Kondo Effect in Quantum Dots

Seminar: Nanoscopic Systems

29. 7. 2005

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Outline

1. What is the Kondo effect?
2. Calculation of the Kondo effect for a single magnetic impurity
3. ″Poor Man's Scaling″ - A renormalization group approach
4. Investigation of the Kondo effect in quantum dots
5. Conclusion

1. What is the Kondo effect?

- Resistivity is dominated by phonon scattering for $T \gg 0$
- In most metals the resistivity decreases monotonically for $T \to 0$
- But: resistance minimum in some metals for $T \to 0$
- **Kondo effect**: Resonant spin flip scattering at local magnetic impurities
- Influences transport properties

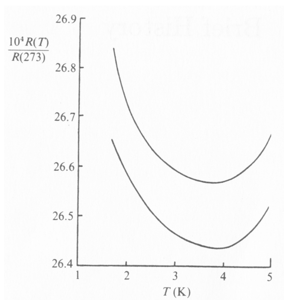


Figure 1: Minimum in the resistivity of Au (de Haas, de Boer and van den Berg, 1934)

2. Calculation for a single local magnetic impurity

Hamiltonian

Kondo's assumption:
a local magnetic moment associated with a spin S
which is coupled via an exchange interaction with the conduction band electron.

$$
\begin{aligned}
H &= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} J(\omega) \left(S^+ s^- + S^- s^+\right) + J_z(\omega) S_z s_z \\
&= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} \sum_{k,k'} J(\omega) \left(S^+ c^\dagger_{k\downarrow} c_{k'\uparrow} + S^- c^\dagger_{k\uparrow} c_{k'\downarrow}\right) + J_z(\omega) S_z \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow}\right)
\end{aligned}
$$

S = local impurity spin   s = conduction electron spin

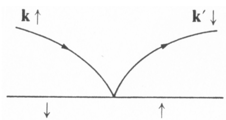


Figure 2: Spin flip scattering of a localized impurity moment by a conduction electron

Perturbative approach

- $T > 0 \Longrightarrow$ expectation values can't be taken with respect to the ground state
- Appropriate: **Matsubara Method**

Starting point: $H = H_0 + V(t)$ with

$$V(t) = \frac{1}{2} J_1(\omega) \left(S^+ s^- + S^- s^+ \right) + J_z(\omega) S_z s_z$$

Generalized **Wick Theorem** for n particle Green's function:

$$\langle T_\tau (UVW...XYZ) \rangle^{(0)} = \{fully\ contracted\ terms\}$$

Problem:

- Wick's theorem only valid for operators, whose commutator is a c-number
- Not the case for the impurity spin,
  obeying the standard commutation relations of angular momentum

Pseudo fermion method

Representation of $S^{\pm}$, S_z through canonical field operators

In formulas: $\vec{S} = \sum_{\sigma\sigma'} f_\sigma^\dagger \vec{S}_{\sigma\sigma'} f_{\sigma'}$

for example:

$$S_z|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle \quad \text{corresponds to} \quad \frac{1}{2}\left(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow\right)|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle$$

Problem: artificially enlarged Fock space
$\Longrightarrow$ project out the unphysical part with the following constraint

$$Q = \sum_\sigma f_\sigma^\dagger f_\sigma = 1$$

All physical relevant quantities depend on the partition function :

$$Z_c = \lim_{\lambda\to\infty} tr\left[Q\, e^{-\beta(H+\lambda(Q-1))}\right]$$

Evaluation of Wick's theorem

Two particle interaction using the pseudo fermions:

$$V(t) \quad = \quad \sum_{klmn} \frac{1}{2} v(kl;nm)\, f_k^\dagger f_l\, c_m^\dagger c_n \qquad\qquad k,l,m,n \in \{\uparrow,\downarrow\}$$

Two particle correlation function looks like:

$$\propto \quad \left\langle T_\tau \left(\widehat{V}\, f_{k_1}^\dagger f_{l_1}\, c_{m_1}^\dagger c_{n_1}\, \widehat{V}\, f_{k_2}^\dagger f_{l_2}\, c_{m_2}^\dagger c_{n_2}\, f_k^\dagger f_l\, c_m^\dagger c_n \right) \right\rangle$$

Remember:

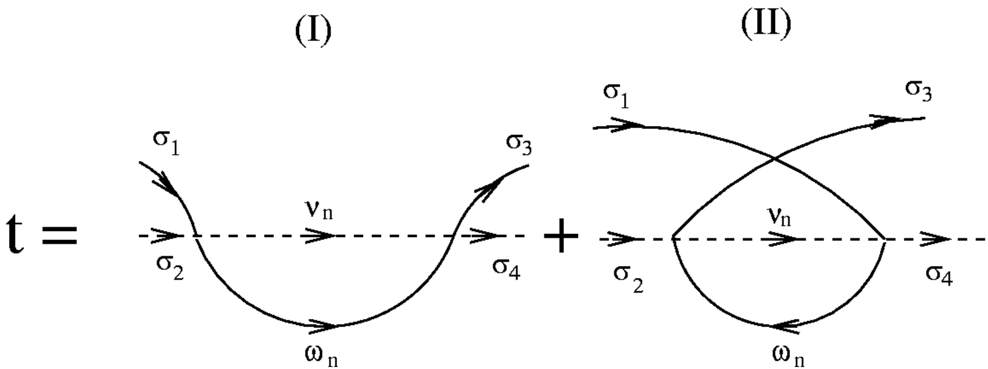
- any contraction between a pseudo and a fermion operator = 0
- $contraction(f_k f_l^\dagger) \propto \delta_{kl}$

$\Longrightarrow$ **just two fully contracted terms survive,**

corresponding to two diagrams

Diagrams

The scattering matrix is defined as the sum of diagram (I) and (II)



- Solid lines: bare electron operators
- Dashed lines: impurity pseudo fermion operators

Evaluation of the diagrams

Vertex part of the diagrams:

$$\begin{aligned}(I) \quad = \quad & -\frac{1}{\beta}\frac{1}{4}\sum_{\sigma,\tau,\omega_n,k}\left[J_1\left(\langle\tau|S^+|\sigma_2\rangle\langle\sigma|s^-|\sigma_1\rangle + \langle\tau|S^-|\sigma_2\rangle\langle\sigma|s^+|\sigma_1\rangle\right) + 2J_z\langle\tau|S^z|\sigma_2\rangle\langle\sigma|s^z|\sigma_1\rangle\right] \\ & \cdot\left[J_1\left(\langle\sigma_4|S^+|\tau\rangle\langle\sigma_3|s^-|\sigma\rangle + \langle\sigma_4|S^-|\tau\rangle\langle\sigma_3|s^+|\sigma\rangle\right) + 2J_z\langle\sigma_4|S^z|\tau\rangle\langle\sigma_3|s^z|\sigma\rangle\right] \\ & \cdot G_{k\sigma}(i\omega_n)g_\tau(i\omega - i\omega_n)\end{aligned}$$

$$\begin{aligned}(II) \quad = \quad & -\frac{1}{\beta}\frac{1}{4}\sum_{\sigma,\tau,\omega_n,k}\left[J_1\left(\langle\tau|S^+|\sigma_2\rangle\langle\sigma_3|s^-|\sigma\rangle + \langle\tau|S^-|\sigma_2\rangle\langle\sigma_3|s^+|\sigma\rangle\right) + 2J_z\langle\tau|S^z|\sigma_2\rangle\langle\sigma_3|s^z|\sigma\rangle\right] \\ & \cdot\left[J_1\left(\langle\sigma_4|S^+|\tau\rangle\langle\sigma|s^-|\sigma_1\rangle + \langle\sigma_4|S^-|\tau\rangle\langle\sigma|s^+|\sigma_1\rangle\right) + 2J_z\langle\sigma_4|S^z|\tau\rangle\langle\sigma|s^z|\sigma_1\rangle\right] \\ & \cdot G_{k\sigma}(i\omega_n)g_\tau(-i\omega + i\omega_n)\end{aligned}$$

where the free Matsubara Green's functions for electrons and pseudo fermions are :

$$G_{k\nu}(i\omega_n) = \frac{1}{i\omega_n - \epsilon_k} \qquad g_\tau(i\nu_n) = \frac{1}{i\nu_n - \lambda}$$

Simplifications

- Sum over Matsubara Frequencies
  Fermionic Matsubara Frequencies correspond to singularities of Fermi distribution
  $\Longrightarrow$ The sum can be replaced by a contour integral:

$$(I) \propto -\frac{1}{\beta}\sum_{\omega_n}\frac{1}{i\omega_n-\epsilon_k}\cdot\frac{1}{i\omega-i\omega_n-\lambda}=\oint\frac{dz}{2\pi i}f(z)\frac{1}{z-\epsilon_k}\cdot\frac{1}{i\omega-z-\lambda}=\frac{f(-\lambda)-f(\epsilon_k)}{i\omega-\epsilon_k-\lambda}$$

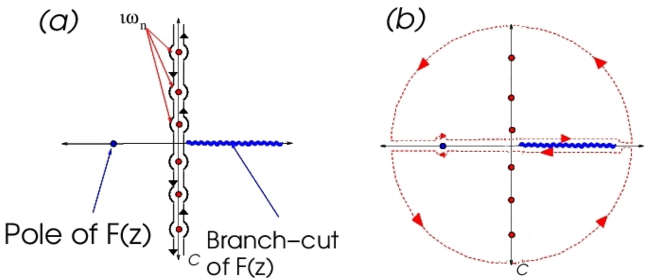


Figure 3: $\frac{1}{\beta}\sum_n F(i\omega_n)=-\oint\frac{dz}{2\pi i}F(z)f(z)$

Further simplifications

- Pseudo fermion energy is gauged to get rid of the λ in the denominator Constraint Q allows a U(1) gauge symmetry for this energy

  $\left(f' = e^{i\alpha} f \Rightarrow f'^{\dagger} f' = f^{\dagger} f\right)$

$$i\omega \rightarrow \omega + \lambda \qquad\qquad i\omega \rightarrow \omega - \lambda$$

- Project out unphysical part by $\lambda \rightarrow \infty$, using $\lim_{\lambda\rightarrow\infty} f(-\lambda) = 1$

$$(I) \quad \longrightarrow \quad \sum_k \frac{1 - f(\epsilon_k)}{\omega - \epsilon_k}$$

$$(II) \quad \longrightarrow \quad \sum_k \frac{f(\epsilon_k)}{\omega - \epsilon_k}$$

- Evaluation of the spin sum using
  - Completeness relations
  - Spin algebra

Second order term of the scattering matrix

$$t^{(2)} = \frac{1}{2} J^2 \langle \sigma_4 | \vec{S} | \sigma_2 \rangle \langle \sigma_3 | \vec{s} | \sigma_1 \rangle \sum_k \frac{1 - 2f(\epsilon_k)}{\omega - \epsilon_k} + \frac{3}{16} J^2 \langle \sigma_4 | \sigma_2 \rangle \langle \sigma_3 | \sigma_1 \rangle \sum_k \frac{1}{\omega - \epsilon_k}$$

- Evaluation of the k-sum
  (assuming a constant density N(0) for the conduction electrons):

$$\begin{aligned} -\sum_k \frac{1 - 2f(\epsilon_k)}{\omega - \epsilon_k} &= N(0) \int_{-D}^{D} d\epsilon \, \frac{\tanh(\epsilon/2T)}{\epsilon - \omega} \\ &\cong 2N(0) \ln \frac{D}{max(|\omega|, T)} \end{aligned}$$

For electrons near the Fermi surface $(\omega = 0)$ and small temperatures T the result is:

$$t^{(2)} = N(0) J^2 \langle \sigma_4 | \vec{S} | \sigma_2 \rangle \langle \sigma_3 | \vec{s} | \sigma_1 \rangle ln \left(\frac{D}{T} \right)$$

Scattering matrix and resistivity

- The resistivity is connected to the scattering matrix via:

$$\rho(T) \propto |t|^2$$

Scattering matrix:

$$\begin{aligned} t &= J\,\vec{S}\,\vec{s}\left(1 + N(0)\;J\;ln\left(\frac{D}{T}\right)\right) \\ \Longrightarrow\;\rho(T) &\propto \left(1 + 2N(0)\;J\;ln\left(\frac{D}{T}\right)\right) \end{aligned}$$

- Problem:
  This term for the resistivity is divergent for $T \to 0$

- Perturbation theory breaks down,
  when the 2^{nd} order term becomes $\simeq$ 1^{st} order term

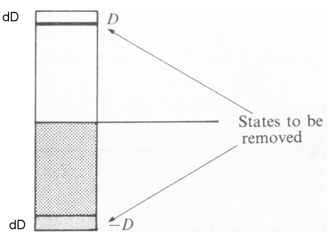
- This limit defines the so called **Kondo temperature**:

$$T_k = De^{-\frac{1}{2N(0)J}}$$

3. "Poor Man's Scaling" - A renormalization group approach

- Anderson's idea:
  Use scaling to continue the perturbative approach to small temperatures $(T < T_K)$
- Idea: reduce the bandwidth D of the conduction band
- Constraint: The underlying physical quantity, the scattering matrix t, stays invariant
- $\Longrightarrow$ Coupling constants $(J_1,\ J_z)$ change with bandwidth D

$$\begin{aligned} t &= V + VP_{dD}G_0t + V(1-P_{dD})G_0t \\ \Rightarrow t &= V' + V'(1-P_{dD})G_0t \qquad\qquad \textit{with} \quad V' = V + P_{dD}G_0V = V + dV \end{aligned}$$



Renormalization

Evaluating the integral for the reduced bandwidth:

$$\int_{int} d\epsilon \frac{\tanh(\epsilon/2T)}{\epsilon-\omega} \quad = \quad \int_{-D}^{D} d\epsilon \, \frac{\tanh(\epsilon/2T)}{\epsilon-\omega} - \int_{-(D-dD)}^{D-dD} d\epsilon \, \frac{\tanh(\epsilon/2T)}{\epsilon-\omega} = 2d(lnD)$$

Change of the potential term

$$dV = -2N(0)\left[\frac{1}{2}J_z J_1 \left(S^+ s^- + S^- s^+\right) + J_1^2 S^z s^z\right] d(lnD)$$

Renormalization Group Equations:

$$\frac{dJ_z}{d\,lnD} \quad = \quad -2N(0)J_1^2 \qquad\qquad \frac{dJ_1}{d\,lnD} = -2N(0)J_z J_1$$

In the physical state $(J_1 = J_z)$ this leads to one analytically soluble differential equation:

$$J(D) = \frac{1}{\frac{1}{J_0} + 2N(0)ln(\frac{D}{D_0})}$$

$\rightarrow$ Divergent for $T = T_K$

Physical consequences

- Low temperature regime corresponds to diverging coupling constant
- Since $J \to \infty$ the impurity and conduction electron spin have to allign antiparallel to minimize the total energy
- For $T \to 0$ local impurity spin forms a singlet with a conduction electron
- Local impurity spin is screened by the conduction electrons
- Behaves like a non-magnetic one
- Saturation of the resistivity becomes explicable

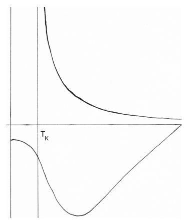


Figure 4: Sketch of the coupling constant and the resistance minimum versus temperature

4. Investigation of the Kondo effect in quantum dots

Quantum Dot

- Small solid-state device
- Single electron transistor (SET)
- Contains confined 'droplet' of electrons
- Integer number of electrons N
- Artificial atom

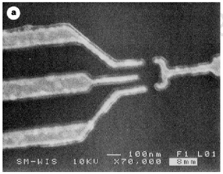


Figure 5: Scanning electron microscope image of a SET

(Picture taken from: D. Goldhaber-Gordon, H. Shtrikman et al.: "Kondo effect in a single-electron transistor", Nature vol 391, 156 (1998).)

Transport in detail

- Tunable tunnel coupling to the leads
- Has a single spin-degenerate energy state ϵ_0
- Occupied by one electron with spin up or down
- First order tunneling is blocked by the coulomb blockade
- Virtual tunnel events with an effective spin-flip are possible
- Successive spin-flip processes screen the local spin on the dot

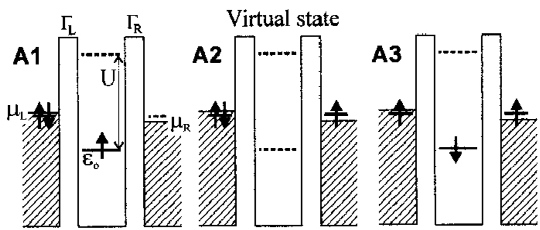


Figure 6: Possible virtual tunnel event

Why is a quantum dot a Kondo system?

- For an odd number of electrons the dot has a net spin magnetic moment
  For an even number of electrons it is no Kondo system
- Individual artificial magnetic impurity
- Spin singlet state is formed between the unpaired localized electron and delocalized electrons in the leads
- Quantum dot has a narrow-resonance in the density-of-states (DOS)
- This Kondo resonance gives rise to enhanced conductance through the dot

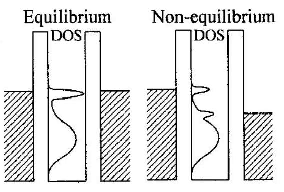


Figure 7: Kondo resonance (Lower energy bump: broadened single-particle state ϵ_0)

Minimum in the conductance

- Minimum in δG strongly resembles the resistance minimum for magnetic impurities
- 3, 5, 7 show Kondo behavior (odd number of electrons)
- 2, 4, 6 are no Kondo systems (even number of electrons)

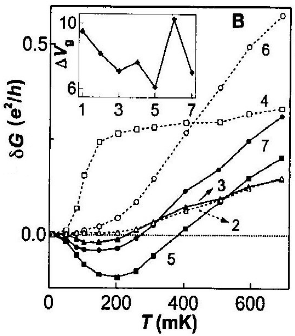


Figure 8: Conductance versus temperature

(Data taken from: Sara M. Cronenwett, T. Oosterkamp, L.Kouwenhoven: "A Tunable Kondo effect in Quantum Dots", Science vol 281, 540 (1998))

5. Conclusion

- Kondo systems show unusual transport properties for low temperatures
- Some metals have a minimum in the resistivity
- Quantum dots have a minimum in the conductance
- This behavior is due to the same physical effect of resonant spin flip scattering
- For even smaller temperatures the localized spin is screened

Advantages of investigating Kondo physics in quantum dots

- The Kondo system can be switched on and off
- A single localized state can be studied instead of a statistical distribution
- T_K can be tuned to experimentally accessible temperatures

References

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