Kondo Effect in Nanostructures

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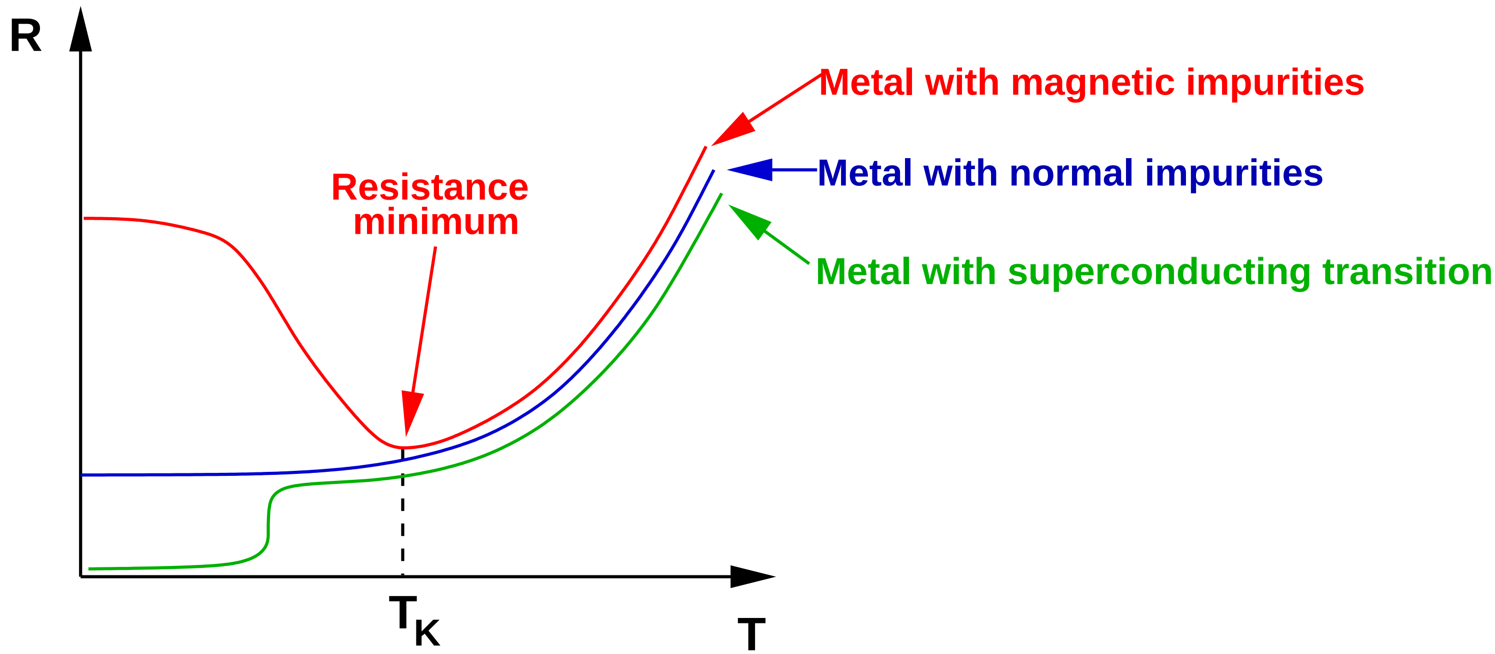
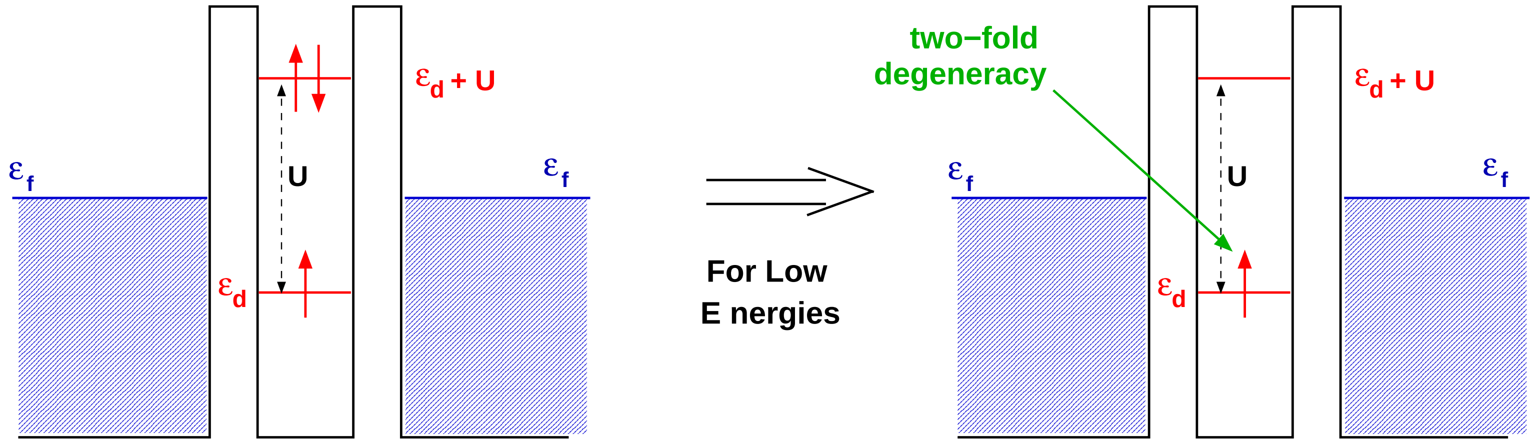
The Kondo-effect



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

From Anderson-model to Kondo-model



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

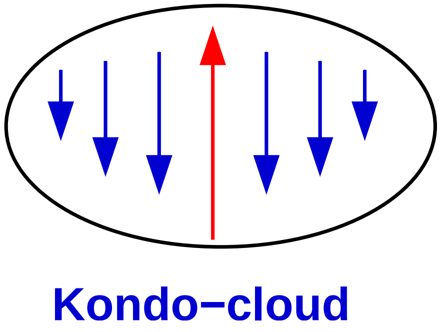
$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_{\sigma\sigma'} \mathbf{S} \cdot c^{\dagger}_{R,\sigma} \tau_{\sigma\sigma'} c_{R,\sigma'}$$

$$\mathbf{J > 0}$$

Antifferomagnetic coupling

between mangetic impurity and host electrons

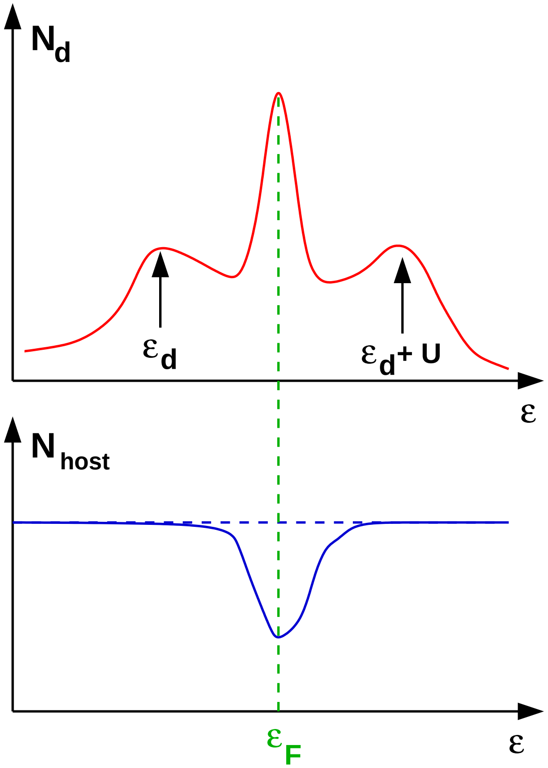
Kondo resonance



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.

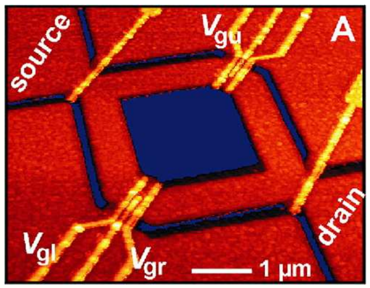
$$E_B \sim T_K$$

For $T < T_K$

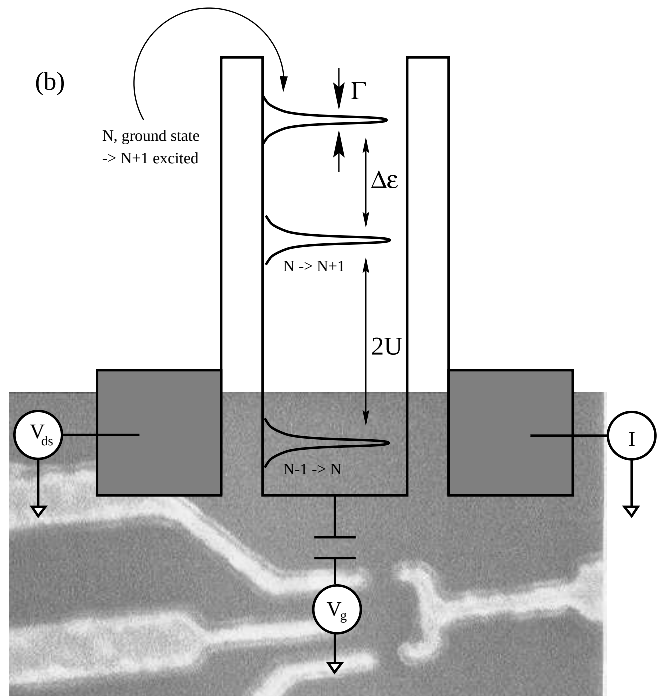


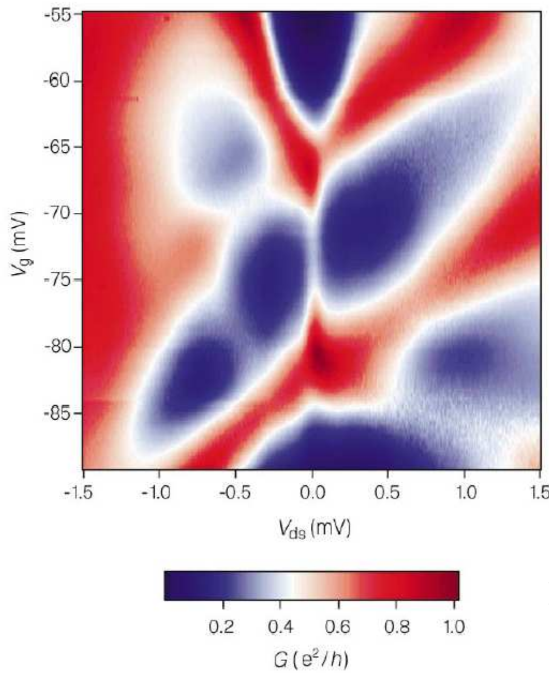
- For the impurity we have a resonant state for $\epsilon = 0$;
- For the host electrons the density of states at the Fermi energy is suppressed $\Longrightarrow$ increase of resistivity.

Nanostructures: Quatum Dots



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

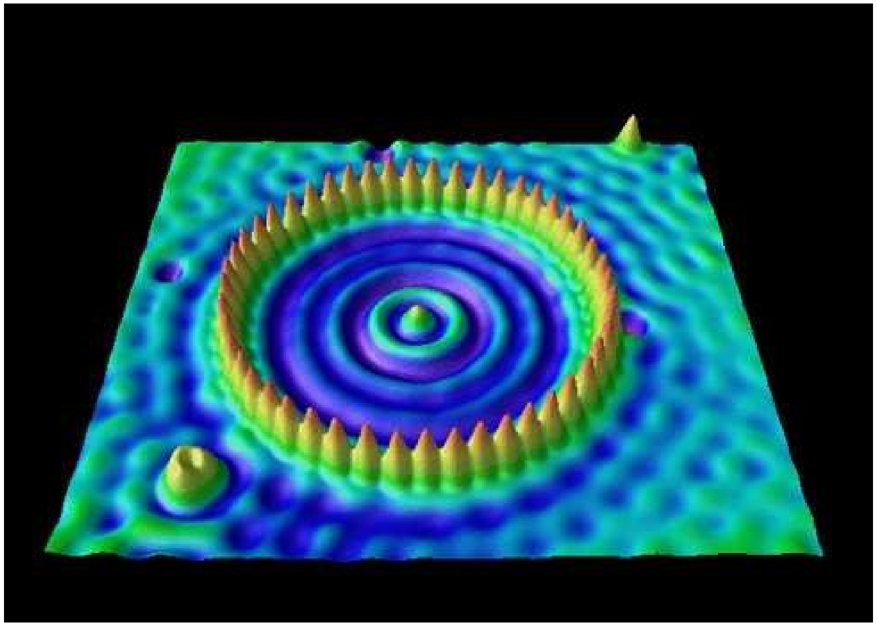




D. Golhaber−Gordon et al. Nature (1998)

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

Nanostructures: Quantum Corrals + Scanning Tunneling Microscopy (STM)



D. Eigler IBM

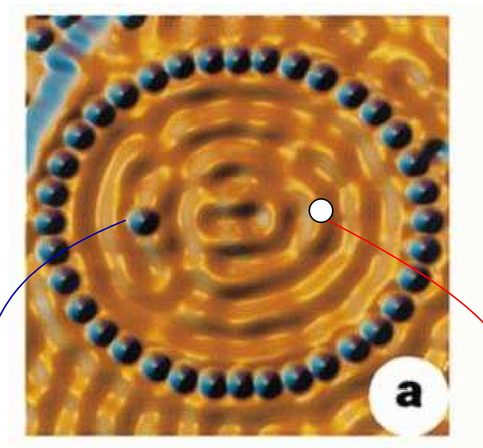
- **Atomic control of impurity position;**
- **By changing the size and/or shape of the corral, we can control the LDOS of conduction electrons;**
- **Direct observation of the LDOS.**

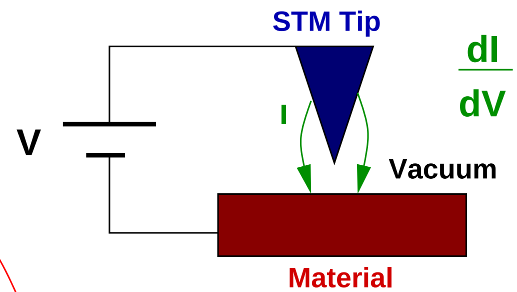
By combining advances in nanofabrication and new probes like STM we can now:

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

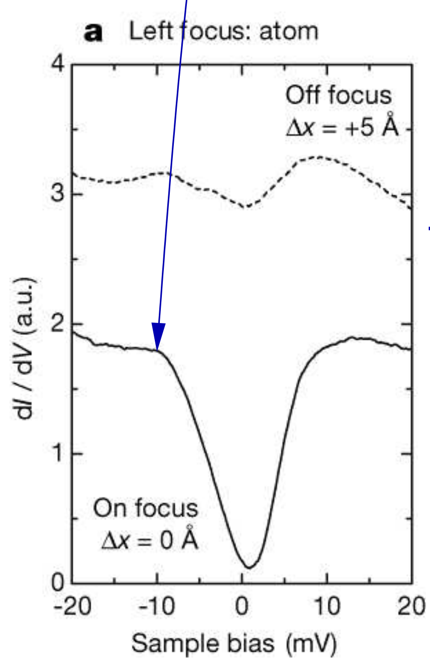
Creation of a quantum candle: Kondo resonance

Manhoran et al.
Nature 403, 512 (2000)

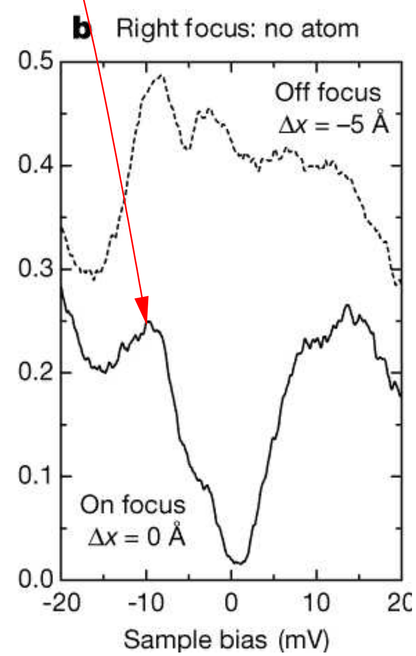




$$\frac{dI}{dV} = N(r,eV)$$



Kondo resonance in occupied focus

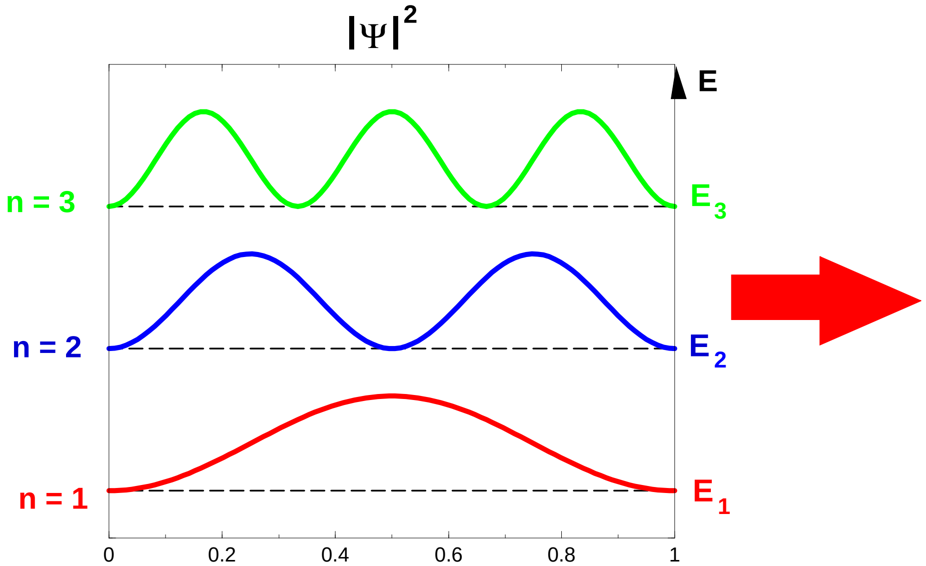


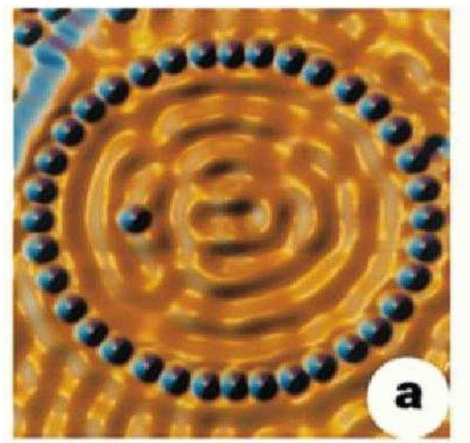
Quantum Image in unoccupied focus

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

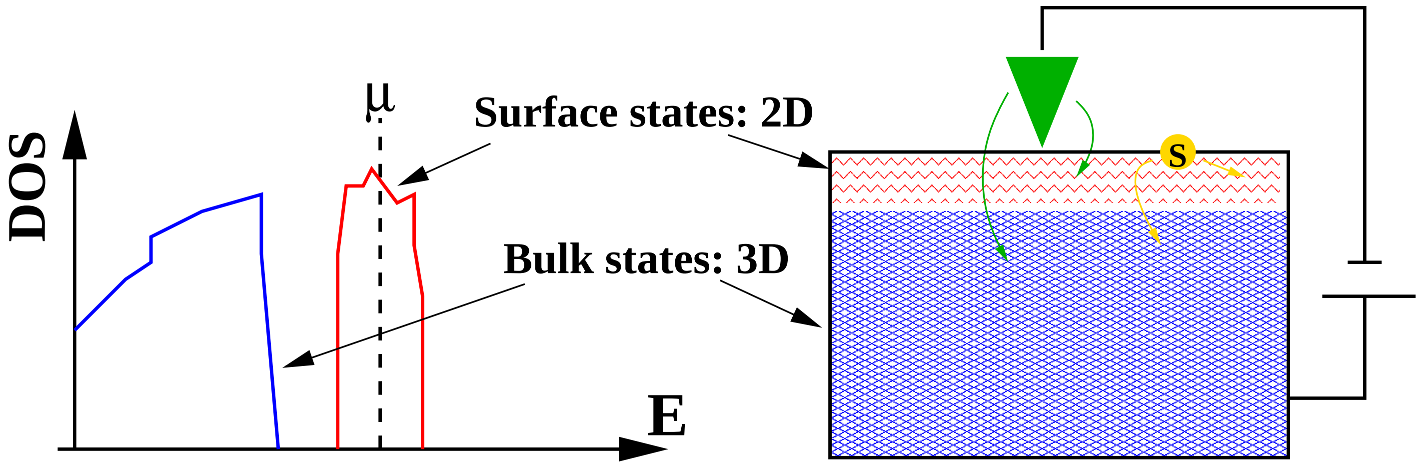
D.K. Morr and N. Stavropoulos, PRL (2004).

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:

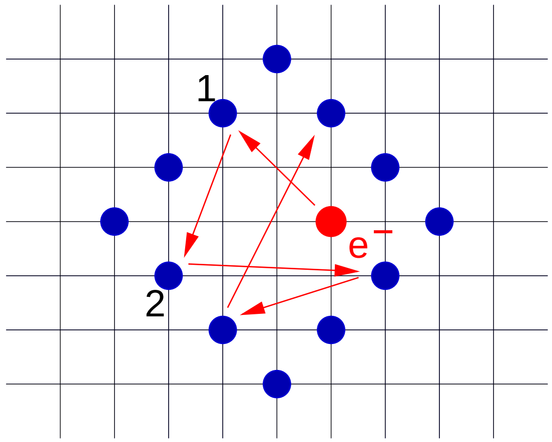
- Coupling surface-bulk states;
- Tip tunneling in part to bulk states;
- Coupling of the Kondo impurity to the bulk states (Knorr et al. PRL (2002))

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.

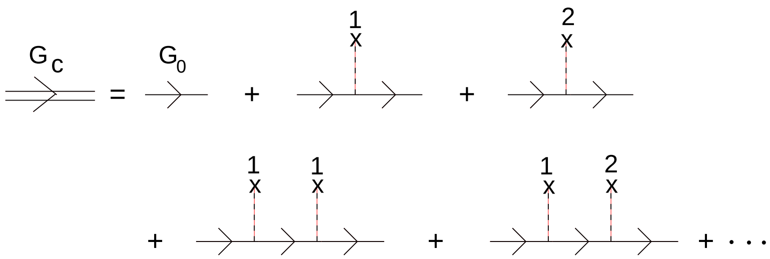


G_c, the Green's function for the conduction electrons in presence of the corral only is given by:

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

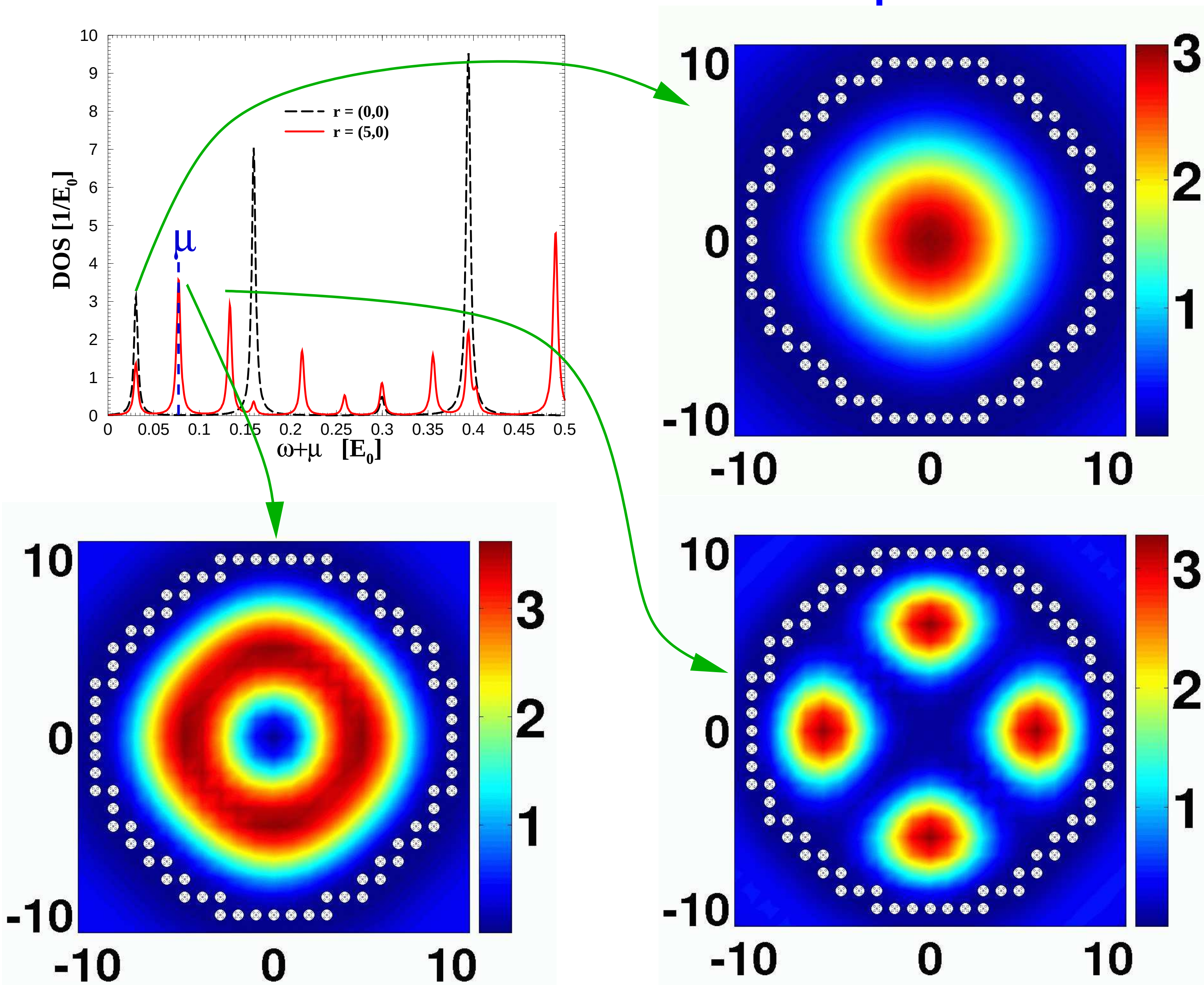
Where the T-matrix satis£es the Bethe-Salpeter equation:

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



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

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:

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

Decoupled using HS transformation

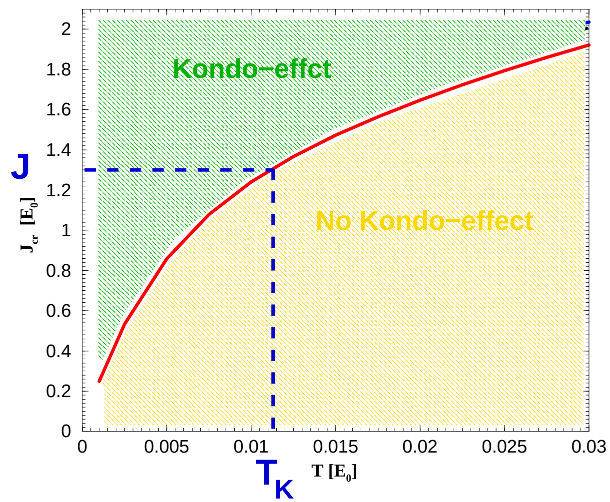
introduce HS field s

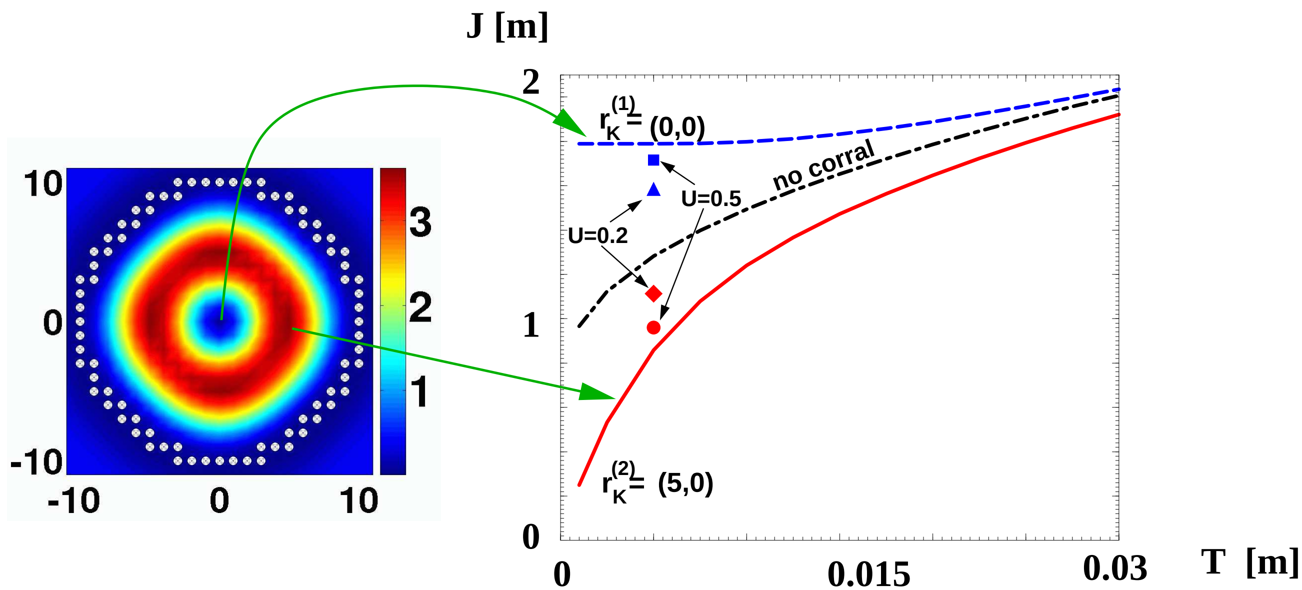
We then find an effective action, S_{eff}, function of two fields:

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

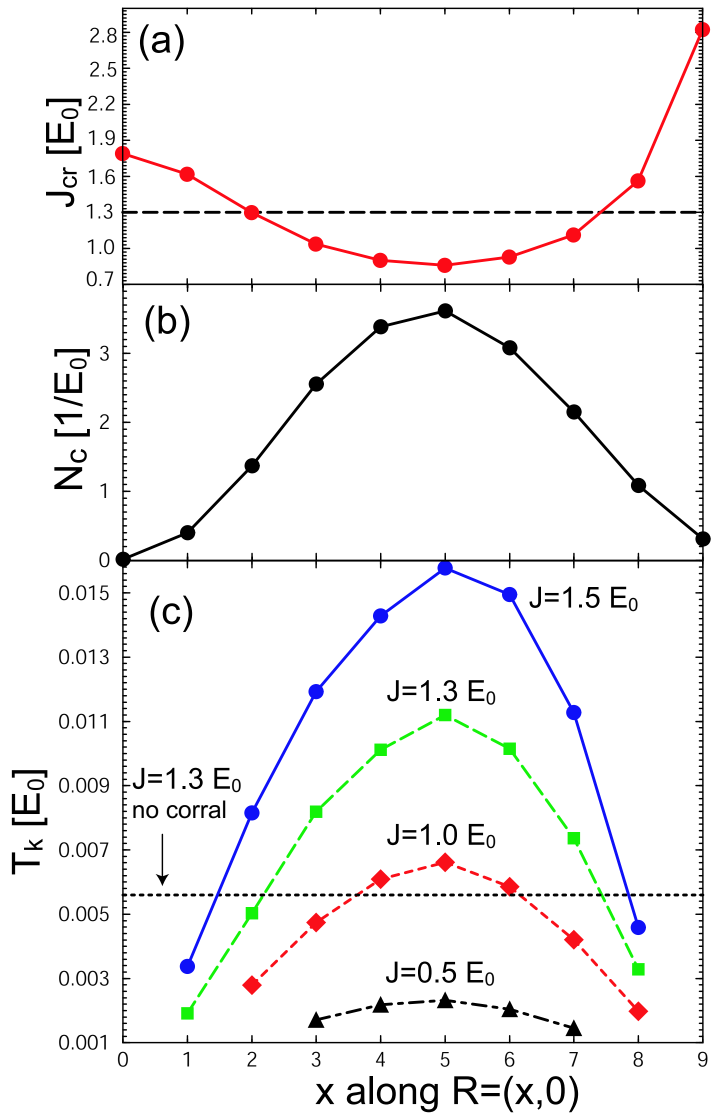
Critical Kondo coupling: J_{cr}

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.

E.R. and Dirk. K. Morr PRL (2006).

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:

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

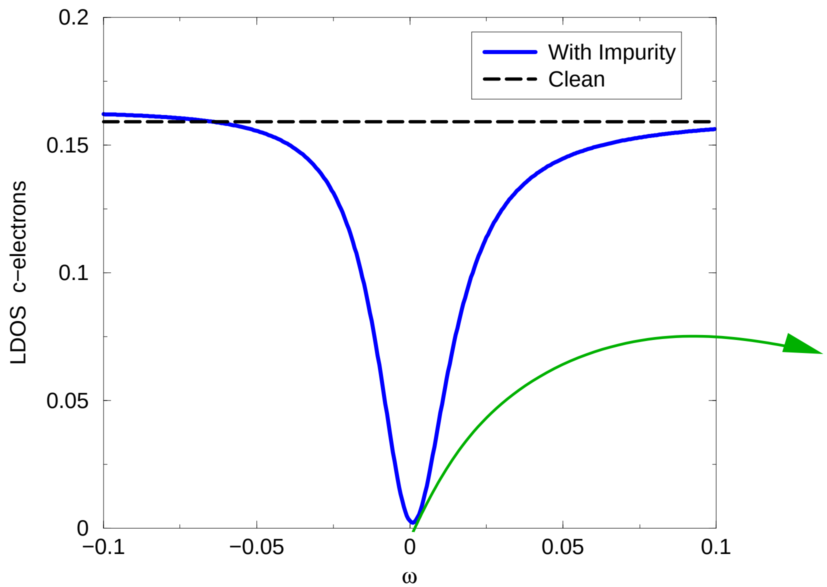
and for the host electrons:

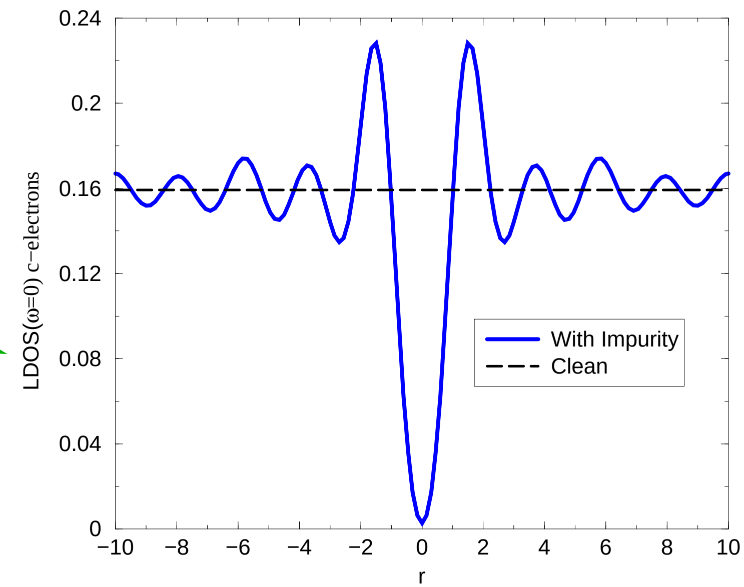
$$\boxed{G(\mathbf{r}, \mathbf{r}, i\omega_n) = G_c(\mathbf{r}, \mathbf{r}, i\omega_n) + s^2 G_c(\mathbf{r}, \mathbf{R}, i\omega_n) F(\mathbf{R}, i\omega_n) G_c(\mathbf{R}, \mathbf{r}, i\omega_n)}$$

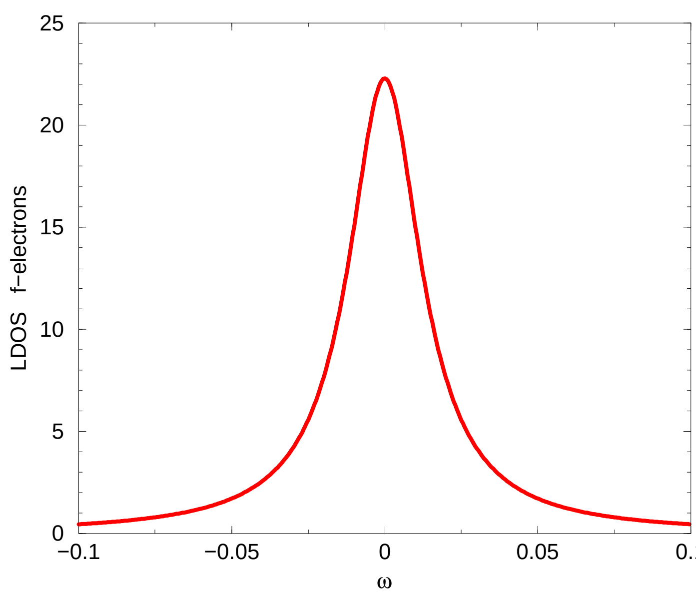
and then:

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

No corral

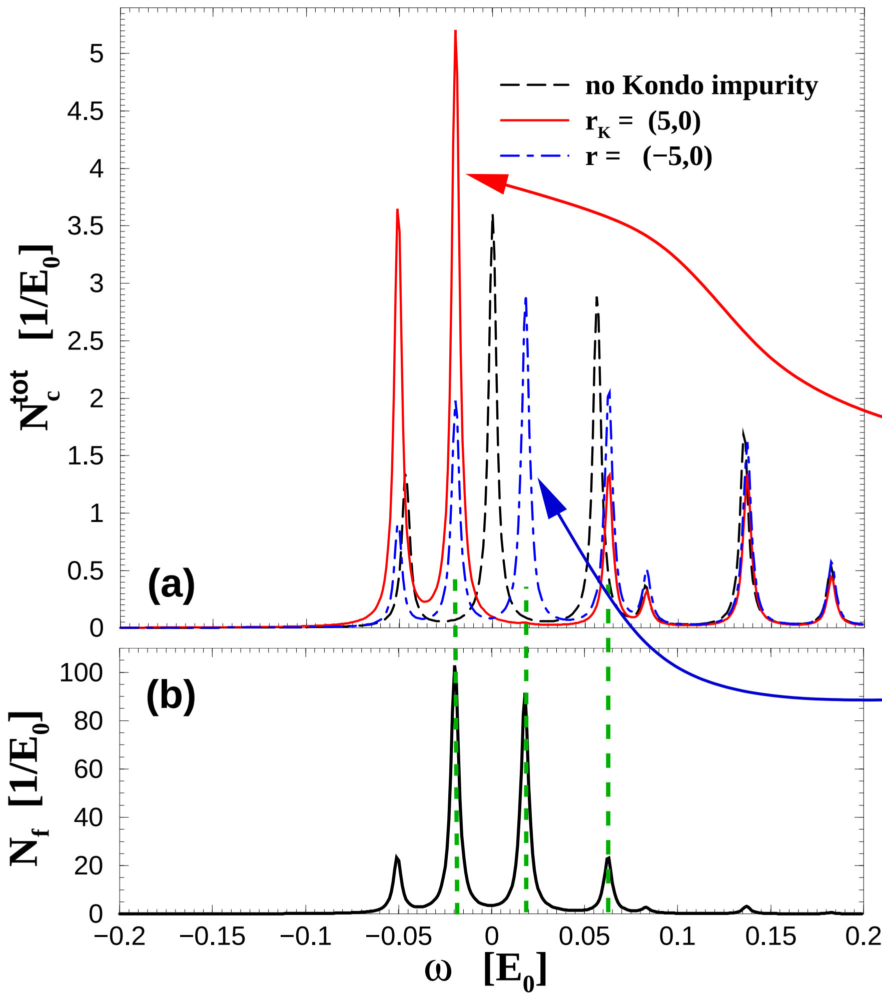




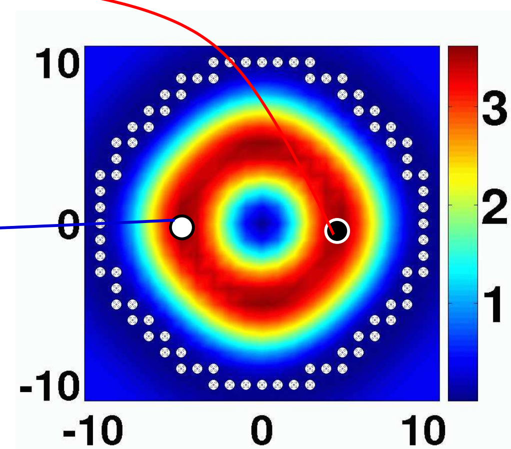


- Simple dip for c−electrons
- Peak for f−electrons
- Simple oscillations in real space

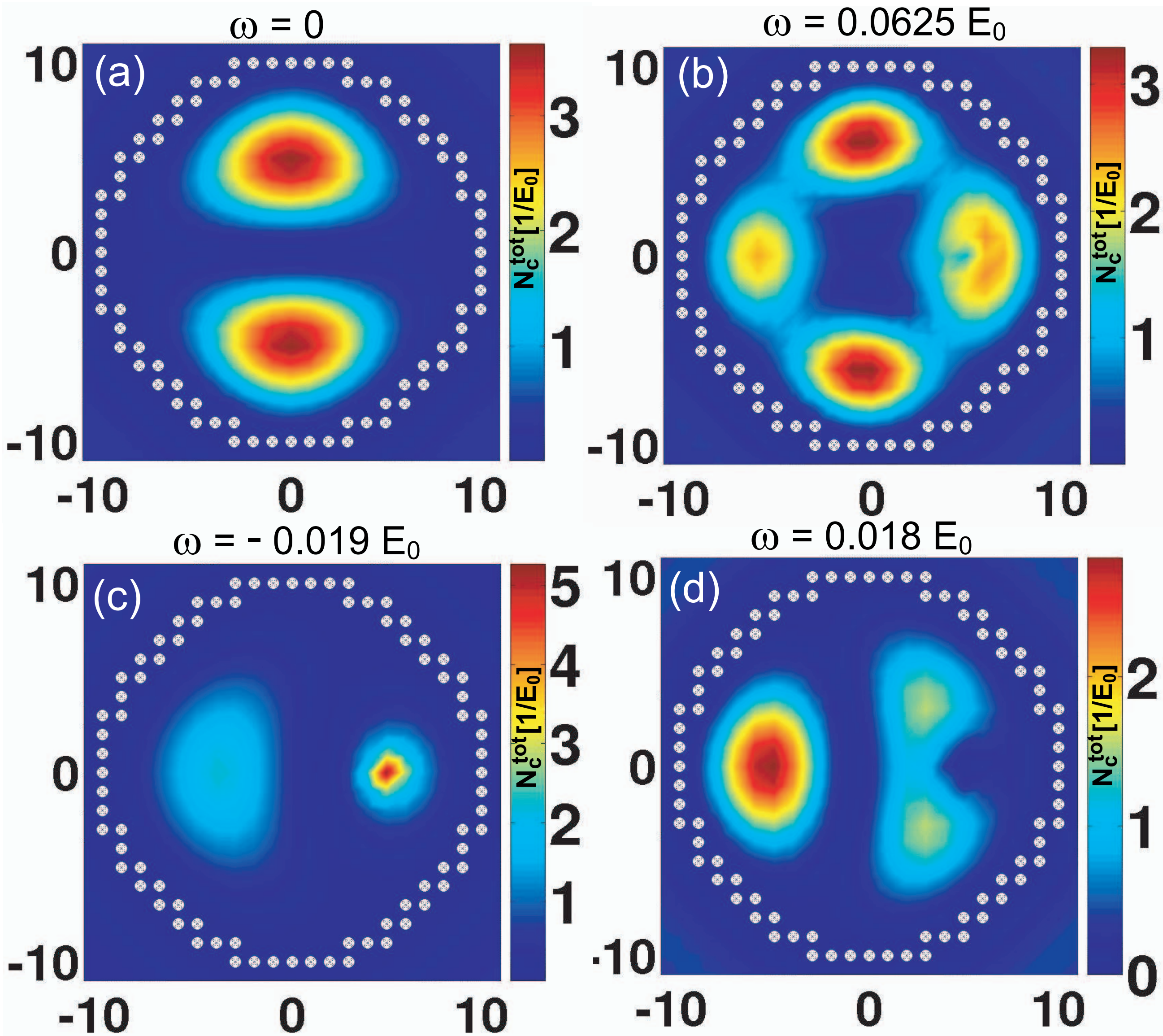
Kondo Resonances



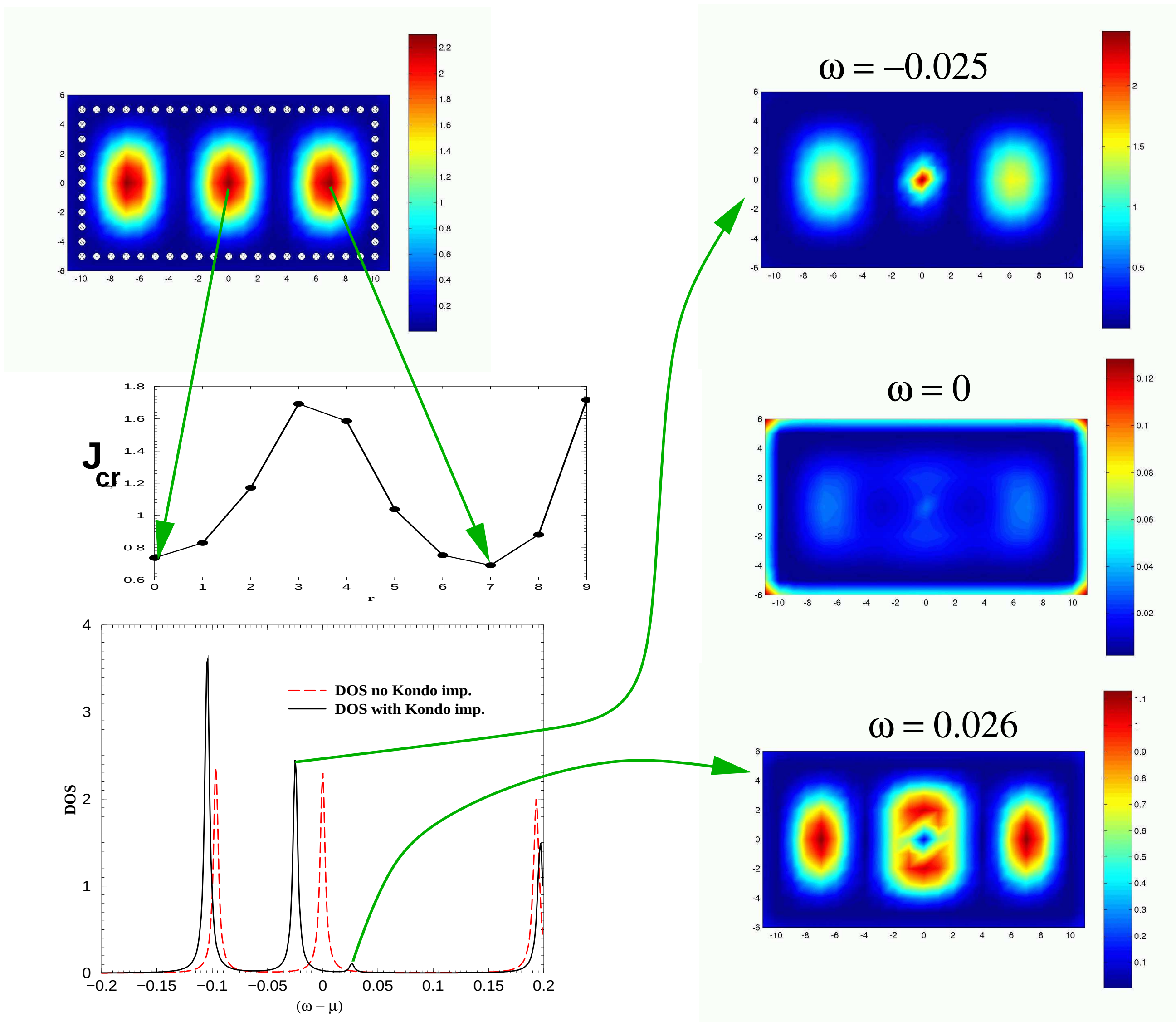
- Original mode decreased in amplitude; suppression of LDOS at $\omega = 0$
- Kondo resonaces also away from the magnetic impurity
- Additional resonances
  N modes ⟶ N + 1 Kondo resonances



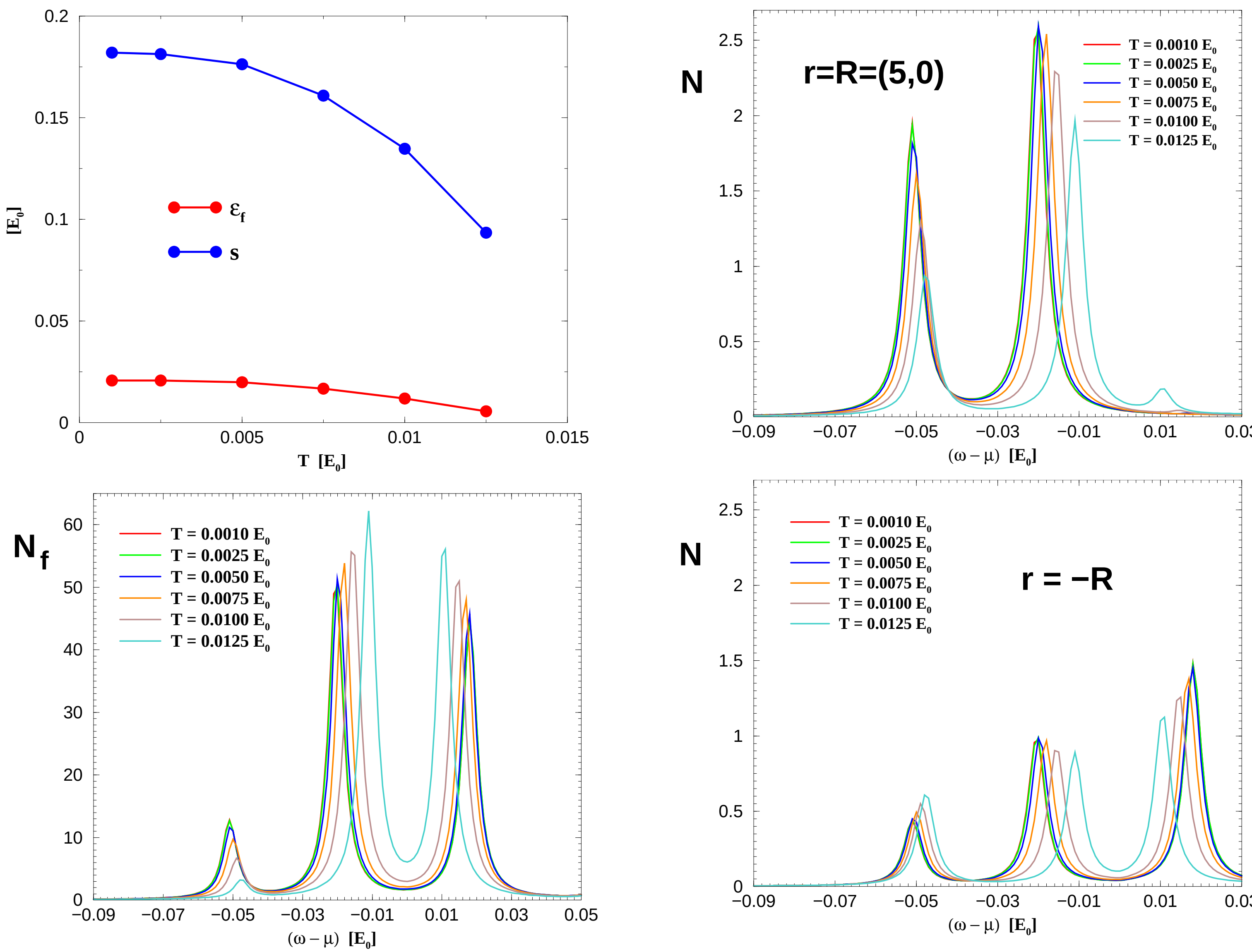
Spatial structure of Kondo resonances



Different geometries

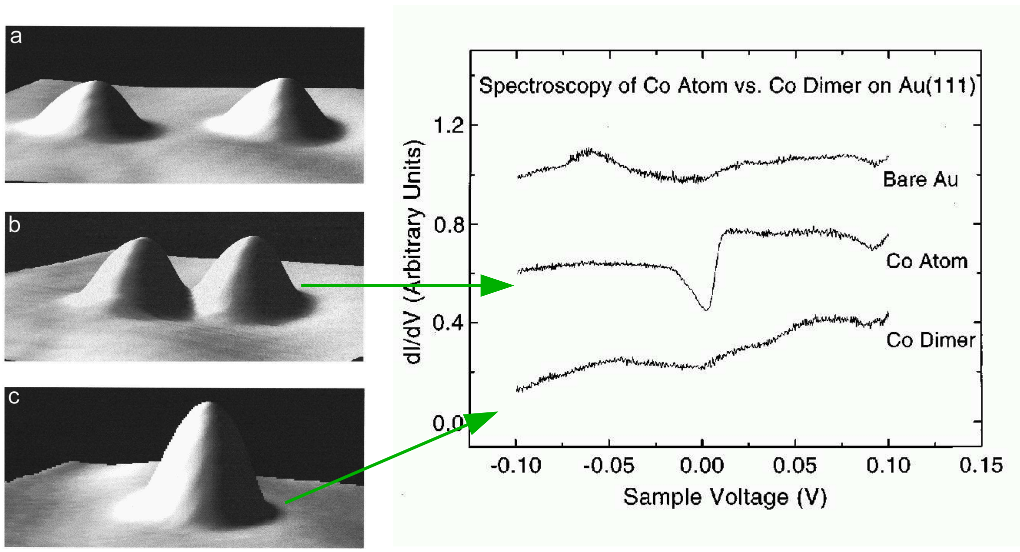


Temperature dependence of Kondo resonances

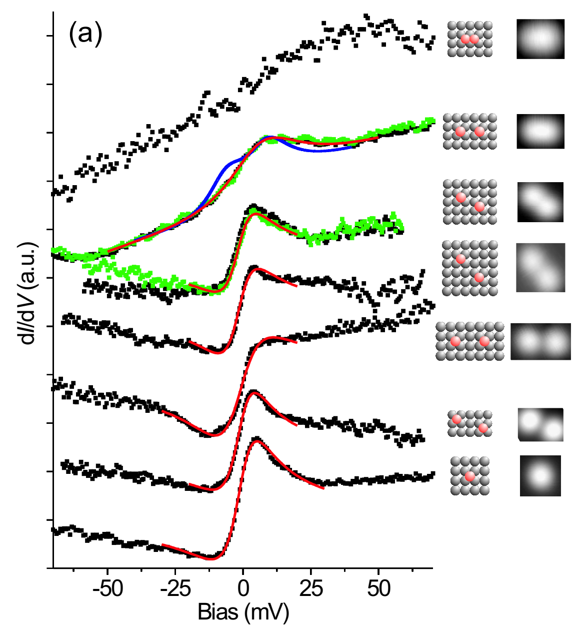


Future Directions

There are many possible extensions of the work presented. Motivated by recent experiments



W. Chen et al. PRB, 60 R8529 (1999)



P.Wahl et al PRL (2006)

we are now considering the problem of two or more impurities inside the corral.

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!