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

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Enrico Rossi

Collaborators: Dirk K. Morr, Roy H. Nyberg
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.


- **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 $\rightarrow$ 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.

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

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

\[ J \sum_{\sigma\sigma'} S \cdot \hat{c}_{R,\sigma}^\dagger \hat{t}_{\sigma\sigma'} \hat{c}_{R,\sigma'} \]

\( J > 0 \)

Antiferromagnetic coupling between magnetic impurity and host electrons
**Kondo resonance**

The antiferromagnetic interaction $\mathbf{J}$ 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 $\rightarrow$ increase of resistivity.
Nanostructures: Quantum Dots

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


- tune $\epsilon_d$;
- tune width of energy level, $\Gamma$;
- tune $U$;
Nanostructures: Quantum Corrals + Scanning Tunneling Microscopy (STM)

D. Eigler  IBM

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

- 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.

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Creation of a quantum candle: Kondo resonance

Manhoran et al.

Kondo resonance in occupied focus

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

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).

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:

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

free electrons  corral scatterers  magnetic impurity
non-magnetic

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:

\[
G_c(r, r', i\omega_n) = G_0(r - r', i\omega_n) + \sum_{j,l} G_0(r - r_j, i\omega_n) T_{jl}(i\omega_n) G_0(r_l - r', i\omega_n)
\]

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

\[
\text{DOS } \frac{1}{E_0} \quad r = (0,0) \quad r = (5,0)
\]

\[\mu\]

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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:

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

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

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

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;
- $\epsilon_f$: 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.
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 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:

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

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Spatial structure of Kondo resonances

\[
\omega = 0
\]

(a)

\[
\omega = 0.0625 \, E_0
\]

(b)

\[
\omega = -0.019 \, E_0
\]

(c)

\[
\omega = 0.018 \, E_0
\]

(d)
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);**

- **Charge density wave (CDW)**
  - ARPES, STM: J. Tranquada

- **Phonon**
Impurities as probes of collective behavior

\[
H = H_0 - JS \cdot s_c(R) + V_0 n_c(R)
\]

\[
\langle s_z(r) \rangle = \langle s_c^z(r) \rangle + \langle S_{imp}^z \rangle \delta_{r,R}; \quad \delta\langle n(r) \rangle = \langle \delta n_c(r) \rangle + \delta_{r,R}
\]

\begin{align*}
\chi_s(q, \omega = 0) &= \frac{\chi_0}{(\xi_s^{-2} + (q - Q)^2)} \\
\chi_c(q, \omega = 0) &= \frac{\chi_0}{(\xi^{-2} + q^2)}
\end{align*}

\[
Q = (\pi, \pi) \quad \xi_s = \xi_c = 5 \ a_0
\]
Model

\[ \mathcal{H} = \sum_{\mathbf{r}, \mathbf{r}', \alpha} t_{\mathbf{r} \mathbf{r}'} c_{\mathbf{r}, \alpha}^\dagger c_{\mathbf{r}', \alpha} + \sum_{\mathbf{r}, \mathbf{r}'} \left[ \Delta(\mathbf{r}, \mathbf{r}') c_{\mathbf{r}, \uparrow}^\dagger c_{\mathbf{r}', \downarrow}^\dagger + h.c. \right] \\
- \sum_{\mathbf{r}, \sigma, \sigma'} \left[ g_s \langle s_z(\mathbf{r}) \rangle \sigma_{\alpha \beta} - g_c \langle \delta n(\mathbf{r}) \rangle \delta_{\alpha \beta} \right] c_{\mathbf{r}, \alpha}^\dagger c_{\mathbf{r}', \beta}^\dagger \]

Interaction of conduction electrons with droplet pinned by impurity

where

\[ \langle s_z(\mathbf{r}) \rangle = \langle s_z^c(\mathbf{r}) \rangle + \langle S_{\text{imp}}^z \rangle \delta_{\mathbf{r}, \mathbf{R}} \]
\[ \delta \langle n(\mathbf{r}) \rangle = \langle \delta n_c(\mathbf{r}) \rangle + \delta_{\mathbf{r}, \mathbf{R}} \]

- 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 \( \max |\Delta(\mathbf{r}, \mathbf{r}')| = 30 \text{ meV} = 0.1 \ t \) 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 $\rightarrow$ High Resolution for the LDOS at low energies.
  - The superconducting order parameter $\Delta_0$ is assumed fixed: not calculated self consistently

- **Bogoliubov de Gennes (BdG)**
  - $\Delta_0$ is calculated self-consistently
  - Limited to small size systems $\rightarrow$ Low Resolution for LDOS at low energies
BdG approach

Within the BdG approach one solves the eigenvalue equation:

\[
\sum_{r'} \begin{pmatrix} H_{rr'}^+ & \Delta_{rr'} \\
\Delta_{rr'}^* & -H_{rr'}^-
\end{pmatrix} \begin{pmatrix} u_{r',n} \\
v_{r',n}
\end{pmatrix} = E_n \begin{pmatrix} u_{r,n} \\
v_{r,n}
\end{pmatrix}
\]

where

\[
H_{rr'}^{\pm} = t_{rr'} + (\pm g_s \langle s_z (r) \rangle - g_c \langle V(r) \rangle - \mu) \delta_{r,r'}
\]

and \( \Delta_{rr'} \) is calculated self consistently:

\[
\Delta_{rr'} = -\frac{V}{2} \sum_n (u_n(r)v_n(r') + u_n(r')v_n(r)) \tanh \left( \frac{E_n}{2k_BT} \right),
\]

The LDOS at \( r \) is finally given by:

\[
N(\omega, r) = \sum_n \left[ u_n^2(r) \delta(\omega - E_n) + v_n^2(r) \delta(\omega + E_n) \right]
\]
T-matrix results

**Spin Droplet**

\[ g_s \langle S^z_{\text{imp}} \rangle = 400 \text{ meV}; \quad g_c = 0 \]

**Charge Droplet**

\[ g_s \langle S^z_{\text{imp}} \rangle = 0; \quad g_c = 400 \text{ meV} \]
BdG result for $\Delta_0$: magnetic case

Single Impurity

Spin-droplet

$\Delta_0$ 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 $\Delta_0$.
  At the center we have effective decrease of scattering strength.
- BdG results show $\pi$ phase shift at $\approx 10 a_0$ from center.

Only minor differences
Spin-droplet: spin resolved results
Effect of magnetic field

\[ \langle S_{imp}^z \rangle = \frac{CH}{T + \Theta}; \quad H_0 \rightarrow 2H_0 \implies \langle S_{imp}^z \rangle \text{ two times bigger} \]

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.
Conclusions

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

- **Magnetic impurity** $\rightarrow$ **Spin-droplet**
- **Charge impurity** $\rightarrow$ **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 $\Delta_0$: charge case

Single Impurity

charge-droplet

$\Delta_0$ recovers in only 2-3 lattice spacings.