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 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

\[ H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\mathbf{k}\sigma} \left( c_{d\sigma}^{\dagger} c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^{\dagger} c_{d\sigma} \right) \]

\[ H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + J \sum_{\sigma\sigma'} S \cdot c_{R,\sigma}^{\dagger} \tau_{\sigma\sigma'} c_{R,\sigma'} \]

\( J > 0 \)

Antiferromagnetic 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 $\implies$ increase of resistivity.
Nanostructures: Quantum Dots

GaAs Quantum Dot.


- tune $\epsilon_d$;
- tune width of energy level, $\Gamma$;
- 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.

Kondo resonance in occupied focus

Quantum Image in unoccupied focus

\[
\frac{dl}{dV} = N(r,eV)
\]
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).

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:

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

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

We solve the problem in two steps:

Step 1: Compute the eigenmodes of quantum corral using

Generalized scattering theory


Step 2: Calculate effect of magnetic impurity using

large-N expansion

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:

$$G_c(r, r', i\omega_n) = G_0(r - r', i\omega_n) + \sum' G_0(r - r_j, i\omega_n) T_{jl}(i\omega_n) G_0(r_l - r', i\omega_n)$$

Where the $T$-matrix satisfies the Bethe-Salpeter equation:

$$T_{ij}(i\omega_n) = U\delta_{ij} + U\sum_l G_0(r_i - r_l, i\omega_n) T_{li}(i\omega_n).$$

$$N_c(r, \omega) = -\frac{2}{\pi} \text{Im}[G_c(r, r, \omega + i\delta)]$$
LDOS for corral with No Kondo impurities

DOS $[1/E_\mu]$ for different positions $r = (0,0)$ and $r = (5,0)$.
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 $S$ of the magnetic impurity in terms of fermionic operators, $f_m^\dagger, f_m$:

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

with the constraint:

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

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

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

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;
- $\epsilon_f$: Lagrange multiplier to impose the constraint.
Critical Kondo coupling: $J_{cr}$

For the fields $s$ and $\epsilon_f$ 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.
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 find the values of $s$ and $\epsilon_f$. 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:

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

and for the host electrons:

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

and then:

$$N_f(R, \omega) = -\frac{N}{\pi} \text{Im}[F(R, \omega + i\delta)]; \quad N(r, \omega)^{\text{tot}} = -\frac{2}{\pi} \text{Im}[G(r, r, \omega + i\delta)];$$
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 $\rightarrow N + 1$ Kondo resonances

### Figure

- (a) Suppression of LDOS at $\omega = 0$
- (b) Kondo resonances also away from the magnetic impurity

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Spatial structure of Kondo resonances

\( \omega = 0 \)

\( \omega = 0.0625 \ E_0 \)

\( \omega = -0.019 \ E_0 \)

\( \omega = 0.018 \ E_0 \)
Different geometries

\[ J_{cr} \]

\[ \omega = -0.025 \]

\[ \omega = 0 \]

\[ \omega = 0.026 \]

DOS no Kondo imp.

DOS with Kondo imp.
Temperature dependence of Kondo resonances

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Future Directions

There are many possible extensions of the work presented. Motivated by recent experiments, we are now considering the problem of two or more impurities inside the corral.

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

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!