Impurity-Induced States in 2DEG and d-wave Superconductors

Symposium on “Quantum Phenomena”

Condensed Matter Theory Center

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Outline

- **Impurity induced states in 2DEG**

  States induced by a quantum corral, formed by non-magnetic impurities, and a magnetic impurity inside the corral, on 2D metallic host materials. For $T < T_K$ the magnetic impurity gives rise to a Kondo resonance. In this problem impurities play a double role:

  - **The magnetic impurity induces a strongly correlated state;**
  - **The impurities form the corral that allows me to probe in detail some of the properties of the correlated state.**

  Reference: E.Rossi, D. K. Morr, PRL **97***, 236602 (2006).*

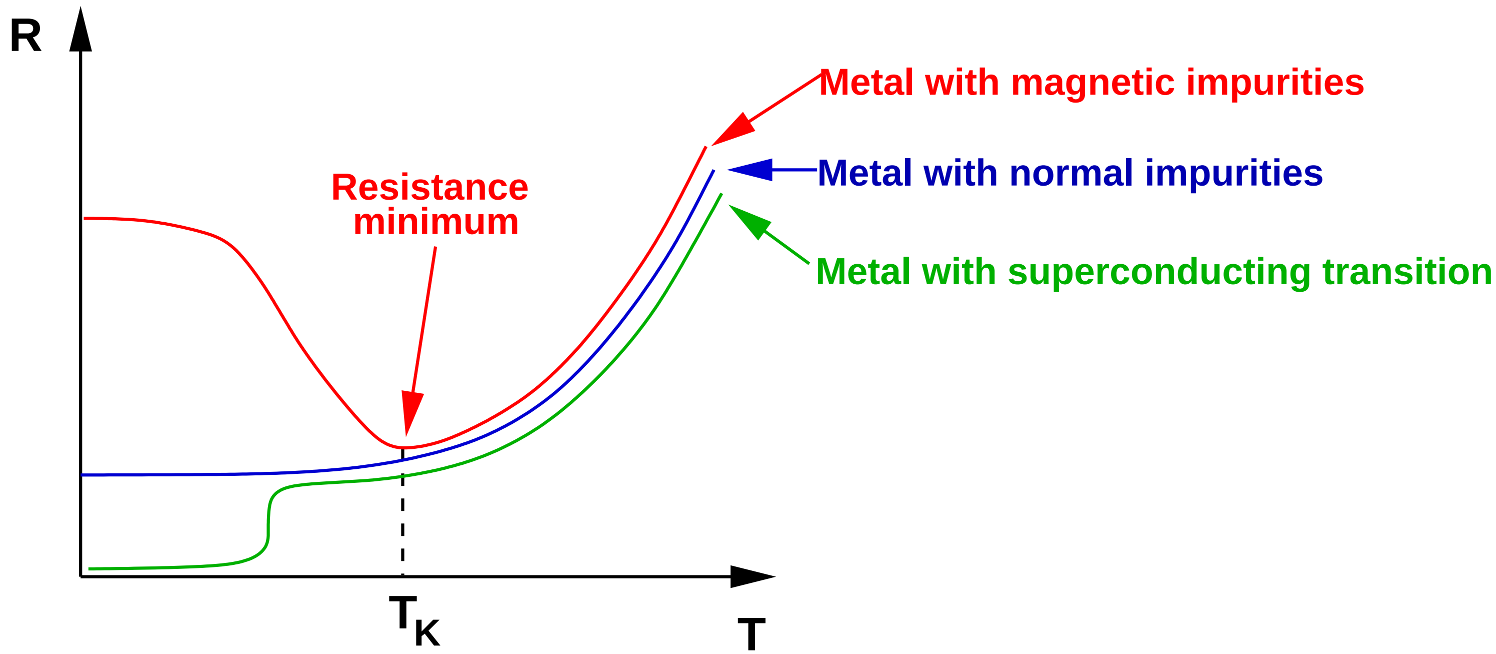
- **Impurity induced states in d-wave superconductors**

  Electronic states induced by an isolated impurity coupled to a collective mode. The impurity pins the collective mode $\longrightarrow$ I have a static mode. Different static modes induce qualitatively different fingerprints in the local density of states (LDOS).

  - **Impurities used to identify nature of collective mode.**

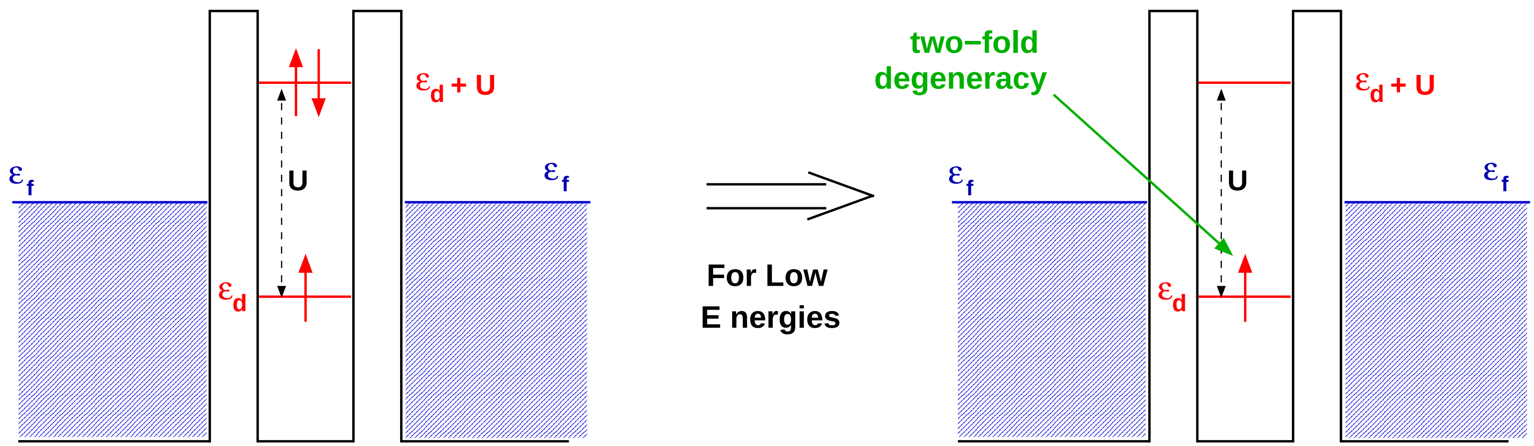
  Reference: Roy H. Nyberg, E. Rossi, D.K. Morr, arXiv:cond-mat/0703684

The Kondo-effect



- 1930's: Discovered experimentally;
- 1964: Using perturbation theory Kondo explains existence of minimum, but his calculation gives R diverging for $T \to 0$;
- 1970's: Renormalization approach by Anderson and Wilson provides adequate theoretical framework for understanding of the Kondo-effect.

From Anderson-model to Kondo-model



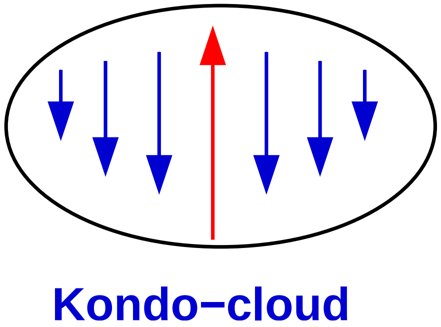
$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\sigma} \epsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\mathbf{k}\sigma} \left(c^\dagger_{d\sigma} c_{\mathbf{k}\sigma} + c^\dagger_{\mathbf{k}\sigma} c_{d\sigma} \right)$$

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_{\sigma\sigma'} \mathbf{S} \cdot c^\dagger_{R,\sigma} \tau_{\sigma\sigma'} c_{R,\sigma'}$$

$$\mathbf{J > 0}$$

Antifferomagnetic coupling
between magnetic impurity and host electrons

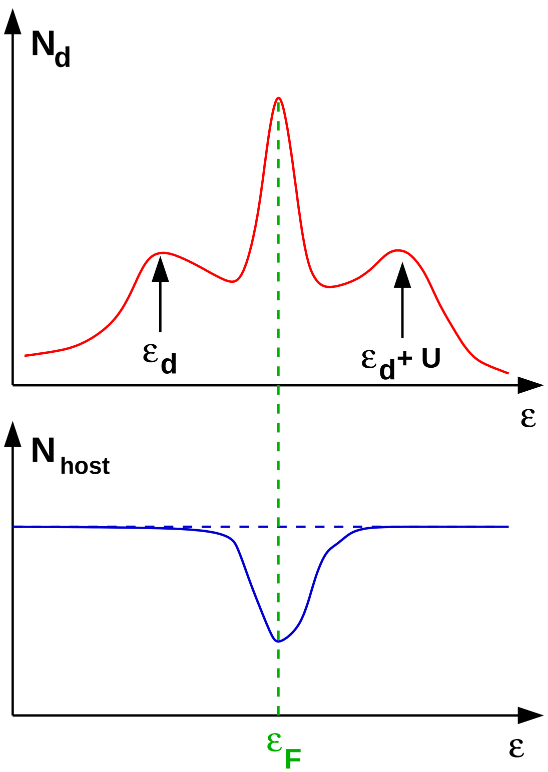
Kondo resonance



The antiferromagnetic interaction **J** can form a bound state of energy E_B between the local spin and one made up from the conduction electron states.

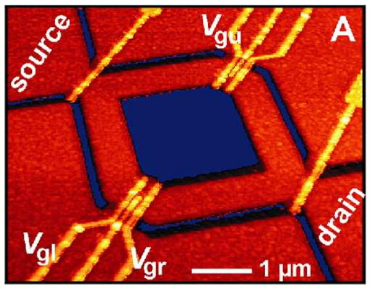
$$E_B \sim T_K$$

For $T < T_K$

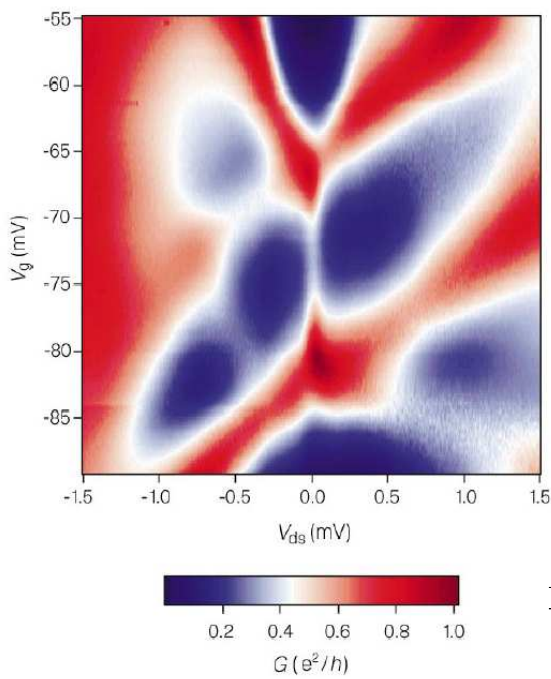


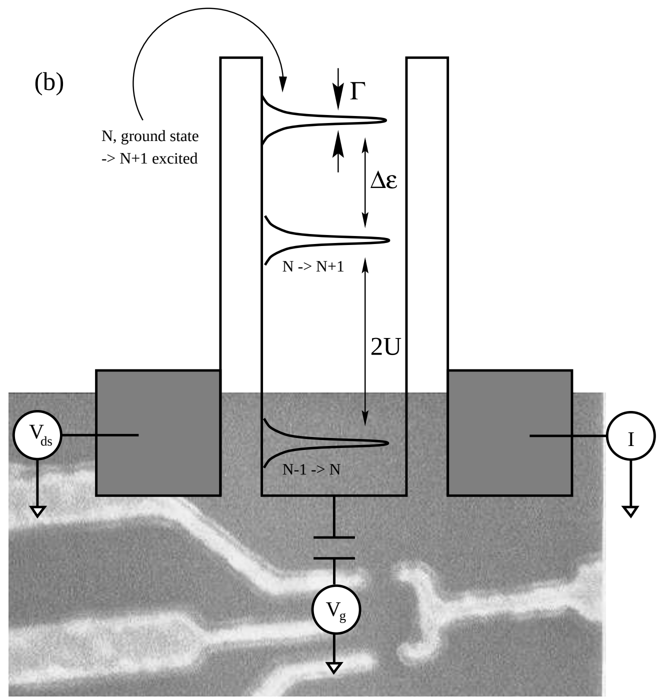
- For the impurity we have a resonant state for $\epsilon = 0$;
- For the host electrons the density of states at the Fermi energy is suppressed $\Longrightarrow$ increase of resistivity.

Nanostructures: Quantum Dots



GaAs Quantum Dot.
S.M. Cronenwett et. al Science (1998)

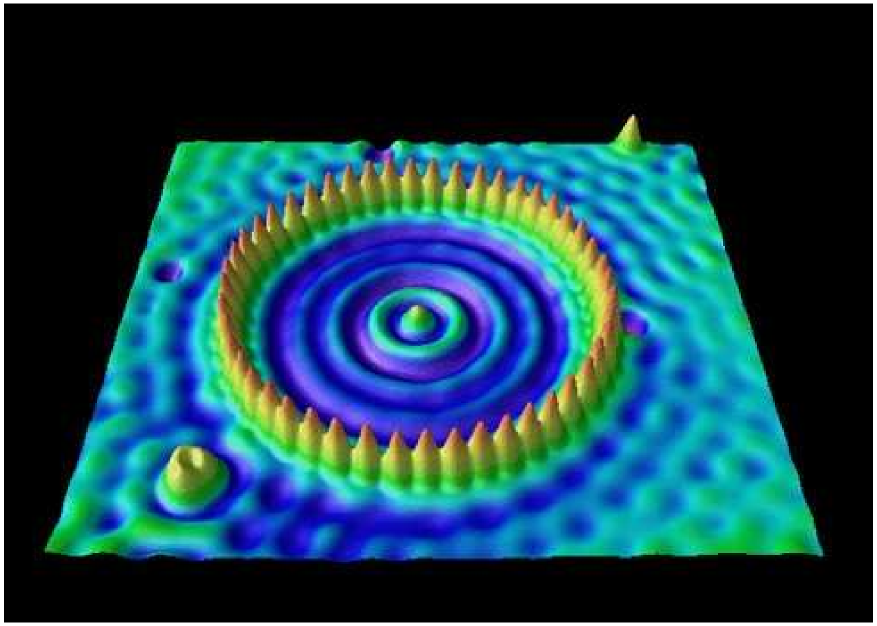




- **tune ϵ_d;**
- **tune width of energy level, Γ;**
- **tune U;**

D. Golhaber−Gordon et al. Nature (1998)

Nanostructures: Quantum Corrals + Scanning Tunneling Microscopy (STM)



D. Eigler IBM

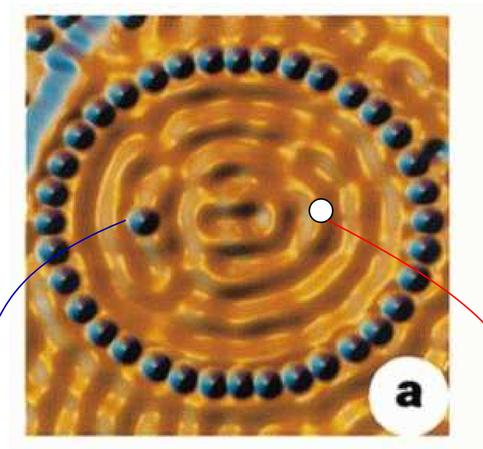
- **Atomic control of impurity position;**
- **By changing the size and/or shape of the corral, we can control the LDOS of conduction electrons;**
- **Direct observation of the LDOS.**

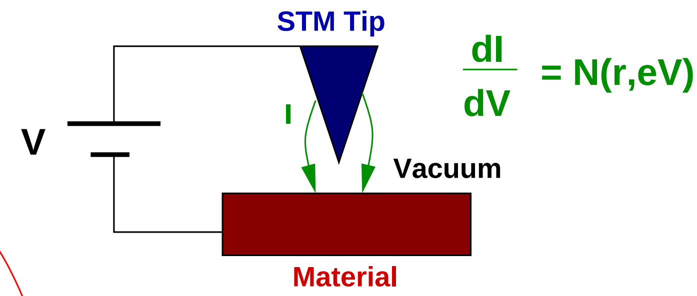
By combining advances in nanofabrication and new probes like STM we can now:

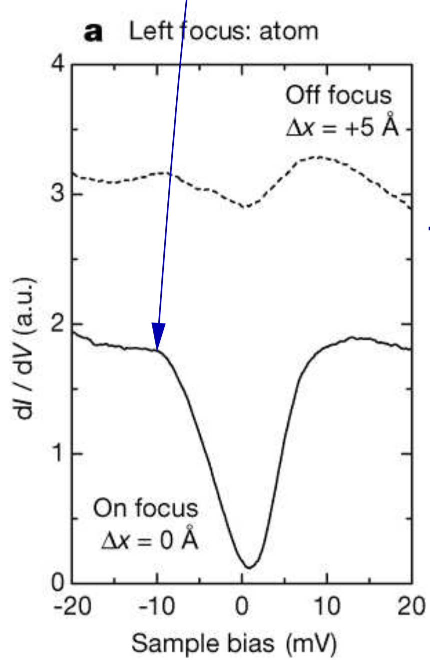
- Control the parameter governing the Kondo-effect;
- Observe *directly* the Kondo-effect.

Creation of a quantum candle: Kondo resonance

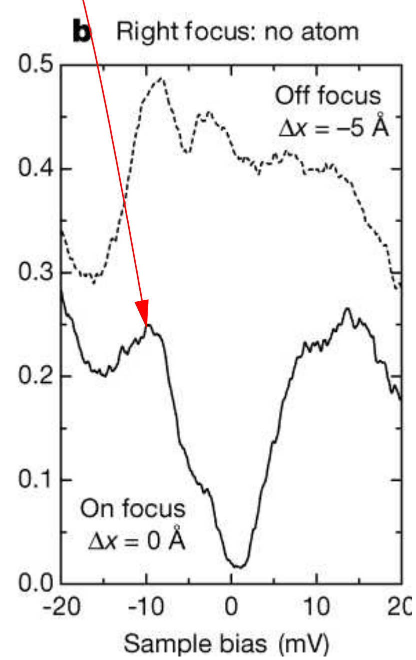
Manhoran et al.
Nature 403, 512 (2000)







Kondo resonance in occupied focus

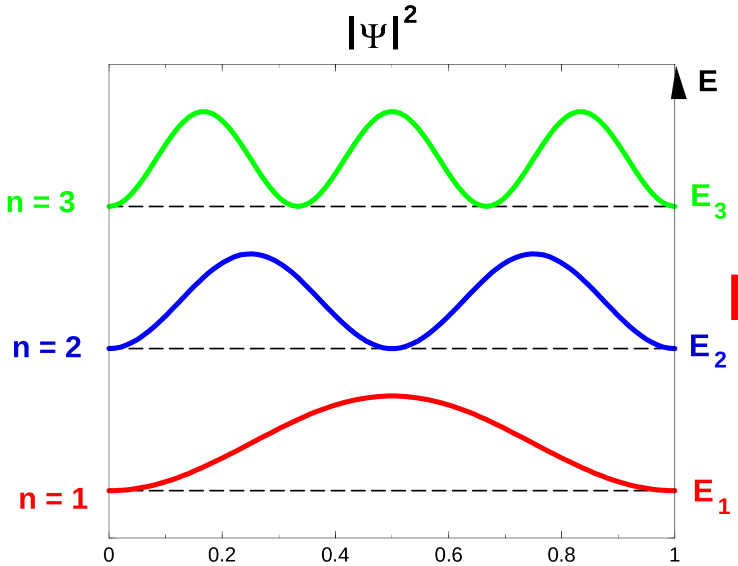


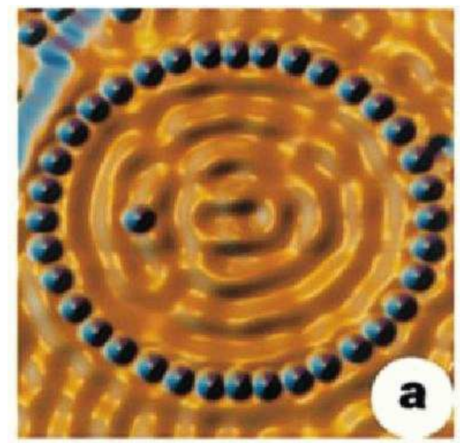
Quantum Image in unoccupied focus

Corral eigenmodes and quantum images

Quantum images are projected through corral eigenmodes

Fiete *et al.*, PRL (2001); Agam and Schiller, PRL (2001); Porras *et al.* PRB (2001); Aligia, PRB (2001).





Manoharan et al.
Nature 403, 512 (200)

Important unsolved questions:

- How does the Kondo effect emerge inside a quantum corral?
- How does the Kondo effect depend on the position of the magnetic impurity?
- What is the form of the Kondo resonance in space and energy in a quantum corral?

Theoretical approach

We model the system with the following Hamiltonian:

$$H = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + U_0 \sum_{I=1..N_c,\sigma} c^\dagger_{I,\sigma} c_{I,\sigma} + J\mathbf{S} \cdot c^\dagger_{R,\alpha} \sigma_{\alpha\beta} c_{R,\beta}$$

free electrons — corral scatterers non-magnetic — magnetic impurity

We consider a two-dimensional host metal on a square lattice with dispersion $\epsilon_{\mathbf{k}} = k^2/2m - \mu$, where μ is the chemical potential. In the following we set the lattice constant a_0 to unity and use $E_0 \equiv \hbar^2/ma_0^2$ as our unit of energy.

We solve the problem in two steps:

Step 1: Compute the eigenmodes of quantum corral using

Generalized scattering theory

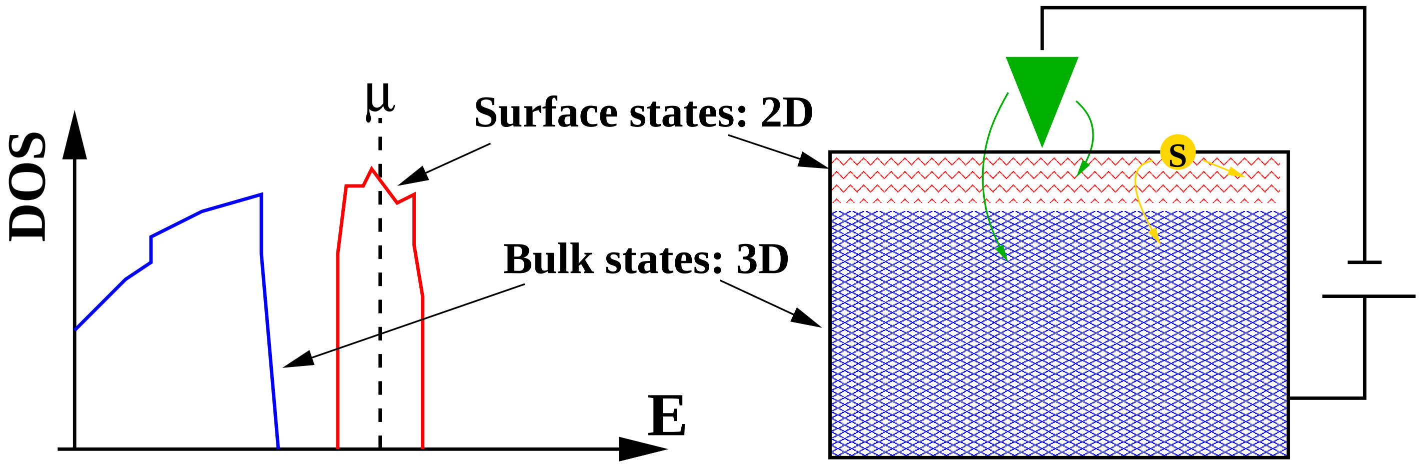
D.K. Morr and N. Stavropoulos, PRL (2004).

Step 2: Calculate effect of magnetic impurity using

large-N expansion

N. Read and D. M. Newns, J. Phys. C (1983).

Surface States and Bulk States



The presence of the bulk states might complicate the analysis, because we can have:

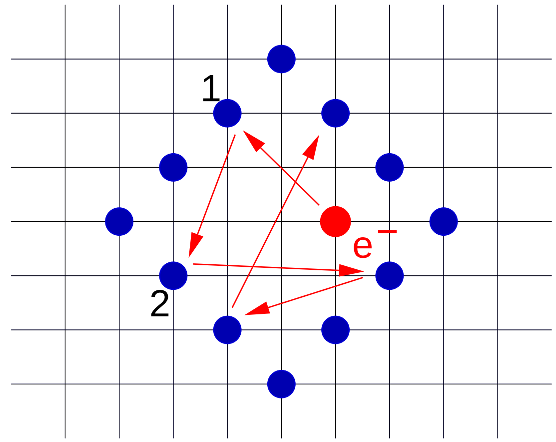
- Coupling surface-bulk states;
- Tip tunneling in part to bulk states;
- Coupling of the Kondo impurity to the bulk states (Knorr et al. PRL (2002))

However we can reduce these effect can minimized:

- Use ultrathin film (few atomic layers) grown on insulating or semiconducting substrates (S.J. Tang et al. PRL (2006));
- Presence of corral should enhance relative importance of surface states with respect to bulk states. The mirage experiment shows 2D character of the states on Cu(111) surface inside a corral.

Generalized Scattering theory

The host electrons undergo multiple scattering with the atoms forming the quantum corral.

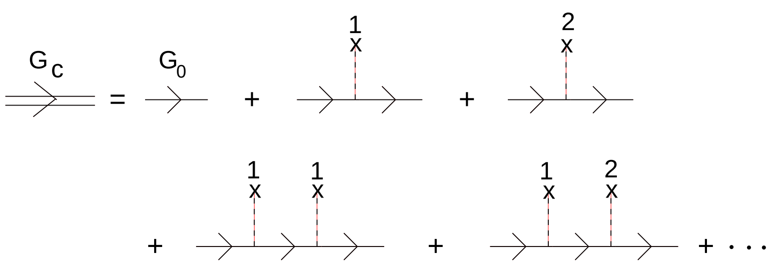


G_c, the Green's function for the conduction electrons in presence of the corral only is given by:

$$G_c(\mathbf{r}, \mathbf{r}', i\omega_n) = G_0(\mathbf{r} - \mathbf{r}', i\omega_n) + \sum_{j,l}{}' G_0(\mathbf{r} - \mathbf{r}_j, i\omega_n)\, T_{jl}(i\omega_n) G_0(\mathbf{r}_l - \mathbf{r}', i\omega_n)$$

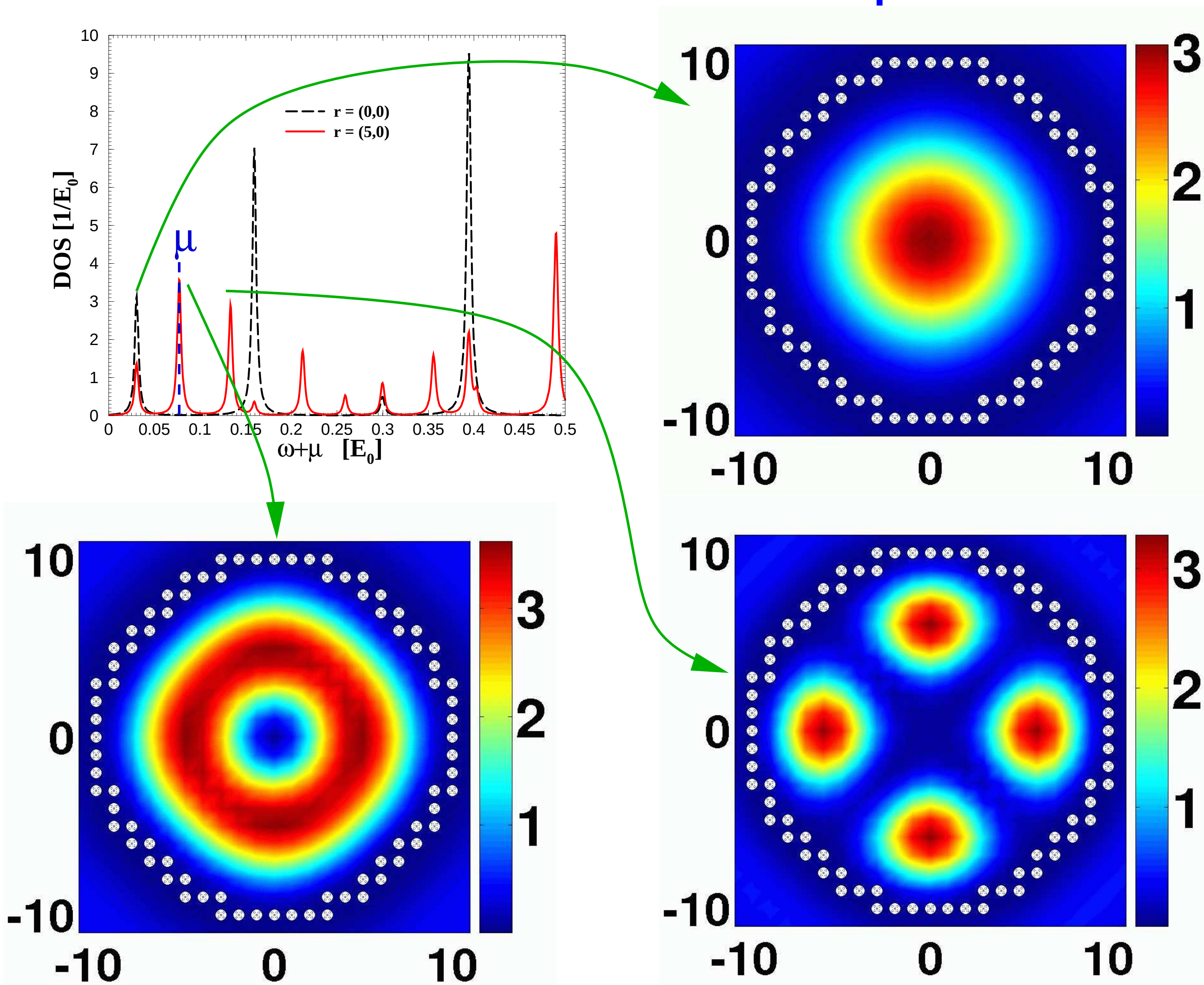
Where the T-matrix satis£es the Bethe-Salpeter equation:

$$T_{ij}(i\omega_n) = U\delta_{ij} + U\sum_l{}' G_0(\mathbf{r}_i - \mathbf{r}_l, i\omega_n) T_{li}(i\omega_n).$$



$$N_c(\mathbf{r}, \omega) = -\frac{2}{\pi}\mathrm{Im}[G_c(\mathbf{r}, \mathbf{r}, \omega + i\delta)]$$

LDOS for corral with No Kondo impurities



Large-N expansion

We know that the perturbation analysis in the Kondo coupling, **J**, breaks down. In the *large-N* expansion we express the spin $\mathbf{S}$ of the magnetic impurity in terms of fermionic operators, $f_m^\dagger$, f_m:

$$\mathbf{S} = \frac{N-1}{2}\mu_B \sum_{m=1}^{N} f_m^\dagger f_m$$

with the constraint:

$$|\mathbf{S}| = \frac{N-1}{2}\mu_B \Longrightarrow n_f \equiv \sum_{m=1}^{N} f_m^\dagger f_m = 1.$$

In our case $|\mathbf{S}| = 1/2$ and then $N = 2$. We can then rewrite the Hamiltonian in the form:

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U_0 \sum_{I=1..N_c,\sigma} c_{I,\sigma}^\dagger c_{I,\sigma} + J \sum_{\alpha\beta} c_{R,\beta}^\dagger f_\alpha^\dagger f_\beta c_{R,\alpha}$$

Decoupled using HS transformation

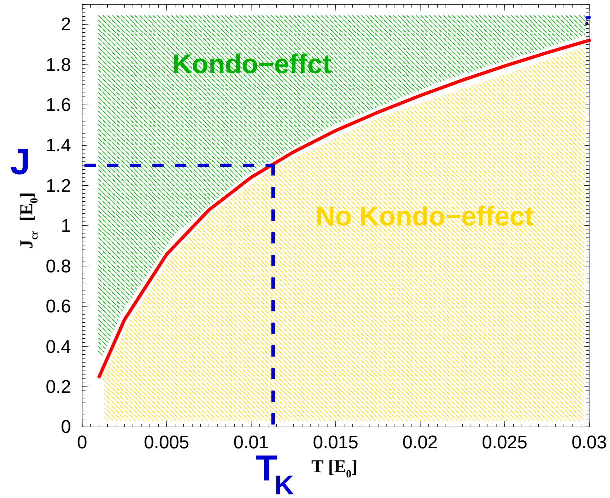
introduce HS field s

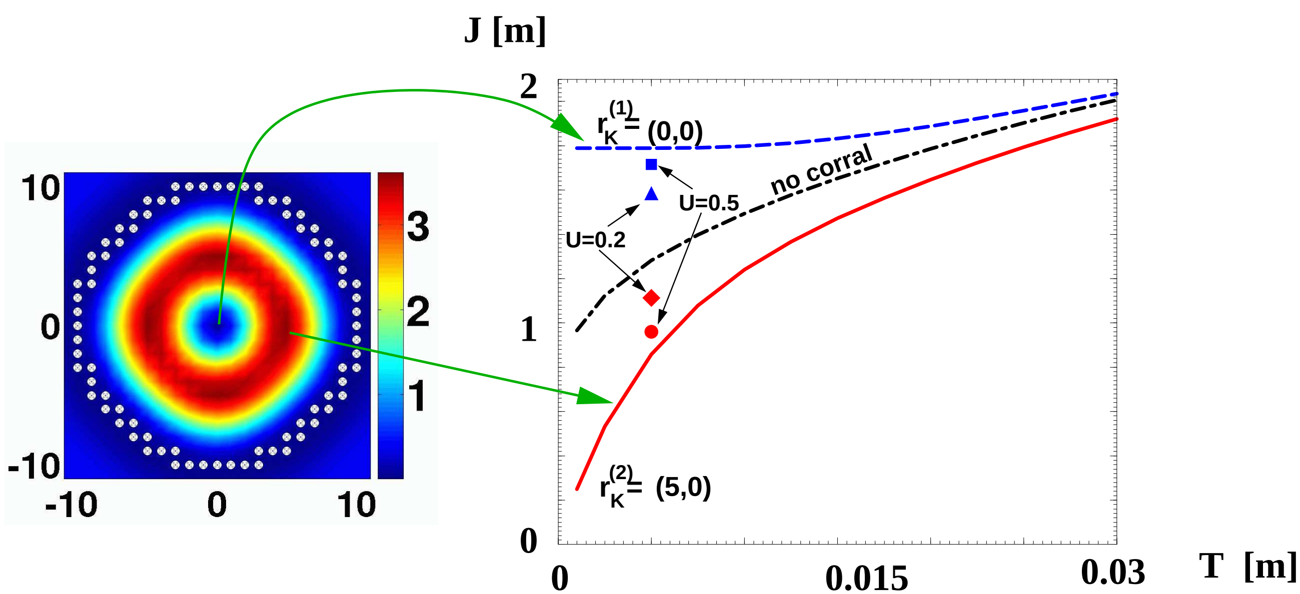
We then find an effective action, S_{eff}, function of two fields:

- s: The hybridization of f electrons with host electrons;
- ϵ_f: Lagrange multiplier to impose the constraint.

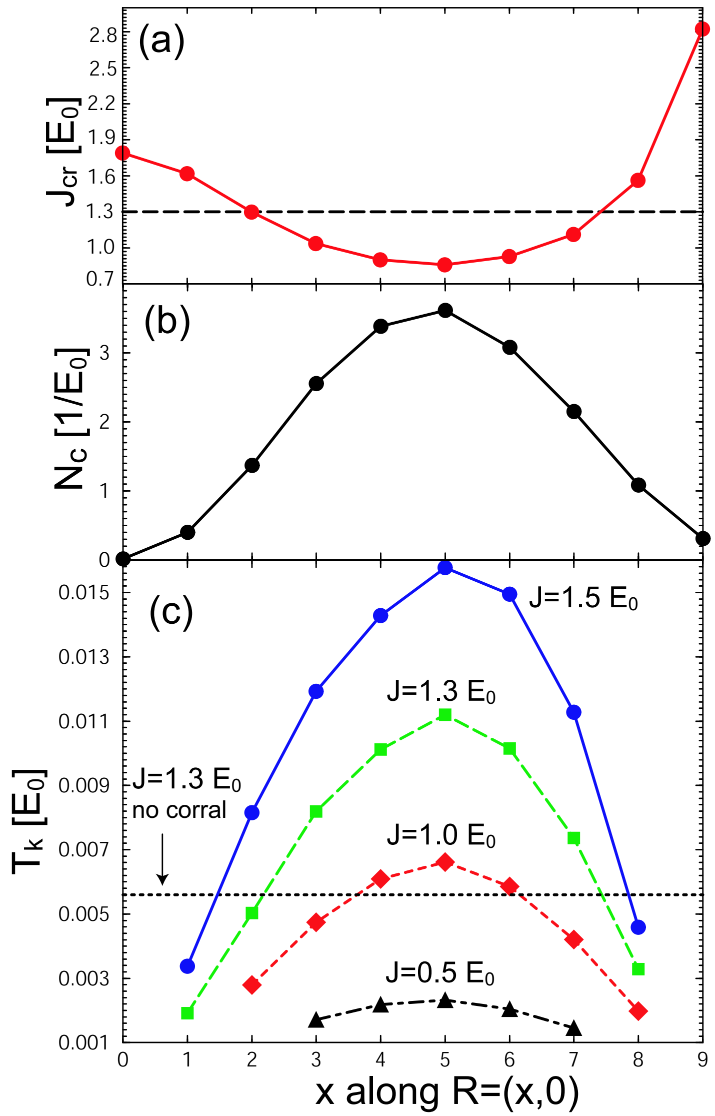
Critical Kondo coupling: J_{cr}

For the fields s and ϵ_f we then take the mean fields values, obtained by minimizing S_{eff} on the saddle point. Approximation is exact in the limit $N \to \infty$. Solve the saddle point equations for different values of T and J. In the *large-N* approach for fixed T there is a minimum value of J, J_{cr}, for which the saddle point equations admit a solution.





Spatially Dependent Kondo-effect



- For fixed T we can see the dependence of J_{cr} on the position of the magnetic impurity inside the corral. In particular we see that J_{cr} is minimum where the conduction electron LDOS is maximum.
- For fixed J we can tune T_K by moving the impurity inside the corral. In particular T_K is maximum where the conduction electron LDOS is maximum.
- Using the spatial dependence of J_{cr}, T_K we can:
  - Turn on and off the Kondo-effect by simply moving the magnetic impurity inside the corral;
  - Increase or decrease T_K with respect to the case with no corral.

LDOS with Kondo Impurity

For a given J and $T < T_K$ solving the saddle point equations we £nd the values of s and ϵ_f. Once we know these values we can calculate the LDOS of the f electrons and of the host electrons taking into account the Kondo coupling. For the f electrons we have the Green's function:

$$F(\mathbf{R}, i\omega_n) = \frac{1}{i\omega_n - \epsilon_f - s^2 G_c(\mathbf{R}, \mathbf{R}, i\omega_n)}$$

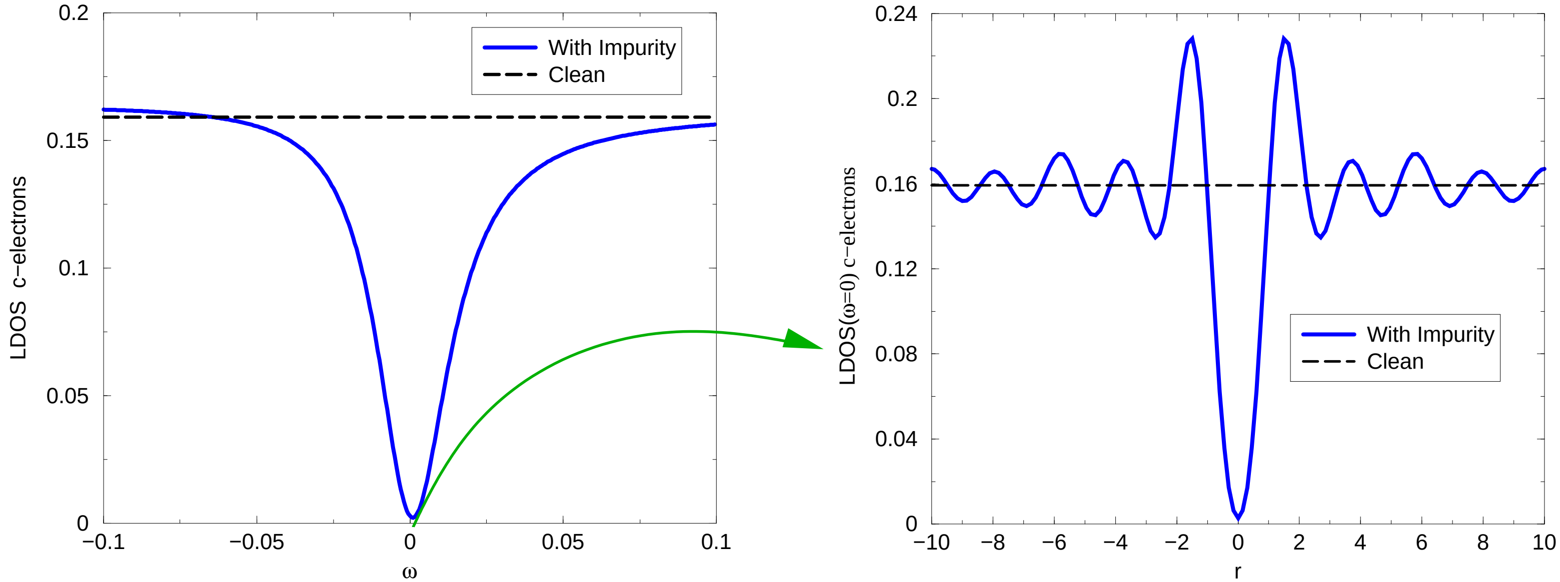
and for the host electrons:

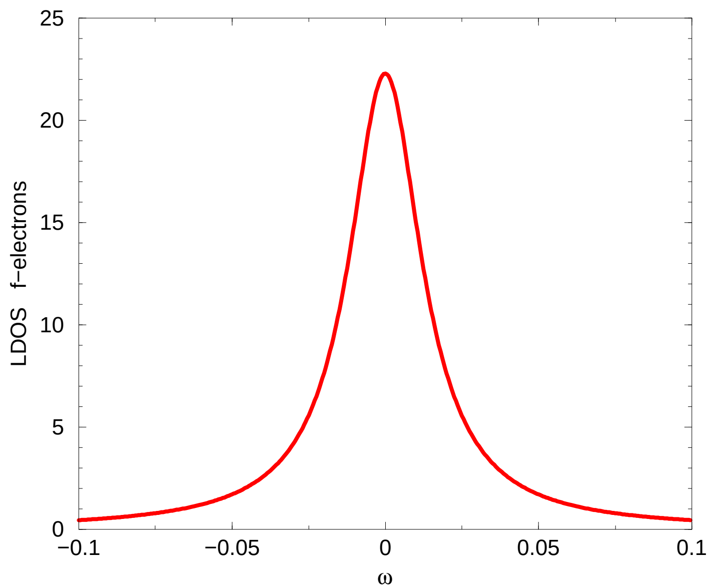
$$G(\mathbf{r}, \mathbf{r}, i\omega_n) = G_c(\mathbf{r}, \mathbf{r}, i\omega_n) + s^2 G_c(\mathbf{r}, \mathbf{R}, i\omega_n) F(\mathbf{R}, i\omega_n) G_c(\mathbf{R}, \mathbf{r}, i\omega_n)$$

and then:

$$N_f(\mathbf{R}, \omega) = -\frac{N}{\pi}\mathrm{Im}[F(\mathbf{R}, \omega + i\delta)]; \qquad N(\mathbf{r}, \omega)^{tot} = -\frac{2}{\pi}\mathrm{Im}[G(\mathbf{r}, \mathbf{r}, \omega + i\delta)];$$

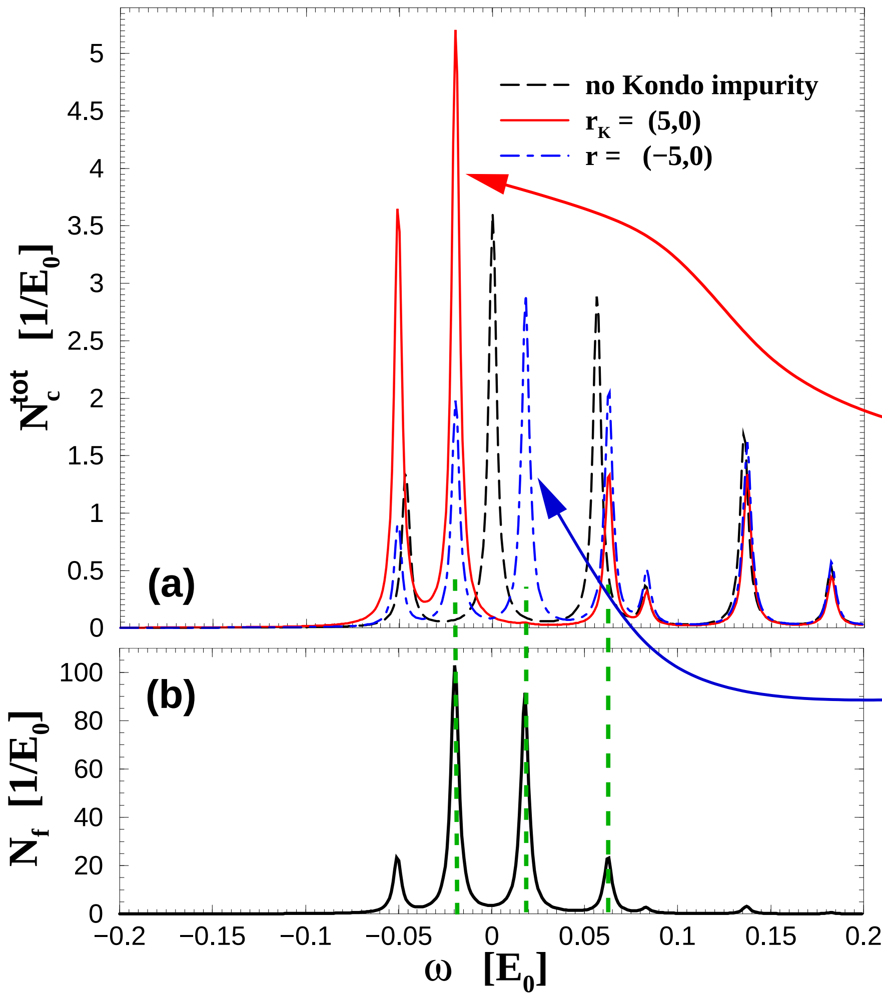
No corral



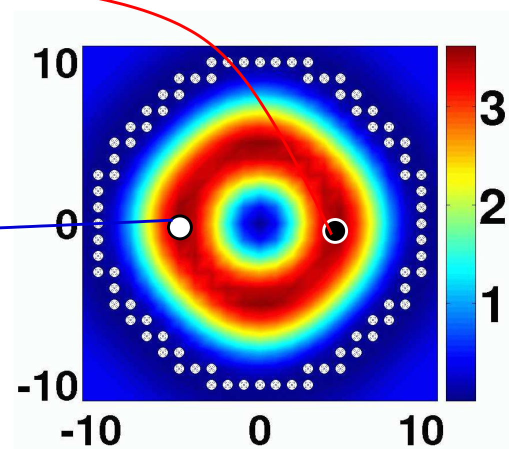


- **Simple dip for c−electrons**
- **Peak for f−electrons**
- **Simple oscillations in real space**

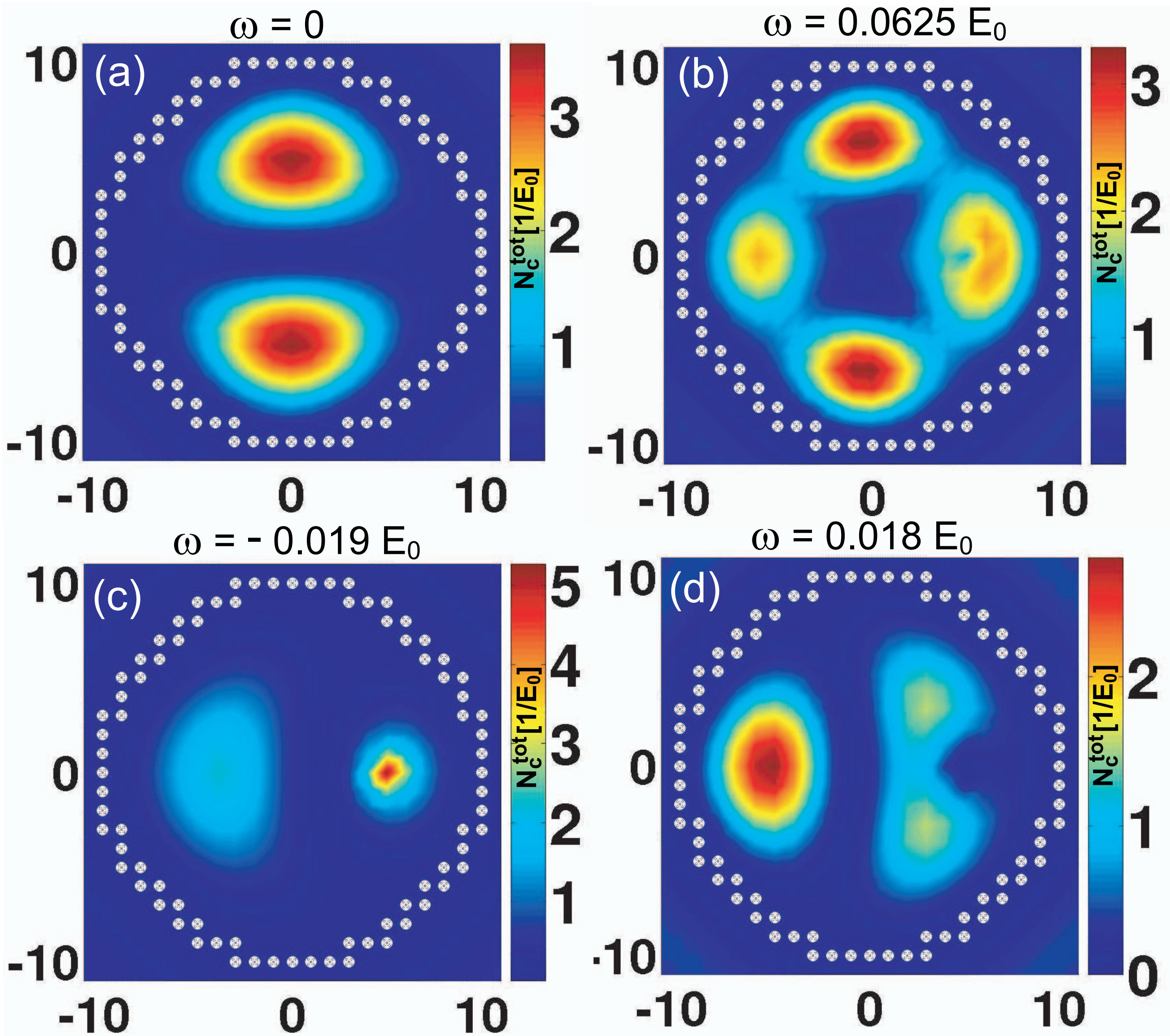
Kondo Resonances



- Original mode decreased in amplitude; suppression of LDOS at $\omega = 0$
- Kondo resonances also away from the magnetic impurity
- Additional resonances
  N modes ⟶ N + 1 Kondo resonances



Spatial structure of Kondo resonances



Conclusions

We showed that the spatial structure of the corral's low energy eigenmode leads to:

- Spatial variations in the critical coupling J_{cr}, in particular J_{cr} is minimum where LDOS is maximum;
- Spatial variations of the Kondo temperature T_K, in particular T_K is maximum where LDOS is maximum
- Spatial dependence of the relation between J_{cr} and T

Quantum Corrals: a new probe for the Kondo effect!

Identifying collective modes in d-wave SC via impurities. Motivation

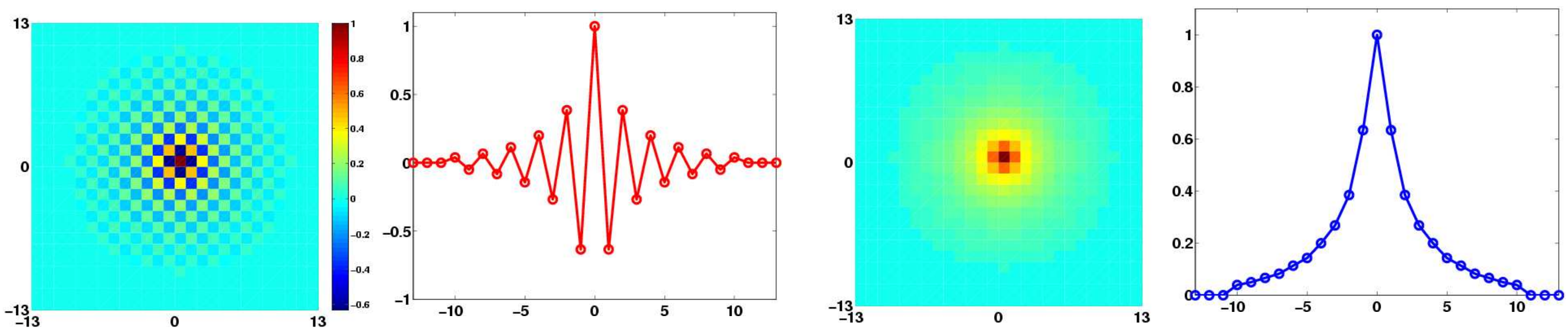
The nature of collective modes in High T_c superconductors is one of the most important and controversial issues in condensed matter physics.

- **Magnetic in Nature: Spin Density Wave (SDW);**
  - ARPES: J.C. Campuzano *et al.*, PRL (1999)
  - NMR experiments with Ni impurities: J. Bobroff *et al.*, PRL (1997)
- **Charge density wave (CDW)**
  - ARPES, STM: J. Tranquada
- **Phonon**
  - ARPES: G.H. Gweon *et al.*, Nature (2004).
  - STS: J. Lee *et al.*, Nature (2006).

Impurities as probes of collective behavior

$$H = H_0 - J\mathbf{S}\cdot\mathbf{s}_c(\mathbf{R}) + V_0 n_c(\mathbf{R})$$

$$\langle s_z(\mathbf{r})\rangle = \langle s_c^z(\mathbf{r})\rangle + \langle S_{imp}^z\rangle\delta_{\mathbf{r},\mathbf{R}}; \qquad \delta\langle n(\mathbf{r})\rangle = \langle \delta n_c(\mathbf{r})\rangle + \delta_{\mathbf{r},\mathbf{R}}$$



static spin mode:

spin droplet

static charge mode:

charge droplet

$$\chi_s(\mathbf{q},\omega=0) = \frac{\chi_0}{(\xi_s^{-2} + (\mathbf{q}-\mathbf{Q})^2)} \qquad \chi_c(\mathbf{q},\omega=0) = \frac{\chi_0}{(\xi_c^{-2} + \mathbf{q}^2)}$$

$$\mathbf{Q} = (\pi,\pi) \qquad \xi_s = \xi_c = 5\ a_0$$

Model

$$\mathcal{H} = \sum_{\mathbf{r},\mathbf{r}',\alpha} t_{\mathbf{r}\mathbf{r}'} c^{\dagger}_{\mathbf{r},\alpha} c_{\mathbf{r}',\alpha} + \sum_{\mathbf{r},\mathbf{r}'} \left[\Delta(\mathbf{r},\mathbf{r}') c^{\dagger}_{\mathbf{r},\uparrow} c^{\dagger}_{\mathbf{r}',\downarrow} + h.c. \right]$$

$$- \sum_{\mathbf{r},\sigma,\sigma'} \left[g_s \langle s_z(\mathbf{r}) \rangle \sigma^{z}_{\alpha\beta} - g_c \langle \delta n(\mathbf{r}) \rangle \delta_{\alpha\beta} \right] c^{\dagger}_{\mathbf{r},\alpha} c_{\mathbf{r},\beta}$$

Interaction of conduction electrons with droplet pinned by impurity

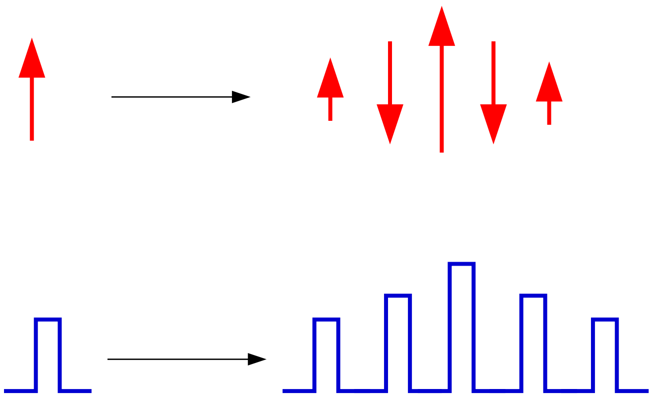
where

$$\langle s_z(\mathbf{r}) \rangle = \langle s^{z}_{c}(\mathbf{r}) \rangle + \langle S^{z}_{imp} \rangle \delta_{\mathbf{r},\mathbf{R}}$$

$$\delta \langle n(\mathbf{r}) \rangle = \langle \delta n_c(\mathbf{r}) \rangle + \delta_{\mathbf{r},\mathbf{R}}$$

- Hopping parameters t and chemical potential chose to reproduce the dispersion observed in High T_c superconductors.
- For $\Delta(\mathbf{r},\mathbf{r}')$ we assume d-wave symmetry with $\max|\Delta(\mathbf{r},\mathbf{r}')| = 30\ \mathrm{meV} = 0.1\ \mathrm{t}$ between nearest neighbors sites.

Theoretical approach



We treat the droplet as a set of single impurities

- **T-matrix**

  Same approach as shown previously to treat non-magnetic impurities for Kondo-corral problem.

  – We can treat infinite system-sizes$\Longrightarrow$ High Resolution for the LDOS at low energies.

  – The superconducting order parameter Δ_0 is assumed fixed: not calculated self consistently

- **Bogoliubov de Gennes (BdG)**

  – Δ_0 is calculated self-consistently

  – Limited to small size systems $\Longrightarrow$ Low Resolution for LDOS at low energies

BdG approach

Within the BdG approach one solves the eigenvalue equation:

$$\sum_{\mathbf{r}'} \begin{pmatrix} H^{+}_{\mathbf{r}\mathbf{r}'} & \Delta_{\mathbf{r}\mathbf{r}'} \\ \Delta^{*}_{\mathbf{r}\mathbf{r}'} & -H^{-}_{\mathbf{r}\mathbf{r}'} \end{pmatrix} \begin{pmatrix} u_{\mathbf{r}',n} \\ v_{\mathbf{r}',n} \end{pmatrix} = E_n \begin{pmatrix} u_{\mathbf{r},n} \\ v_{\mathbf{r},n} \end{pmatrix}$$

where

$$H^{\pm}_{\mathbf{r}\mathbf{r}'} = t_{\mathbf{r}\mathbf{r}'} + (\pm g_s \langle s_z(\mathbf{r})\rangle - g_c \langle V(\mathbf{r})\rangle - \mu)\delta_{\mathbf{r},\mathbf{r}'}$$

and $Delta_{\mathbf{r}\mathbf{r}'}$ is calculated self consistently:

$$\Delta_{\mathbf{r}\mathbf{r}'} = -\frac{V}{2} \sum_n \left(u_n(\mathbf{r}) v_n(\mathbf{r}') + u_n(\mathbf{r}') v_n(\mathbf{r})\right) \tanh\left(\frac{E_n}{2k_B T}\right) \; ,$$

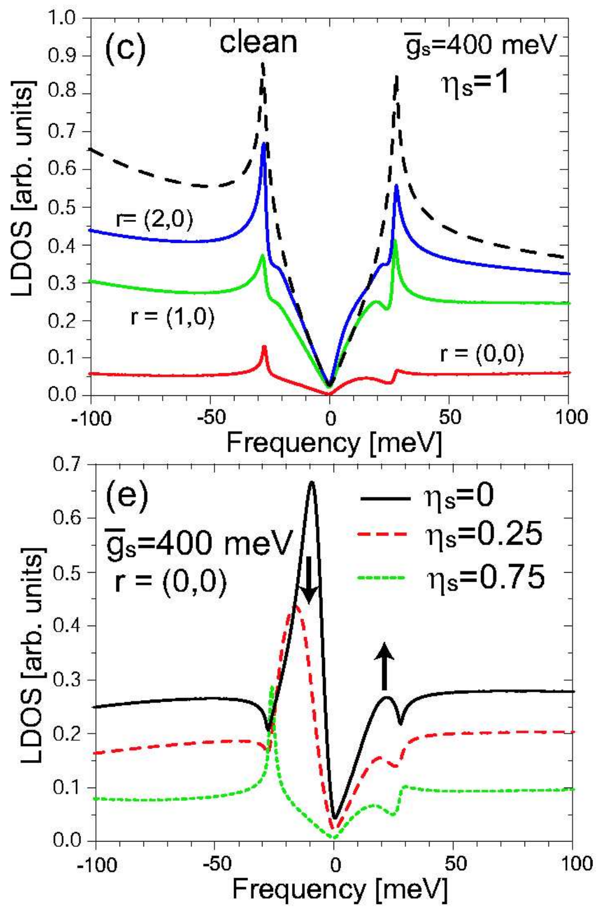
The LDOS at **r** is finally given by:

$$N(\omega, \mathbf{r}) = \sum_n \left[u_n^2(\mathbf{r})\delta(\omega - E_n) + v_n^2(\mathbf{r})\delta(\omega + E_n)\right]$$

T-matrix results

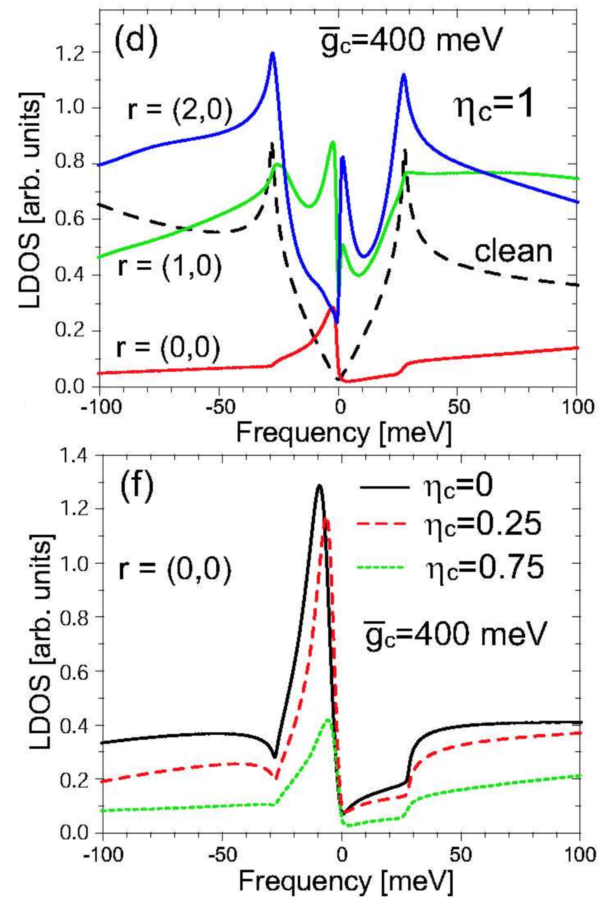
Spin Droplet

$g_s \langle S^z_{imp} \rangle = 400$ meV; $g_c = 0$



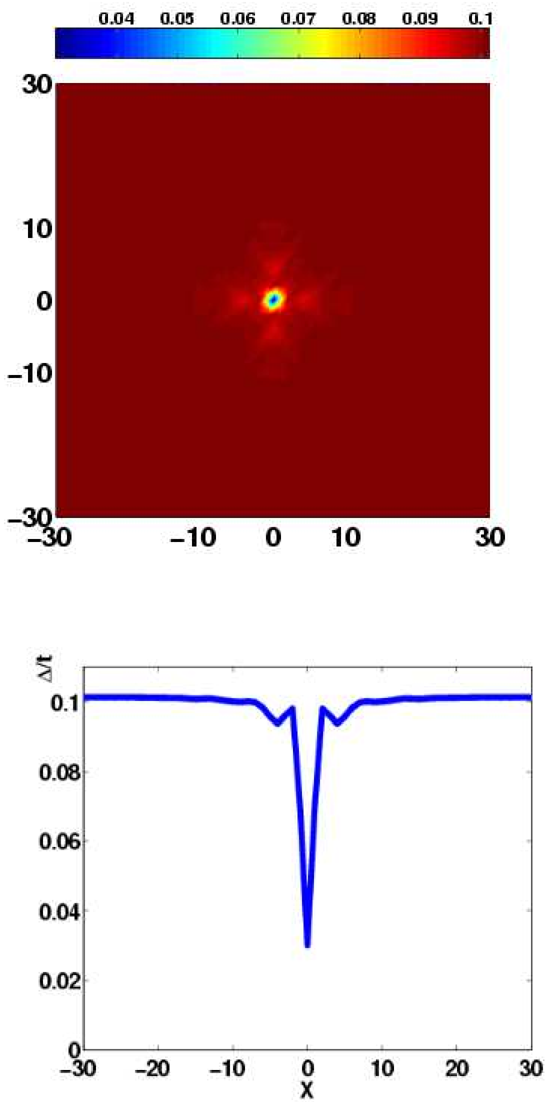
Charge Droplet

$g_s \langle S^z_{imp} \rangle = 0$; $g_c = 400$ meV

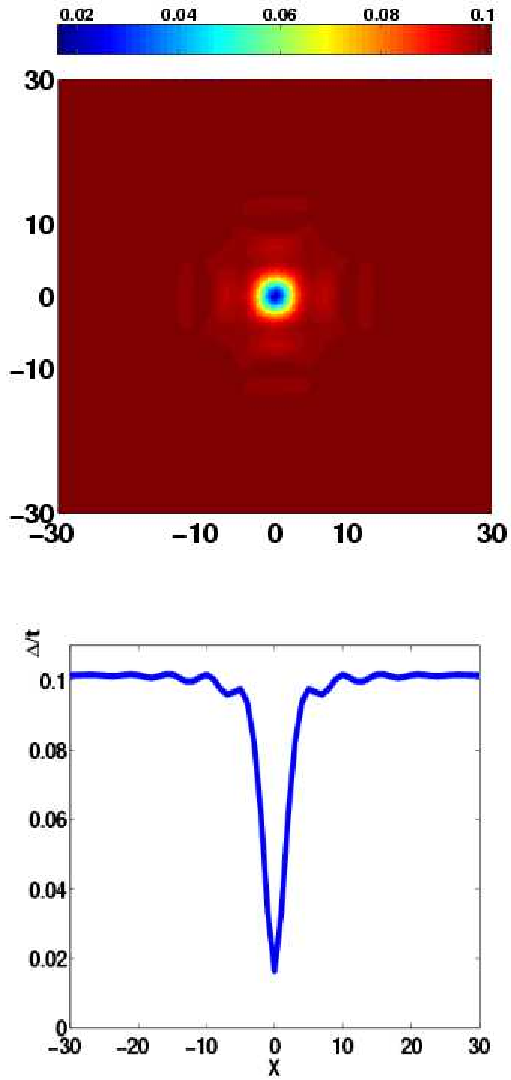


BdG result for Δ_0: magnetic case

Single Impurity



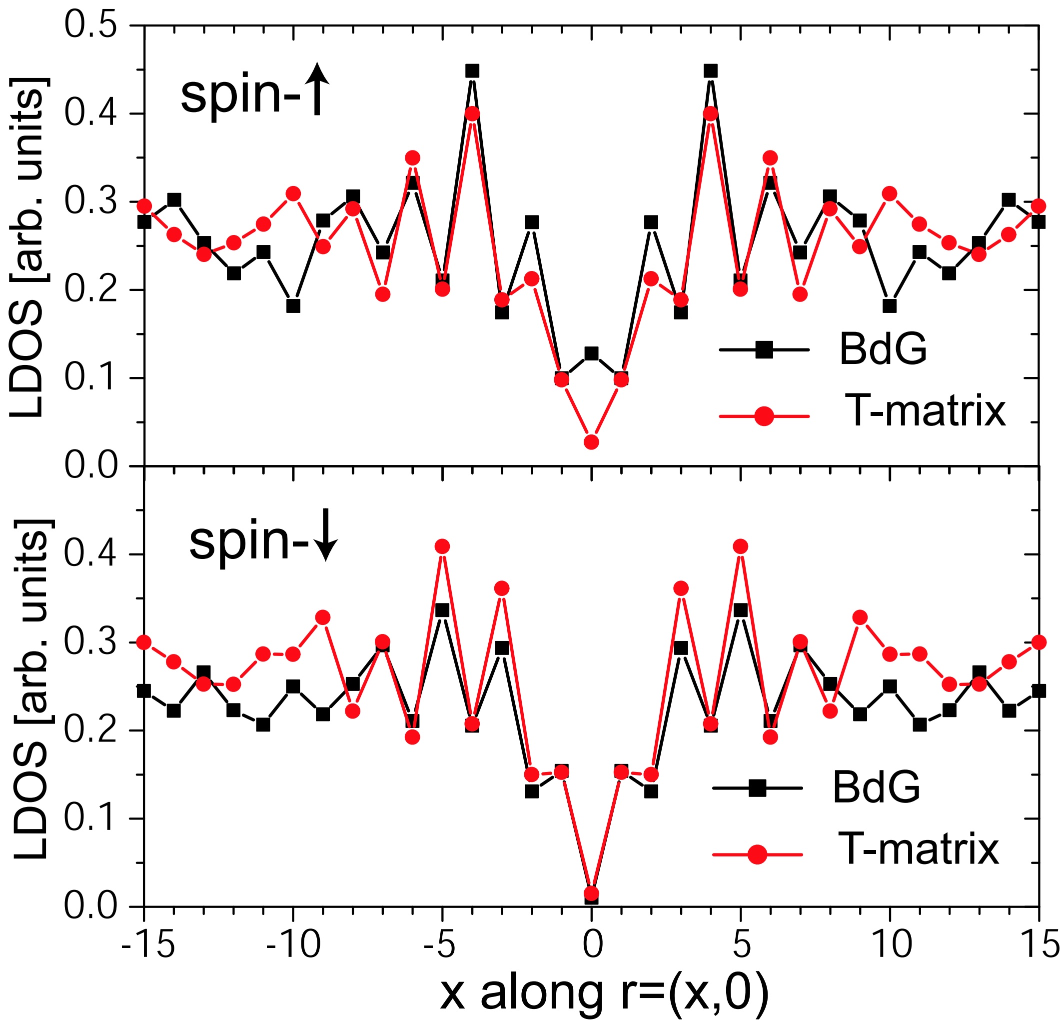
Spin-droplet



Δ_0 recovers in only 2-3 lattice spacings.

Comparison of BdG and T-matrix results

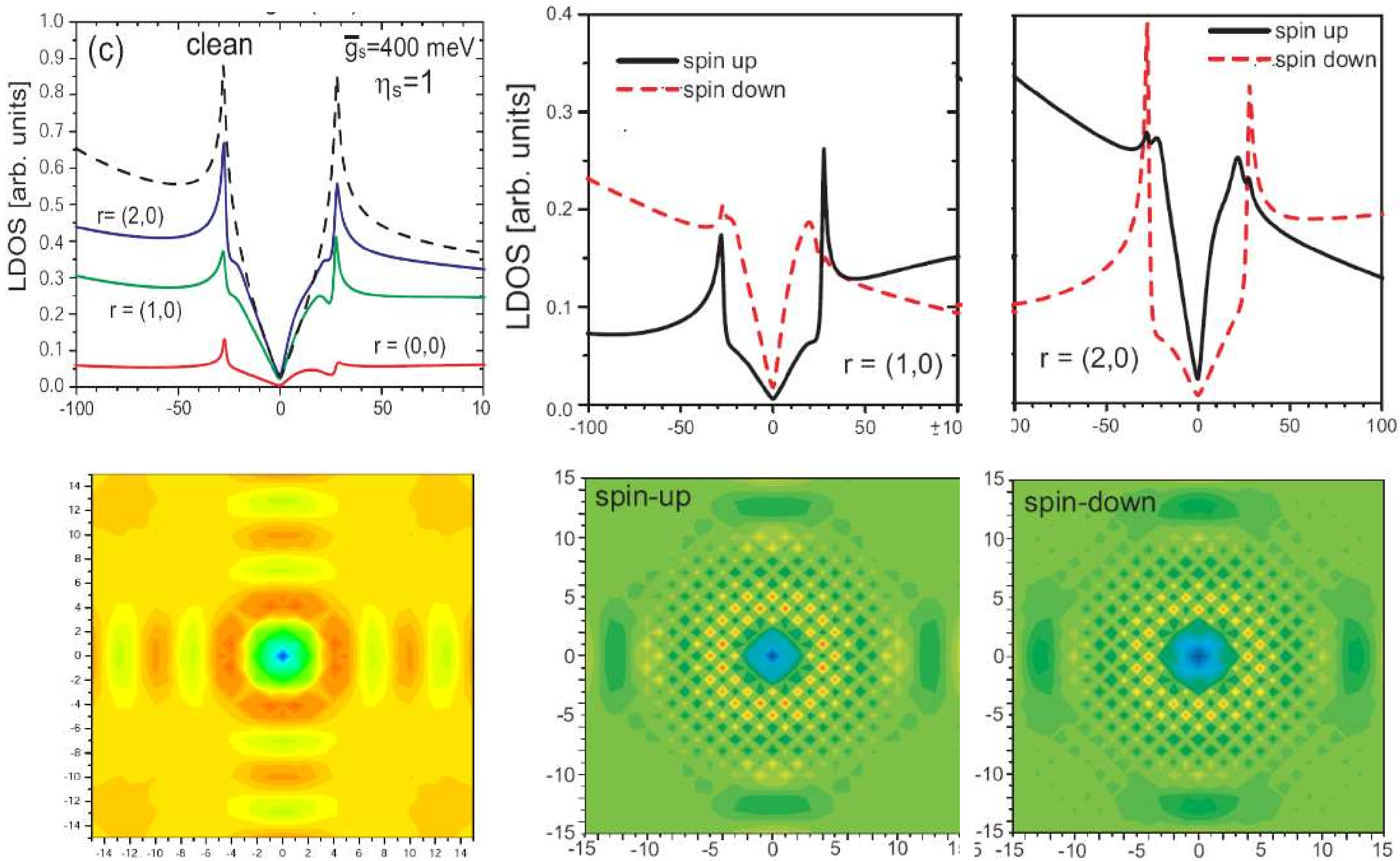
Let's consider for example the LDOS at hole-like coherence peak for a spin-droplet.



- Small deviation at center due to the suppression of $\Delta_0 \longrightarrow$ At the center we have effective decrease of scattering strength.
- BdG results show π phase shift at $\approx 10a_0$ from center.

Only minor differences

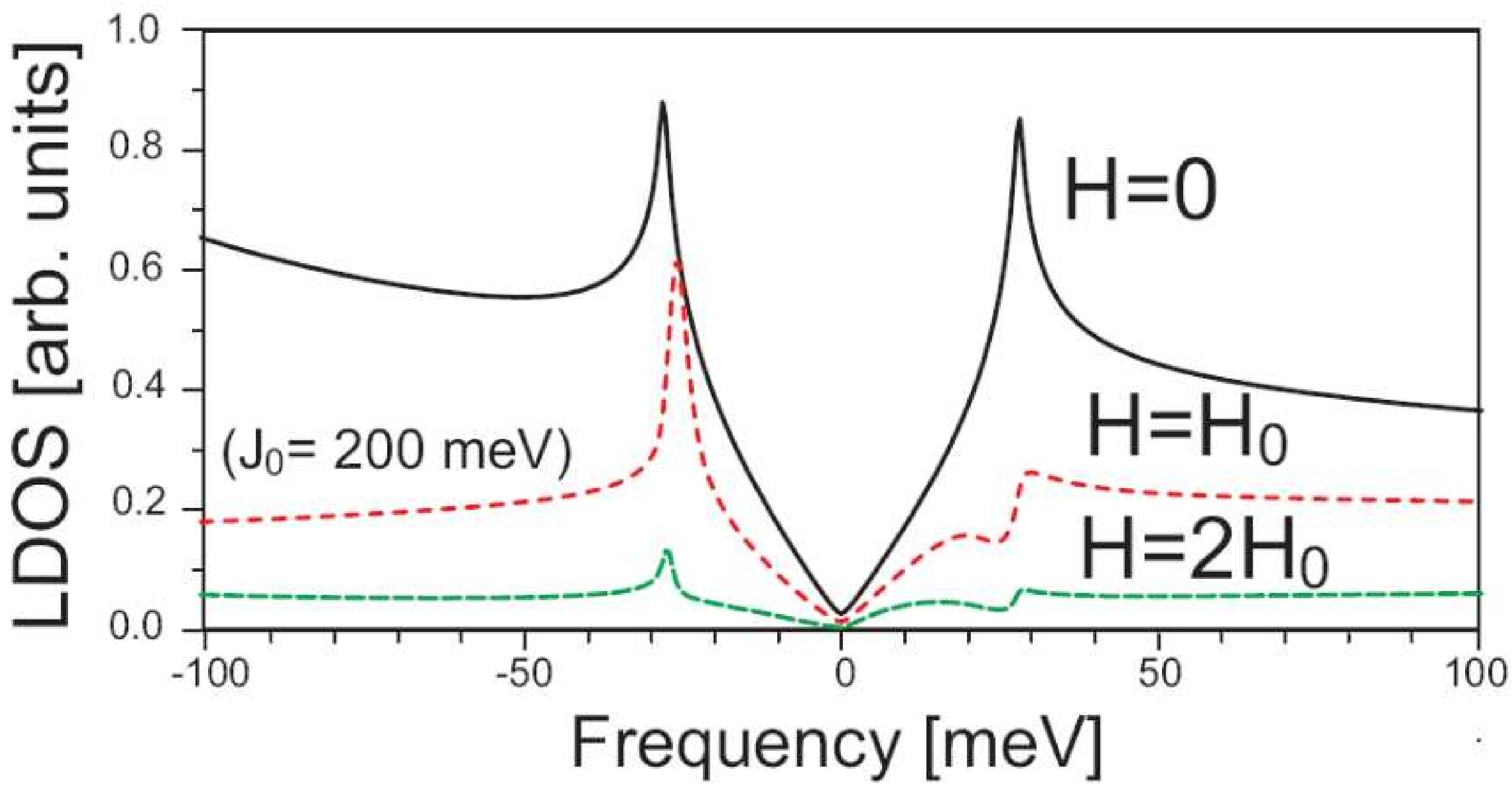
Spin-droplet: spin resolved results



Effect of magnetic field

$$\langle S^z_{imp} \rangle = \frac{CH}{T+\Theta}; \qquad H_0 \longrightarrow 2H_0 \Longrightarrow \langle S^z_{imp} \rangle \ \text{two times bigger}$$

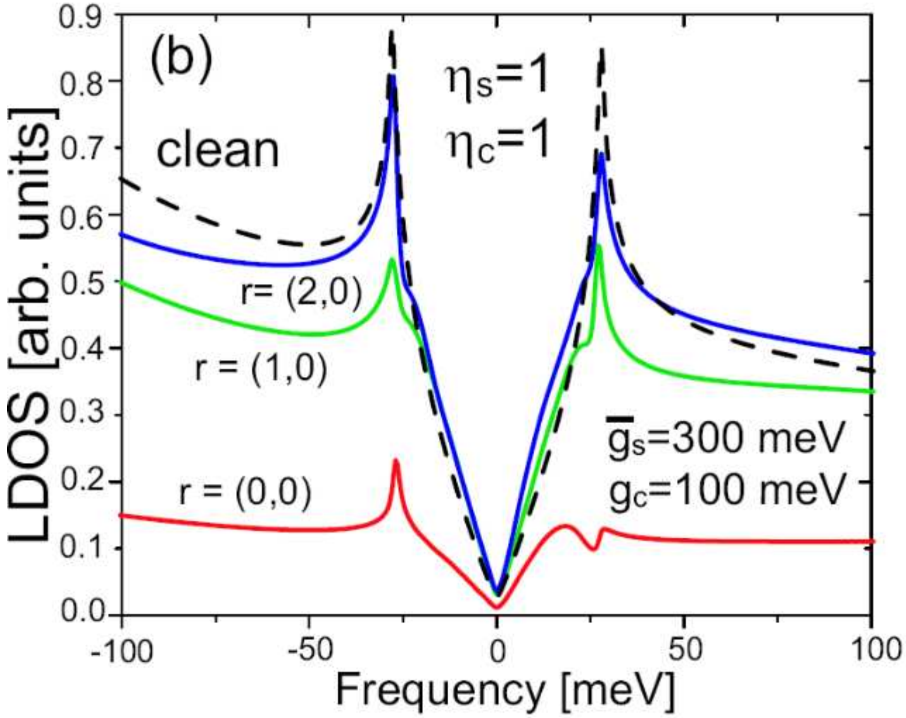
By changing H (or the temperature T) we effectively change the strength of the magnetic impurity and therefore of the spin droplet. A change of H does not change the strength of a charge-droplet.



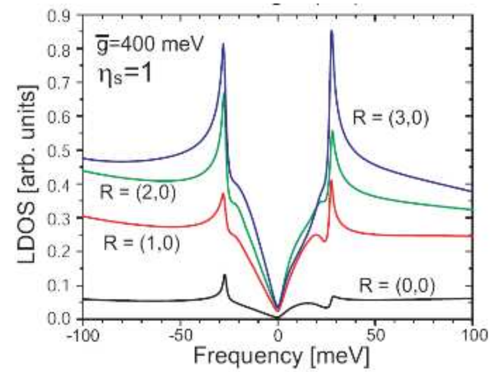
Spin Droplet + Charge Droplet

In general impurities have both spin and charge scattering potential. However if one scattering potential is coupled to a collective mode and the other is not, the effect of the latter on the LDOS is completely negligible (and localized at the site of the impurity). On the other hand we can have a situation when both a spin and a charge collective modes are present.

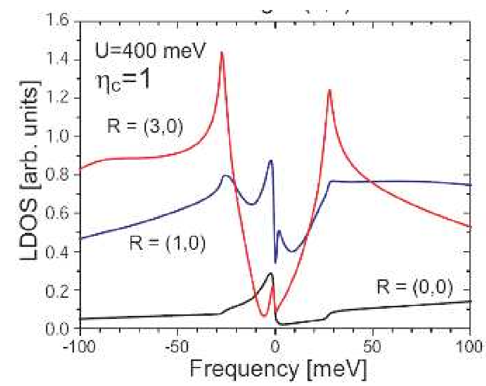
Spin droplet + Charge droplet



Spin Droplet



Charge Droplet



Conclusions

The pinning of a collective mode by an impurity creates a static droplet.

- **Magnetic impurity $\Longrightarrow$ Spin-droplet**
- **Charge impurity $\Longrightarrow$ Charge droplet**

I showed that different droplets cause very different changes in the LDOS. In particular for a spin droplet, close to the center of the droplet:

- LDOS very different from single impurity and charge droplet;
- Impurity state is suppressed;
- Coherence peaks are preserved;
- Strong dependence on H and T;
- Spatial structure of spin-resolved LDOS reflects AF nature of the magnetic mode.

Impurities can be used to uncover the nature of the collective mode!

Final Conclusions

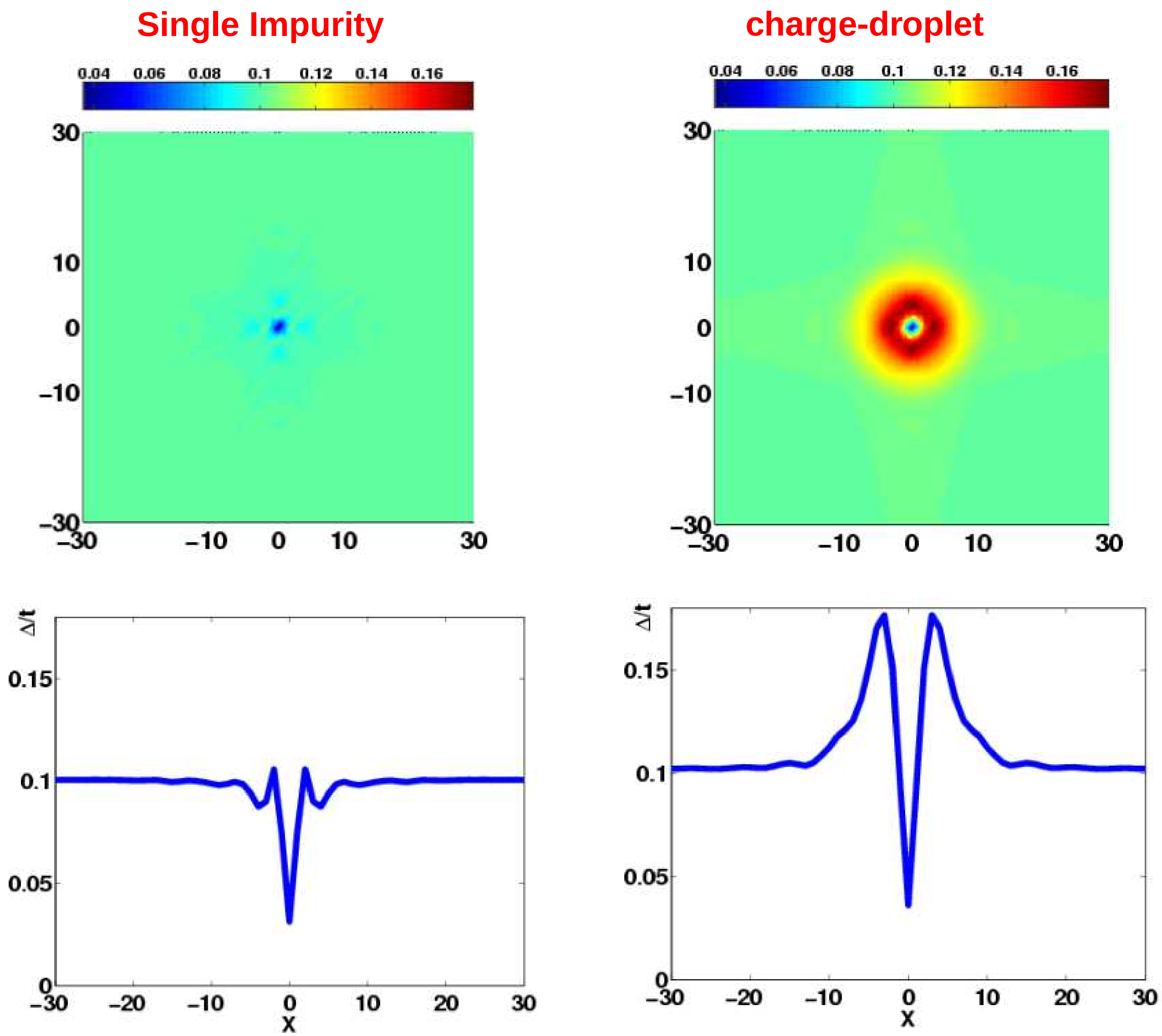
The Physics of impurities in:

- **Low dimensional systems**
- **Nanosystems**
- **Strongly correlated systems**

is very rich and to in many respects still largely unexplored

Thank you!

BdG result for Δ_0: charge case



Δ_0 recovers in only 2-3 lattice spacings.