Kondo effect in mesoscopic and nanoscopic systems

Pablo S. Cornaglia
Centro Atómico Bariloche and Instituto Balseiro,
Comisión Nacional de Energía Atómica, Bariloche, Argentina
Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET),
Argentina
Recap Lecture 1

• Anderson model
• Magnetic moment formation: Stoner criterion
• At second order in the $d$ level-electron bath coupling the Anderson model is equivalent to the Kondo model (are the higher order terms important at low energies?)
• Anderson's poor man's scaling:
  – solves problem for ferromagnetic coupling: free impurity at low energies.
  – suggests a singlet ground state for the antiferromagnetic case, but breaks-down at low energy scales $\sim k_B T_K$
Outline of lecture 2

- Numerical renormalization group
  - Numerical solution of the Kondo problem
- Nozières Fermi liquid theory
  - Low energy effective description
- Slave boson mean field theory
  - Variational solution at low energies (Fermi liquid regime)
References

- K. G. Wilson, Rev. Mod. Phys. **47** 773 (1975)
Wilson's renormalization group (RG)

- In poor's man scaling approach two couplings are considered: $\rho_0 J_{\perp}$, $\rho_0 J_{\parallel}$
  - Other couplings that appear in higher order perturbation theory may be important
- Wilson's RG considers all couplings.
  - There is no need to guess which couplings to use.
  - Renormalizations are performed until a fixed point is reached where the couplings stop changing.
  - An effective Hamiltonian close to the fixed points
Anderson model

\[ H = H_d + H_m + H_V \]

\[ H_d = \epsilon_d (\hat{n}_\uparrow + \hat{n}_\downarrow) + U \hat{n}_\uparrow \hat{n}_\downarrow \]

\[ H_m = \sum_k \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} \]

\[ H_V = \sum_k V_k c_{k\sigma}^\dagger d_\sigma + V_k^* d_\sigma^\dagger c_{k\sigma} \]
renormalization by successive diagonalizations

- Solve exactly by numerical diagonalization the problem of the impurity coupled to a few high energy states.
- At each iteration include extra conduction band states with decreasing energy.
renormalization by successive diagonalizations

- Problems:
  - Too many states to consider at each energy scale in the original Hamiltonian.
  - Exact diagonalization can only be done for a few conduction band states limiting the number of states that can be retained at each iteration.
  - Each extra state increases by a factor 4 the size of the Hilbert space. (Need to discard $\frac{3}{4}$ of the states at each iteration)
  - In this form the procedure does not converge.
Wilson's numerical renormalization group (NRG)

- Wilson's approach: discretize conduction band in a logarithmic way: defines hierarchy of energy scales. Wilson showed that a single electronic state needs to be considered at each energy interval.
- Mapping of the conduction band into a semi-infinite tight-binding chain. Because of the logarithmic discretization, the hopping terms of the chain decrease exponentially. The impurity is coupled to the first site of the chain.
- Iterative diagonalization of the impurity problem starting from the impurity and adding sites to the chain. The exponentially growing Hilbert space is truncated keeping a set of low-lying states.

[K. G. Wilson, RMP 47 773 (1975)]
Logarithmic discretization

\[ a_m = \frac{1}{N_m} \int_{D\Lambda^{-1-m}}^{D\Lambda^{-m}} c_k d\epsilon_k \]

\[ \gamma_n^2 = \int_{D\Lambda^{-1-m}}^{D\Lambda^{-m}} \rho(E) dE \]
Lanczos tridiagonalization

- The model can be brought to a one-dimensional tight binding chain using Lanczos tridiagonalization procedure.
- Change of basis states in the metallic host.
  - Define the normalized state:
    \[ |\phi_0\rangle = f_0^\dagger |0\rangle = \frac{1}{V} \sum_k V_k c_k^\dagger |0\rangle \]
  - where:
    \[ V = \left( \sum_k |V_k|^2 \right)^{1/2} \]
    
    \[ H_V = \sum_k V_k c_{k\sigma}^\dagger d_\sigma + V_k^* d_\sigma^\dagger c_{k\sigma} \]
Lanczos tridiagonalization

- The $d$ level – metal tunneling term simplifies to:
  \[ H_V = V (f_{0\sigma}^\dagger d_\sigma + d_\sigma^\dagger f_{0\sigma}) \]

- Construct an orthonormal basis using:
  \[ H_m |\phi_0\rangle = \epsilon_0 |\phi_0\rangle + t_1 |\phi_1\rangle \quad \langle \phi_0 | \phi_1 \rangle = 0 \]

- with:
  \[ \epsilon_0 = \langle \phi_0 | H_m | \phi_0 \rangle, \quad t_1^2 = \langle \phi_0 | H_m^2 | \phi_0 \rangle - \epsilon_0^2 \]

- and recursively:
  \[ t_{n+1} |\phi_{n+1}\rangle = H_m |\phi_n\rangle - \epsilon_n |\phi_n\rangle - t_n |\phi_{n-1}\rangle \]
  \[ \epsilon_n = \langle \phi_n | H_m | \phi_n \rangle, \quad t_{n+1}^2 = \langle \phi_n | H_m^2 | \phi_n \rangle - \epsilon_n^2 - t_n^2 \]
Lanczos tridiagonalization

- We finally have

\[ H_d = \epsilon_d (\hat{n}_\uparrow + \hat{n}_\downarrow) + U \hat{n}_\uparrow \hat{n}_\downarrow \]

\[ H_V = V (f_{0\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger f_{0\sigma}) \]

\[ H_m = \sum_{n=0} \epsilon_n f_n^\dagger f_n + \sum_{n=0} t_{n+1} (f_n^\dagger f_{n+1} + h.c.) \]

\[ \Delta(E) = \pi V^2 \rho_0(E) \quad \rho_0 \text{ is the density of states at site 0} \]
Wilson's transformation of the conduction band

Logarithmic discretization

Single state on each interval

Mapping to a linear chain

Due to the logarithmic discretization the hoppings decay exponentially:

$$t_n \sim \Lambda^{(1-n)/2}$$

Well separated energy scales.

Each RG step produces a perturbation in the spectrum.
Iterative diagonalization

- The size of the Fock space grows exponentially with the number of sites: $N_{st} = 4^{n+1}$
- Discard highest energy states after each iteration.
- In practice converged results for:
  - $\Lambda = 1.5,...,3$;
  - retaining $N = 400,...,5000$ at each iteration
- There are small systematic errors due to the logarithmic discretization. The precision can be much improved averaging over multiple possible discretizations with the same $\Lambda$.
Numerical renormalization steps

\[ H_{n+1} = \mathcal{R}_\Lambda [H_n] \]

\[ H_{n+1} = \sqrt{\Lambda} H_n + \tilde{\tau}_{n+1} (f_{n+1}^\dagger f_n + f_n^\dagger f_{n+1}) \]

\[ \tilde{\tau}_{n+1} = \Lambda^{(n-1)/2} t_{n+1} \sim 1 \]

The parity of the number of sites in the chain changes at each NRG step. Two steps are necessary in order to obtain a convergence in the spectrum at a fixed point.
Numerical renormalization steps

The Hamiltonian is diagonalized to obtain the eigenenergies and eigenfunctions.

The high energy states are truncated.

A new site is coupled to the chain.
NRG flow for the Anderson model

Three different regimes:
- Free orbital
  \( U = V = 0 \)
- Local moment
  \( J = 0 \)
- Strong coupling.
  \( J \to \infty \)
Fixed points

- **Free orbital:** $k_B T > U, V$
  - The orbital is effectively decoupled
- **Local moment** $k_B T_K \ll k_B T < U, V$
  - Free spin
- **Strong coupling:** $k_B T \ll k_B T_K$
  - Screened spin: no remaining magnetic moment.
  - Energy spectrum identical to that of a system with: $J = \infty$
  - Additive spectrum: Fermi liquid behavior.
At iteration $n$

- Set of eigenfunctions with given quantum numbers:
  - charge, spin and energy: $|Q, S, S_z, E, i\rangle_n$

- The energies span a range of roughly an order of magnitude and allow the calculation of thermodynamic properties at a temperature: $T_n \sim D\Lambda^{-(n-1)/2}$

- For dynamic properties, a broadening of the levels is required due to the discrete spectrum: bad resolution at high energies.
  - Many developments in recent years to improve resolution: some using Oliveira's trick.
Thermodynamic properties

At a given iteration, thermodynamic properties can be calculated at a temperature $T_n \sim D \Lambda^{-\left(n-1\right)/2}$.

![Graph showing thermodynamic properties](image-url)
Thermodynamic properties

At low temperatures Fermi liquid like behavior

Compensated spin (no divergence)

\[ \chi(T \to 0) \propto \frac{1}{k_B T_K} \]

\[ C(T \to 0) = \gamma_{\text{imp}} T \propto \frac{T}{T_K} \]

In the Kondo regime there is a single relevant energy scale: \( k_B T_K \)

Wilson's ratio measures residual interaction between quasiparticles

\[ R = \frac{4(\pi k_B)^2}{3(g \mu_B)^2} \frac{\chi_{\text{imp}}}{\gamma_{\text{imp}}} = 2 \quad \text{(strong coupling } U \to \infty) \]

\[ R = 1 \quad \text{For non-interacting quasiparticles} \]
Dynamic properties

Abrikosov Suhl resonance
Kondo peak
width: $\sim k_B T_K$

$|0\rangle \rightarrow |\sigma\rangle$

$|\uparrow\downarrow\rangle \rightarrow |\bar{\sigma}\rangle$
Dynamic properties

- Kondo peak of width: $\propto k_B T_K$

- And height:
  \[
  A_{d\sigma}(E = 0, T = 0) = \frac{\sin^2(\pi n_{d\sigma})}{\pi \Delta}
  \]

(sum rule)

- Charge fluctuation peaks of reduced height compared to non-interacting results.

- No spin symmetry breaking:
  \[
  A_{d\uparrow}(E, B = 0) = A_{d\downarrow}(E, B = 0)
  \]
Applications

• Interacting impurity in a superconductor, ferromagnetic or pseudogapped host.
  - [Satori et al. 1992], [Martinek et al. 2003], [Ingersent 1996]

• Anderson-Holstein model (coupling to local phonons).
  - [Hewson and Meyer 2002]

• Coupling to a boson bath.
  - [Bulla 2003]

• Coupling to phonon and fermion baths.
  - [Glossop and Ingersent 2008]

• Impurity solver for DMFT (currently limited to at most two conduction bands)
  - [Bulla 1999]
Nozières local Fermi liquid

- Close to the strong coupling fixed point the local moment captures a spin from the conduction band to form a singlet. No spin-flip scattering remains and the energy spectrum can be fitted assuming weakly interacting quasiparticles.
- Based on Anderson's and Wilson's results Nozières constructed a Fermi liquid theory to describe the quasiparticles in terms of the scattering phase shifts.
- The Fermi liquid is described by a set of Landau parameters. Nozières inferred the value of the parameters. e.g. effective mass $\propto 1/T_K$ and scattering phase shift $\delta_0 = \pi/2$

$$A_{d\sigma}(E = 0, T = 0) = \frac{\sin^2(\pi n_{d\sigma})}{\pi \Delta}$$

Slave boson mean field theory

- Variational approach, exact in large $N$ limit: SU($N$) symmetry ($N=2$ for the spin $\frac{1}{2}$ Kondo model).
- Construct a representation of the impurity states extending the Fock space to include auxiliary boson: $b$

\[
[b, b^\dagger]_- = 1 \quad [f_\sigma, f_\sigma^\dagger]\_+ = 1
\]

\[
d_\sigma \rightarrow b^\dagger f_\sigma
\]

\[
|0\rangle \rightarrow b^\dagger |\text{vac}\rangle |0\rangle
\]

\[
| \uparrow \rangle \rightarrow f_\uparrow^\dagger |\text{vac}\rangle |0\rangle
\]

\[
| \downarrow \rangle \rightarrow f_\downarrow^\dagger |\text{vac}\rangle |0\rangle
\]

\[
U = \infty \quad \text{constraint:} \quad b^\dagger b + \sum_\sigma f_\sigma^\dagger f_\sigma = 1
\]

[P. Coleman 1984, Kotliar and Ruckenstein 1986]
Slave bosons $U=\infty$

\[ H_{U=\infty} = \epsilon_d (\hat{n}_\uparrow + \hat{n}_\downarrow) + \sum_k \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k V_k c_{k\sigma}^\dagger d_\sigma + V_k^* d_\sigma^\dagger c_{k\sigma} \]

\[ d_\sigma \rightarrow b^\dagger f_\sigma \]

\[ H = \epsilon_d \sum f_\sigma^\dagger f_\sigma + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} V_k c_{k\sigma}^\dagger b_\sigma^\dagger f_\sigma + V_k^* f_\sigma^\dagger b_\sigma c_{k\sigma} \]

Impose the constraint in the partition function using the representation of the Kronecker delta function:

\[ \delta_{n,0} = \frac{\beta}{2\pi} \int_{-\pi/\beta}^{\pi/\beta} e^{-i\lambda\beta n} d\lambda \quad \beta = \frac{1}{k_B T} \]

\[ Z = \text{Tr} \frac{\beta}{2\pi} \int_{-\pi/\beta}^{\pi/\beta} e^{-\beta H - i\lambda\beta (b^\dagger b + \sum_\sigma f_\sigma^\dagger f_\sigma)} d\lambda \]
Calculate $Z$ in the mean field approximation replacing the Bose operators by their expectation values:

$$r = \langle b \rangle, \quad r = \langle b^\dagger \rangle$$

The effective mean field Hamiltonian has the form:

$$H_{mf} = (\epsilon_d - i\lambda) \sum f^\dagger f + \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} r V_k c^\dagger_{k\sigma} f_{\sigma} + r V^*_k f^\dagger_{\sigma} c_{k\sigma}$$

$$H_{mf} = \tilde{\epsilon}_d \sum f^\dagger f + \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} \tilde{V}_k c^\dagger_{k\sigma} f_{\sigma} + \tilde{V}^*_k f^\dagger_{\sigma} c_{k\sigma}$$

Non interacting model with renormalized parameters
Slave bosons U=\infty

The Free energy can be calculated and minimized using \tilde{\epsilon}_d \text{ and } r \text{ as variational parameters.}

Some general remarks about the solution:

In the Kondo regime \( \langle f_{\sigma}^\dagger f_{\sigma} \rangle \lesssim 1/2 \)

Taking averages on the constraint we get:

\[
r^2 = 1 - \sum_{\sigma} \langle f_{\sigma}^\dagger f_{\sigma} \rangle \ll 1
\]

Resonance at the Fermi level

\[
\langle \langle f_{\sigma}, f_{\sigma}^\dagger \rangle \rangle = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}}
\]

\[
\tilde{\epsilon}_d \lesssim E_F \quad \tilde{\Delta} = \pi r^2 V^2 \rho_0
\]

\[
\langle \langle d_{\sigma}, d_{\sigma}^\dagger \rangle \rangle = r^2 \langle \langle f_{\sigma}, f_{\sigma}^\dagger \rangle \rangle
\]

Kondo peak of width \( \tilde{\Delta} \) and height \( \sim \frac{1}{\pi \Delta} \quad k_B T_K \propto \tilde{\Delta} \)
The effective Hamiltonian is quadratic in the fermion operators: It is a Fermi gas with renormalized parameters.

The Free energy can be calculated and minimized for the parameters: $\lambda$ and $r$

The approach can be formulated in terms of a variational in terms of a Fermi gas: it can only be valid if the ground state is a Fermi liquid. In the Kondo problem it provides a description at low temperatures.
Slave bosons Kondo model

\[ H_K = J(S^+ f_{0\downarrow}^{\dagger} f_{0\uparrow} + S^- f_{0\uparrow}^{\dagger} f_{0\downarrow} + S_z (f_{0\uparrow}^{\dagger} f_{0\uparrow} - f_{0\downarrow}^{\dagger} f_{0\downarrow})) \]

\[ H_K = J(d_{\uparrow}^{\dagger} d_{\downarrow} f_{0\downarrow}^{\dagger} f_{0\uparrow} + d_{\downarrow}^{\dagger} d_{\uparrow} f_{0\uparrow}^{\dagger} f_{0\downarrow} + \frac{1}{2}(d_{\uparrow}^{\dagger} d_{\uparrow} - d_{\downarrow}^{\dagger} d_{\downarrow})(f_{0\uparrow}^{\dagger} f_{0\uparrow} - f_{0\downarrow}^{\dagger} f_{0\downarrow})) \]

Mean field decoupling:

\[ d_{\uparrow}^{\dagger} d_{\downarrow} f_{0\downarrow}^{\dagger} f_{0\uparrow} \rightarrow d_{\uparrow}^{\dagger} \langle d_{\downarrow} f_{0\downarrow}^{\dagger} \rangle f_{0\uparrow} + f_{0\downarrow}^{\dagger} \langle f_{0\uparrow} d_{\uparrow}^{\dagger} \rangle d_{\downarrow} - \langle f_{0\downarrow}^{\dagger} d_{\downarrow} \rangle \langle f_{0\uparrow} d_{\uparrow}^{\dagger} \rangle \]

The Kondo coupling to the band turns into a hopping term:

\[ \tilde{H}_K = \tilde{J} \sum_{\sigma} (d_{\sigma}^{\dagger} f_{0\sigma} + h.c.) \]

\[ \tilde{J} = J \langle d_{\downarrow} f_{0\downarrow}^{\dagger} \rangle = J \langle d_{\uparrow} f_{0\uparrow}^{\dagger} \rangle \]
Slave bosons Kondo model

Using the equation of motion we can write the correlation function:

$$\langle\langle f_{0\sigma}, d_{\sigma}^{\dagger}\rangle\rangle = i\pi\rho_0 \tilde{J} G_{\sigma}(E)$$

In terms of the d-level Green's function and we obtain an equation for $\langle f_0, d_{\sigma}^{\dagger}\rangle$

$$\langle f_{0\sigma}, d_{\sigma}^{\dagger}\rangle = -\frac{1}{\pi} \int_{-D}^{D} dE f(E)\pi \tilde{J} \rho_0 Re[G_{\sigma}(E)]$$

$$G_{\sigma}(E) = \frac{1}{E + i\tilde{\Delta}} \quad \tilde{\Delta} = \pi \langle d_{\downarrow} f_{0\downarrow}^{\dagger}\rangle^2 J^2 \rho_0$$
Slave bosons

\[ \langle f_{0\sigma}, d^\dagger_{\sigma} \rangle = -\frac{1}{\pi} \int_{-D}^{D} dE f(E) \pi \tilde{J} \rho_0 \text{Re}[G_\sigma(E)] \]

\[ \frac{1}{\rho_0 J} = -\int_{-D}^{D} dE f(E) \frac{E}{E^2 + \tilde{\Delta}^2} \]

\[ T = 0 \]

\[ \frac{1}{\rho_0 \tilde{J}} = -\int_{-D}^{0} dE \frac{E}{E^2 + \tilde{\Delta}^2} = \ln \sqrt{1 + (D/\tilde{\Delta})^2} \]

Width of the $T=0$ the resonance

\[ \tilde{\Delta} \sim De^{-1/\rho_0 J} = k_B T_K \]
Slave bosons

Finite temperatures:

\[
\frac{1}{\rho_0 J} = \int_0^D dE \tanh[\beta E/2] \text{Re}[G_\sigma(E)]
\]

\[
\frac{1}{\rho_0 J} \approx \int_0^{2T} dE \frac{\beta E}{2} \text{Re}[G_\sigma(E)] + \int_{2T}^D dE \text{Re}[G_\sigma(E)]
\]

This method gives a spurious transition at \( T \sim T_K \) where the impurity decouples \( \tilde{\Delta}(\sim T_K) = 0 \)

At high temperatures the local spin is free.

\[
\langle d_\sigma f_{0\sigma}^\dagger \rangle
\]
Conclusions Lecture 2

- Numerical Renormalization Group gives a complete solution of the Kondo problem and can be used to study other related model systems.
- At low temperatures, when the ground state is a Fermi liquid, a simple mean field approach can give a semi-quantitative description of the low energy physics.
- The slave boson description can also be extended to study more complex systems [Lechermann 2007]
- Next lecture:
  - Electronic Transport in nanostructures.
  - Molecular transistors: molecular vibrations an the Kondo effect