



Quantum cluster approaches for investigating strongly correlated electronic systems



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Outline

- What are strongly correlated electron systems?
- Why are they interesting?
- Models
- Methods – Dynamical mean field theory and extensions
- Applications
- A peek into Cluster approaches



Strongly correlated electron systems

Various Definitions:

- Kinetic energy \lesssim Inter-electron repulsive potential energy
- Failure of independent-electron description
- Electrons at the edge of magnetism
- Strong competition between itinerancy and localization



Strongly correlated electron systems

Materials :

- Transition metal oxides – High T_c superconductors,
Mott Hubbard/Heisenberg insulators,
Colossal magnetoresistive oxides
(V_2O_3 , $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_7$, YVO_3 ,
 $LaMnO_3$, $LaTiO_3$)
- Rare earth intermetallics – Heavy fermion materials
($CeAl_3$, CeB_6 , $YbRh_2Si_2$, $CeCoIn_5$, $PuCoIn_5$, $CeCu_{6-x}Au_x$)
- 2DEG - Quantum Hall Systems, Graphene (?)



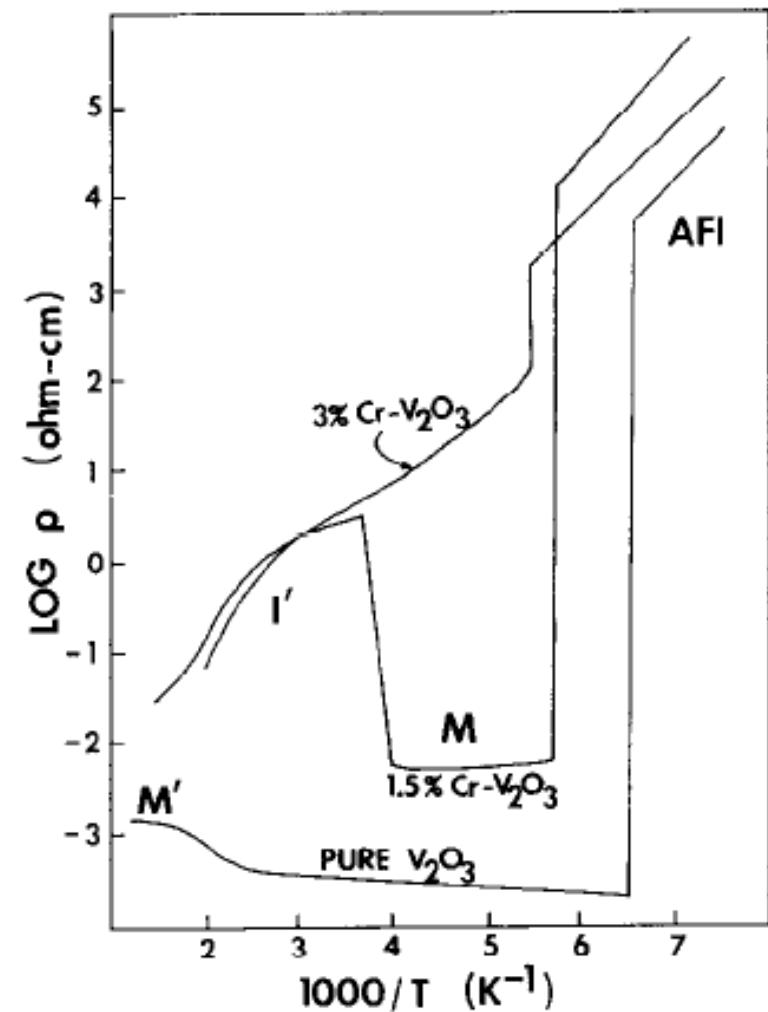
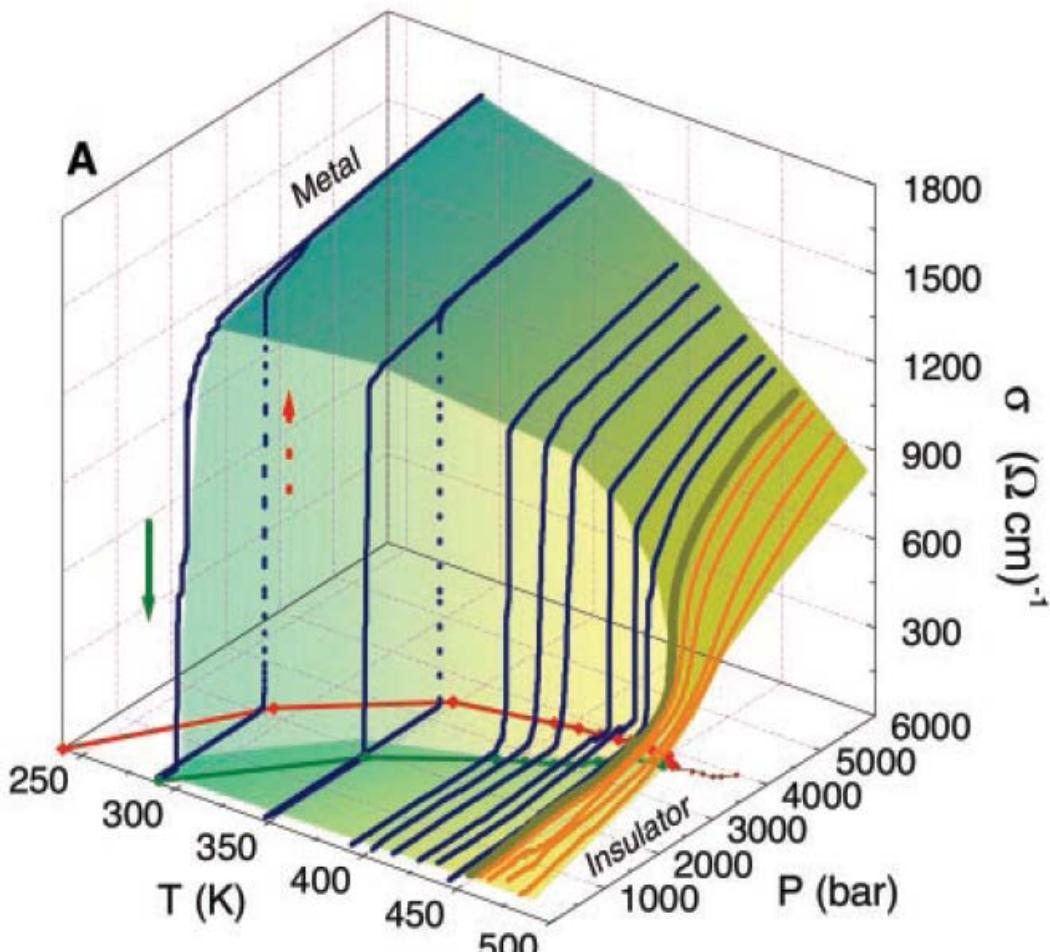
Strongly correlated electron systems

Phenomena :

- **Mott Metal-Insulator Transition** – Just Spectacular, Itinerancy vs Localization
- **High Temperature Superconductivity** – Again spectacular (Spin-Charge Separation, Pseudogap, Striped phases, Bond order, Quantum Critical Point, Non-Fermi Liquid)
- **Colossal Magnetoresistance** – Extreme Sensitivity to perturbations
- **Heavy Electrons** – Extreme examples of Adiabatic Continuity
- **Quantum Critical Points** – Connection to Black Hole Physics and string Theories
- **Fractional Quantum Hall Effect** – Fractional Charges and Statistics



The Mott Transition in V_2O_3

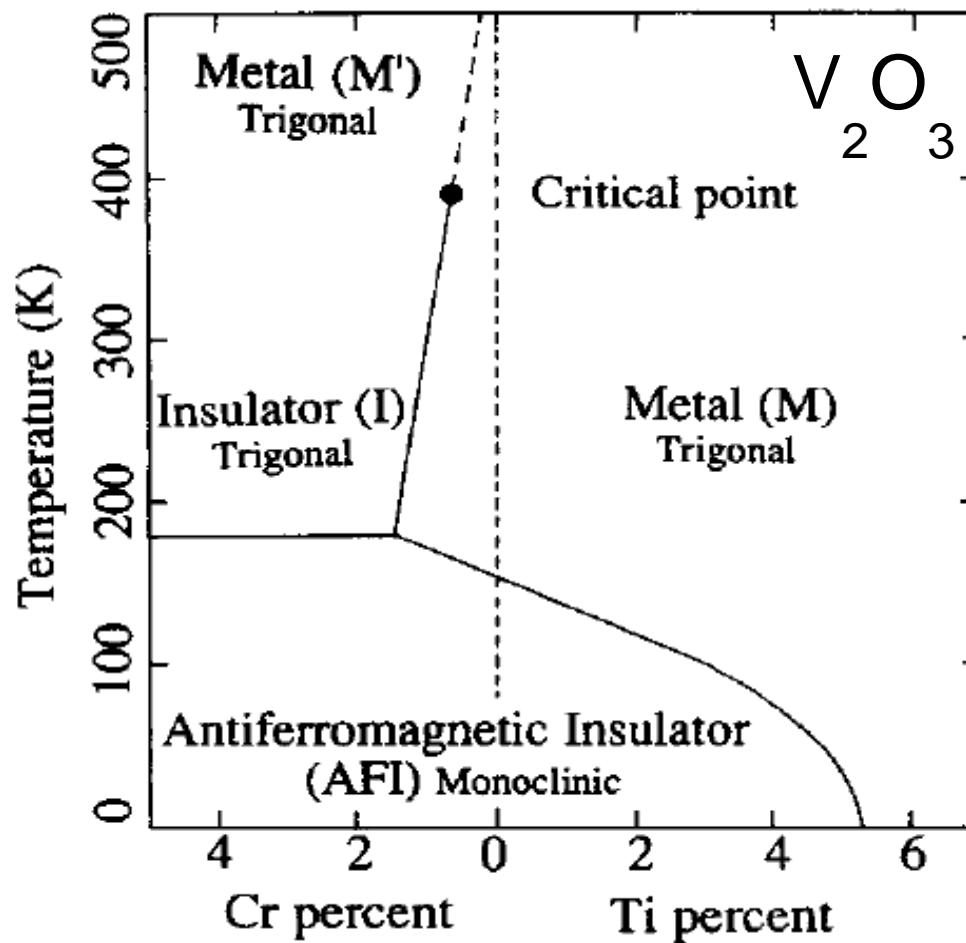


Limelette et al, SCIENCE **302** (2003).

Yethiraj et al, J. Sol. St. Chem, **88**, 53-69 (1990).



The Mott Transition

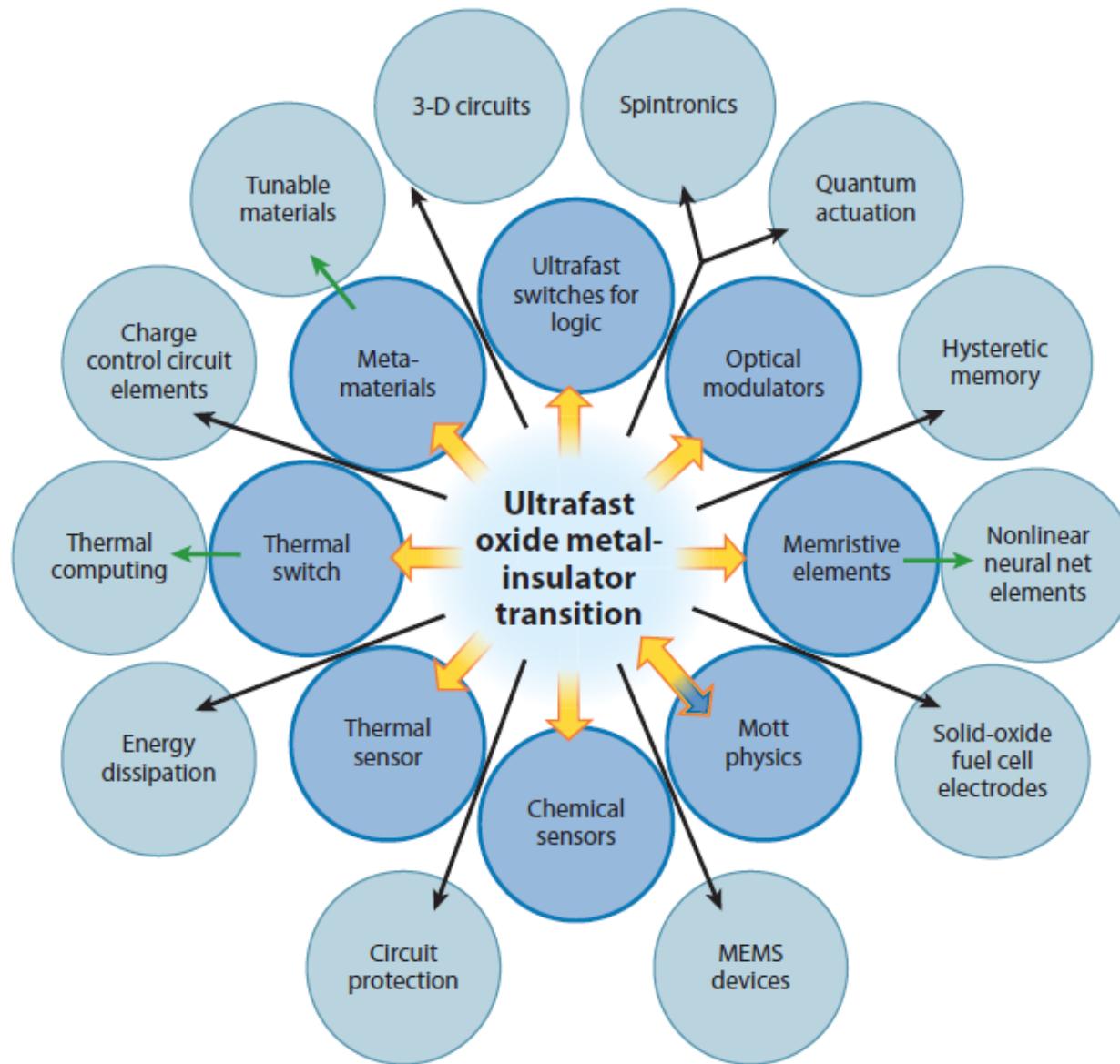


Yethiraj, J. Sol. St. Chem, Vol.88, 53-69
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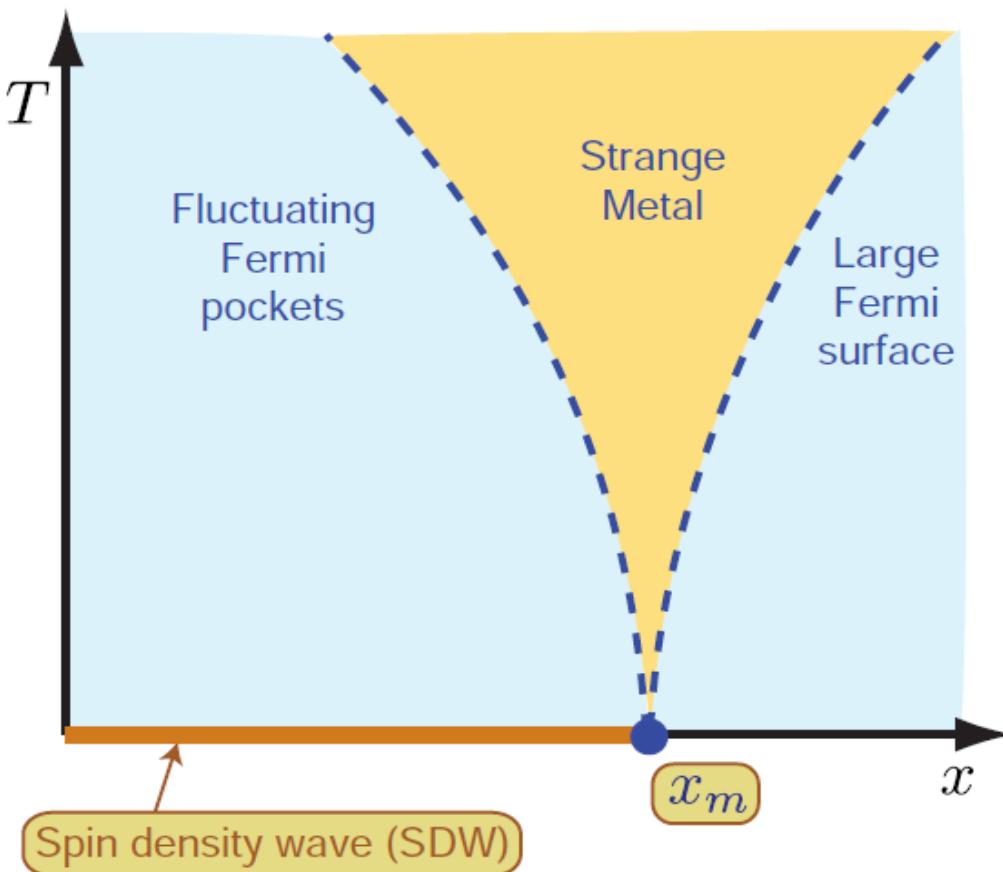
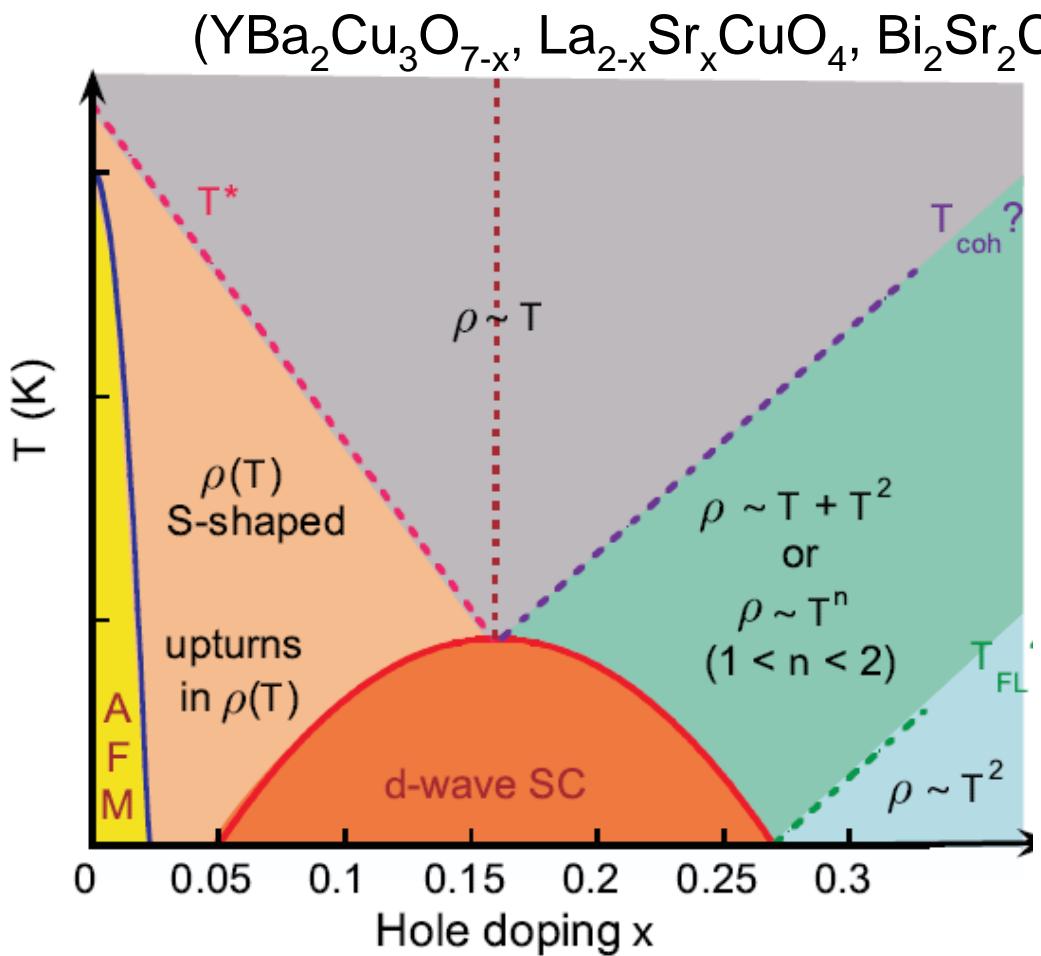
The Mott Transition- Applications

VO_2





High Temperature Superconductors



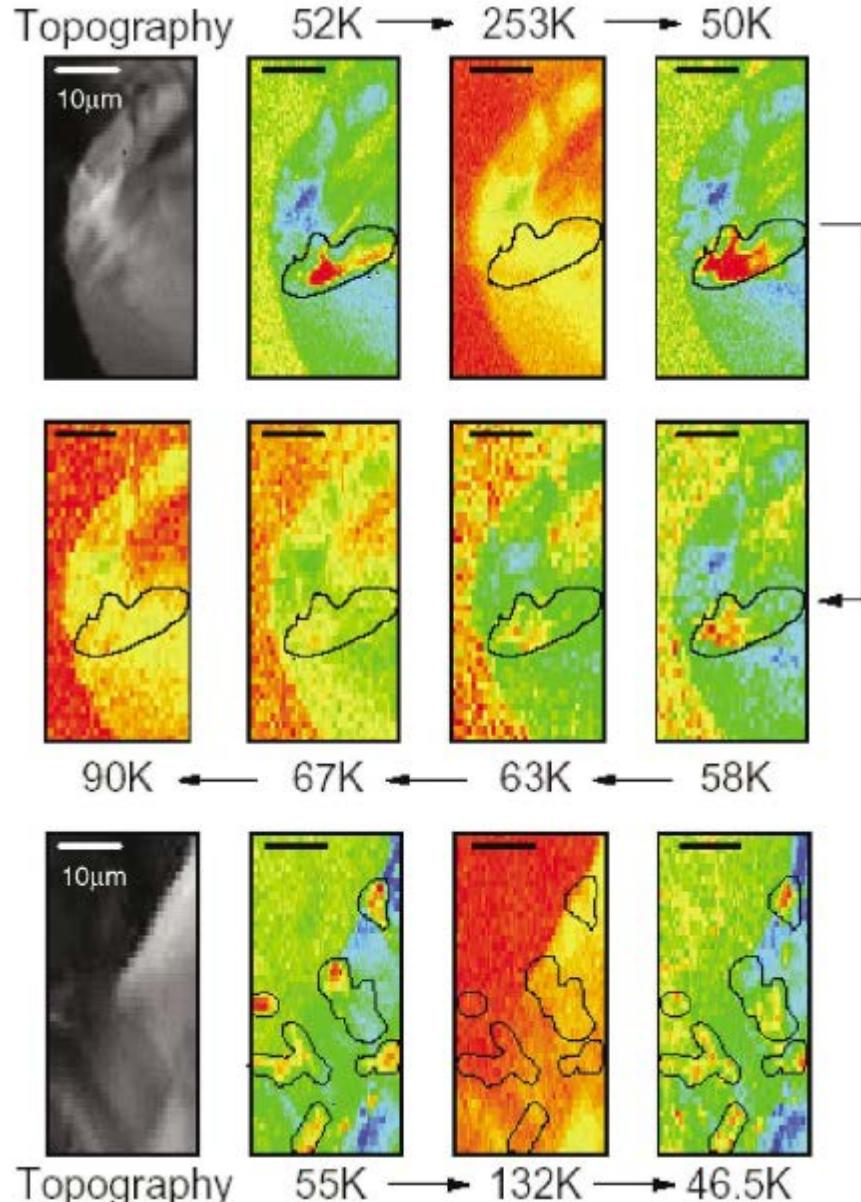
S. Sachdev <http://arxiv.org/pdf/0907.0008>

N. S. Vidhyadhiraja et al, Phys. Rev. Lett. Vol.102, pp.206407 (2009).

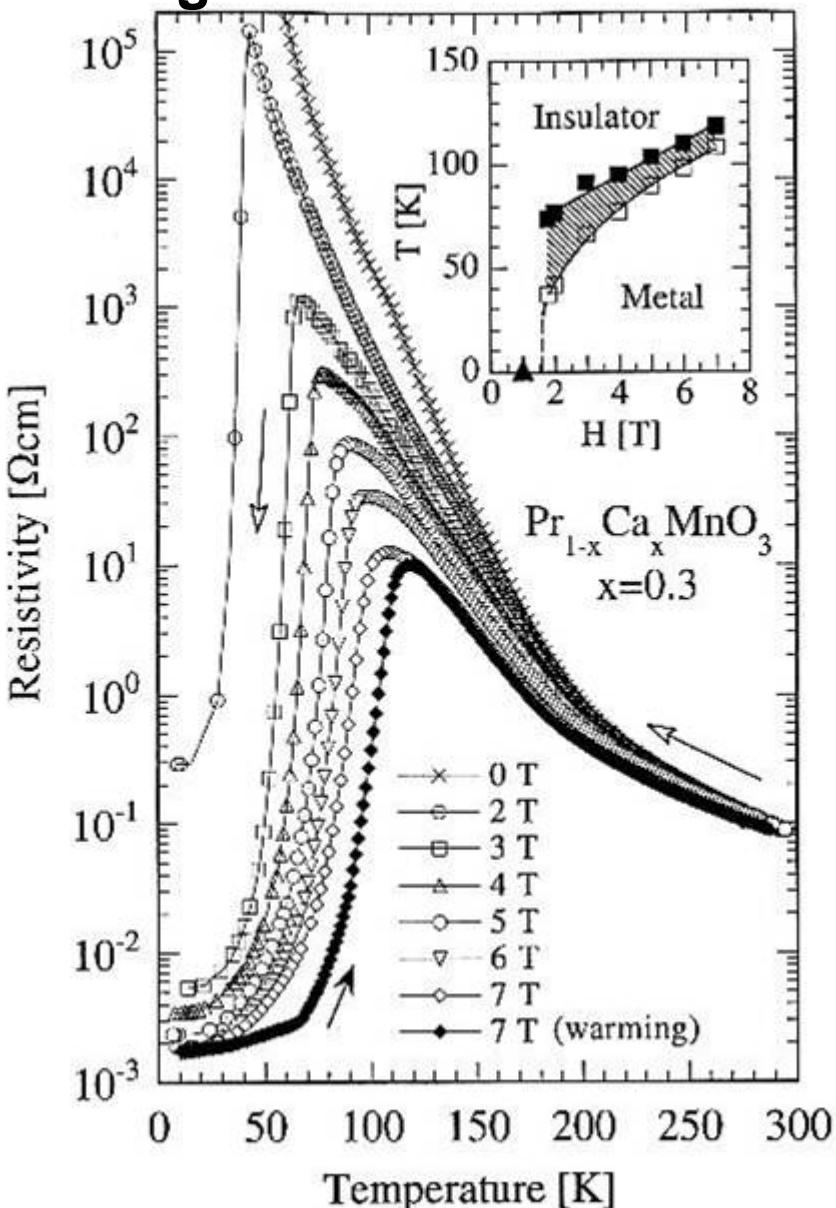


Manganites

(ReMnO_3 ; RE=La, Pr, Sm, Nd, ...)



Electronic Phase Separation and Colossal Magnetoresistance





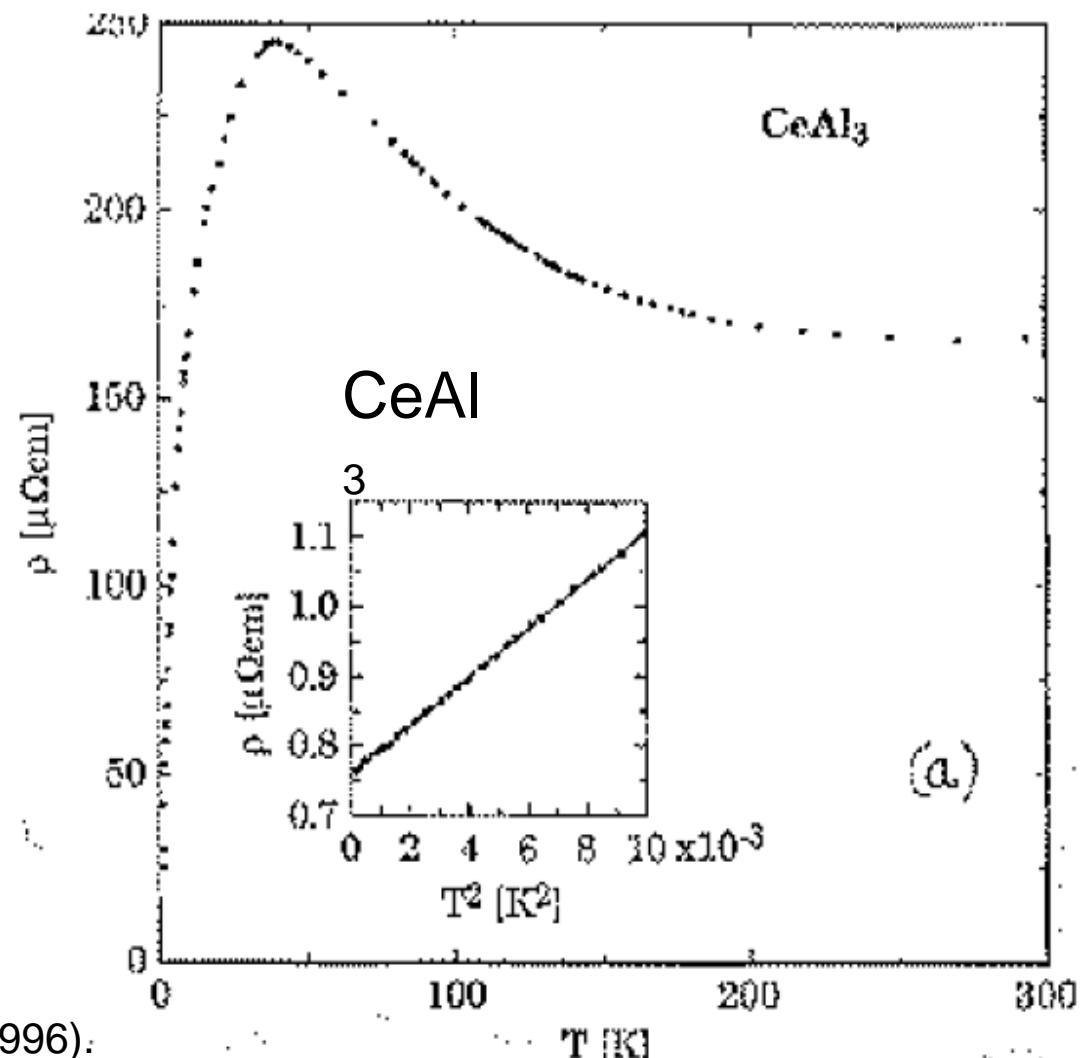
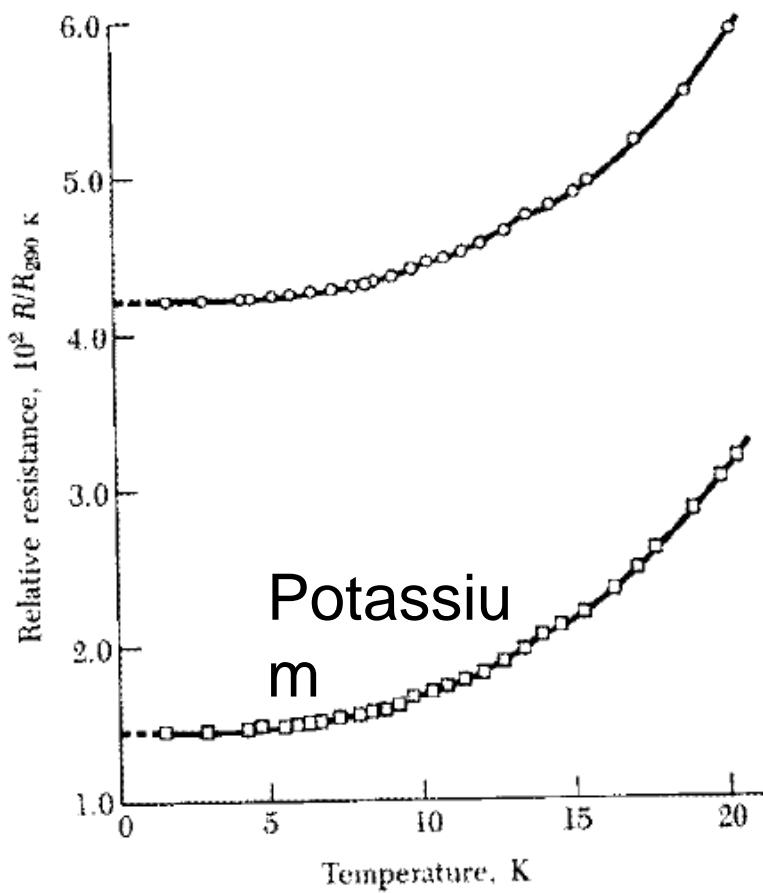
Heavy Fermions

CeAl₃; CePd₃; CeSn₃; CeCoIn₅

CeB₆; CeInCu₂; CePtSi; CeCu₆

YbFe₄Sb₁₂; YbCuAl; YbPtIn

YbAl₃; YbInAu; YbPdSb; YbPtBi

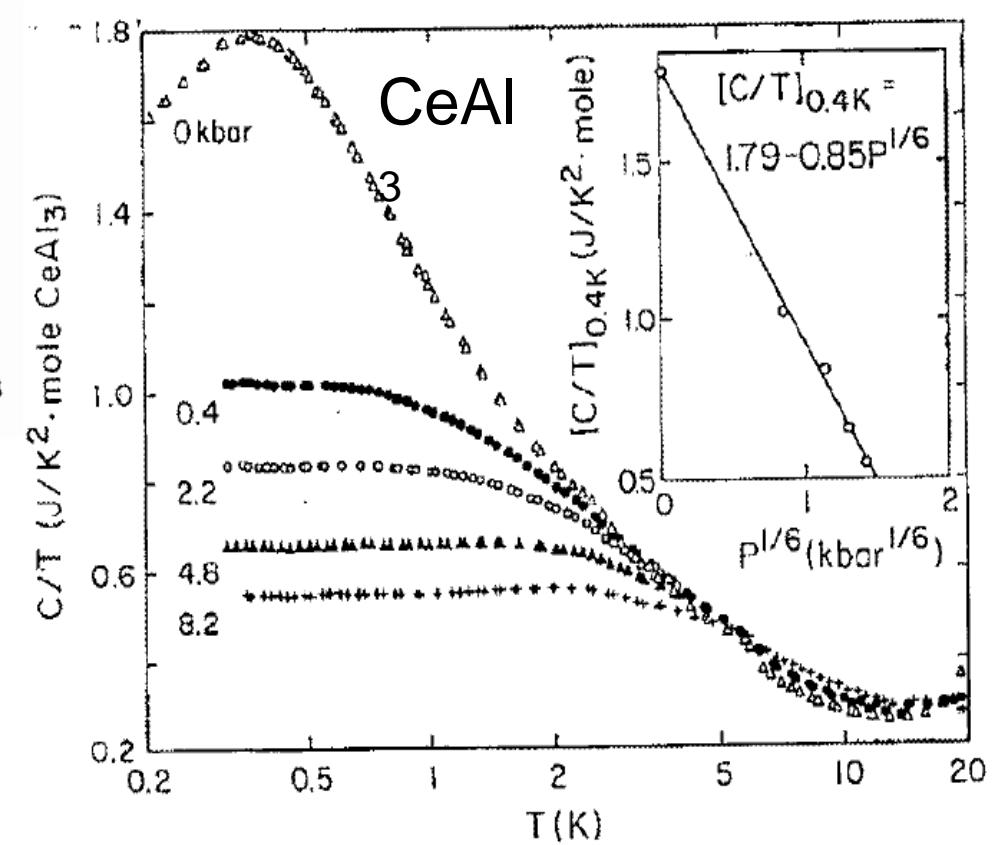
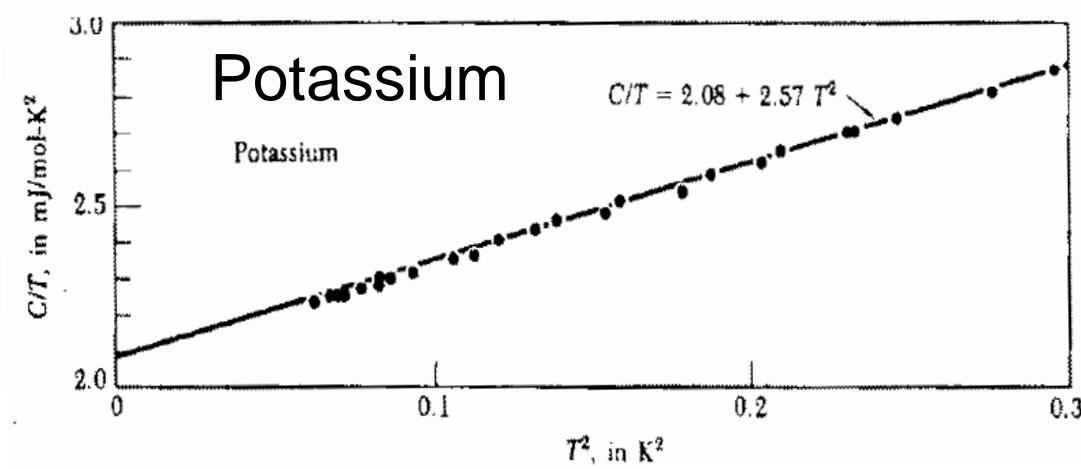


C. Kittel, Introduction to Solid State Physics, (1996).

L.Degiorgi, Rev. Mod. Phys. 71, 687(1999).



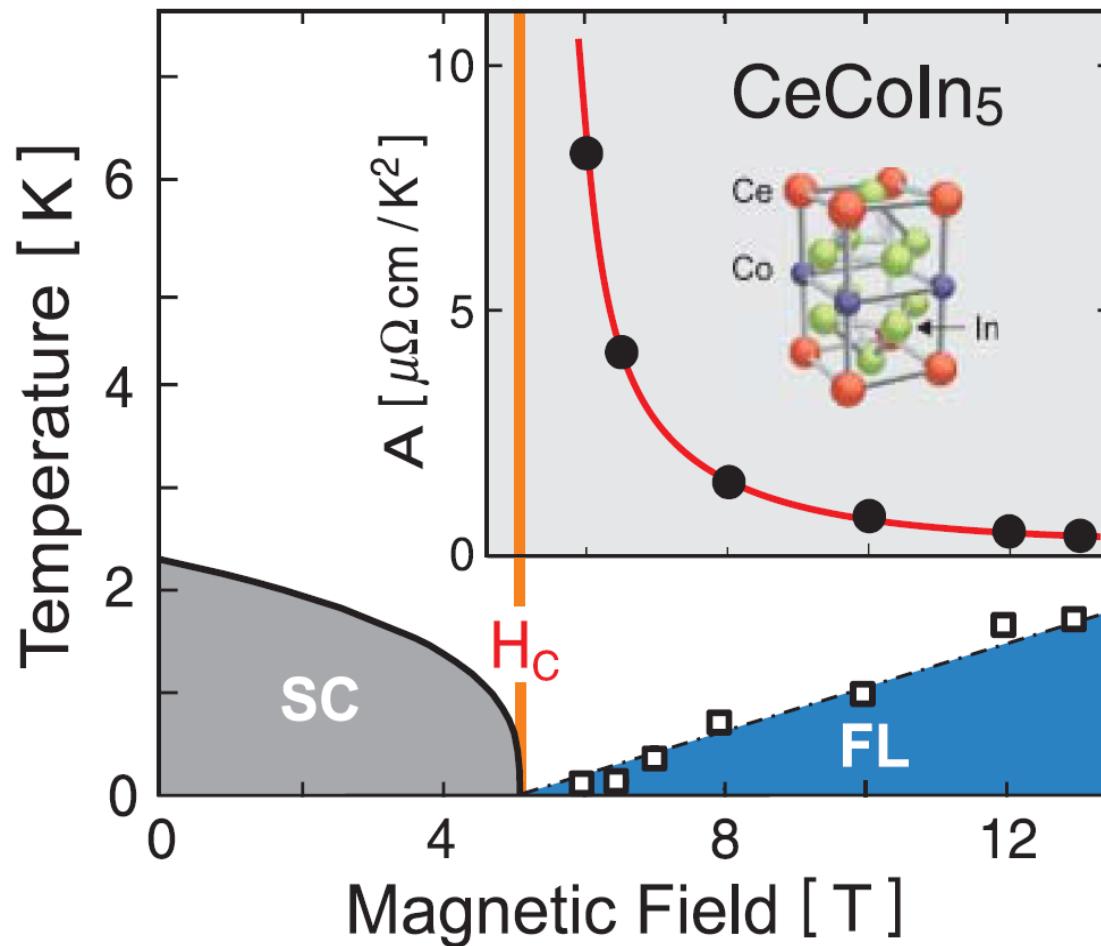
Adiabatic Continuity: Heavy Fermions



C. Kittel, Introduction to Solid State Physics, (1996).
L.Degiorgi, Rev. Mod. Phys. 71, 687(1999).



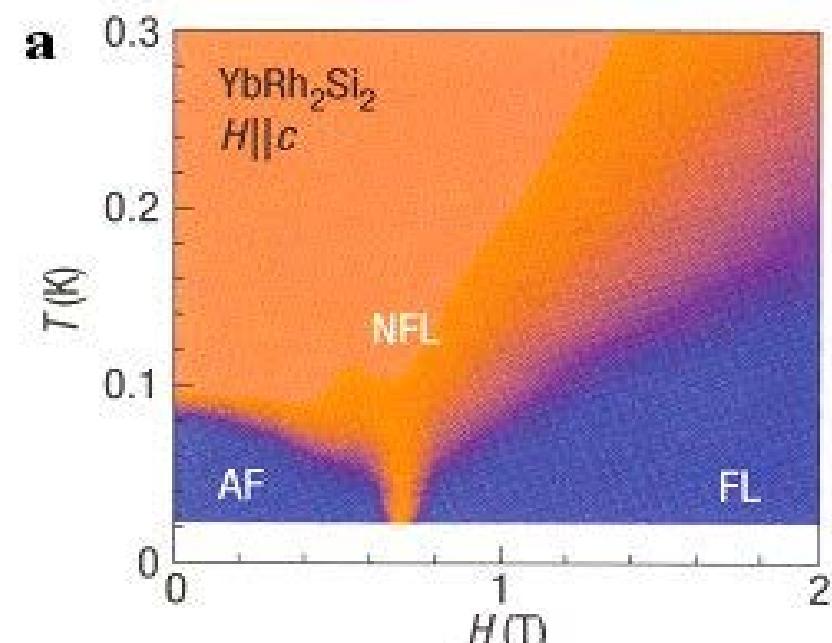
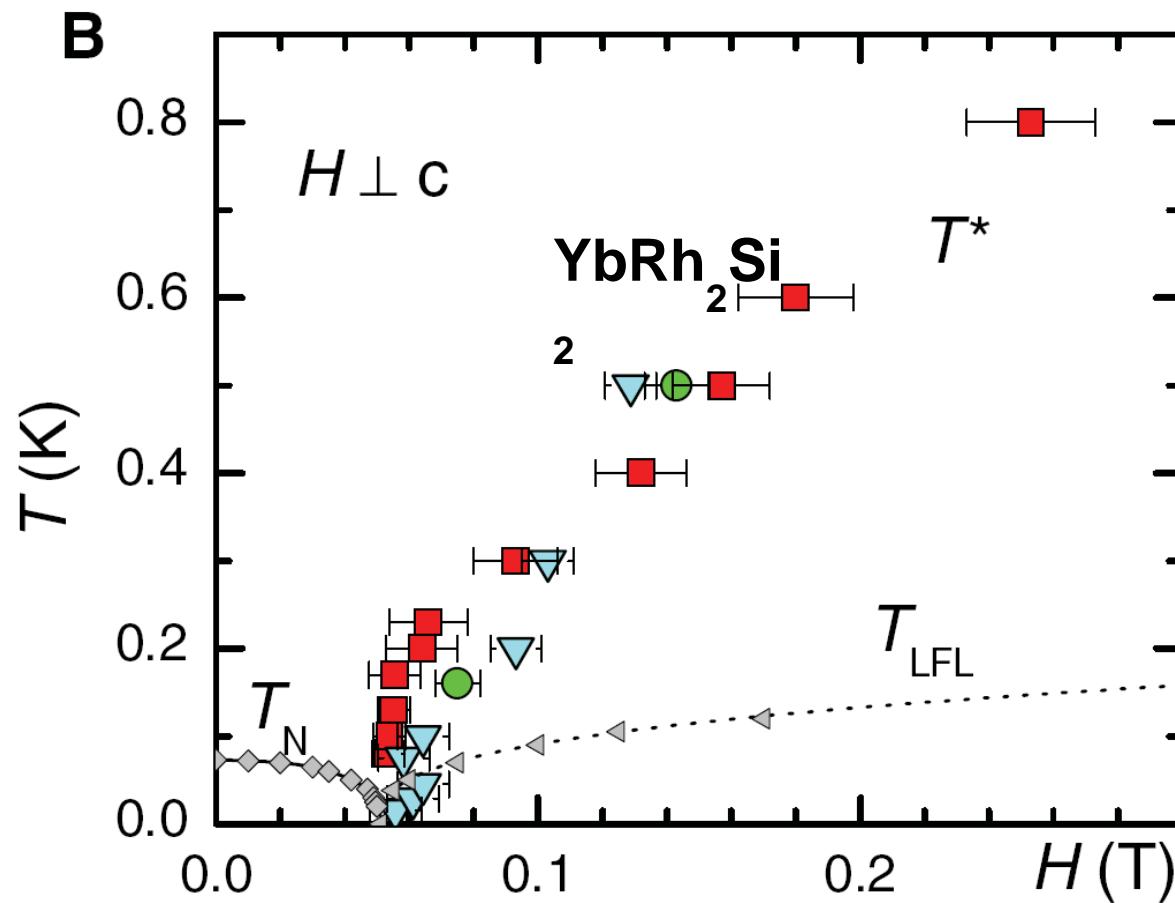
Quantum Critical Points



Tanatar et al, Science 316, no.5829, pp.1320-1322 (2007).



Quantum Critical Points

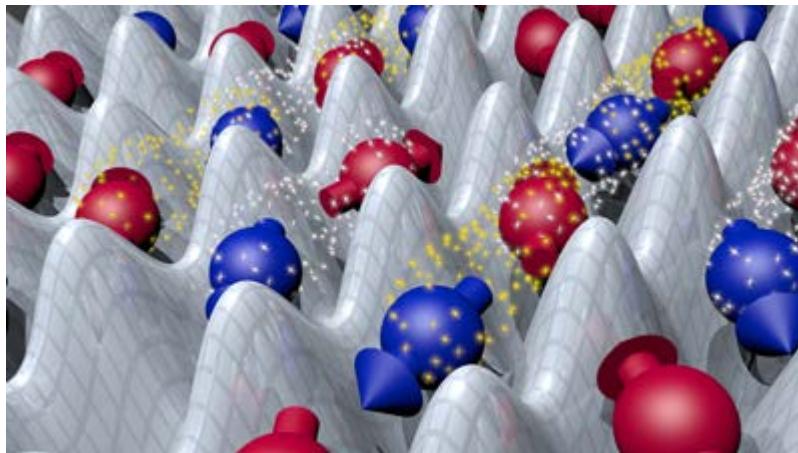


Gegenwart et al, Nature Physics **4**, pp.186-197 (2008).

http://www.scitopics.com/Quantum_Criticality_of_Heavy_Fermions.html

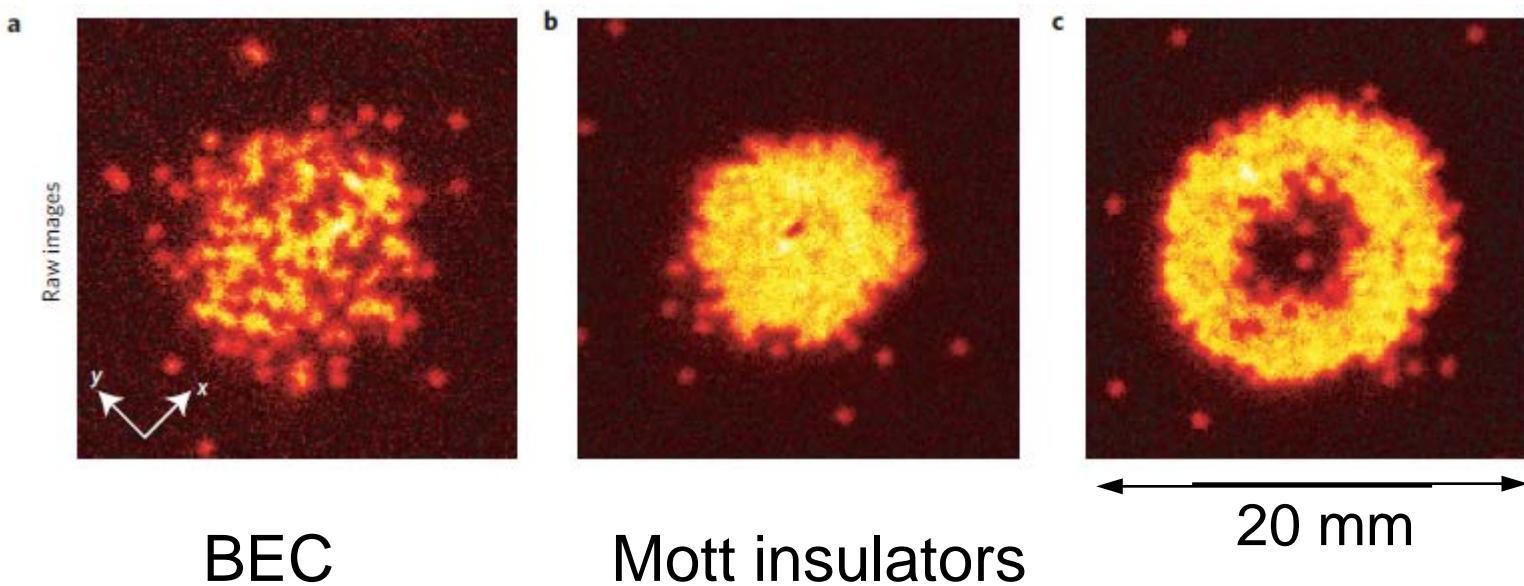


Ultra-cold atomic systems



Quantum magnetism simulated using ultracold fermions.

H.Johnston Physics World May 24 (2013).





Realistic Models for SCES

$$\mathcal{H}_0 = \sum_{i\alpha\sigma} \epsilon_{i\alpha} n_{i\alpha\sigma} + \sum_{ij\alpha\beta\sigma} T_{ij}^{\alpha\beta} (c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + h.c)$$

Tight-binding model with multiple orbitals



Realistic Models for SCES

$$\mathcal{H}_0 = \sum_{i\alpha\sigma} \epsilon_{i\alpha} n_{i\alpha\sigma} + \sum_{ij\alpha\beta\sigma} T_{ij}^{\alpha\beta} (c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + h.c)$$

Tight-binding model with multiple orbitals

$$\mathcal{H}_U = \sum_{i\alpha\sigma} \frac{U}{2} n_{i\alpha\sigma} n_{i\alpha\bar{\sigma}}$$

Electron-electron interaction

$$+ \sum_{i\alpha\sigma \neq \beta\sigma'} \frac{(U - 2J)}{2} n_{i\alpha\sigma} n_{i\beta\sigma'} + \sum_{i\sigma\alpha \neq \beta} \frac{(U - 3J)}{2} n_{i\alpha\sigma} n_{i\beta\sigma} .$$



Realistic Models for SCES

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Parameters are obtained from first principles density functional theory based methods.



Minimal Models

- **Single Impurity Anderson Model** (s-d model, Kondo Model) for dilute magnetic impurities in metals.
- **Hubbard Model** (t-J model, Heisenberg model) for transition metal oxides, cuprate superconductors.
- **Periodic Anderson Model** (Kondo Lattice model) for heavy fermion systems.
- **Holstein-Hubbard Model, Double-exchange model, Falikov-Kimball model, Bose-Hubbard model etc.**



Minimal Models

Hubbard model

$$\hat{H} = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + \epsilon_d \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Periodic Anderson Model

$$\begin{aligned} \hat{H} = & \epsilon_c \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{(i,j),\sigma} c_{i\sigma}^\dagger c_{j\sigma} + V \sum_{i,\sigma} (f_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.}) \\ & + \sum_{i,\sigma} \left(\epsilon_f + \frac{U}{2} f_{i-\sigma}^\dagger f_{i-\sigma} \right) f_{i\sigma}^\dagger f_{i\sigma}. \end{aligned}$$



Solving the models

Wavefunction based approaches are impractical in the thermodynamic limit.



Solving the models

Quantum many body theory approach

Single-particle Green's function or propagator

$$G_{ij;\sigma}(t) = -i \langle 0 | T\{c_{i\sigma}(t)c_{j\sigma}^\dagger(0)\} | 0 \rangle$$

- Density of states (Photoemission)
- Scattering rates and self-energy

Many-particle Green's function or propagator

$$G(t_1, t_2, \dots) = \langle \phi | T \mathcal{A}(t_1) \mathcal{B}(t_2) \cdots \mathcal{R}(t_r) | \phi \rangle$$

- Charge, spin and orbital susceptibilities
- Electrical and thermal conductivities
- Vertex functions
- Binder Cumulant, bond-order



Solving the models

- **Semi-Analytical Methods**

- Slave particles
- Dynamical mean field and cluster methods
- Diagrammatic Perturbation Theory
- Unitary transformations and Flow equation methods

- **Numerical methods**
- Finite Systems :

- Quantum Monte Carlo
- Exact Diagonalization
- Density Matrix RG

- **Exact methods**

- Bethe Ansatz – 1D
- Bosonization – 1D

**Approximation
is inevitable.**



Dynamical mean field theory

Analogous to Curie-Weiss mean field theory

Ising model

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

Trace out all S_i
except S_0

Mean field approximation

$$H_{\text{eff}} = -h_{\text{eff}} S_o$$

Effective field – self consistently determined

$$h_{\text{eff}} = h + J \sum_i m_i = h + z J m$$

Magnetization

$$m = \langle S_o \rangle = \tanh(\beta h + z \beta J m)$$



Dynamical mean field theory

Now the fermionic case

Hubbard model

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Effective single site action

$$S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{o\sigma}^\dagger(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

Dyson's equation

$$\mathcal{G}_0^{-1} = G^{-1} + \Sigma$$



Local lattice Green's function

Impurity Self energy

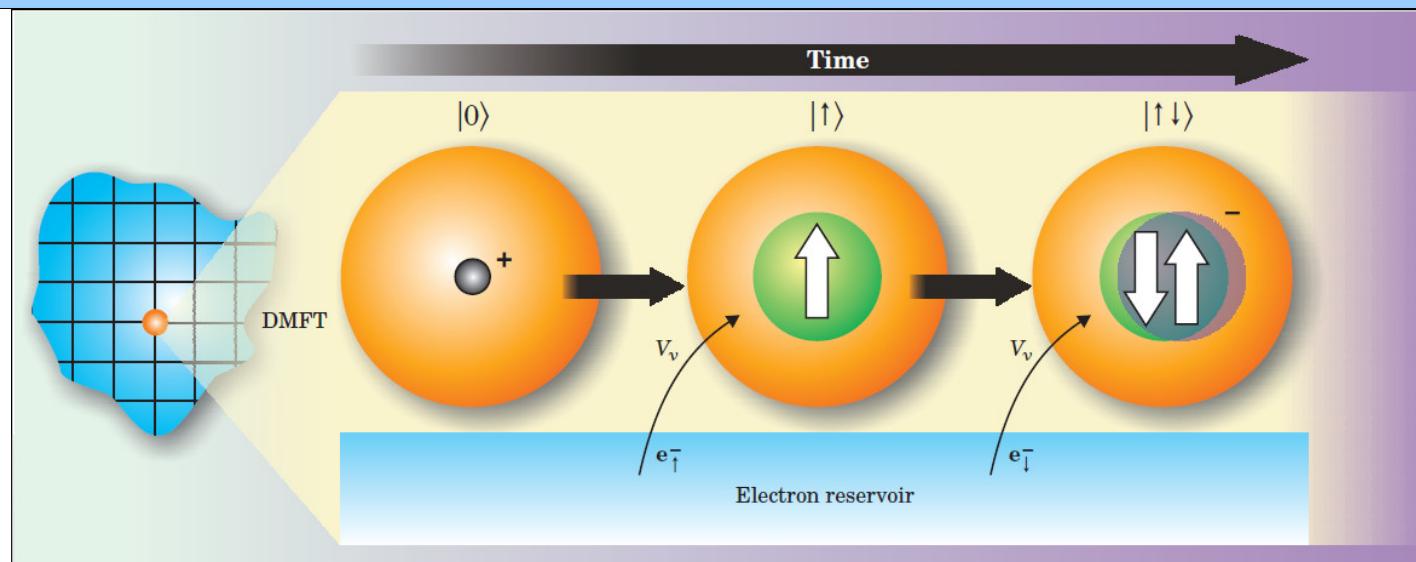
$$\Sigma(z)$$

$$G(z) = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)}{z - \epsilon + \mu - \Sigma(z)}$$



Dynamical mean field theory

- Mean field theory for quantum many body systems on a lattice.
- Maps lattice models to self-consistent impurity models
- Self energy and Vertex function become purely local and momentum independent.
- Ignores spatial fluctuations but accounts for quantum local temporal fluctuations.
- Exact in the limit of infinite dimensions.





Dynamical mean field theory

Now the fermionic case

Hubbard model

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Effective single site action

$$S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{o\sigma}^\dagger(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

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Local lattice Green's function

Impurity Self energy

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$$G(z) = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)}{z - \epsilon + \mu - \Sigma(z)}$$



Impurity solvers

- Static Mean field theories – Hartree Fock, Slave Boson/Particle theories
- Renormalization Group Based Approaches
- Numerical renormalization group, Poor Man's scaling, Functional RG, Perturbative RG, Density Matrix RG
- Diagrammatic Perturbation theory based
- Non-Crossing Approximation, FLEX, IPT, LMA
- Computational – Exact Diagonalization, Quantum Monte Carlo, Configuration Interactions



Integration with first principles DFT

Hamiltonian:

$$\hat{\mathcal{H}} = \hat{H}_{DFT}(\mathbf{k}) + \hat{H}_{int}$$

Green's functions:

$$\hat{G}_{\alpha,\beta} = \sum_{\mathbf{k}} \left([(\omega^+ + \mu) \mathbb{I} - \hat{H}_{DFT}(\mathbf{k}) - \hat{H}_{DC} - \hat{\Sigma}(\omega)]^{-1} \right)_{\alpha,\beta}$$

Occupancy constraint for μ :

$$-\frac{1}{\pi} \text{Im} \int_{-\infty}^0 \text{Tr} \hat{G} = n_{tot}^{DFT}$$



Integration with first principles DFT

- We have developed an open source package that can be used to investigate SCES.
- The package is called MO-IPT and is located at
<http://www.institute.loni.org/lasigma/package/mo-ipt/>
- (Google search: MO-IPT)
- Paper: arXiv:1504.04097.



Dasari



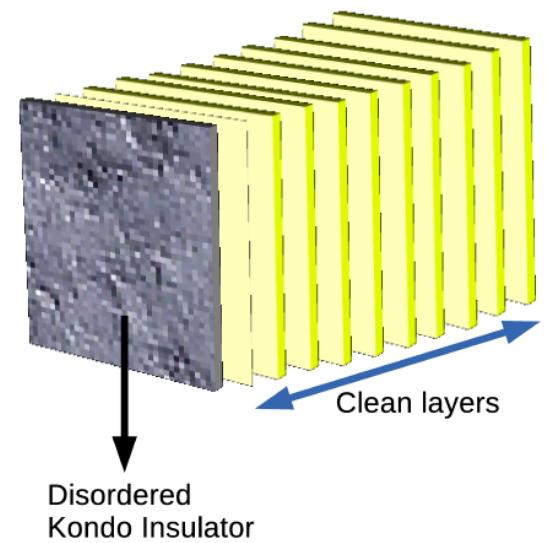
Wasim



Layer-DMFT or Inhomogeneous DMFT

Extension of DMFT to heterostructures, layered and disordered systems

$$\begin{aligned}\mathcal{H} = & - \sum_{ij\alpha\sigma} t_{i\alpha j\alpha}^{\parallel} \left(c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma} + h.c. \right) \\ & + \sum_{i\alpha\sigma} V_\alpha \left(f_{i\alpha\sigma}^\dagger c_{i\alpha\sigma} + h.c. \right) \\ & + \sum_{i\alpha\sigma} \left(\epsilon_{c\alpha} c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma} + \epsilon_{f\alpha} f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} \right) + \\ & + \sum_{\alpha} U_\alpha n_{fi\alpha\uparrow} n_{fi\alpha\downarrow} - \sum_{i\alpha\sigma} t_{\alpha\alpha+1}^{\perp} \left(c_{i\alpha\sigma}^\dagger c_{i\alpha+1\sigma} + h.c. \right)\end{aligned}$$





Layer-DMFT or Inhomogeneous DMFT

Extension of DMFT to heterostructures, layered and disordered systems

$$\hat{G}^{cc}(\omega, \mathbf{k}^{\parallel}) = \begin{pmatrix} \lambda_1 - \epsilon(\mathbf{k}^{\parallel}) & -t_{\perp} & 0 & \dots \\ -t_{\perp} & \lambda_2 - \epsilon(\mathbf{k}^{\parallel}) & -t_{\perp} & \dots \\ 0 & -t_{\perp} & \lambda_3 - \epsilon(\mathbf{k}^{\parallel}) & \dots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \lambda_N - \epsilon(\mathbf{k}^{\parallel}) \end{pmatrix}^{-1},$$

$$\lambda_{\alpha} = \omega^{+} - \epsilon_{c\alpha} - \Sigma_{c\alpha}, \quad \omega^{+} = \omega + i\delta$$

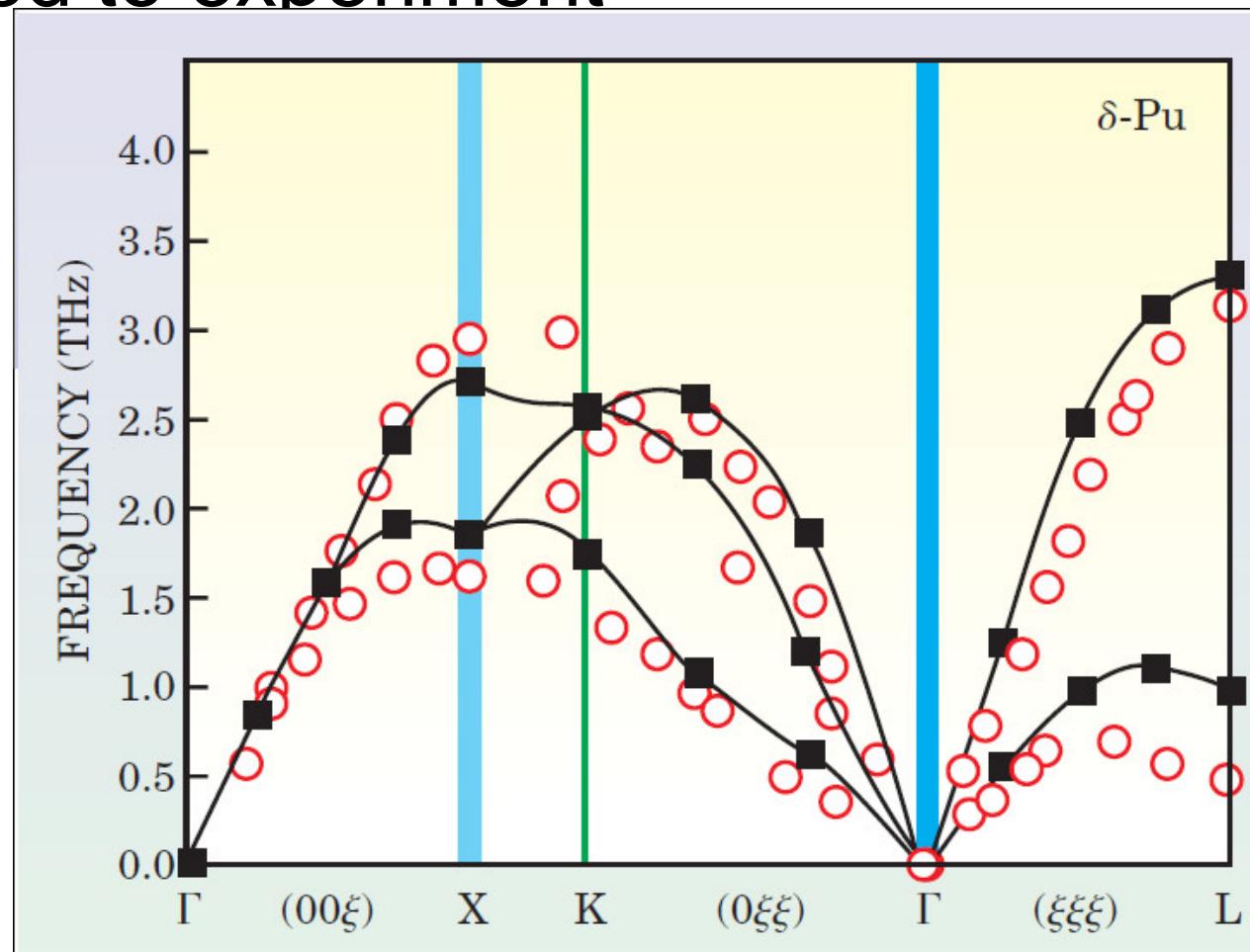


**Sudeshn
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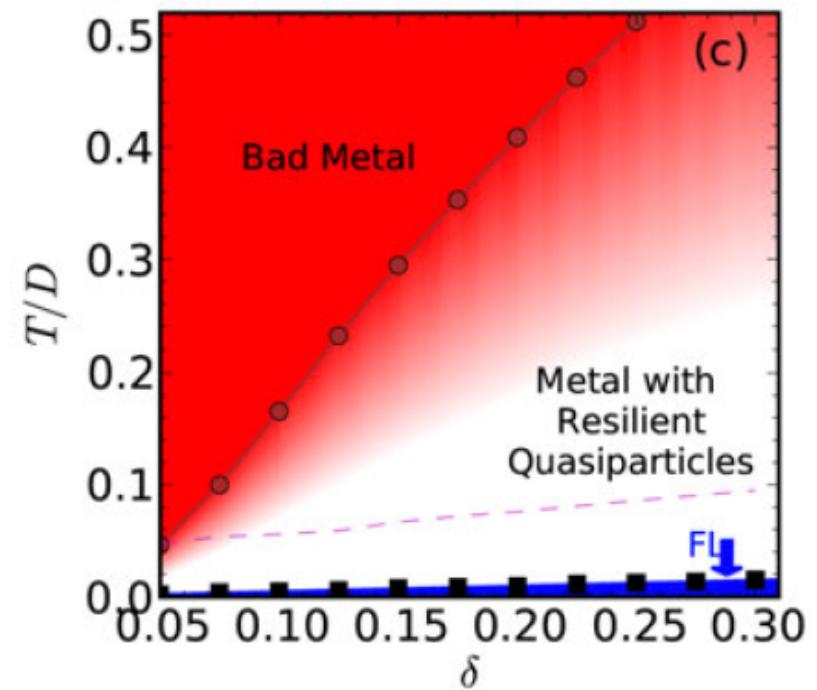
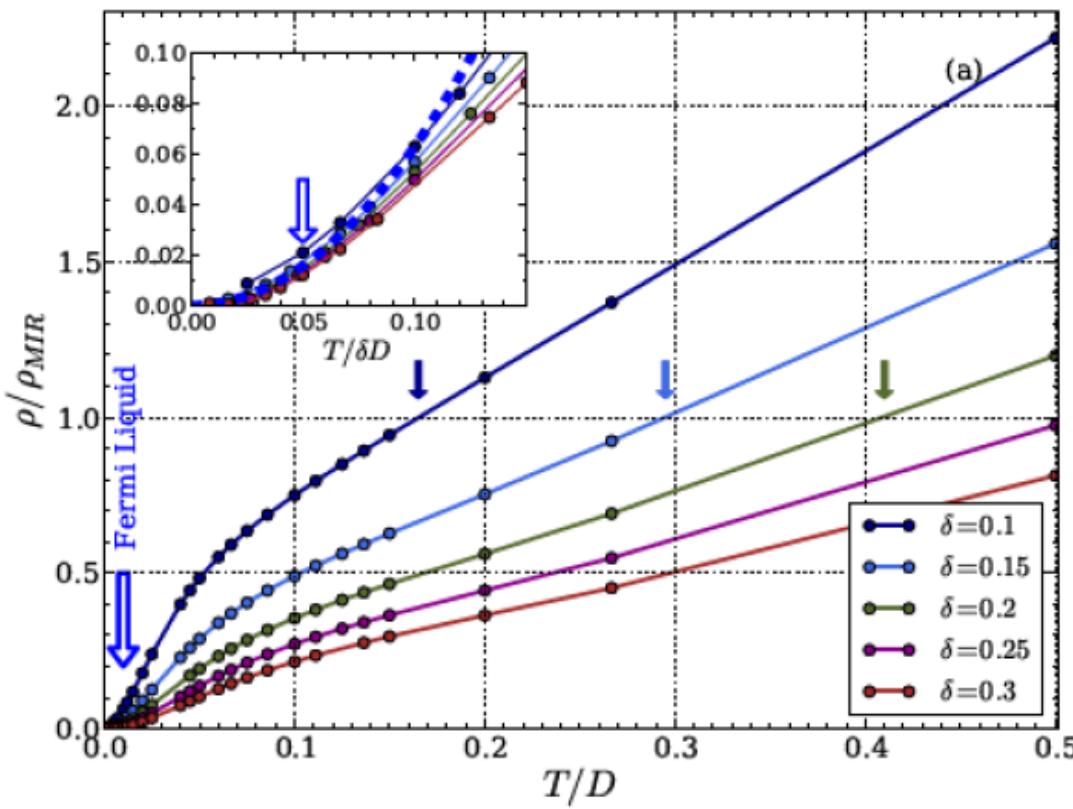
Elemental Plutonium

Phonon spectrum computed with DMFT and compared to experiment





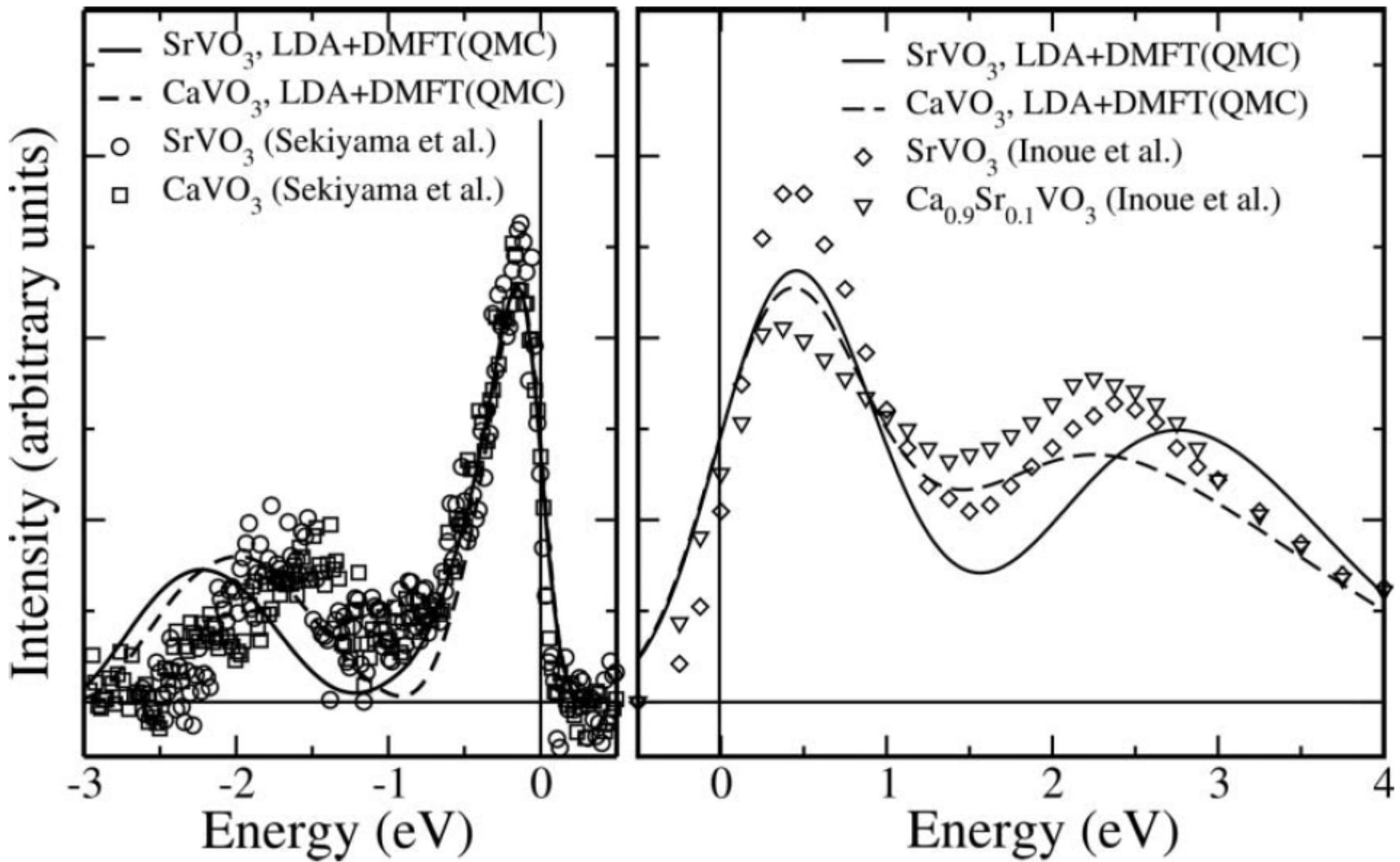
Strange-metal in Cuprates



Resistivity in the hole-doped single-band Hubbard model



SrVO₃



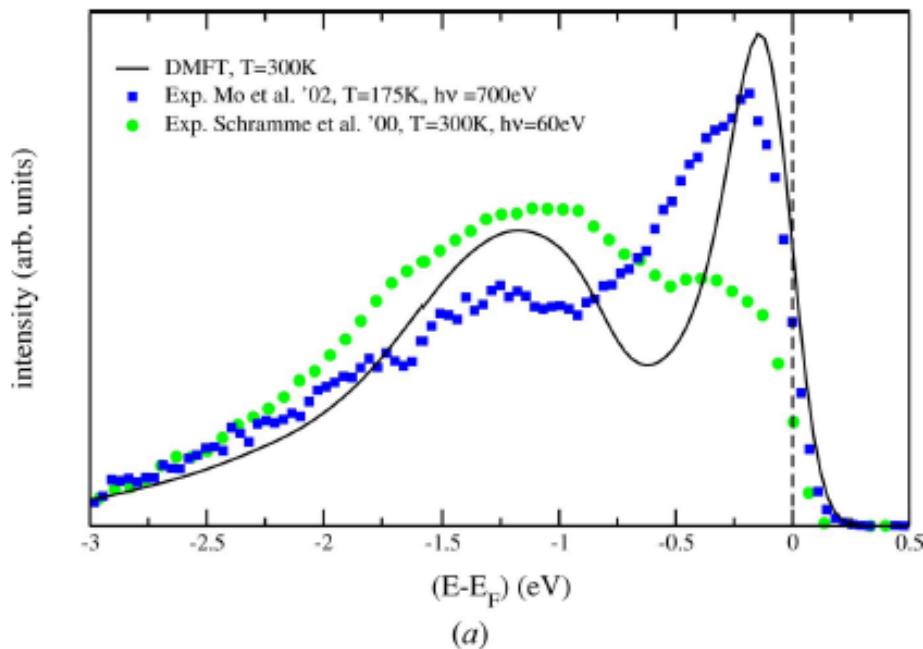
Anisimov and Lukyanov Acta Crys. Sec. C (2014)..

N.Dasari et al, arXiv:1504.04097.

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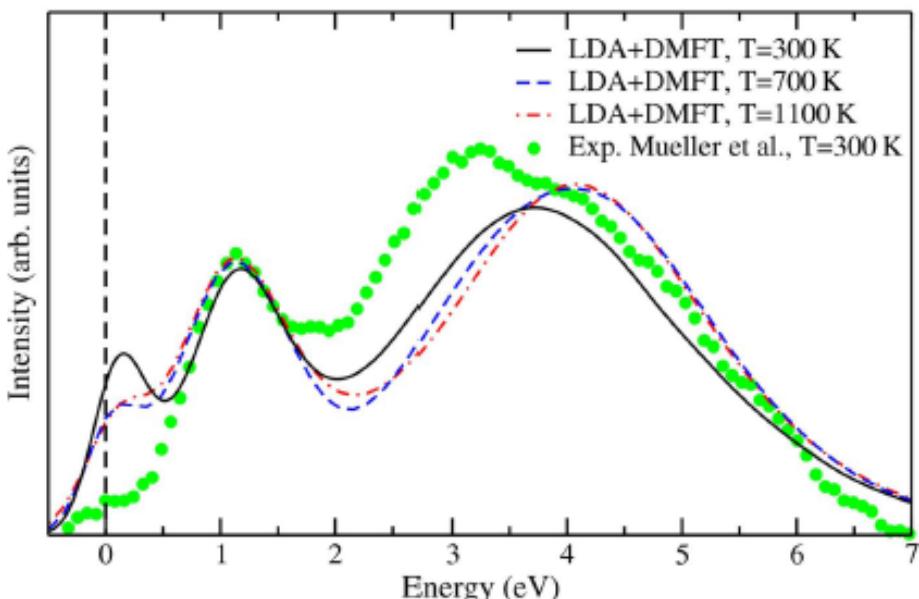


V_2O_3



(a)

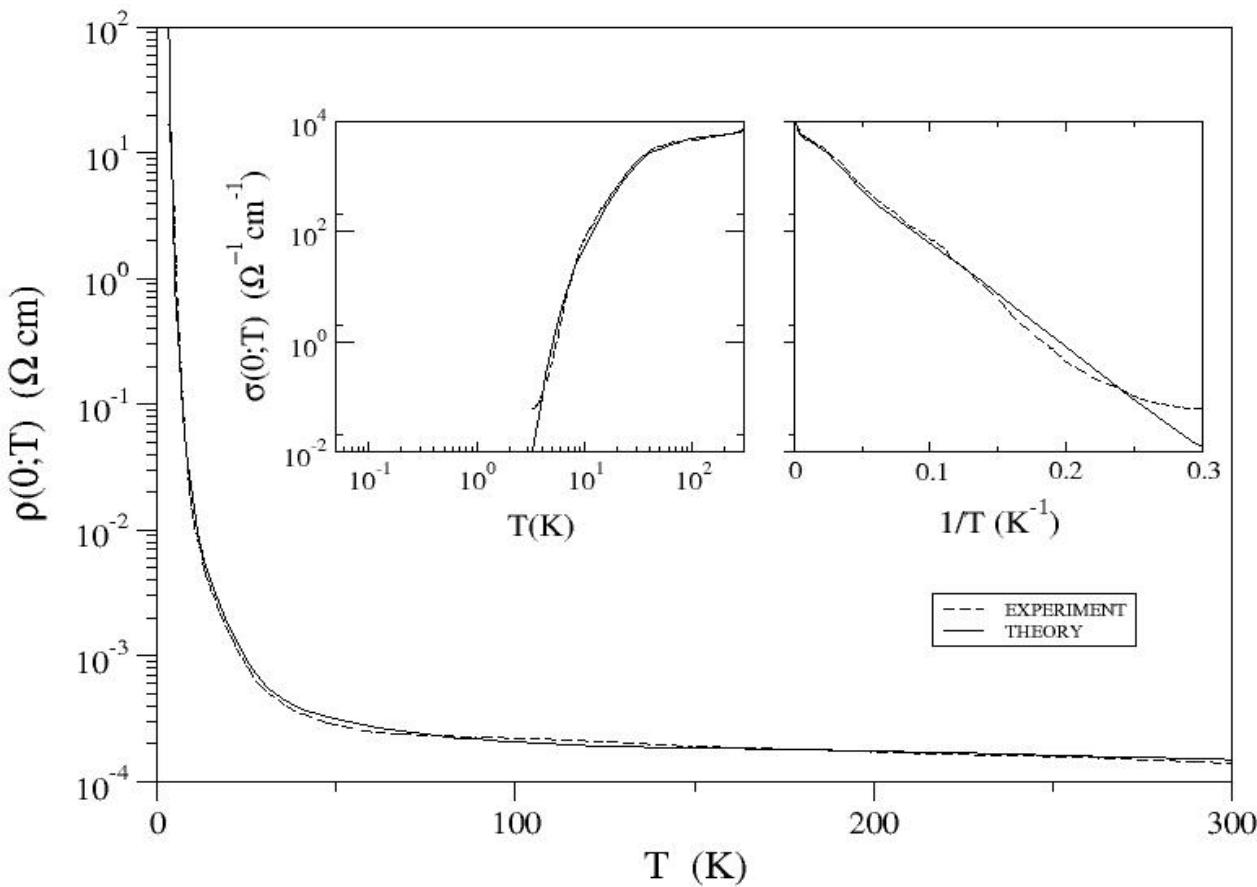
Photoemission
spectra



X-ray absorption
spectra



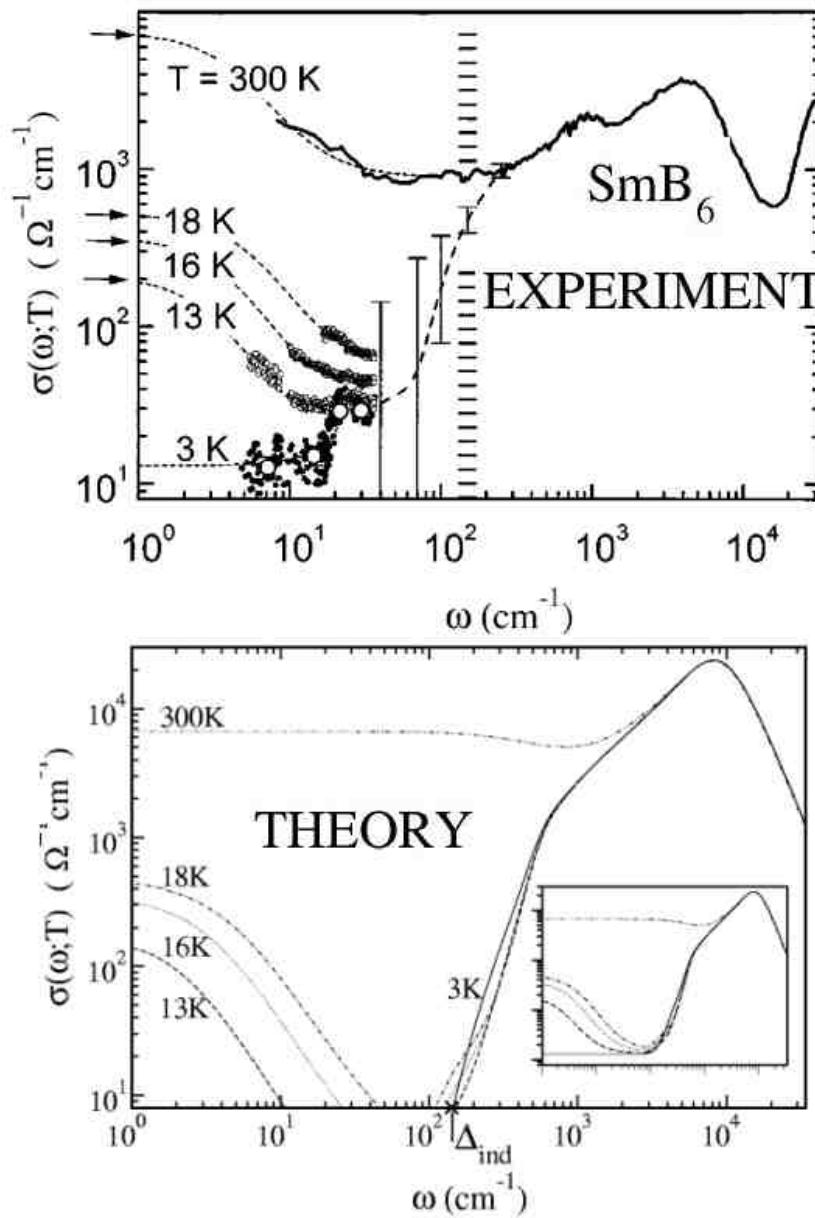
Heavy fermions



SmB_6
DC Resistivity

$$\Delta_g = 8.75 \text{ meV} = 101 \text{ K}$$

N. S. Vidhyadhiraja et al J. Phys. Condens. Matter Vol.15 pp.4045-4087 (2003).
Gorshunov et al Phys. Rev. B, Vol.59, pp.1808-1814 (1999).



SmB₆

Optical conductivity

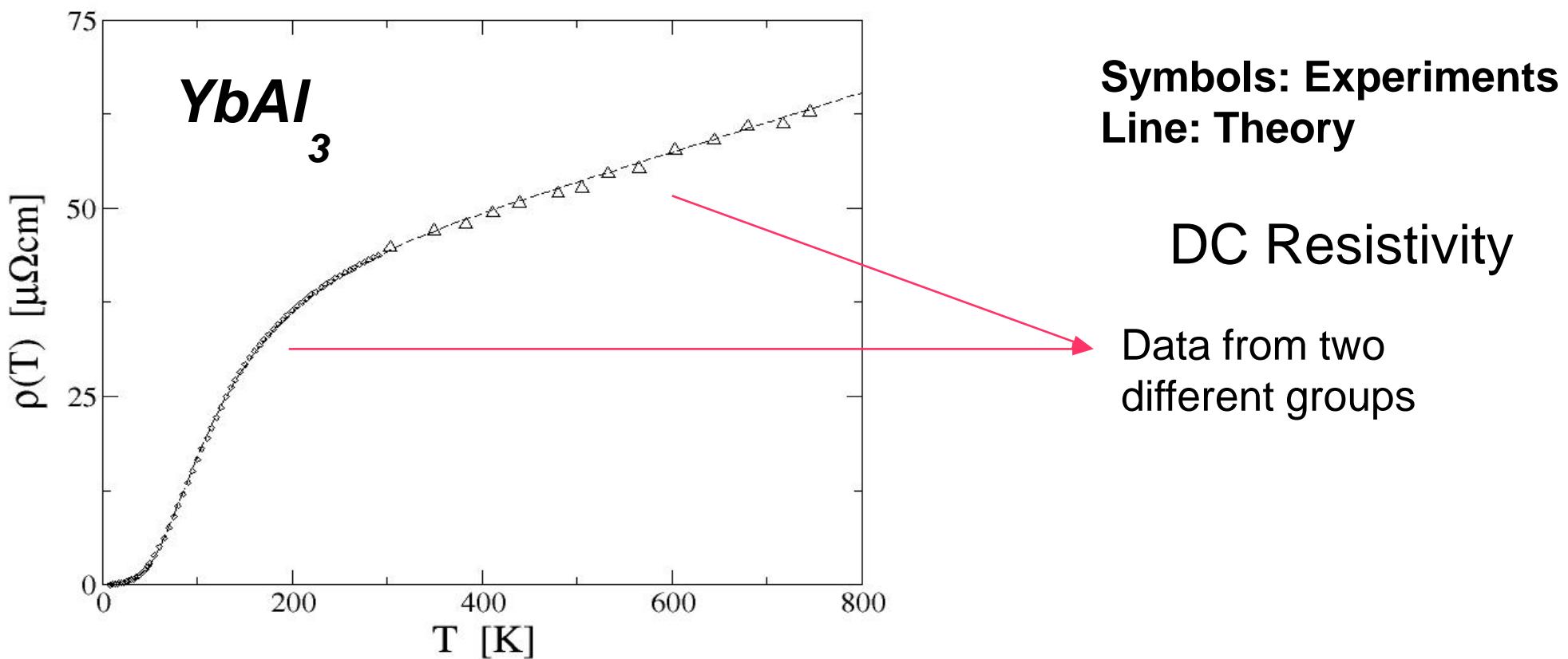
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Gorshunov et al PRB (1999);

N. S. Vidhyadhiraja et al J. Phys. Condens. Matter Vol.15 pp.4045-4087 (2003).



Heavy Fermions – Dynamical Mean Field Theory

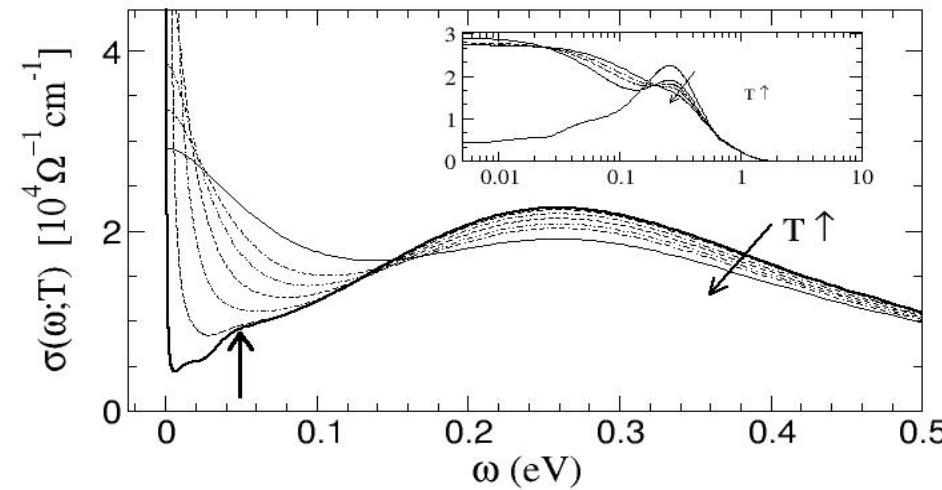


Rowe et al J. Phys. D: Appl. Phys Vol. 35 pp.2183-2186 (2002).
N.S.Vidhyadhiraja , Logan J. Phys. Condens. Matter Vol.17 pp.2959-2976 (2005);

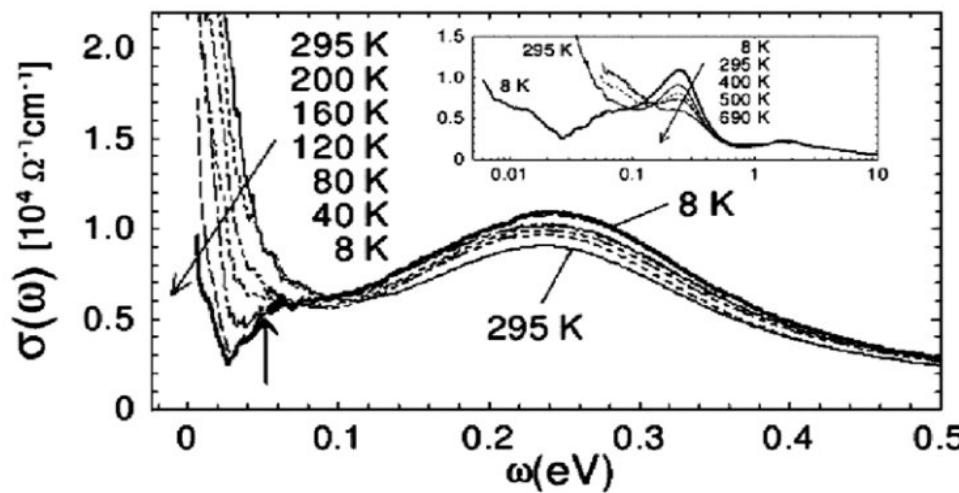


YbAl_3

Optical conductivity



Theory



Experiment

Okamura et al J. Phys. Soc. Japan Vol.73 pp.2045 (2004).
NSV , Logan J. Phys. Condens. Matter Vol.17 pp.2959-2976 (2005);



Heavy Fermions – Dynamical Mean Field Theory

**SmB_6 , YbB_{12} , $Ce_2Bi_4Pt_3$, CeB_6 , $CeAl_3$, $CeCoIn_5$,
 $YbAl_3$, $CeOs_4Sb_{12}$, $CeFeGe_3$, $CeRhSi_2$, $Ce_2Ni_3Si_5$
 $Ce_{1-x}La_xB_6$, $Ce_{1-x}La_xAl_3$**

***Spectral Dynamics, DC and Optical transport,
Thermodynamics, Magnetotransport***



Dynamical Cluster approaches

Map the lattice onto a cluster embedded in a self-consistent medium

$$\begin{aligned}\Delta(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &= \sum_{\mathbf{r}} \exp [i\mathbf{r} \cdot (\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)] \\ &= N\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4},\end{aligned}$$

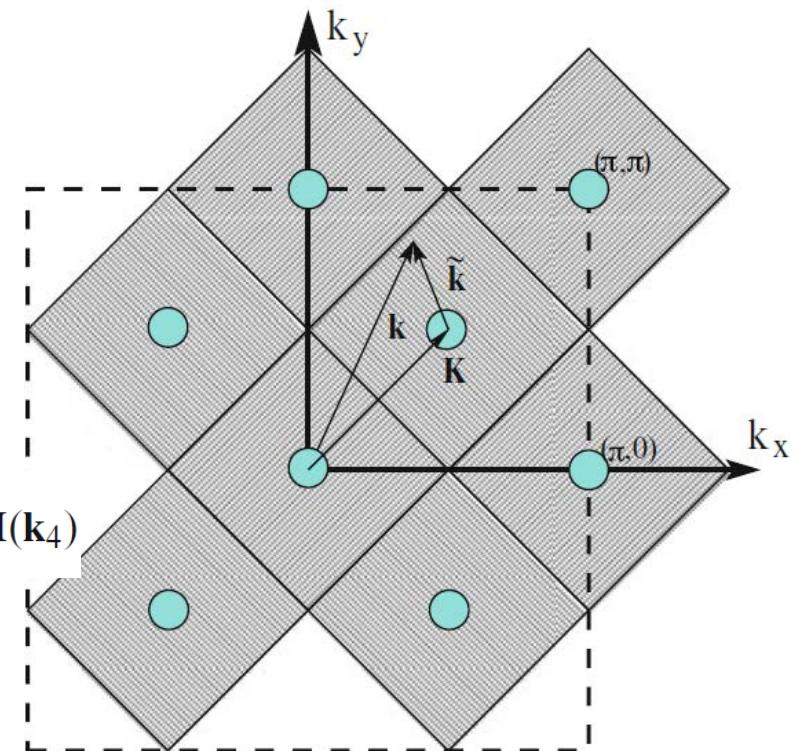
Momentum conservation is replaced by

$$\Delta_{D \rightarrow \infty}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = 1 + \mathcal{O}(1/D).$$

In DMFT and

$$\Delta_{\text{DCA}}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = N_c \delta_{\mathbf{M}(\mathbf{k}_1)+\mathbf{M}(\mathbf{k}_2), \mathbf{M}(\mathbf{k}_3)+\mathbf{M}(\mathbf{k}_4)}$$

In dynamical cluster approximation.





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- Students: D.Parihari, Himadri Barman, Naushad Kamar, Pramod Kumar, N. Dasari, Wasim Mondal, Sudeshna Sen, Rukhsan-ul-Haq, Swagata Acharya.
- Special thanks to Erica Carlson for hosting me.
- Funding: DST India, NSF, APS-IUSSTF.