The Abdus Salam International Centre for Theoretical Physics

2157-16

Workshop on Principles and Design of Strongly Correlated Electronic Systems

2 - 13 August 2010

Defects, Density of States and Differential Conductance in Heavy-Fermion Systems

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Defects, Density of States and Differential Conductance in Heavy-Fermion Materials

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Principles and Design of Strongly Correlated Electron Systems
ICTP Trieste, 5 August 2010

Collaborators:

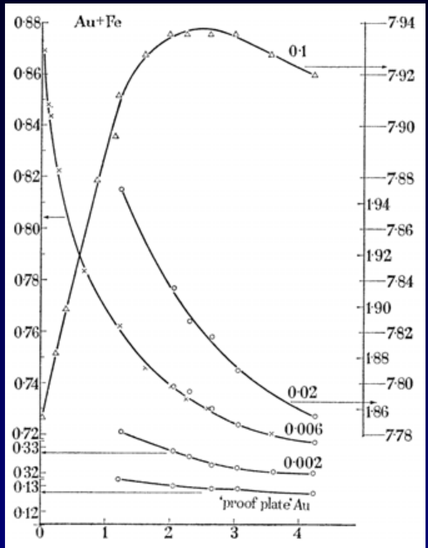
Theory: • J. Figgins (UIC)

Experiment:
- H. Manoharan (Stanford)
- J.C. Davis (Cornell)

J. Figgins and D.K.M.:
1) PRL **104**, 187202 (2010);
2) arXiv:1001.3875

The puzzle: a resistance minimum in metals

ρ [$\mu\Omega$cm]



T [K]

MacDonald *et al.,* Proc. Roy. Soc. **266**, 161 (1962)

resistance minimum due scattering of electrons by magnetic impurities

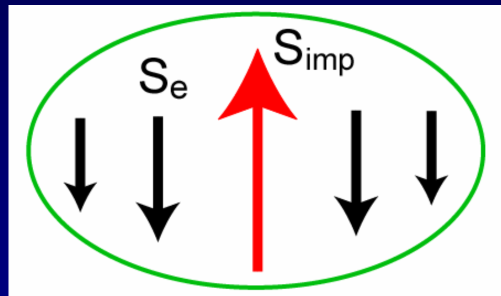
screening of the impurity spin below

$$T_K = De^{-1/JN_0}$$

J. Kondo: Prog. Theor. Phys. **32,** 37 (1964)

Kondo Hamiltonian

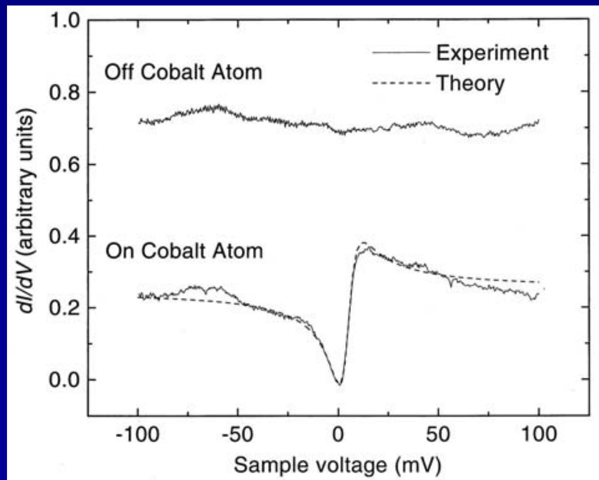
$$H_K = J\,\mathbf{S}_{imp}\cdot\mathbf{s}_e$$



$S_{tot} = 0$

spectroscopic signature: Kondo resonance in dI/dV

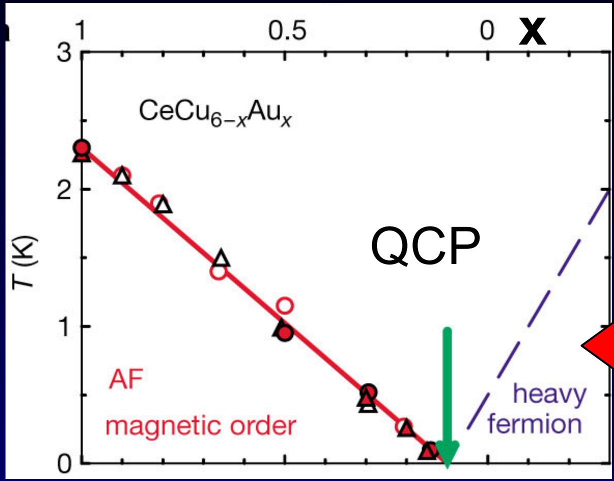
V. Madhavan *et al*, Science **280**, 567 (1998)



Renormalization Group
K.G. Wilson
RMP 47, 773 (1975)

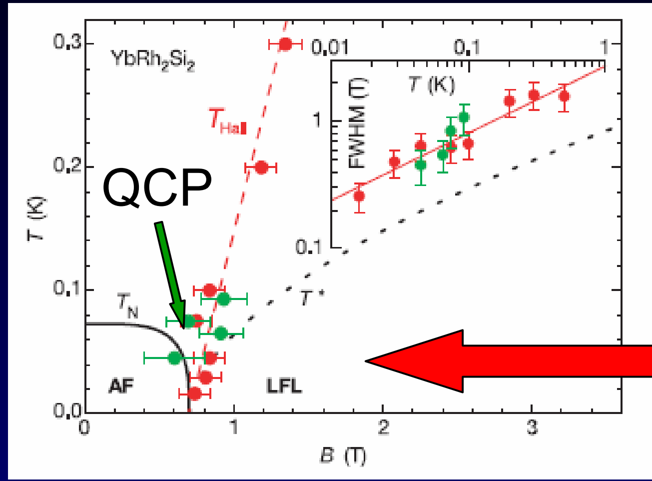
Large-N expansion
Read and Newns
J. Phys. C **16**, 3273 (1983)

The Conundrum of Heavy-Fermion Materials



Kondo lattice

Schroeder *et al.*, Nature **407**, 351 (2000)



Kondo lattice

Paschen *et al.*, Nature **432**, 811 (2004)

Non-Fermi-liquid properties at the quantum critical point

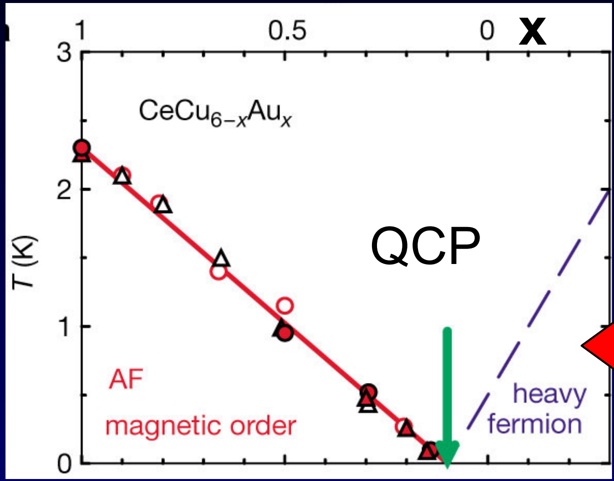
FL: $\Delta\rho \sim T^2$, $\gamma = C/T = const.$

NFL: $\Delta\rho \sim T^n \quad n < 2$, $\gamma \sim \ln(T_0/T)$

Origin: quantum critical behavior, competition between AFM ordering and the Kondo screened phase, ….???

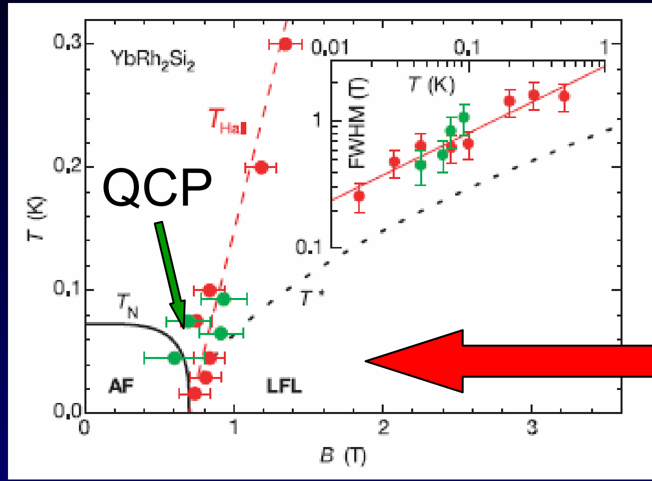
Coleman, Fulde, Kotliar, Norman, Pepin, Sachdev, Schofield, Senthil, Si, Vojta,….

The Conundrum of Heavy-Fermion Materials



Kondo lattice

Schroeder *et al*., Nature **407**, 351 (2000)



Kondo lattice

Paschen *et al*., Nature **432**, 811 (2004)

required:

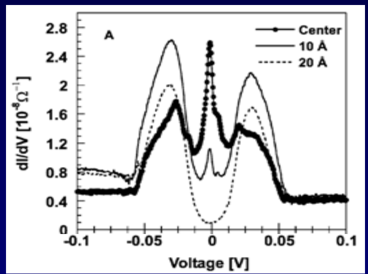
detailed insight into the complex electronic and magnetic structure of heavy-fermion materials

defects as microscopic probes

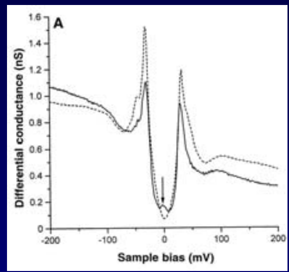
Defects as Microscopic Probes in the Cuprates

- unconventional SC symmetry

defects induce resonant states
Salkola *et al.*, PRL 77, 1841 (1996)

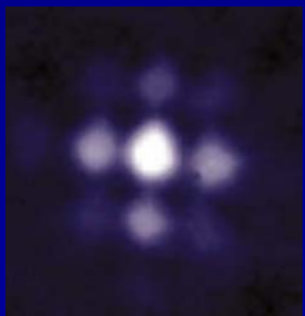


A.Yazdani et al.,
PRL 83, 176 (1999)



Hudson et al.
Science **285**, 88 (1999)

- SC gap structure



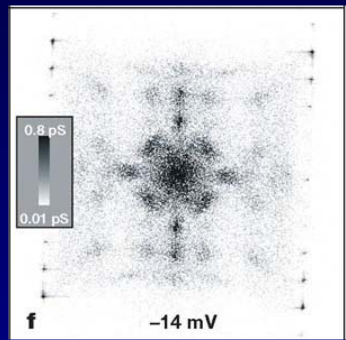
probing
line nodes

Hudson et al.
Nature **411**,
920 (2001)

- SC gap structure & Fermi surface

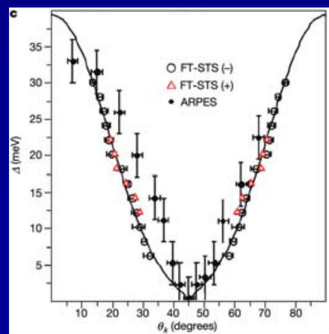
quasi-particle interference

Wang and Lee, PRB **67**, 020511(R) (2003)
Capriotti et al., PRB **68**, 014508 (2003)

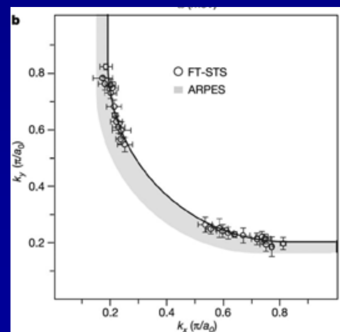


FT-LDOS

McElroy *et al.*,
Nature **422**,
592 (2003)



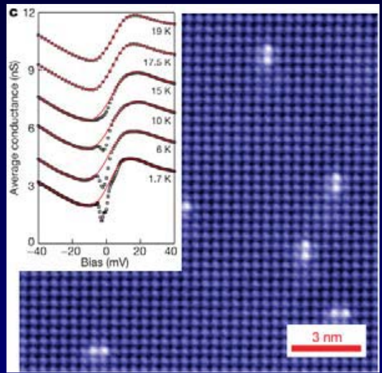
SC gap structure



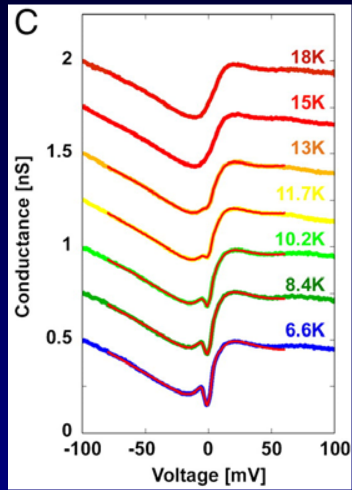
Fermi surface

Defects: Unveiling Strong Correlations in Heavy-Fermion Materials

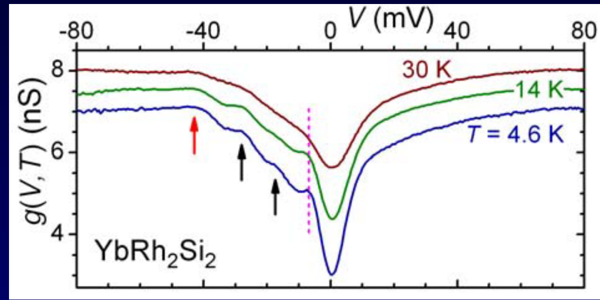
first STM experiments on heavy-fermions: URu_2Si_2 and $YbRh_2Si_2$



Schmidt *et al.*
Nature **465**, 570 (2010)

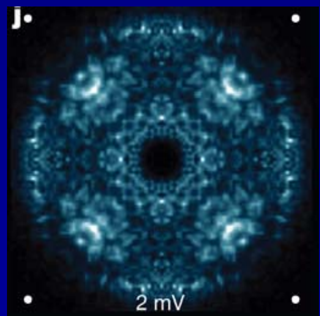


Aynajian et al.
PNAS **107**,
10383 (2010)



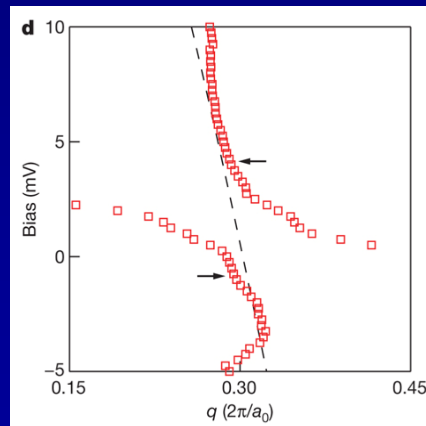
Wirth *et al.,* unpublished

FT-LDOS



Schmidt *et al.*
Nature **465**, 570-576 (2010)

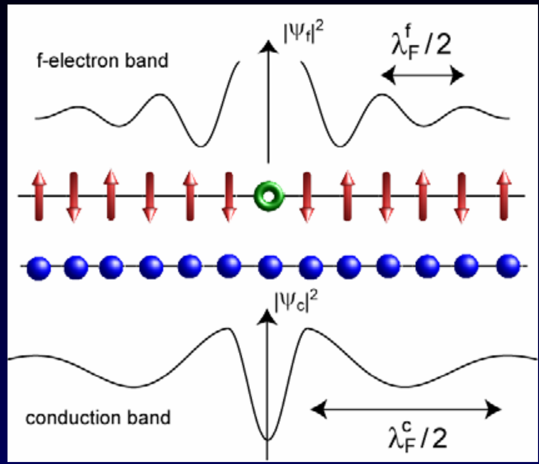
first QPI analysis
in heavy-fermions



bandstructure

Questions:

- can defects provide insight into the complex structure of heavy-fermions?
- do defects discriminate between electronic and magnetic correlations?



defects are created by ⇒

- removing a magnetic atom (Kondo hole)
- replacing a magnetic atom by a non-magnetic one

How does one describe the removal of a correlated magnetic atom?

First attempts:

R. Sollie and P. Schlottmann, J. Appl. Phys. 69, 5478 (1991)
R. Freytag and J. Keller, Z. Phys. B **80**, 241 (1990)

Recently:

R.K. Kaul and M. Vojta, Phys. Rev. B **75**, 132407 (2007)

Defects in Heavy Fermion Materials

J. Figgins, D.K.M., arXiv:1001.3875

$$H = -\sum_{i,j,\sigma} t_{ij} c^{+}_{i,\sigma} c_{j,\sigma}$$ conduction electrons

$$+ J \sum_{i} \mathbf{S}_{imp}(\mathbf{R}_i) \cdot \mathbf{s}_e(\mathbf{R}_i)$$ Kondo coupling

$$+ I \sum_{i,j} \mathbf{S}_{imp}(\mathbf{R}_i) \cdot \mathbf{S}_{imp}(\mathbf{R}_j)$$ magnetic interaction

$$+ U_0 \, n_c(\mathbf{R}_0)$$ non-magnetic impurity

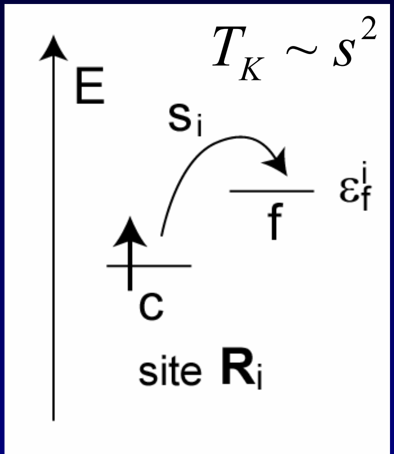
SU(N) spin representation via fermions

$$\mathbf{S}_{imp} = \sum_{\alpha,\beta} f^{+}_{\alpha} \, \mathbf{\Gamma}_{\alpha\beta} \, f_{\beta} \qquad \mathbf{s}_e = \sum_{\alpha,\beta} c^{+}_{\alpha} \, \mathbf{\Gamma}_{\alpha\beta} \, c_{\beta}$$

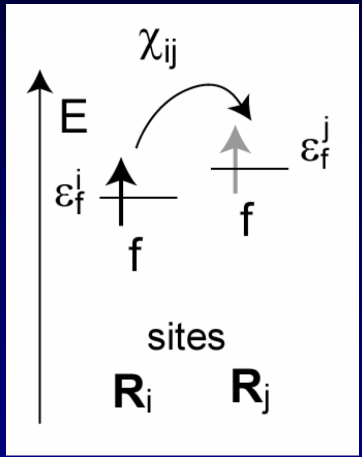
⇒ large-N expansion

decoupling of the Hamiltonian via (non-) local mean-fields

hybridization
electronic correlations

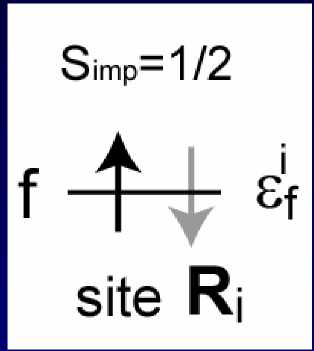


magnetic bond variable
magnetic correlations



local constraint

$$n_f = 1$$



valence fluctuations
are forbidden

We can now study a variety of systems:

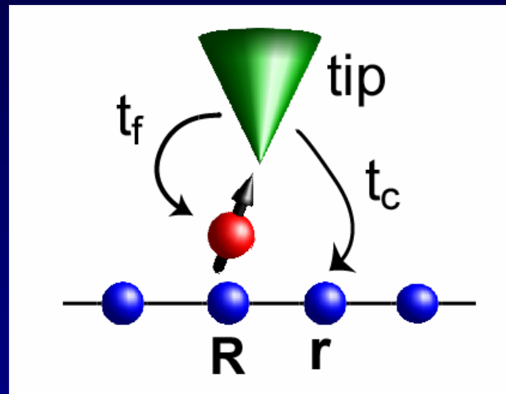
- defects in Kondo lattices
- disordered Kondo lattices
- Kondo systems with different magnetic atoms
- effects of dissipation
- Kondo droplets

What do STM experiments measure in Heavy-Fermion Materials?

J. Figgins and D.K.M., PRL **104**, 187202 (2010)

Let us first consider a single magnetic (Kondo) atom

U. Fano, PR **124**, 1866 (1961).
V. Madhavan *et al*., Science **280**, 567 (1998).
J. Li, *et al*., PRL **80**, 2893 (1998).
O. Ujsaghy *et al*., PRL **85**, 2557 (2000).
N. Knorr *et al.,* PRL **88**, 096804 (2002).
V. Madhavan *et al.,* PRB **64**, 165412 (2001).
A. A. Aligia and A.M.Lobos, J.PCM **17**, S1095 (2005).

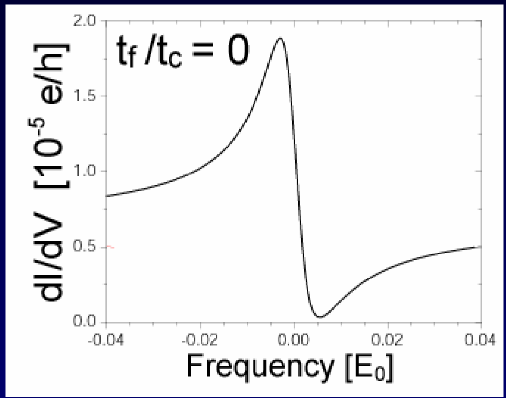


two tunneling paths → quantum interference

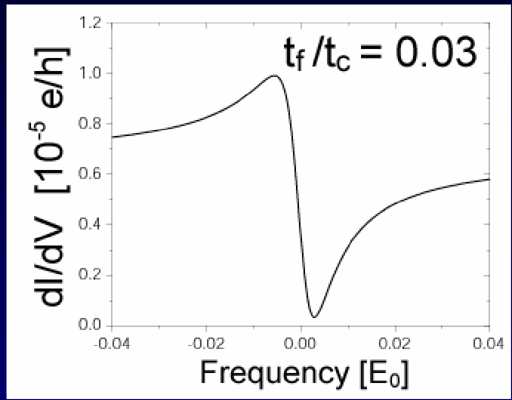
$$\frac{dI}{dV} = \frac{2\pi e}{\hbar} N_t \left[t_c^2 N_c(r,V) + t_f^2 N_f(R,V) + 2 t_c t_f N_{cf}(r,R,V) \right]$$

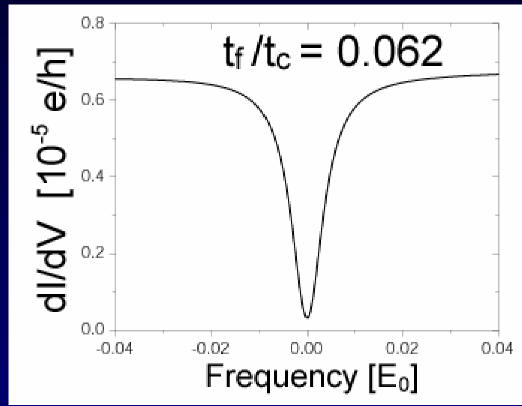
quantum interference

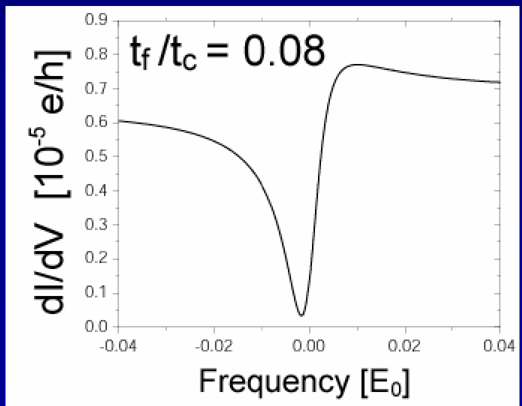
How does Quantum Interference determine the dI/dV-Lineshape?



~ conduction LDOS

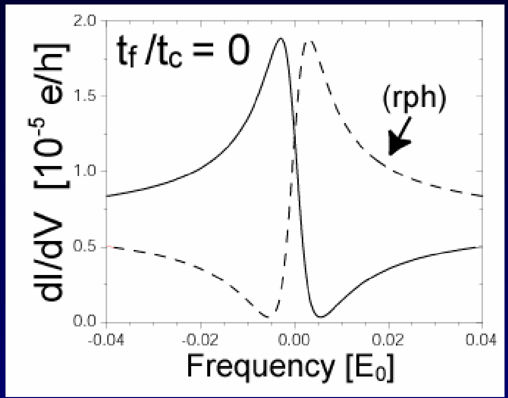




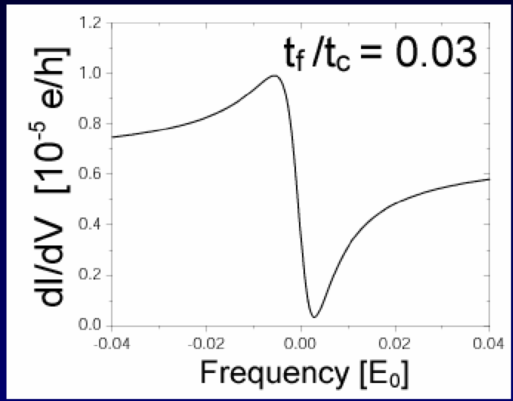


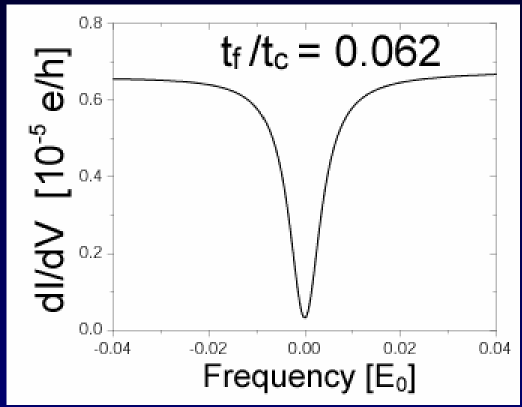
quantum interference effects are crucial in understanding the asymmetry of dI/dV

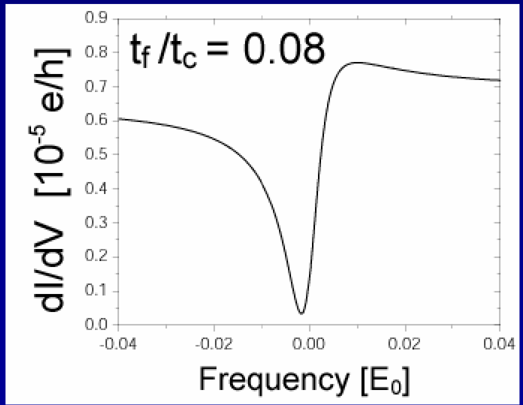
How does Quantum Interference determine the dI/dV-Lineshape?



~ conduction LDOS





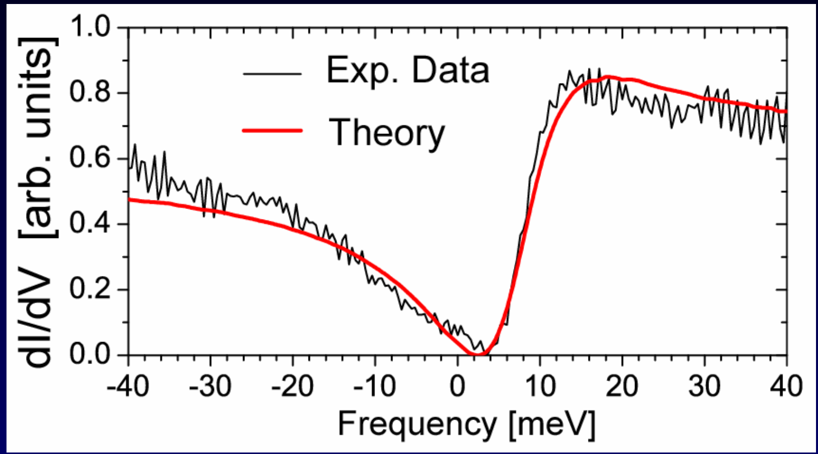


quantum interference effects are crucial in understanding the asymmetry of dI/dV

…as well as the bandstructure

Microscopic explanation of the experimental STM data

V. Madhavan, *et al.*, PRB **64**, 165412 (2001)



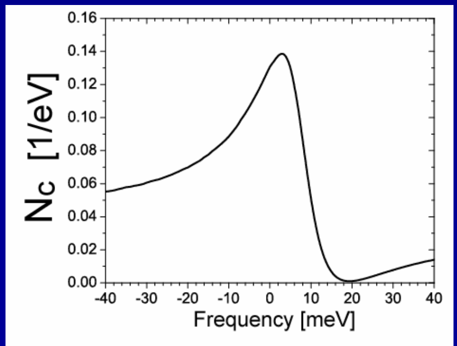
Co on Au(111)

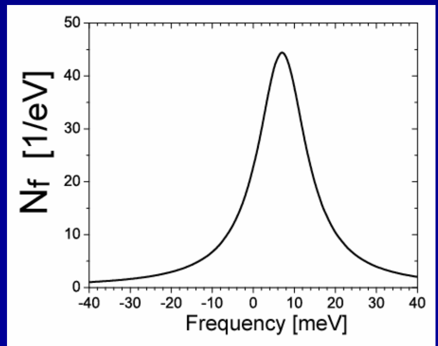
Kondo coupling $J=1.39$ eV

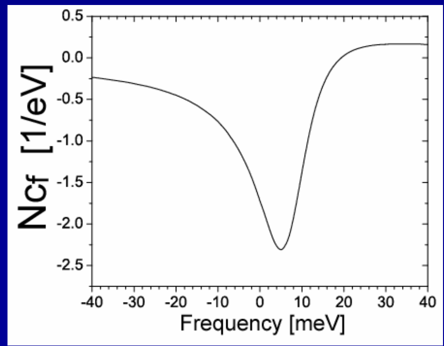
tunneling amplitudes $t_f / t_c = 0.066$

spin $S_{Co}=3/2$

electronic and magnetic structure/correlations







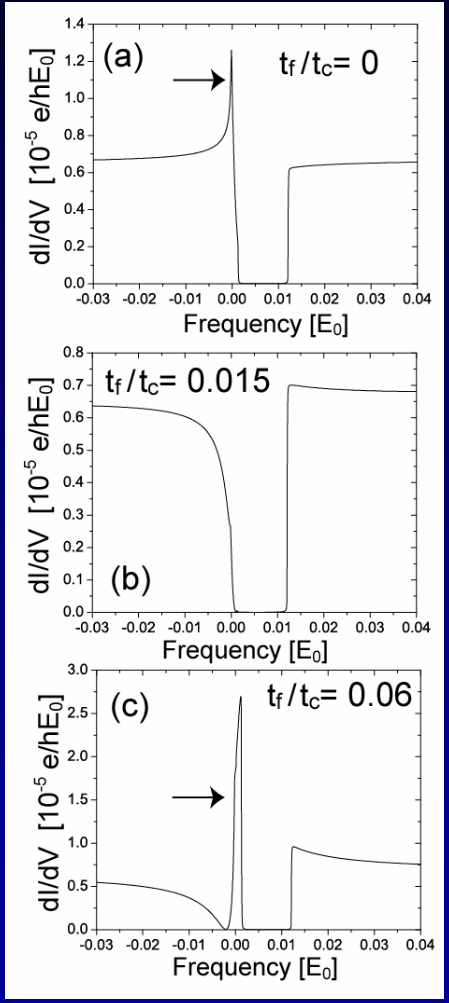
dI/dV in Heavy-Fermion Materials

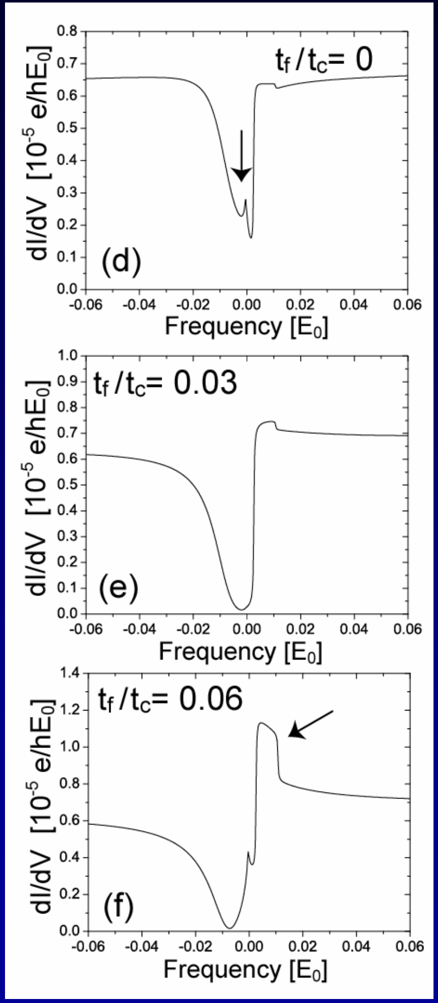
J. Figgins, D.K.M.
PRL **104**, 187202 (2010)

M. Maltseva et al.,
PRL **103**, 206402 (2009)

magnetic interactions significantly affect the form of the differential conductance

insight into the strength of magnetic correlations





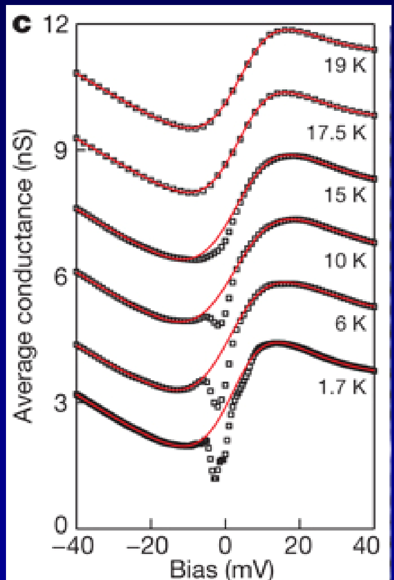
weak magnetic coupling
I/J=0.001

strong magnetic coupling
I/J=0.015

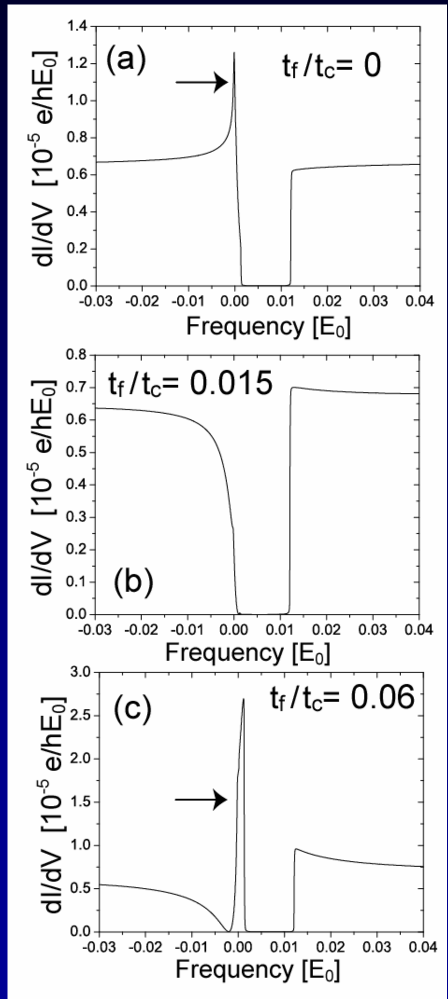
dI/dV in Heavy-Fermion Materials

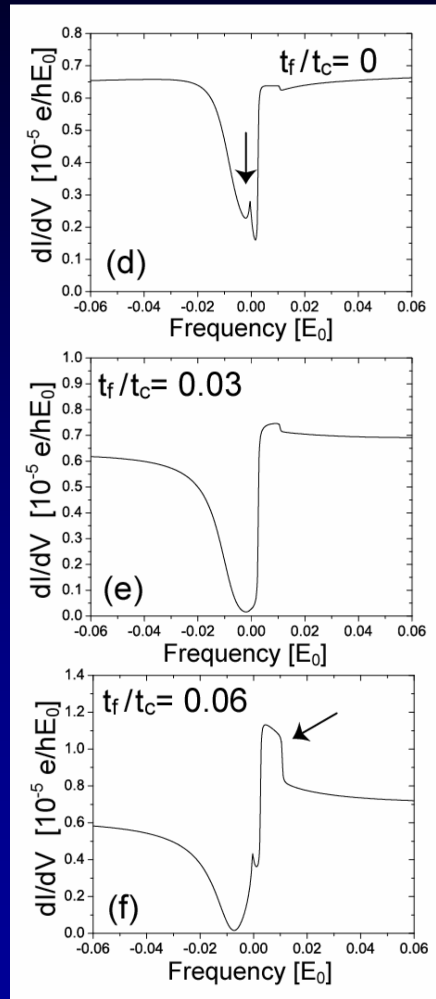
J. Figgins, D.K.M.
PRL **104**, 187202 (2010)

M. Maltseva et al.,
PRL **103**, 206402 (2009)



Schmidt *et al.*
Nature **465**, 570 (2010)

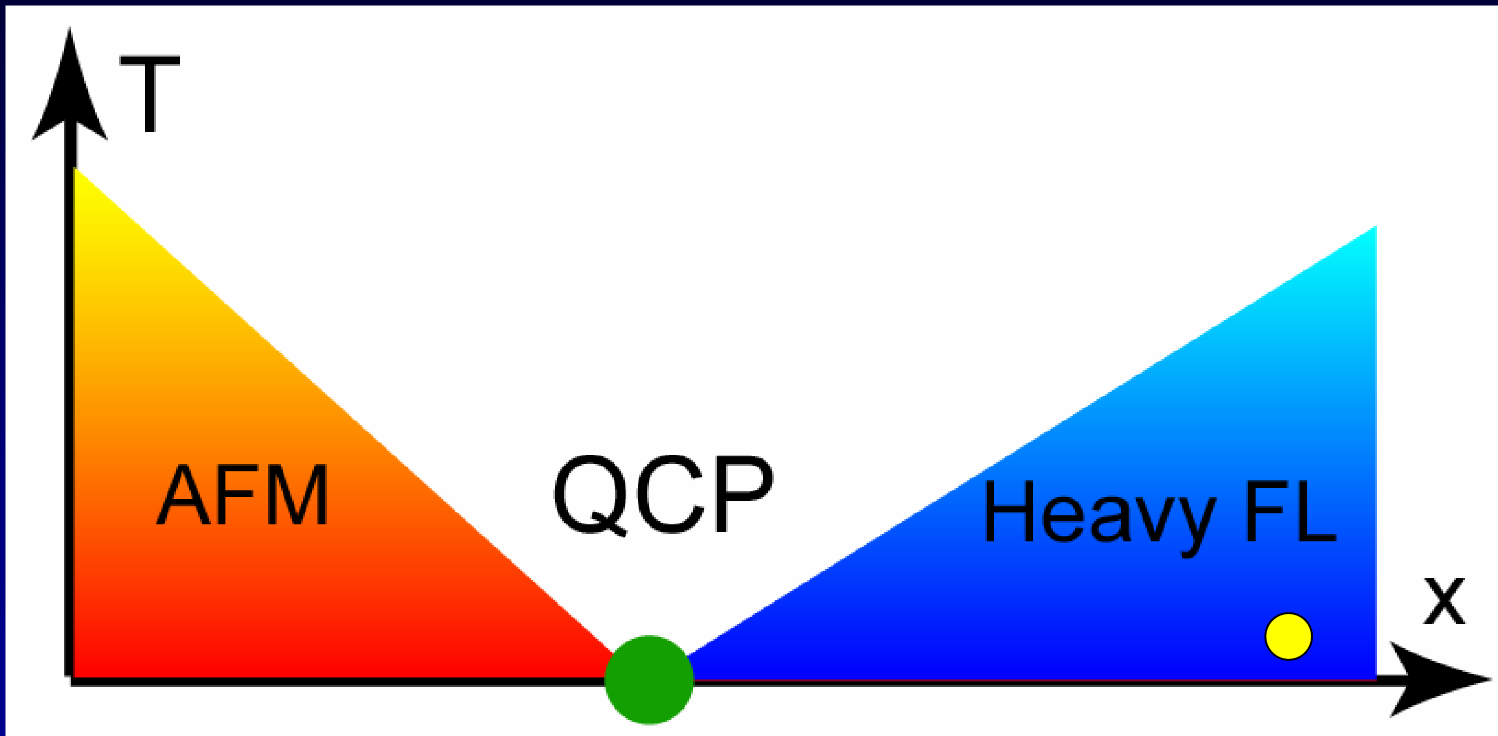




weak magnetic coupling
I/J=0.001

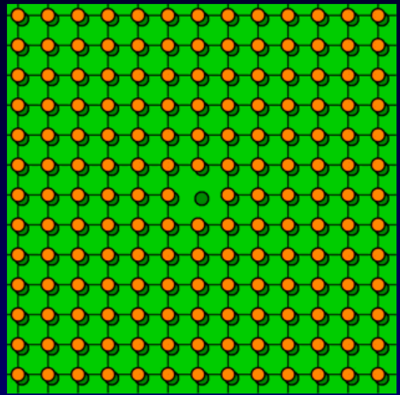
strong magnetic coupling
I/J=0.015

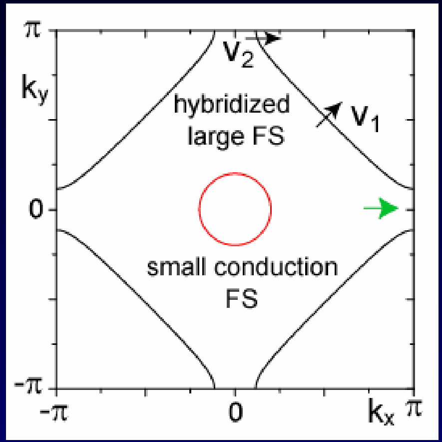
Defects in Heavy Fermion Systems



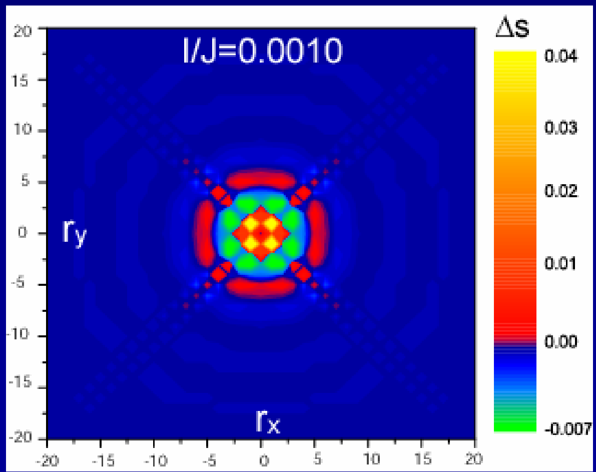
The Kondo Hole in the Kondo Lattice

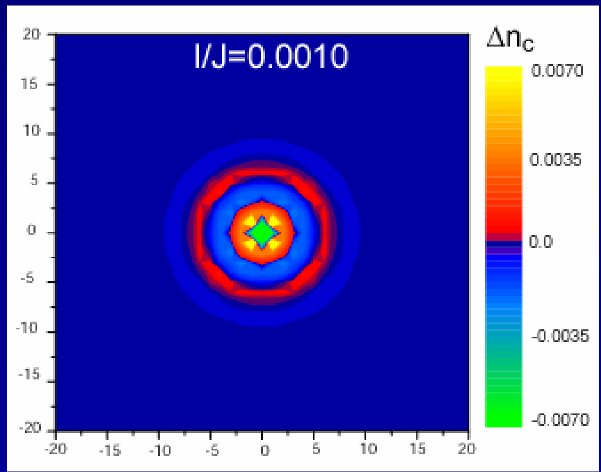
J.Figgins, and D.K.M., arXiv:1001.3875





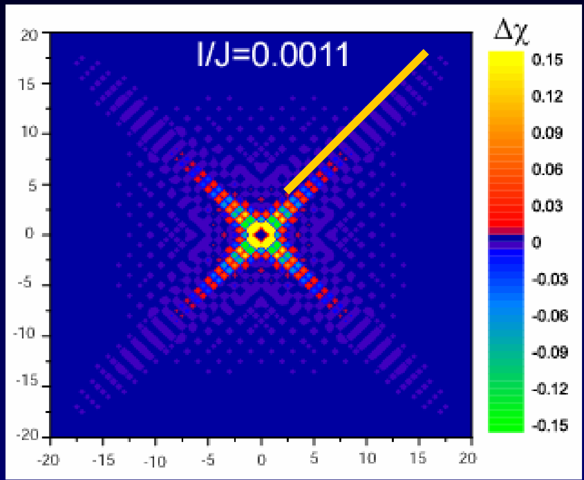
perturbations in the electronic correlations

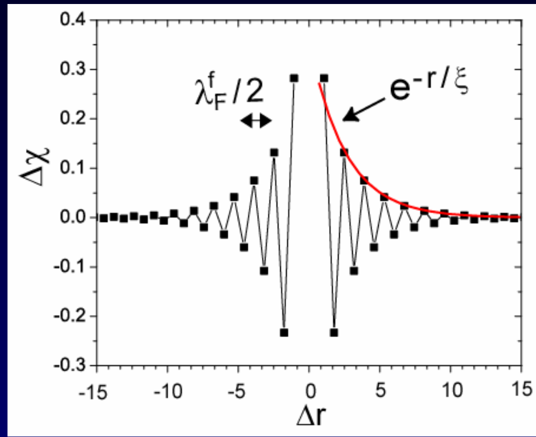


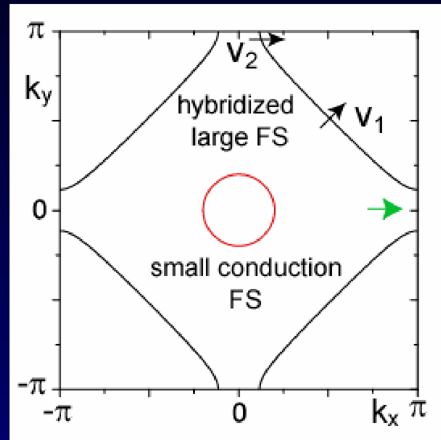


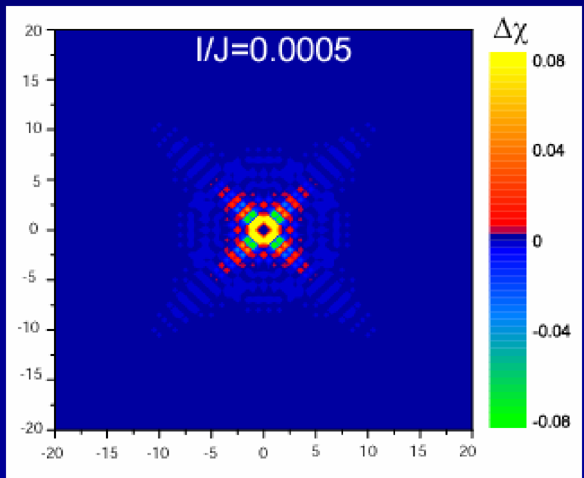
screening increases the local conduction electron density

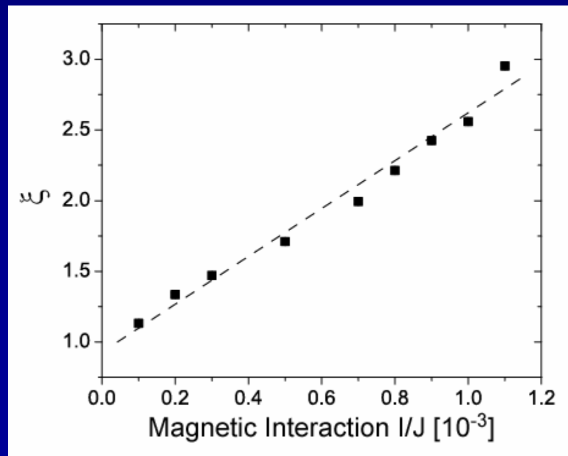
perturbations in the magnetic correlations





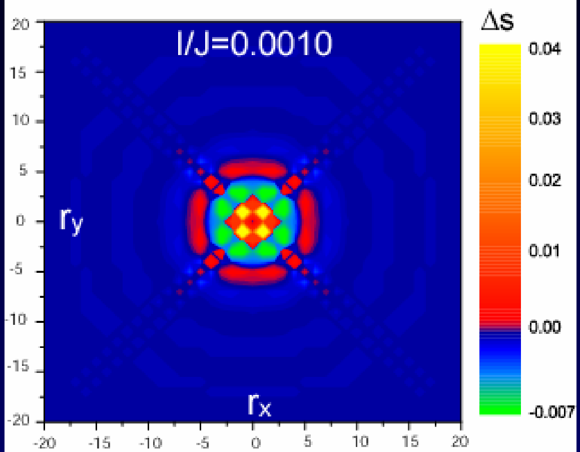


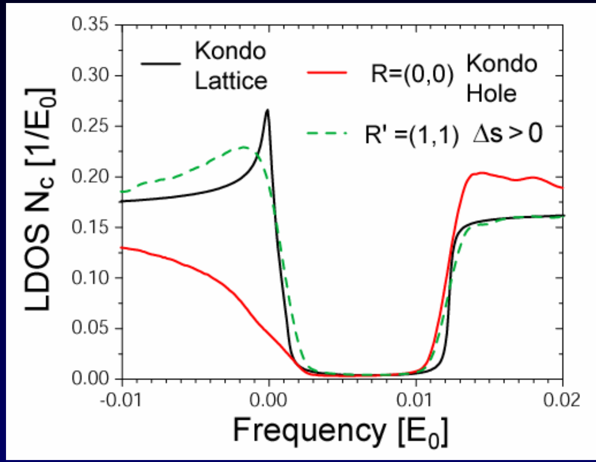




perturbations grow in real space with increasing magnetic interactions

Spectroscopic Signatures

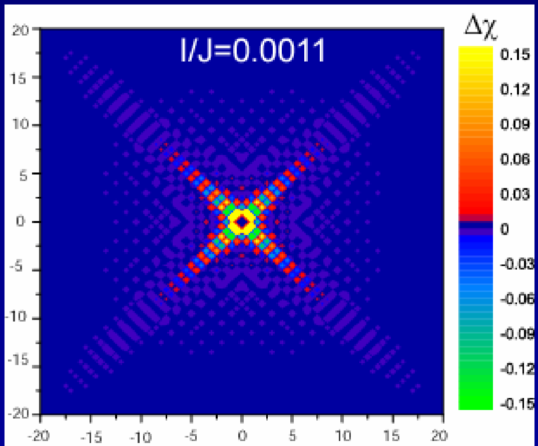


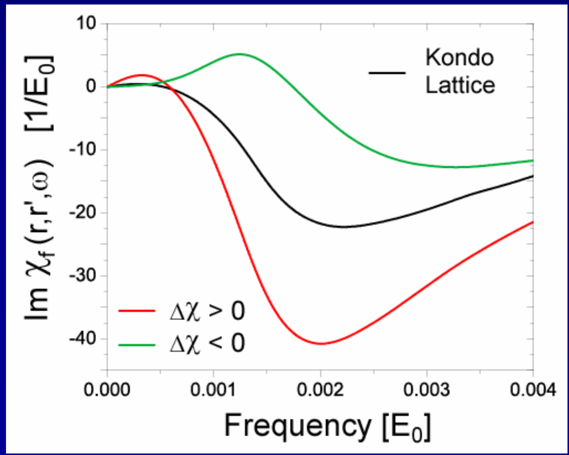


at T=0

$$n_c(r) = \int_{-\infty}^{0} d\omega \, N_c(r,\omega)$$

LDOS reflects the spatial form of electronic correlations





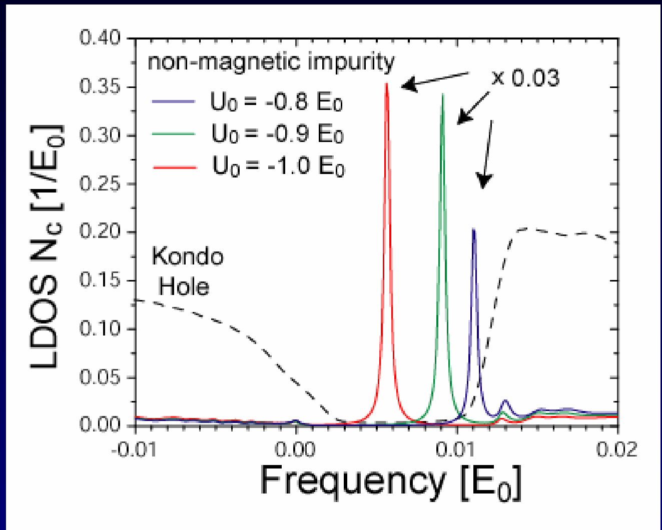
magnetic resonance force microscopy:

D. Rugar

P.C. Hammel

spin susceptibility reflects the spatial magnetic correlations

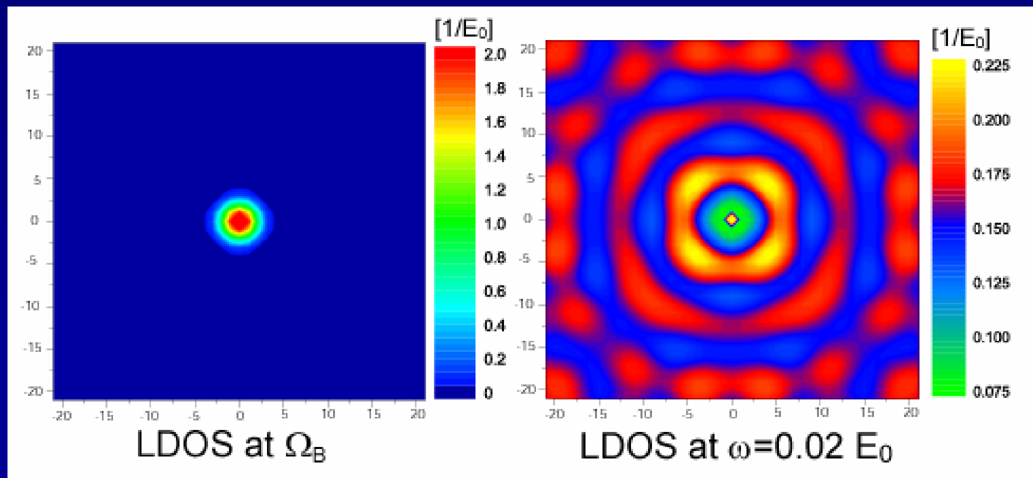
Effects of Non-Magnetic Impurities



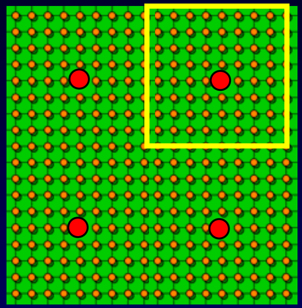
non-magnetic impurities can induce states inside the hybridization gap

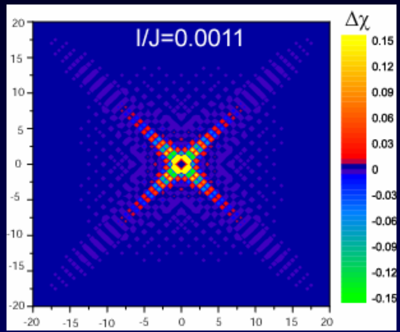
if $U_0 < 0$ and $|U_0| > U_c$

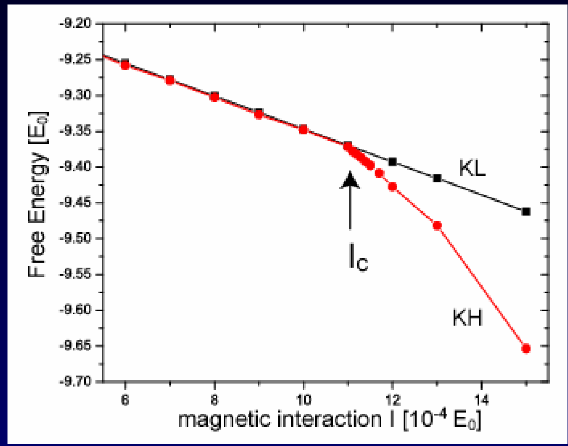
bound state possesses f-electron character



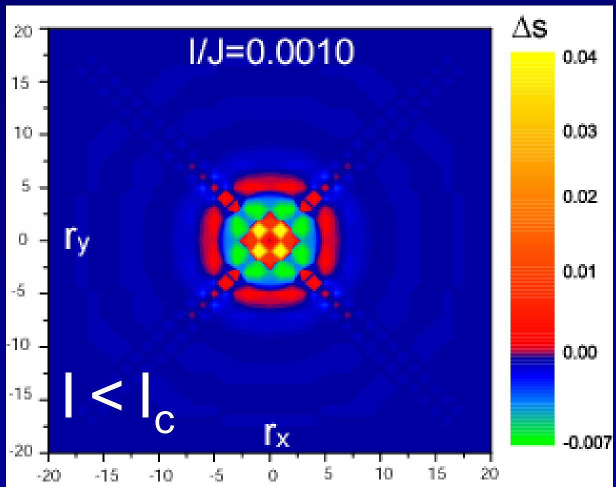
Phase Transition in Kondo Hole Arrays

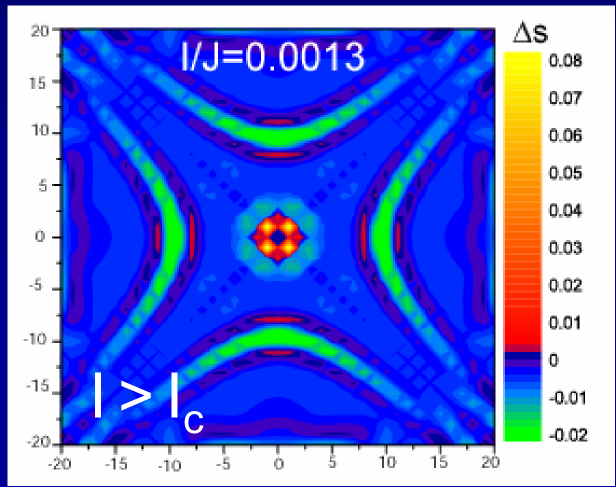






first order phase transition driven by quantum interference effects





transition to a highly inhomogeneous ground state

Open Questions

- Can defects discriminate between electronic and magnetic correlations in real space?

- Can defects provide insight into the competition between Kondo screening and AFM ordering?

- Do the effects of defects/disorder grow with increasing magnetic interactions (as one approaches the QCP)?

- Quantum interference driven phase transitions?