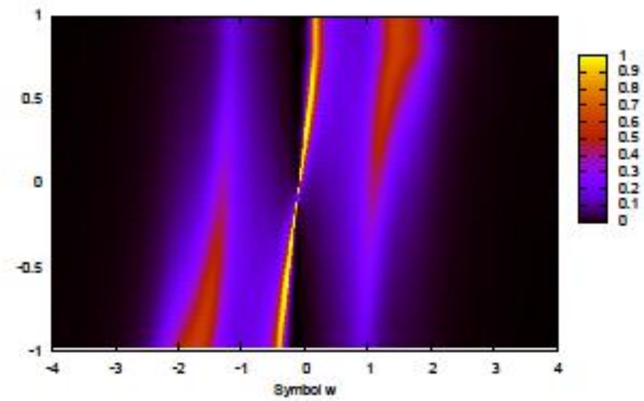
ρ(ω)





k





ω

ω

quasiparticles → coherent

Hubbard bands → incoherent

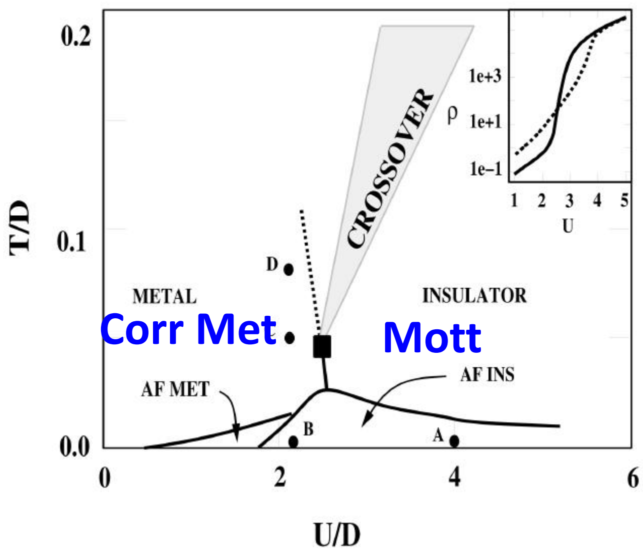
IPT tutorial

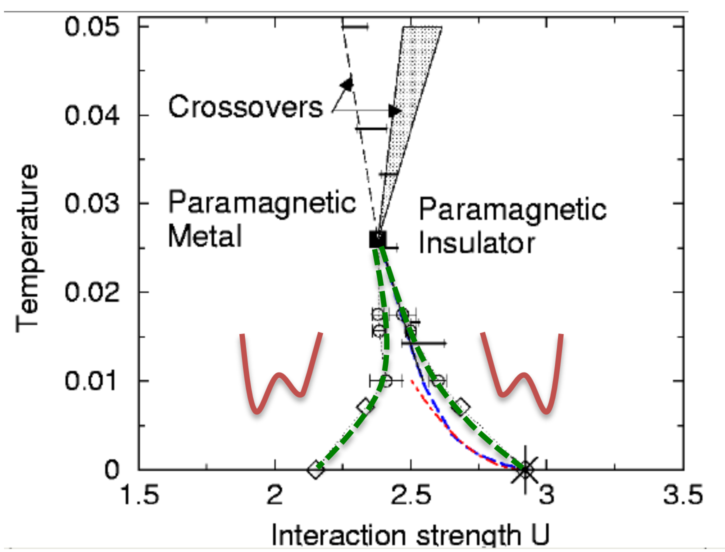
https://drive.google.com/drive/folders/1dENgL58Q0wImpRd2Mnw3TfrSCYR3fkeg?usp=sharing

Hands-on excercise
Unix, Windows, Mac, Phyton
Source (original) fortran77

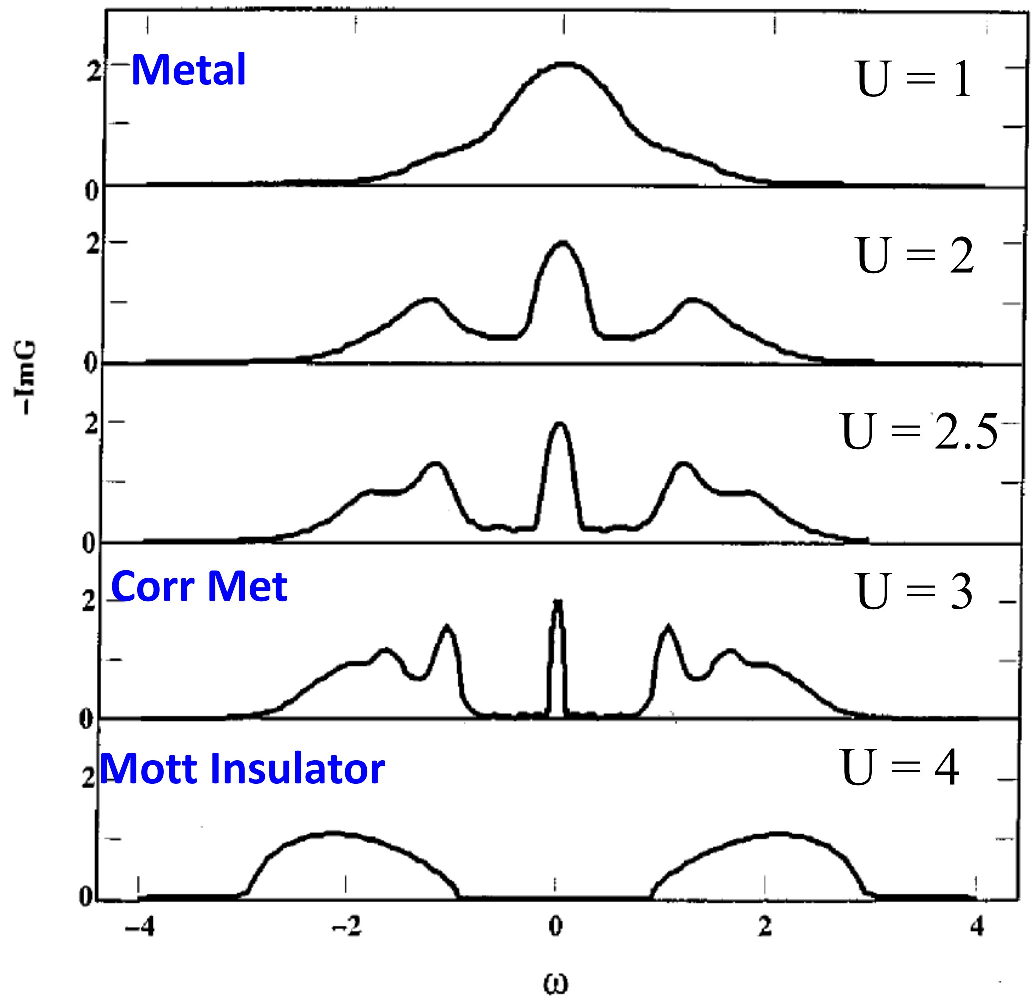
DMFT of the Mott – Hubbard transition

A. Georges et al. RMP ‘96



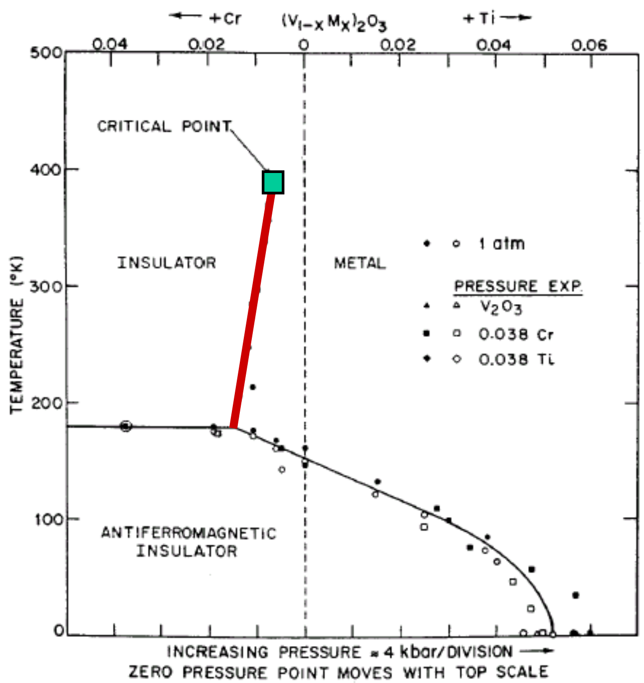


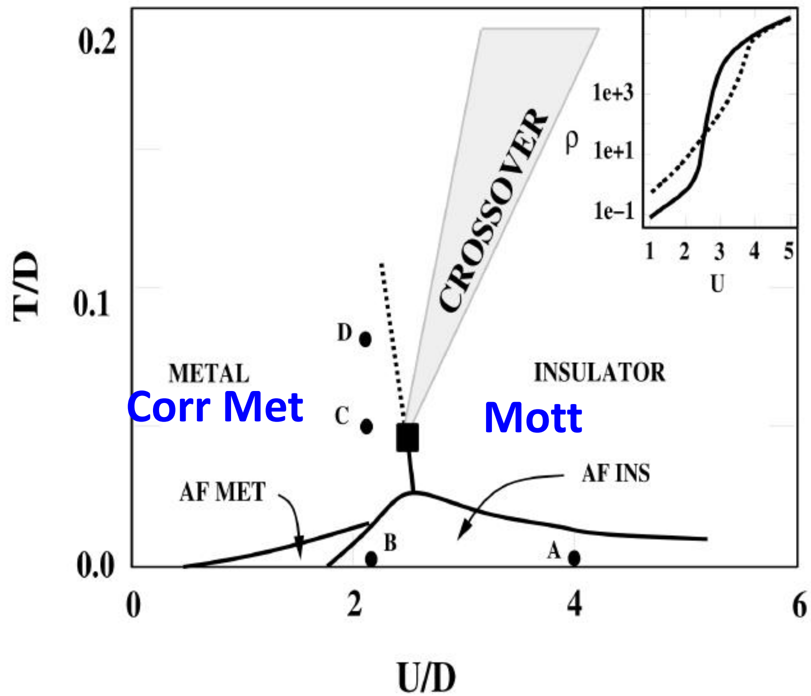
XYZ, MR, Kotliar et al PRL ’91



Coexistance region: 2 solutions

Phase diagram of V_2O_3



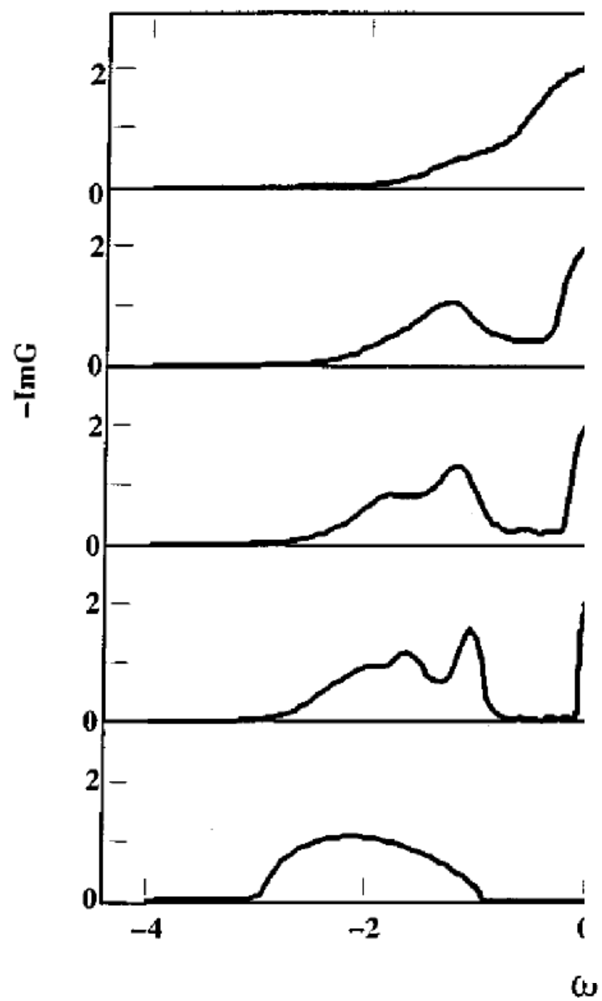


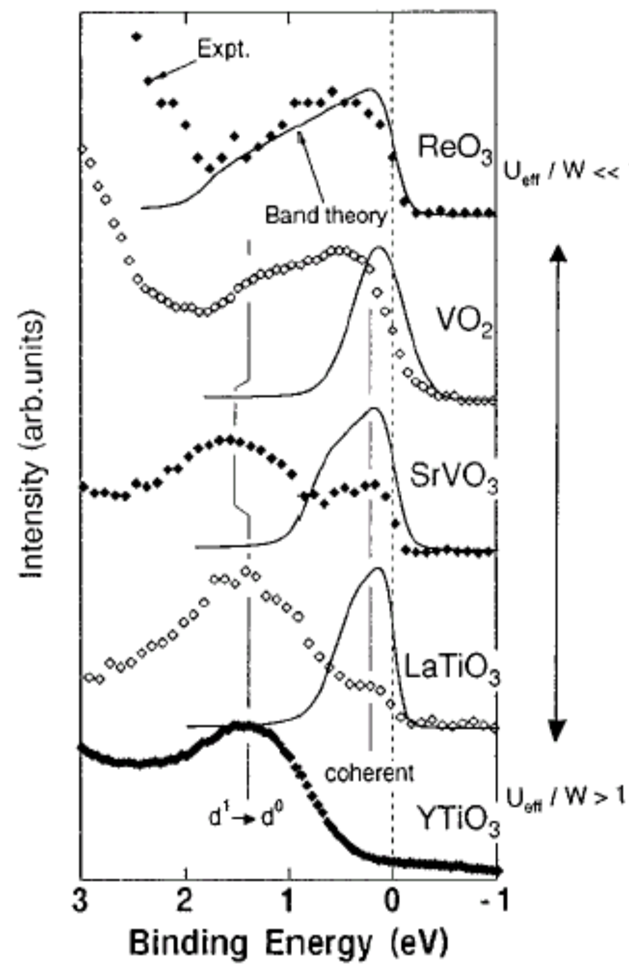
pressure or chemical substitution

McWhan et al PRB '71 '73

MR, Kotliar et al PRB '94 PRL'95

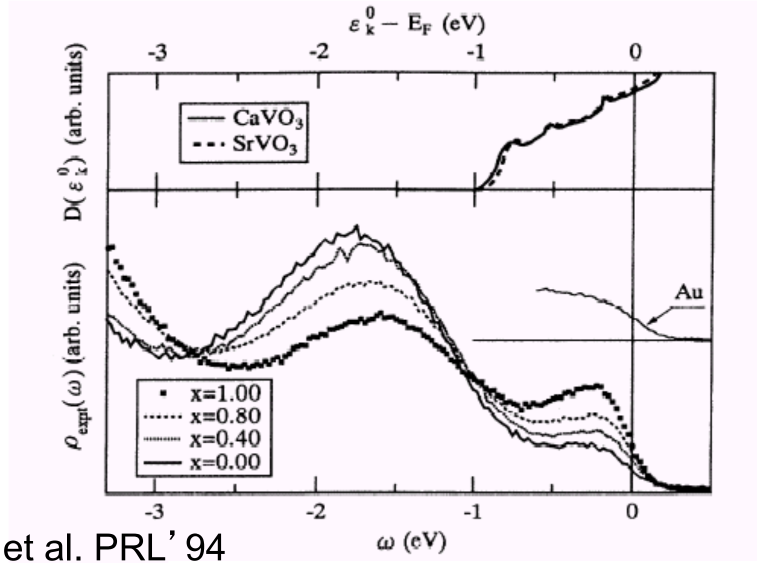
Mott Transition as function of U/W





A Georges & G Kotliar, PRB '92
MR, XY Zhang & G Kotliar, PRL '93

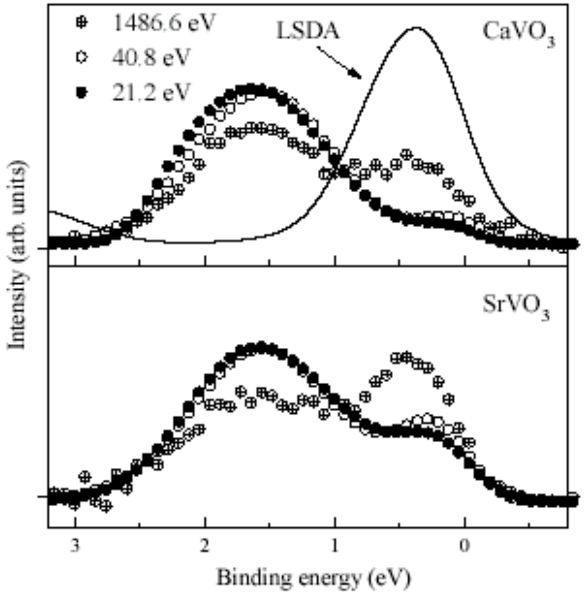
$Sr_{1-x}Ca_xVO_3$ photoemission... where is the qp-peak?

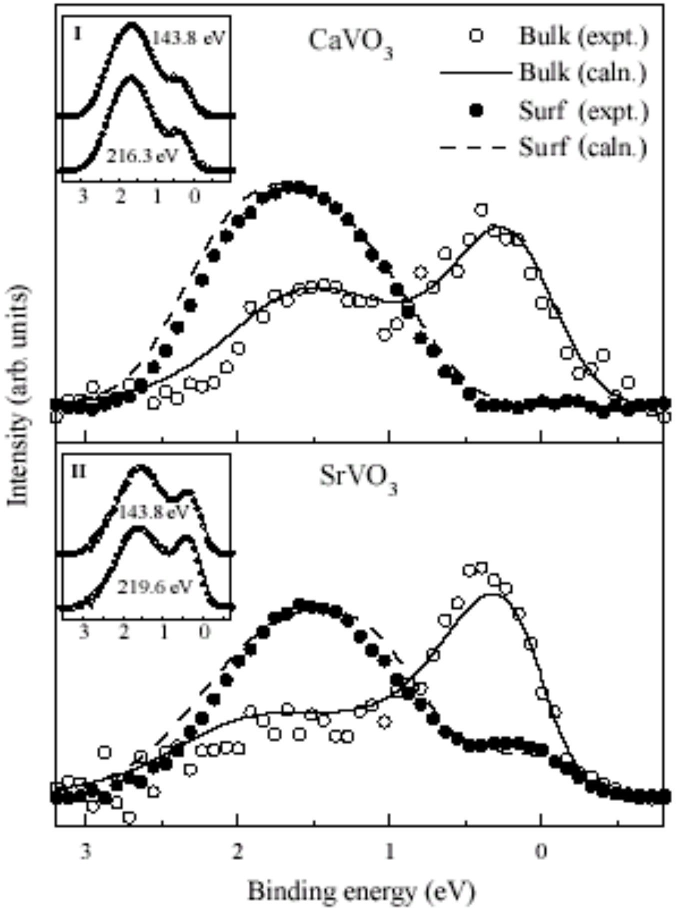


Inoue et al. PRL' 94

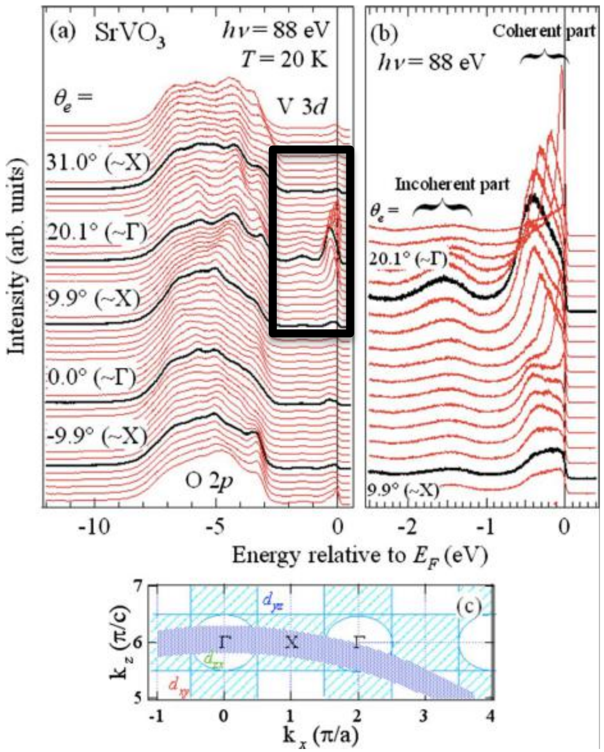
high $h\nu$ spectroscopy

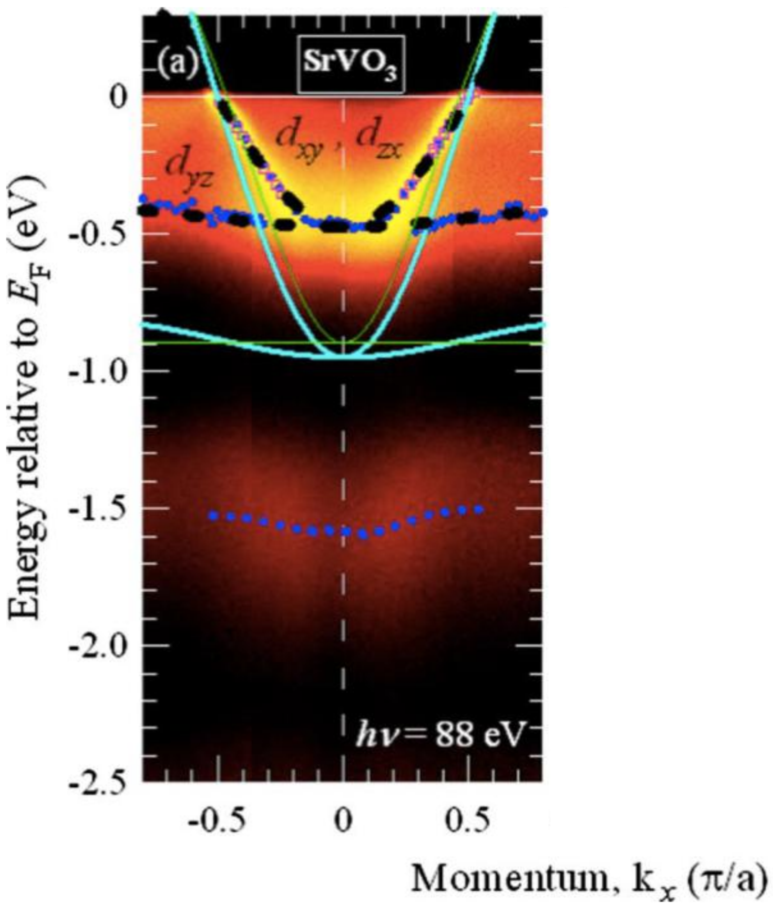
Maiti, Sarma, MR, Inoue et al. EPL' 01



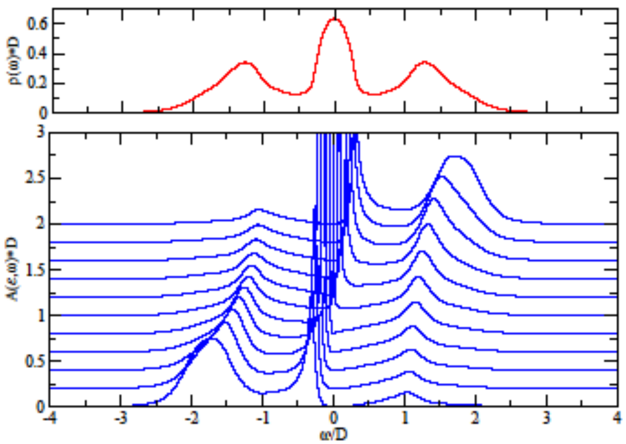


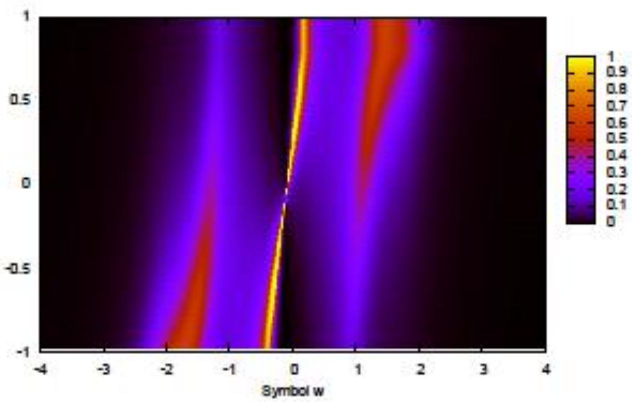
Heavy coherent quasiparticles and Incoherent Hubbard Bands

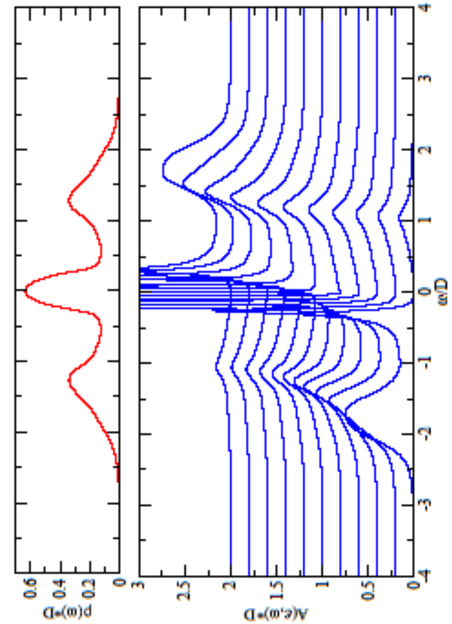


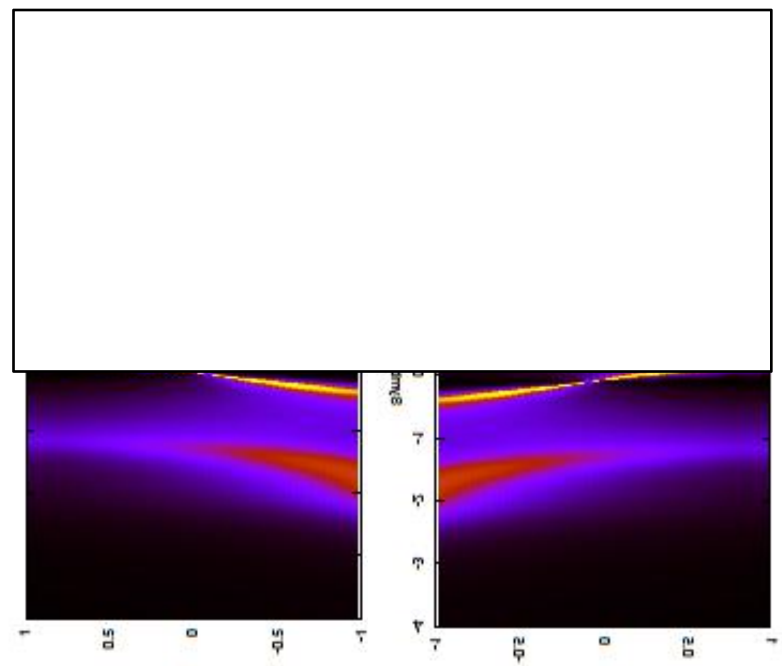


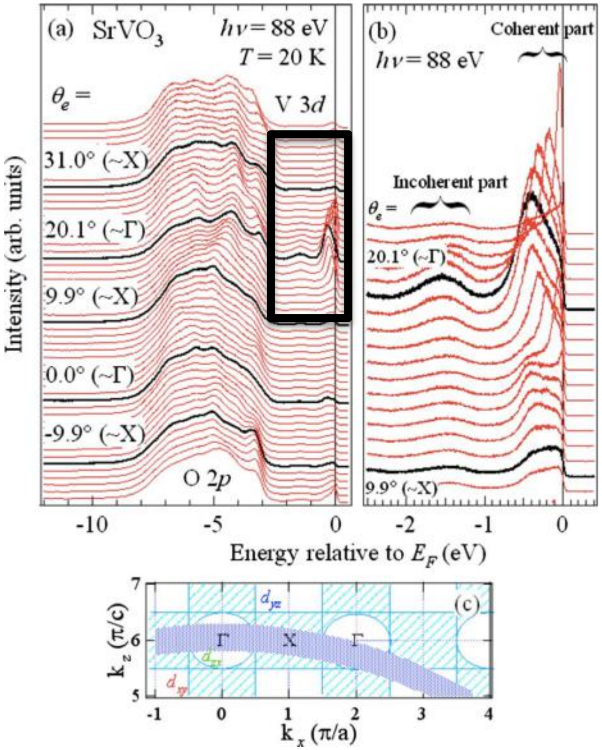
Takizawa, Sordi, MR, et al PRB ’09


ρ(ω)*D
A(ε,ω)*D
ω/D

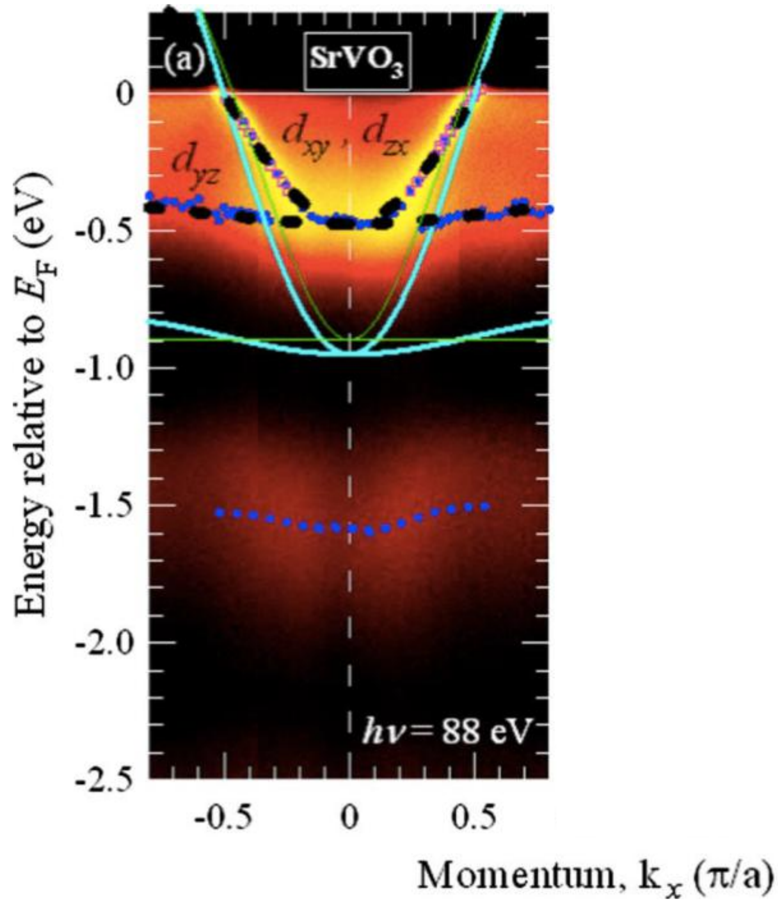

Symbol w


ρ(ω)*D
A(ε,ω)*D
ω/D

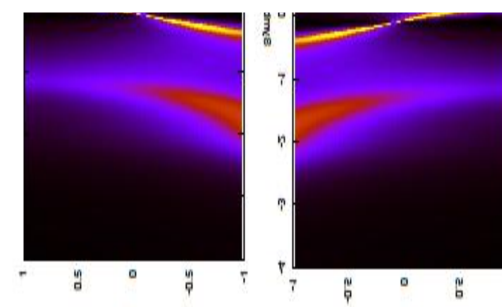




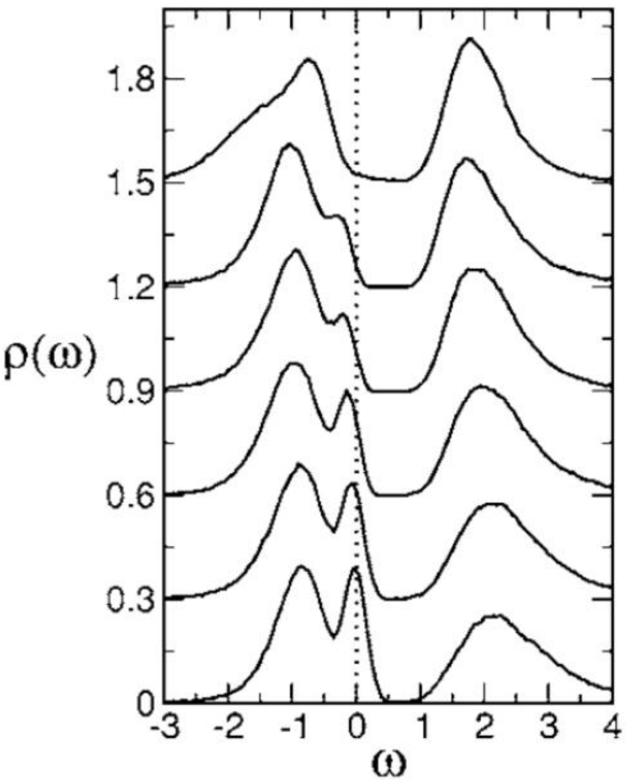
(a) SrVO3
hν = 88 eV
T = 20 K
θe =
V 3d
31.0° (~X)
20.1° (~Γ)
9.9° (~X)
0.0° (~Γ)
-9.9° (~X)
O 2p
Intensity (arb. units)
(b)
hν = 88 eV
Coherent part
Incoherent part
θe =
20.1° (~Γ)
9.9° (~X)
-10
-5
0
-2
-1
0
Energy relative to EF (eV)
(c)
dyz
dzx
dxy
Γ
X
Γ
kz (π/c)
kx (π/a)

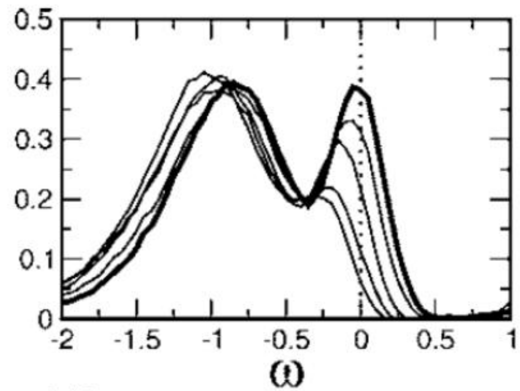


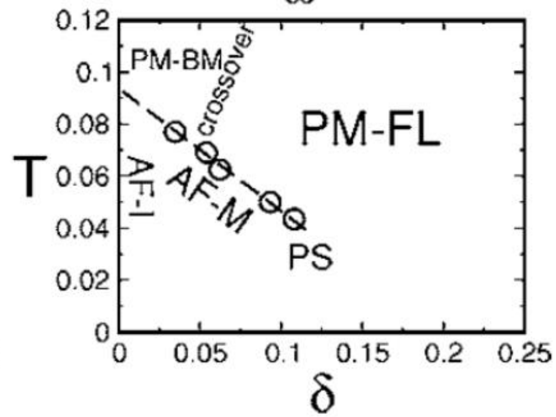
(a)
SrVO3
dyz
dxy, dzx
Energy relative to EF (eV)
0
-0.5
-1.0
-1.5
-2.0
-2.5
hν = 88 eV
-0.5
0
0.5
Momentum, kx (π/a)

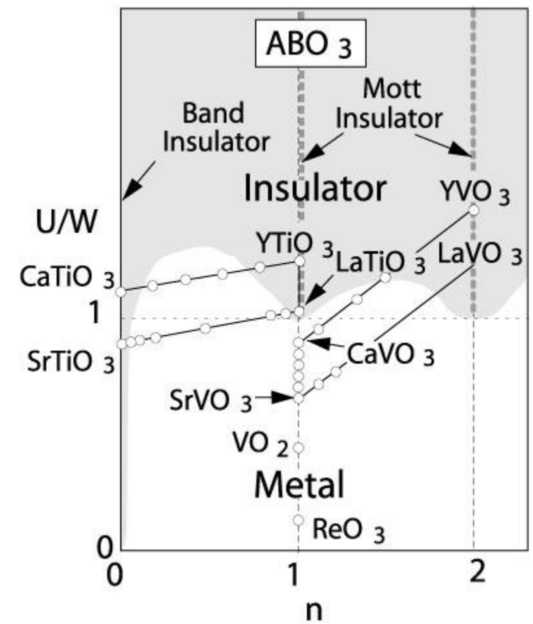


Doping driven transition



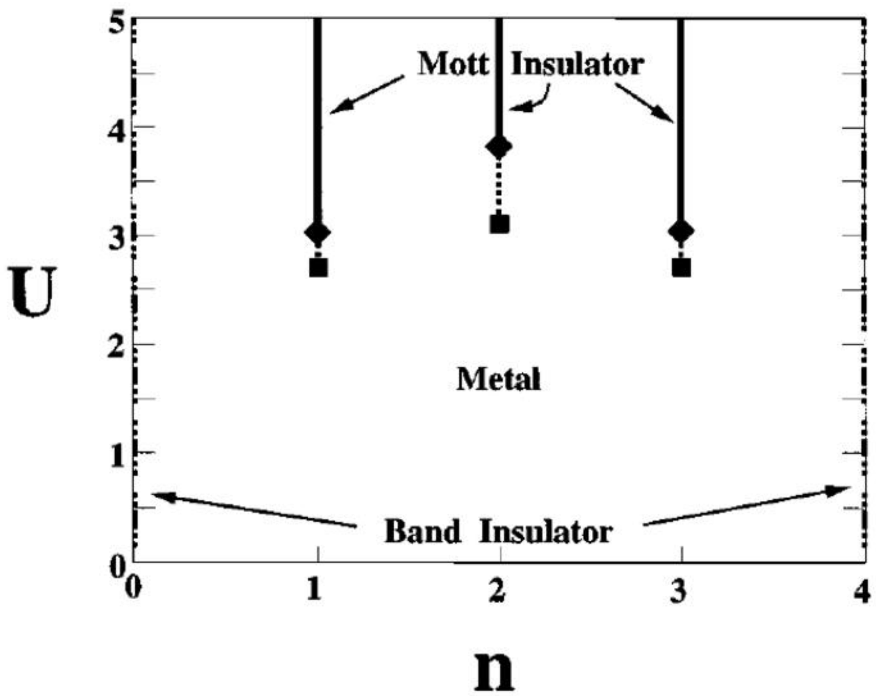


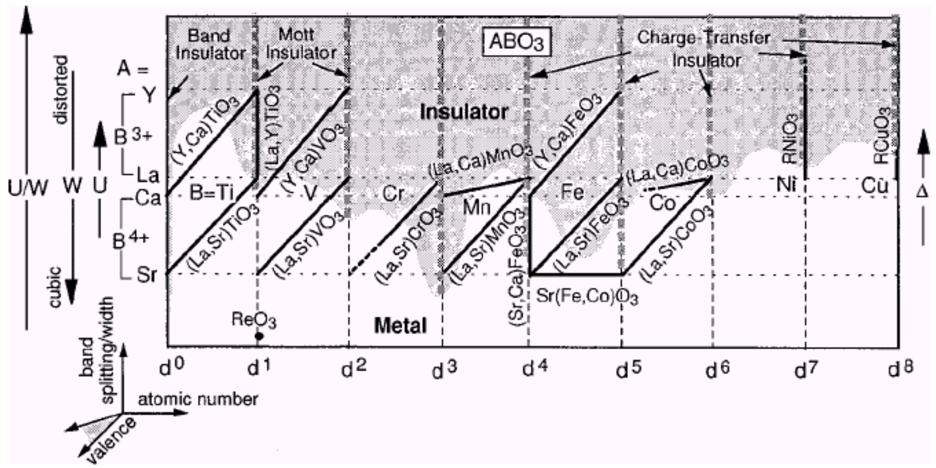




Camjayi, Chitra & MR, PRB(RC) ‘06

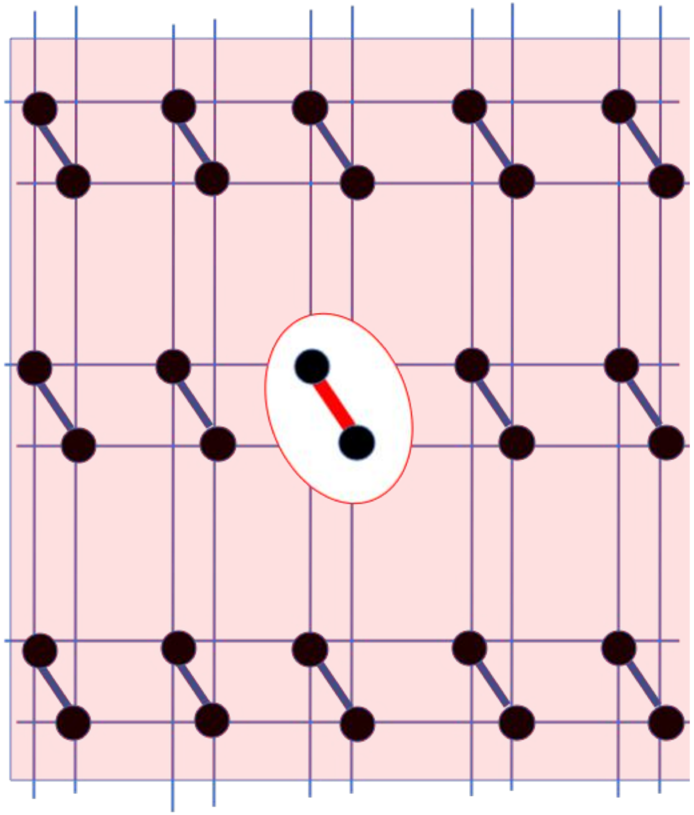
Multi-orbital Hubbard model (degenerate band case)

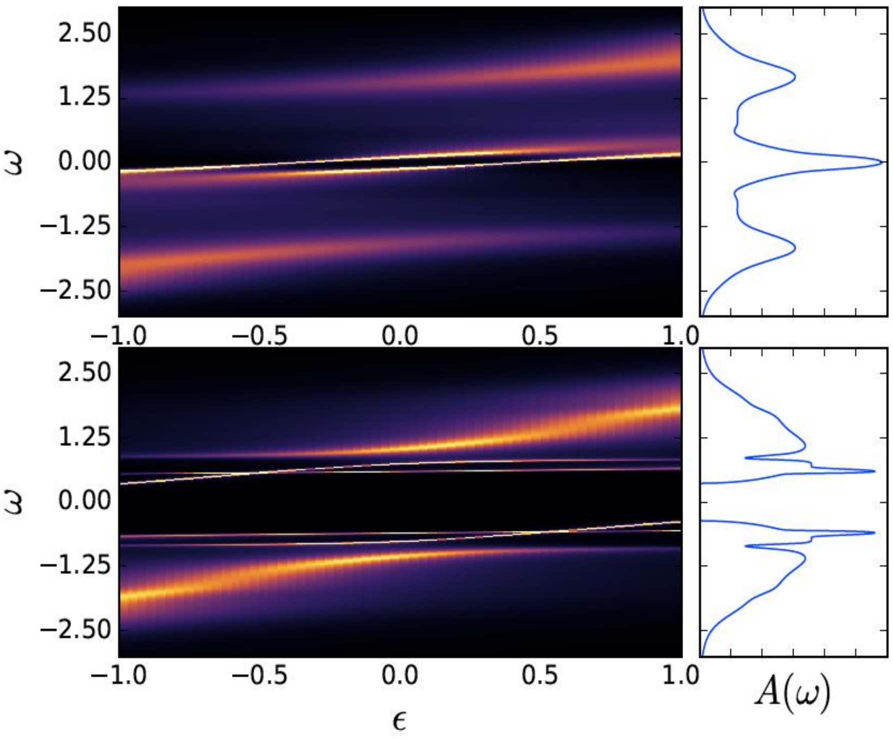




MR PRB(RC) '97

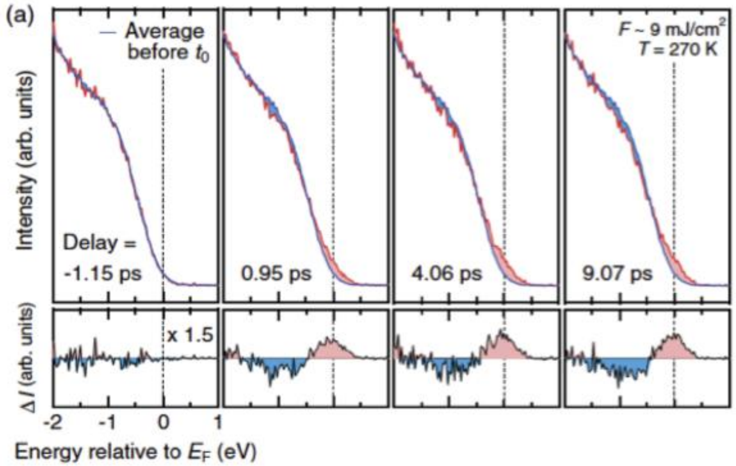
Cluster extensions
Dimer Hubbard model



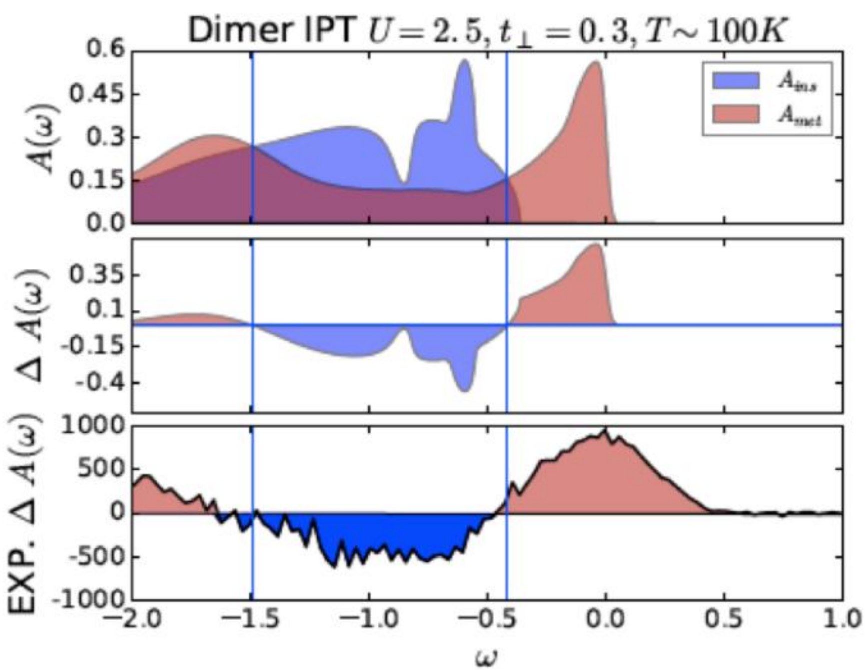


Moeller et al PRB '99
Najera et al PRB '17

Out-of-equilibrium



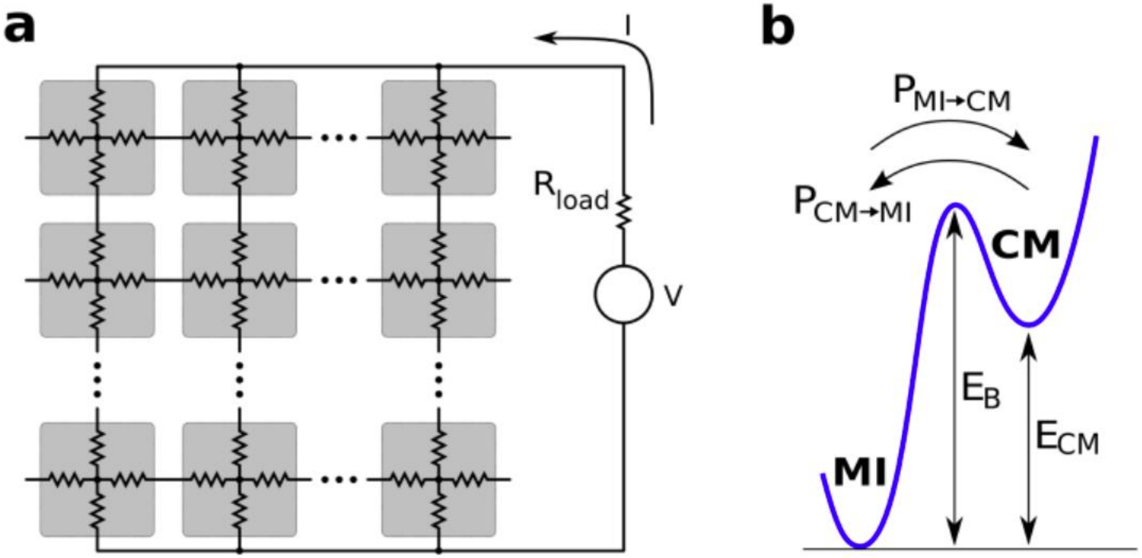
pump-probe photoemission in VO2
Shin et al PRB'14



DMFT of DHM

Najera PhD Thesis '17

Universality of Mott transition under an electric field
Mottronics
Artificial neurons for Artificial Intelligence hardware



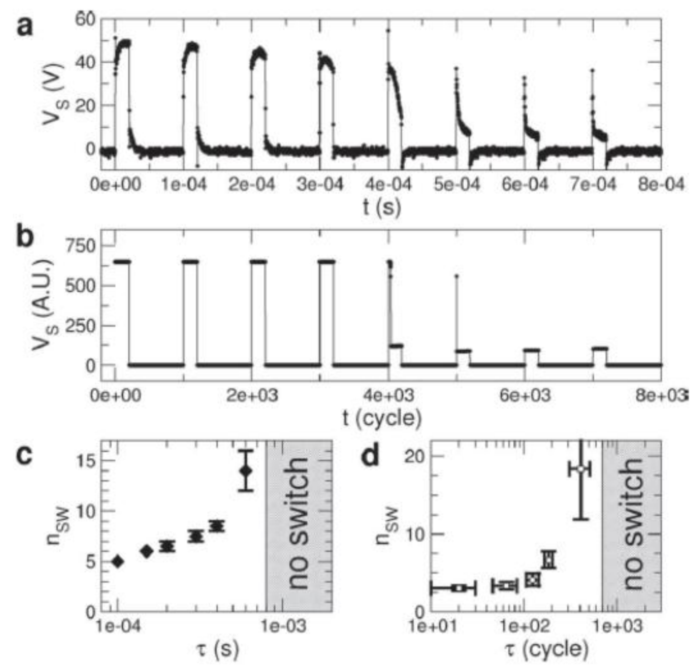
Two states: MI – Mott insulator

CM – Correlated metal

$R_{MI} >> R_{CM}$

$P_{MI\text{->}CM}$ and $P_{CM\text{->}MI}$ are transition probabilities

$$P_{MI\rightarrow CM} = \nu e^{-(E_B - q\Delta V)/kT} \qquad P_{CM\rightarrow MI} = \nu e^{-(E_B - E_{CM})/kT}$$



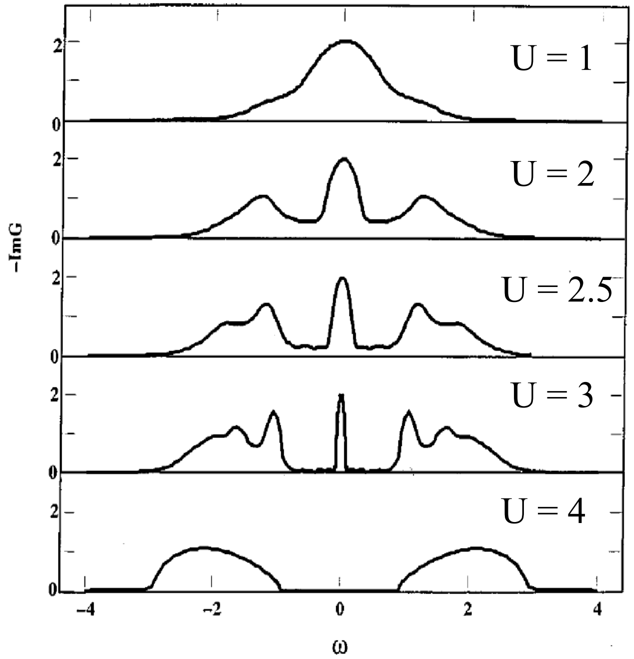
P. Stoliar et al Adv. Mater. ‘13

Stoliar et al. Adv Func Mat ‘17

Del Valle et al Nature ‘19

IPT tutorial

https://drive.google.com/drive/folders/1dENgL58Q0wImpRd2Mnw3TfrSCYR3fkeg?usp=sharing



Hands-on excercise
Unix, Windows, Mac, Phyton
Source (original) fortran77