Lectures: Condensed Matter II
1 – Electronic Transport in Quantum dots
2 – Kondo effect: Intro/theory.
3 – Kondo effect in nanostructures

Luis Dias – UT/ORNL
Lectures: Condensed Matter II

1 – Electronic Transport in Quantum dots
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Lecture 3: Outline

- Quantum Dots: brief review.
- Kondo effect: Review.
- Kondo effect in quantum dots.
- Kondo effect in Single Molecule Transistors.
- Kondo effect in Surfaces (STM, “quantum mirage”).
- Kondo effect in carbon nanotubes.
"The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of simple extrapolation of the properties of a few particles.

Instead, at each level of complexity entirely new properties appear and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other."

Phillip W. Anderson, “More is Different”, *Science* 177 393 (1972)
Can you make “atoms” out of atoms?

Electrostatically confine electrons within a small (nanometer-size) region.

2D Electron gas

“Quantum dot”

GaAs $\text{Al}_x\text{Ga}_{1-x}\text{As}$

from Charlie Marcus’ Lab website (marcuslab.harvard.edu)
Making “artificial atoms” (?) out of atoms

Discrete levels: we might be tempted to call them “artificial atoms”.

BUT: different energy/length scales!

Strong charging (U) → Many-body correlations

Confining in 0D

Strong charging (U) → Many-body correlations
What are Quantum Dots?

Semiconductor Quantum Dots:

- Devices in which electrons are **confined** in nanometer size volumes.

- Sometimes referred to as “artificial atoms”.

- “Quantum dot” is a generic label: **lithographic QDs**, self-assembled QDs, colloidal QDs have different properties.
Coulomb Blockade in Quantum Dots

Even N  Odd N

conductance

$E_c$  $V_{\text{gate}}$

Coulomb Blockade in Quantum Dots
Coulomb Blockade in Quantum Dots

\[ V_{\text{gate}} \]

Even \( N \)

Odd \( N \)

Even \( N \)

conductance

\[ E_c \]

\[ E_c \]

\[ E_c \]

Coulomb Blockade in Quantum Dots
“Coulomb Diamonds” (Stability Diagram)

Coulomb Blockade in Quantum Dots


\[ eV_{\text{sd}} \]

\[ eV_{\text{gate}} \]
Kondo effect

$\xi_K \sim \frac{v_F}{k_B T_K}$

$\rho/\rho_{4.2K}$

$1%$ Fe

Mo$_{10.2}$Nb$_{8.8}$
Mo$_{9.9}$Nb$_{8.1}$
Mo$_{8.8}$Nb$_{2.2}$
Mo$_{7.7}$Nb$_{3.3}$

Resistivity decreases with decreasing $T$ (usual)
Resistivity increases with decreasing $T$ (Kondo effect)

Characteristic energy scale: the Kondo temperature $T_K$

$T_K$ is the temperature at which the resistivity becomes constant.
Kondo problem: s-d Hamiltonian

Kondo problem: s-wave coupling with spin impurity (s-d model):

\[
H_K = \sum_{k_s} \epsilon_{k_s} \hat{n}_{k_s} + J \sum_{k_s; k'_s'} c_{k_s}^\dagger (\mathbf{S} \cdot \vec{\sigma})_{s s'} c_{k'_s'}
\]
Kondo’s explanation for $T_{\text{min}}$ (1964)

- **Perturbation theory in $J^3$:**
  - Kondo calculated the conductivity in the linear response regime

\[
R_{\text{imp}}^{\text{spin}} \propto J^2 \left[ 1 - 4J \rho_0 \log \left( \frac{k_B T}{D} \right) \right]
\]

\[
R_{\text{tot}} (T) = aT^5 - c_{\text{imp}} R_{\text{imp}} \log \left( \frac{k_B T}{D} \right)
\]

\[
T_{\text{min}} = \left( \frac{R_{\text{imp}} D}{5ak_B} \right)^{1/5} c_{\text{imp}}^{1/5}
\]

- **Only one free parameter:** the Kondo temperature $T_K$
  - Temperature at which the perturbative expansion **diverges.**

\[
k_B T_K \sim D e^{-1/2J \rho_0}
\]
A little bit of Kondo history:

- Early ‘30s: Resistance minimum in some metals
- Early ‘50s: Theoretical work on impurities in metals “Virtual Bound States” (Friedel)
- 1961: Anderson model for magnetic impurities in metals
- 1964: s-d model and Kondo solution (PT)
- 1970: Anderson “Poor’s man scaling”
- 1974-75: Wilson’s Numerical Renormalization Group (non PT)
- 1980: Andrei and Wiegmann’s exact solution

Kenneth G. Wilson – Physics Nobel Prize in 1982 "for his theory for critical phenomena in connection with phase transitions"
Renormalization Procedure

\[ H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_{\sigma} f_{N+1\sigma}^\dagger f_{N\sigma} + f_{N\sigma}^\dagger f_{N+1\sigma} \]

- Iterative numerical solution.
- Renormalize by \( \Lambda^{1/2} \).
- Keep low energy states.

\[ H_{N+1} \]

\[ \gamma_n \sim \frac{\xi_n}{H_N} \Lambda^{-n/2} \]

\[ H_{N+1} \]

\[ \gamma_1 \gamma_2 \gamma_3 \ldots \]
Anderson Model

\[ H = \epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_k \epsilon_k \hat{n}_{k\sigma} + t \sum_k c_{d\sigma}^\dagger c_{k\sigma} + h.c. \]

with

\[ \hat{n}_{d\sigma} = c_{d\sigma}^\dagger c_{d\sigma} \]
\[ \hat{n}_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma} \]

- \( e_d \): energy level
- \( U \): Coulomb repulsion
- \( e_F \): Fermi energy in the metal
- \( t \): Hybridization
- \( D \): bandwidth

- \( e_d \): position of the level \((V_g)\)
- \( U \): Charging energy
- \( e_F \): Fermi energy in the leads
- \( t \): dot-lead tunneling
- \( D \): bandwidth
NRG on Anderson model: LDOS

- Single particle peaks at $\varepsilon_d$ and $\varepsilon_d + U$. 
- Many body peak at the Fermi energy: *Kondo resonance* (width $\sim T_K$).
- NRG: good resolution at low $\omega$ (log discretization).
History of Kondo Phenomena

- Observed in the ‘30s
- Explained in the ‘60s
- Numerically Calculated in the ‘70s (NRG)
- Exactly solved in the ‘80s (Bethe-Ansatz)

So, what’s new about it?

Kondo correlations observed in many different set ups:

- Transport in quantum dots, quantum wires, etc
- STM measurements of magnetic structures on metallic surfaces (e.g., single atoms, molecules. “Quantum mirage”)
- ...

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Kondo correlations observed

- Transport in quantum dots
- STM measurements of magnetic surfaces (e.g., single atoms, molecular junctions)
- ...
Kondo Effect in Quantum Dots

Revival of the Kondo effect

Leo Kouwenhoven and Leonid Glazman

1. The Kondo effect in metals and in quantum dots

Coulomb Blockade in Quantum Dots

\[ E_c \]

\[ V_g \]

Even N  Odd N

conductance

V_g
Coulomb Blockade in Quantum Dots

$V_g$, $E_c$

Even N, Odd N, Even N

Kondo Effect in Quantum Dots

\[ \text{Conductance (} G \text{)} \sim E_c \]

- \( T > T_K \): Coulomb blockade (low \( G \))
- \( T < T_K \): Kondo singlet formation
- Kondo resonance at \( E_F \) (width \( T_K \)).
- New conduction channel at \( E_F \):
  Zero-bias enhancement of \( G \)

Kondo effect in Quantum Dots


Semiconductor Quantum Dots:

- Allow for systematic and controllable investigations of the Kondo effect.

- QD in $N_{\text{odd}}$ Coulomb Blockade valley: realization of the Kondo regime of the Anderson impurity problem.

Kondo Effect in CB-QDs

N_{ODD} valley: Conductance rises for low T (Kondo effect)

Kondo Temperature $T_k$: only scaling parameter ($\sim 0.5K$, depends on $V_g$)

Examples of “fundamental” physics (in the “More is Different” sense) we can learn from quantum dots:

- **Strongly correlated effects**: Charging effects due to electron-electron interactions are dominant in QDs.

- **Quantum effects** (spin, tunneling, discreet energy levels, interference) probed in a very controllable way.

- **Quantum Many-body physics**:
  - Kondo effect, Quantum phase transitions, …
Kondo Effect in **Double QDs**

- Tunability of **intradot** and **interdot** parameters (couplings, gate voltage).
- Prospects for experimental probe of many-body phenomena, e.g:
  - SU(4) Kondo, RKKY interactions,...
  - Non-Fermi liquid physics (2-ch Kondo)
  - **Quantum phase transitions.**

**“Side dot” configuration**


**“Parallel” configuration**


Two-channel Kondo effect.

- Spin 1/2 coupled to two independent bands: 2-channel Kondo model ("overscreened").
- Non-Fermi-liquid (NFL) behavior for $J_1 = J_2$.
- Impurity entropy (NFL): $S_{\text{imp}} = k_B \log(\sqrt{2})$ (NRG, Bethe ansatz).
- Recent expts in q-dots.

Kondo effect in Single Molecule Transistors

- Single molecule transistors: $C_{60}$ molecules “caught” between electrodes (break junction).
- Zero-bias peak as a function of gate voltage: correct Kondo scaling.
- Correct behavior vs. Bias.
- $T_K > 50K$.

Transport in molecular junctions.

- Coulomb blockade effects.
- Features consistent with vibrational modes in dI/dV.
- Kondo signatures.

Kondo effect in Single Molecule Transistors


From Dan Ralph’s webpage:
http://people.ccmr.cornell.edu/~ralph/

- Similar expts (D. Ralph’s group).
- Supression of the Kondo resonance in the presence of a magnetic field (top left, black curve, B=10T) and magnetic leads (top right, parallel [green] and antiparallel [blue] magnetizations).
Kondo effect in surfaces (STM images).

- Magnetic (Co, Fe) atoms on metallic surfaces! Right ingredients for Kondo.
- In this case, Kondo is marked by a dip at zero-bias conductance (dl/dV at V=0).
Kondo effect surfaces: STM measurements.

- STM atomic manipulation: can build local structures ("quantum corals").
- Elliptical shape: imaging (top) and dI/dV measurements (bottom).
- Cobalt atoms on Cu(111) shown.

Kondo effect surfaces: STM measurements.

- One extra atom placed in one foci: a peak in the dIdV appears in the other focus although NO ATOM is there! (“quantum mirage”).
- Theory: “focusing” of Kondo-scattered surface electrons*.

*Schiller and Agam, PRL 86 484 (2001)
Magnetic impurities on metallic surfaces: Kondo + STM

Kondo/Fano phenomenology quite generic:

- Early experiments: Co on Au(111)

- Co on Cu(111): “Quantum mirage”

- Co on different surfaces: Cu(100), Ag(111), Ag(100),...

- Magnetic *molecules* on Cu(111): Control of the Kondo temperature by atomic manipulation.

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Kondo: Magnetic molecules on surfaces

V. Iancu, A. Deshpande, Saw W. Hla
Nano Lett. 6 820 (2006)

STM measurements

Co $d_{3z^2-1}$ level (at $\sim-0.7$ eV)

Zero-bias dip: Kondo effect. $T_K \sim 130-170$K
First-principles calculations (GW): hints for a microscopic model.

Model: Anderson-like Hamiltonian

\[
H = H_{\text{Molecule}} + H_{\text{Mol-Surface}}
\]

\[
H_{\text{Molecule}} = \sum_{\sigma} E_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\sigma} E_M \hat{n}_{M\sigma}
\]

\[
H_{\text{Mol-Surf}} = \sum_{\mathbf{k},\sigma} V_{d\mathbf{k}} c_{d\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} V_{M\mathbf{k}} c_{M\sigma}^\dagger c_{\mathbf{k}\sigma} + \text{h.c.}
\]

\[
V_{d(M)\mathbf{k}} = \langle \phi_{d(M)} | \hat{H} | \psi_{\mathbf{k}} \rangle
\]

OK!

GW: Molecular level’s “Co-like” levels

OK!

S=1/2 model

LUMO

\[ E_{d} = 2 \text{ eV} \]

\[ U=6.3 \text{ eV} \]

HOMO

\[ E_{M} = 1.8 \text{ eV} \]

Not easy to calculate with GW!
NRG calculations (Kondo temperature).

Kondo effect In Carbon nanotubes.

- Carbon nanotubes deposited on top of metallic electrodes.
- Quantum dots defined within the carbon nanotubes.
- More structure than in quantum dots: “shell structure” due to orbital degeneracy.


Gleb Filkenstein’s webpage: http://www.phy.duke.edu/~gleb/
Kondo effect In Carbon nanotubes.

- Temperature behavior is Kondo-like.
- Interesting *merging of the four shells* at high $V_g$ ("SU(4)" Kondo instead of the usual SU(2) Kondo).
- NRG calculations* support that picture.

More “Theory-Experiment ballgame”

Transmission Phase Shift of a Quantum Dot with Kondo Correlations

Theory
(Gerland et al. PRL 84 3710 (2000))

Experiment
(Ji, Heiblum et al. Science 290 779 (2000))
More “Theory-Experiment ballgame”

Transmission Phase Shift of a Quantum Dot with Kondo Correlations

Theory (Gerland et al. PRL 84 3710 (2000))

(c) For arbitrary temperatures ($\approx \Gamma$), the only approach which gives reliable results for $\mathcal{G}_{d\sigma}(E)$ for all $\Gamma, U, \varepsilon_d$ is the numerical renormalization group (NRG).
Theory-Experiment ballgame

Phase Evolution in a Kondo-Correlated System

Experiment
(Ji, Heiblum et al.
Science 290 779 (2000))

Experiment
(Ji et al. Science 290 779 (2000))
Summary: Lectures on strongly correlated phenomena in nanostructures.

- **Lecture 1**: Quantum Dots.
- **Lecture 2**: Kondo effect/NRG.
- **Lecture 3**: Kondo effect in nanostructures.

Nanostructures display an array of strongly correlated phenomena: (Kondo and 2ch Kondo effects (= non-Fermi-liquid behavior), interplay of spin and vibrational effects... quantum phase transitions, SU(4) Kondo effect).

Opportunity: *controlled* studies of all these features.

*Thanks for your attention.*