Kondo effect in Quantum Dots: the role of Mesoscopic Fluctuations

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Kondo effect in metals

1934: resistance minima in Au

Dependant of the density of impurity (here Fe).

Figure 1 The minimum in the electrical resistivity of Au (de Haas, de Boer and van den Berg, 1934).
Kondo interpretation of the resistance minima

Prog. Theor. Phys. (1964)

Coupling with a magnetic impurity

\[ H_{\text{Kondo}} = + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \vec{s}'(0) \cdot \vec{S} \]

\[ \vec{S} \equiv \text{impurity spin} \]

\[ \vec{s}'(0) \equiv \sum_{k,\sigma,\sigma'} \left| \phi_k(0) \right|^2 c_{k\sigma}^\dagger c_{k\sigma'} \vec{\sigma}_{\sigma,\sigma'} \]

\[ R(T) = aT^5 + c_{\text{imp}}(R_0 - R_1 \ln (k_B T / D)) \]

\[ R_0 \sim J^2 \]

\[ R_1 \sim J^3 \]

\[ D \equiv \text{bandwidth} \]
Beyond third order perturbations

*Abrikosov, Physics, (1965)*

- order 3 > order 2 → what about higher order terms?
- “leading log” approximation → parquets diagrams

order \((n+2)\) of perturbations

\[ J^{n+2} \left( \ln \left( \frac{D}{T} \right) \right)^n \]

- need for resummation → scaling laws
Anderson’s Poor Man Scaling

\[ H_{\text{int}} = +J \vec{s}(0) \cdot \vec{S} \]

\[ J_{\text{eff}}(T) = \frac{J^0}{1 - J^0 \rho_0 \ln \frac{D}{T}} \]

\[ T_K^0 = D \exp\left(-\frac{1}{J_\rho_0}\right) \equiv \text{Kondo temperature} \]

\[ \delta J = J^2 \frac{\phi_\beta(0)^2}{\epsilon_\beta} \]

\[ \frac{\delta J}{\delta D} = J^2 \frac{\rho_{\text{loc}}(D)}{D} \]
Scaling behavior: e.g. (local) susceptibility

Parameters: \( J, \rho, D, T \)  

Dimensionality \( \rightarrow (J \rho) \& (T/D) \)

Scaling \( J(D) \rightarrow T \chi(T) = f(T/T_K^0) \)

\[ T_K^0 = De^{-1/J \rho} \]

\[ \chi_{loc} = \frac{\delta S_z}{\delta B} \]
**Anderson impurity model**

\[ H_{\text{And}} = H_{\text{band}} + H_{\text{imp}} + V \sum_{\alpha\sigma} [\phi^{\ast}_\alpha(0)c_{\alpha\sigma}^\dagger c_{d\sigma} + \text{h.c.}] \]

\[ H_{\text{band}} = \sum_{\alpha,\sigma} \epsilon_{\alpha} c_{\alpha\sigma}^\dagger c_{\alpha\sigma} \]

\[ H_{\text{imp}} = \sum_{\sigma} \epsilon_d c_{d\sigma}^\dagger c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} \]

\[ U + 2e_d \rightarrow \text{mapping to Kondo} \]

\[ J = 8V^2/U \]
Kondo Physics and Quantum dots

Spin-1/2 Kondo Effect

Odd N QD coupled to leads is a 1-Ch KP  

Charge Fluctuation Kondo Effect

Glazman & Raikh, Ng & Lee

Goldhaber-Gordon et. al.

Experiment  Cross-section of a single impurity
Kondo Physics and Quantum dots

Spin-1/2
Kondo Effect

Charge Fluctuation
Kondo Effect

Mapping to Kondo Problem (Matveev)

\[ Q \rightarrow S_z \]
\[ V_g \rightarrow B \]
\[ C_{diff} = \frac{\delta Q}{\delta V_g} \rightarrow \chi_{loc} = \frac{\delta S_z}{\delta B} \]

Experiment → Effect of B field on a single impurity
Mesoscopic fluctuations

Interference effects
(sensitive to field $B$)
→ wavefunction fluctuations

Van der Wiel et al., Science (2000)
Mesoscopics I: fluctuations of the “Quantum impurity” parameters

**BGS conjecture**: [Bohigas, Giannoni, Schmit, prl (1984)]
quantum systems whose classical analogue are chaotic show the same fluctuation properties as predicted by the corresponding Gaussian Ensemble (GOE for TRI, GUE for TRNI).

→ **Wavefunctions**: Porter-Thomas distribution

\[
P \left( A = \frac{|\Psi|^2}{\langle |\Psi|^2 \rangle} \right) = \begin{cases} 
  e^{-A} & \text{for CUE} \\
  \frac{1}{\sqrt{2\pi A}} e^{-A/2} & \text{for COE}
\end{cases}
\]
fluctuations of the impurity parameters

HAMILTONIAN

\[ \hat{H}_{dot} = \sum_{j\sigma} \varepsilon_j \hat{c}_j^\dagger \hat{c}_j \hat{\sigma} + E_C (\hat{n} - N)^2 \]

Effect of RANDOMNESS on Kondo Effect?
Fluctuations depend qualitatively on \( N_{ch} \).
\[ N_{ch} = N_L + N_R \]
(Our Emphasis!)

- Semiconductor QD: One channel per lead for effective tunneling contact. \( N_{ch} = 2 \)
- Metallic QD: Many channels that tunnel through an oxide barrier. \( N_{ch} \gg 1 \)

\[ \hat{H}_{leads} = \sum_{ik\sigma} (\varepsilon_k + E_i) \hat{c}_{i k \sigma}^\dagger \hat{c}_{i k \sigma} \]

\( i \) is channel index

\[ \hat{H}_T = \sum_{jik\sigma} (t_{ij} \hat{c}_{i k \sigma}^\dagger \hat{c}_{j \sigma} + h.c.) \]

Looks like \( N_{ch} \)-channel impurity problem
BUT for \( S = 1/2 \). Rotate channels: only one channel couples to the dot.

Glazman and Raikh (1989)
.... fluctuations of the impurity parameters ....

**EXPRESSION FOR CONDUCTANCE**

Problem is equivalent to single channel $S = 1/2$ Kondo independent of $N_{ch}$.

Expression for the Kondo conductance with $N_l$ and $N_r$ channels in leads:

$$ G_K = \frac{2e^2}{h} \frac{\sum_{i \in L} \Gamma_i \sum_{i \in R} \Gamma_i}{(\sum_{i \in L,R} \Gamma_i)^2} f(T/T_K) $$

$T_K$ independent prefactor

$\Gamma_i$ fluctuate according to RMT.

$f(T/T_K)$ is a universal function for 1-channel $S = 1/2$ Kondo Problem:

$$ f(T/T_K) \equiv \int d\omega (-df/d\omega)^{1/2} \sum_s [-\pi \text{Im} T_\sigma(\omega)] $$


Pustilnik and Glazman (2001)
fluctuations of the impurity parameters ..... 

$$T^D_{K} = \Delta \left( \frac{\Gamma}{U} \right)^{1/2} \text{Exp}\left[ -\frac{\pi |x(x + 1)| U}{2 \Gamma} \right]$$ where \( \Gamma = \sum \Gamma_i, a = \frac{U}{2 \Gamma}, x = \frac{\varepsilon_0}{U} \)

\[ \Longrightarrow \text{Using RMT for } \Gamma. \text{ Moments of } t_K = T_K / \Delta, \]

\[ \langle t^n_K \rangle = \frac{2(aN)^{N/2}}{(N/2 - 1)!} \left( \frac{\pi |x(x + 1)| n}{2aN} \right)^{n+N/4} K_{n+N/2}^{n+N} \left( \sqrt{2 \pi anN |x(x + 1)|} \right) \]

Distribution of \( T_K \)

For \( N_{ch} = 50 \)

For \( N_{ch} = 4 \)

Moments of \( T_K \)

\[ \langle T_K \rangle \]

\[ \langle (T_K - \langle T_K \rangle)^2 \rangle^{1/2} \]

\[ \langle (T_K - \langle T_K \rangle)^3 \rangle^{1/3} \]
...... fluctuations of the impurity parameters ..... 

Kaul, Ullmo, Baranger, prb 68, 161305(R) (2003)

FLUCTUATIONS OF PREFACTOR

For Many channels, can define a regime where \( T = 0 \)
OR if \( N_l \gg N_r, T_K \) fluctuations are small:

\[
G = \frac{2e^2}{h} \frac{\sum_{i \in L} \Gamma_i \sum_{i \in R} \Gamma_i}{(\sum_{i \in L,R} \Gamma_i)^2}
\]

Using RMT distributions for \( \Gamma_i \):

\[
P(g) = \frac{1}{\beta(N_l, N_r)} \frac{k(g)^{N_l/2-1} + k(g)^{N_r/2-1}}{(k(g) - 1)(1 + k(g))^{N_l+N_r/2-3}}
\]

\[
k(g) = -1 + \frac{1}{2g} + \frac{1}{2} \sqrt{\frac{1}{g^2} - \frac{4}{g}}
\]

and \( G = 4(2e^2/h) g \)
Mesoscopic Kondo problem

What would be the effect of the mesoscopic fluctuations of the electron sea on the Kondo physics?
  e.g.: renormalization scheme, scaling law, etc …

2-dots system
(stolen from Goldhaber-Gordon webpage)
**Mesoscopic Kondo Problem**

\[
\hat{H}_{\text{int}} = \sum_{k_1k_2} J \vec{S} \cdot (c_{\sigma_1k_1}^{\dagger} \sigma_{\sigma_1\sigma_2} c_{\sigma_2k_2})
\]

\[
\hat{H}_{\text{int}} = \sum_{\lambda_1\lambda_2} J \phi_{\lambda_1}^{*}(0) \phi_{\lambda_2}(0) \vec{S} \cdot (c_{\sigma_1\lambda_1}^{\dagger} \sigma_{\sigma_1\sigma_2} c_{\sigma_2\lambda_2})
\]

\[
\rho_{\text{loc}}(\epsilon) = \sum_{\alpha} |\phi_{\alpha}(0)|^2 \delta(\epsilon - \epsilon_{\alpha})
\]

- No Mapping to Clean Problem
- New Confinement Energy Scales \((E_{\text{TH}})\)
Quantum Monte Carlo Calculations

Traditional algorithm: Hirsch & Fye:
- “practical” only for Anderson model
- $U$ (ie cutoff) cannot be taken too large

→ New spin chain QMC algorithm:
impurity coupled to the electron gas locally →
tridiagonalize the free electron term to convert to a
fermion chain form (K.G. Wilson)

\[ H_0 = \sum_{\alpha \sigma} \varepsilon_{\alpha} c_{\alpha \sigma}^{+} c_{\alpha \sigma} \]
\[ \rightarrow \quad H_0 = \sum_{i \sigma} (\alpha_i f_{i \sigma}^{+} f_{i \sigma} + \beta_{i \sigma} f_{i+1 \sigma}^{+} f_{i+1 \sigma} + \beta_{i+1 \sigma} f_{i+1 \sigma}^{+} f_{i \sigma}) \]

Use efficient cluster algorithms to simulate these spin-chain
Hamiltonian (no sign problem)
Update using the continuous time path-integral directed loop algorithm (A.W. Sandvik)

Two updates:
- occupation number update
- spin flip update

- Computer time to obtain susceptibility with a fixed ratio of error grows as $1/T^2$.
- Correlation functions & Matsubara Green function efficiently calculated.
- Size of the system can be significantly increased with logarithmic blocking.

Yoo, Chandrasekharan, Kaul, Ullmo, Baranger, *prb* 71, 201309 (R) (2005)
Numerical simulations: quantum dot models

- Chaotic quantum dots → RMT model
  (realizations = random choice of energies and w.f according to RMT statistics)
- Integrable quantum dots
  – rectangular billiard
  – circular billiard
  (realizations = position of the impurity, chemical potential)
Numerical simulations: chaotic quantum dot

QMC data:

\[ \chi_{loc} = \frac{\delta S_z}{\delta B} \]

\[ \rho_{sm}(\omega) = \frac{\omega}{\pi} \int_{-\infty}^{\infty} d\epsilon \frac{\rho_{loc}(\epsilon)}{\omega^2 + \epsilon^2} \]
Anderson’s poor man’s scaling (1 loop RG): including mesoscopic fluctuations

\[ \delta J = J^2 \frac{|\phi_\alpha(0)|^2}{\epsilon_\alpha} \]

Exact density of state

\[ \rho_{\text{loc}}(\epsilon) = \sum_\alpha |\phi_\alpha(0)|^2 \delta(\epsilon - \epsilon_\alpha) \]

Finite temperature formalism (1 loop RG, Abrikosov parquet resummation)

\[ \rho_{\text{sm}}(\omega) = \frac{\omega}{\pi} \int_{-\infty}^{\infty} d\epsilon \frac{\rho_{\text{loc}}(\epsilon)}{\omega^2 + \epsilon^2} \]

(realization dependant)
Fluctuation of Kondo temperature

Running coupling constant

\[ J_{\text{eff}}(T) = \frac{J^0}{1 - J^0 \int_T^D \rho_{\text{sm}}(\omega) \frac{d\omega}{\omega}} \]

Realization dependant Kondo temperature

\[ T_K[\rho_{\text{sm}}(\omega)] \quad \text{s.t.} \quad J^0 \int_{T_K}^D \rho_{\text{sm}}(\omega) \frac{d\omega}{\omega} = 1 \]
Fluctuation of Kondo temperature

- N.B: even in the bulk

\[ 1 = J \rho_0 \ln \left( \frac{D}{T_K} \right) \]

is a poor approximation

- However, we only expect to describe fluctuations

\[ J^0 \int_{T_K^0 + \delta T_K}^{D} \left( \rho^0 + \delta \rho_{\text{sm}}(\omega) \right) \frac{d\omega}{\omega} = J^0 \int_{T_K^0}^{D} \rho^0 \frac{d\omega}{\omega} \]
Comparison with QMC: chaotic model


Symbols $\rightarrow$ QMC

Lines $\rightarrow f(T/T_k)$

$$T_k = T_k[\rho_{sm}(\omega)]$$
Comparison with QMC: integrable quantum dots

Square

\( J_{\rho} = 0.25, \ \frac{T_K}{D} = 0.0091 \)

circle

\( J_{\rho} = 0.22, \ \frac{T_K}{D} = 0.0046 \)
Relation to classical dynamics

*Mesoscopic fluctuations* of the local density of state related to closed *classical trajectories*

\[
\rho_{\text{loc}}(\mathbf{r}_o; \epsilon) = -\frac{1}{\pi} G(\mathbf{r}_o, \mathbf{r}_o; \epsilon)
\]

\[
\delta G(\mathbf{r}_o, \mathbf{r}_o; \epsilon) = \frac{1}{i\hbar} \frac{1}{\sqrt{2\pi\hbar}} \sum_{j: \mathbf{r}_o \rightarrow \mathbf{r}_o} \sqrt{D_j} \exp \left( \frac{i}{\hbar} S_j(\epsilon) - i\eta_j \frac{\pi}{2} \right)
\]

\[
S_j = \int p \cdot dr \equiv \text{action}
\]

\[
D_j^{-1} = v_F^2 \left( \frac{\partial r_{\perp}^f}{\partial p_{\perp}^i} \right) \equiv \text{stability}
\]

\[
\eta_j \equiv \text{Maslov index}
\]
Relation to classical dynamics: Kondo temperature

\[ \rho_{\text{sm}}(\omega) = \rho_{\text{loc}}(\mu + i\omega) \]

→ “analytical continuation” of classical dynamics (basically \( \frac{dS}{dE} = t \))

\[ \frac{\delta T_K}{T_K^0} \approx \frac{\sqrt{2\pi\hbar}}{\pi m} \sum_{t_j < \frac{\hbar}{T_K^0}} \sqrt{D_j} \sin \left[ \frac{1}{\hbar} S_j(\epsilon) - \eta_j \frac{\pi}{2} - \frac{3\pi}{4} \right] \log \left( \frac{T_K^0 t_j}{\hbar} \right) \]
Relation to classical dynamics: typical size of fluctuations

sum rule (conservation of classical probability):

\[
\sum_j \frac{D_j}{(2\pi \hbar)^d} \delta(t - t_j) = \bar{\rho} P_{\text{cl}}(t)
\]

\[
\frac{\langle \delta T_K^2 \rangle}{T_K^0} \approx \frac{2\Delta V}{\pi \hbar} \int_{T_K^0}^{D_{\text{cut}}} \frac{d\omega_1'}{\omega_1'} \frac{d\omega_2'}{\omega_2'} \int_0^\infty dt P_{\text{cl}}(t) e^{-(\omega_1' + \omega_2')t/\hbar}
\]

\[
\approx \alpha \frac{\Delta}{T_K^0}
\]

for chaotic systems \(\alpha = (4/\pi) \ln 2\)

\(P_{\text{cl}}(t) = \) classical probability of return
Scaling properties

- In the low temperature regime → clearly no
- In the high temperature regime
  
  parameters: \( \rho (\omega), J^0, T \)
  → after renormalization: \( J_{\text{eff}}(T), \rho_{\text{sm}}(T) \)
  → dimensionality: \( T \chi(T) = F(J_{\text{eff}}(T) \cdot \rho_{\text{sm}}(T)) \)
  → same as bulk Kondo pb, at temperature \( \bar{T}(T) \)

\[
J_{\text{eff}}(T) \cdot \rho_{\text{sm}}(T) = J_{\text{eff}}(\bar{T}). \rho_0
\]

\[
T \chi(T) = f(\bar{T}(T)/T_0^K)
\]  

(not necessarily universal)
Summary

• Quantum dots provide experimentally tunable “artificial atoms” that naturally leads to quantum impurity problems, but these later involve mesoscopic fluctuations.

• In the quantum impurity → “just” fluctuations ..

• In the conduction electrons → qualitative modification of the renormalization process
  • One Parameter Scaling destroyed
  • High-T regime follows from Poor-Man’s Scaling
What did we learn?

- **Quantitative level:**
  Explicit expressions for the fluctuations (e.g. of $T_k$)
  $\rightarrow$ scale of the fluctuations, etc …

- **Qualitative level**
  - One loop RG accurate for $T \gg T_k$ (sort of expected).
  - **One parameter scaling** destroyed at low temperature (idem)
  - One loop RG accurate for $T \sim T_k$ (much less)
  $\rightarrow$ bridge to low $T$ (**Fermi liquid**)
What else?

- Low temperature regime:
  - $T \ll \Delta$: ground state spin, etc...
  - $\Delta \ll T \ll T_K$: Fermi liquid picture?
- “Rigorous” theory of the semiclassical + high-T limit.
- Other observables (conductance).
- Coupling with the orbital motion.
- “Chaotic” renormalization flow.
Kondo Physics and Quantum dots

Different realization of quantum dots

**Metal Particles**  
**Semi-Conductor Heterostructures**

Bolotin et. al.  
Goldhaber-Gordon et. al.
Mesoscopic fluctuations

≡ fluctuations of wavefunctions / energies / etc.. associated to interference effects.

stadium billiard

bicircular billiard
CB Peak Heights: Q. Chaos and Meso Fluctuations

Chaotic confinement:

\[ E_{Th} \]

\[ \varepsilon_\alpha < E_{Th} \]

\[ \varepsilon_\alpha, \phi_\alpha(r) \Rightarrow RMT \]

Folk et. al.

Chang, Baranger et. al.
Quantum Monte Carlo Calculations

Kondo

\[ H_{\text{Kondo}} = + \sum_{k, \sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} - J \vec{s}(0) \cdot \vec{S} \]

Anderson

\[ H_{\text{And}} = H_{\text{band}} + H_{\text{imp}} + V \sum_{\alpha, \sigma} \left[ \phi^*_\alpha(0) c_{\alpha\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right] \]

\[ H_{\text{band}} = \sum_{\alpha, \sigma} \epsilon_\alpha c_{\alpha\sigma}^\dagger c_{\alpha\sigma} \]

\[ H_{\text{imp}} = \sum_{\sigma} \epsilon_d c_{d\sigma}^\dagger c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} \]