Part 1: Quantum impurity problems and theoretical background

Part 2: Kondo effect and RG. 1d chain formulation and iterative diagonalization

Part 3: Logarithmic discretization and truncation. The RG in NRG

Part 4: Physical quantities. Results and discussion.
Part 2: Kondo effect and the Renormalization Group

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Overview: Part 2

- Kondo effect
- Perturbation theory
- Perturbative scaling
- Mapping to 1d chain
- Iterative diagonalization
Magnetic impurities

- Resistance of metals:
- Experiments reveal low-temperature minimum

![Graph showing temperature vs. resistance](image)

\[ \frac{10^4 R(T)}{R(273)} \]

\[ R = C_{\text{phonon}} T^5 + R_{\text{impurity}} \]

De Hass, de Bour, de Berg (1934)

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Quantum impurity problems: Part 2
Magnetic impurities

- Resistance minimum an impurity effect
  \[ T_{\text{min}} \propto (C_{\text{imp}})^{1/5} \]
- Conduction electrons scatter off impurities

Iron concentration in Mo_{0.8}Nb_{0.2}

M. Sarachik et al. 1964
Recap: Kondo model

- Scattering from magnetic impurities
  - Single spin-$\frac{1}{2}$ impurity
  - Bath of non-interacting conduction electrons
  - AF Exchange coupling

$$H_K = H_{host} + J \vec{S}_{imp} \cdot \vec{S}_0$$

$$\sum_{k\sigma} \epsilon_k C_{k\sigma}^\dagger C_{k\sigma}$$

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Quantum impurity problems: Part 2

J. Kondo, Prog. Theor. Phys. 32, 37 (1964)
The Kondo problem

- 3rd order perturbation theory in J:

\[ R = C_{\text{phonons}} T^5 + R_{\text{impurity}} + C_{\text{imp}} \left( J^2 + \rho J^3 \log \left( \frac{D}{T} \right) \right) \]

Resistance minimum

\[ T_{\text{min}} \propto \left( C_{\text{imp}} \right)^{1/5} \]
The Kondo problem

- Obviously: perturbation theory fails at low $T$:

$$\rho J^3 \log(D/T) > J^2 \Rightarrow T_K = D e^{-1/\rho J}$$

- What happens below $T_K$?

- What is the ground state?
Scaling and Renormalization

- Look at physics at a lower energy scale

Diagrams:
- Bulk conduction electron states
- Impurity
- Band-edge states (integrate out)
Map to a Kondo model of the same form


Consider a sequence of Hamiltonians with different effective (renormalized) parameters
Fixed points

- Special values of the parameters produce NO renormalization → “fixed points”

- Kondo model:
  - Local Moment (LM) fixed point: $J = 0$
  - Strong coupling (SC) fixed point: $J = \infty$
RG fixed points

- Small J: weak coupling
  - free impurity local moment

... $t_2$ $t_1$ $t_0$

bath in 1d chain representation... more on this later!

impurity

free spin-1/2

see Alex Hewson’s book “The Kondo Problem…” CUP (1997)
**RG fixed points**

- **Large J:** strong coupling state
  - Impurity forms spin-singlet with conduction electrons

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Quantum impurity problems: Part 2

see Alex Hewson’s book “The Kondo Problem…”
CUP (1997)
Scaling and Renormalization

- Look at physics on **successively** lower energy scales


\[ \frac{d \rho J}{d \ln D} = -2(\rho J)^2 + \ldots \]

\[ D e^{-1/\rho J} = \tilde{D} e^{-1/\rho \tilde{J}} \sim k_B T_K \]
For (initially) weak coupling, perturbative scaling indicates that coupling $J$ grows under RG.
- So: when coupling is initially small...

  ... it grows under RG and becomes large

many-body singlet ground state
(complicated real-space structure)
Need a non-perturbative approach!

- Must be able to handle large energy scales: $D$, $J$ etc.
- ... and exponentially small scales, $T_K$
- Exploit RG character of the problem
(very) brief description of NRG:

- Logarithmic discretization of bath
- Mapping to 1d chain
- Iterative diagonalization
- Successive Hilbert-space truncation
NRG: preliminaries

- 1d chain representation
  - Any non-interacting system can be mapped to a 1d tight-binding chain: \textit{“Tridiagonalization”}
Recap: real-space representation

- **Host metal: non-interacting tight-binding model**

\[
H_{host} = \sum_{\sigma} \sum_{<i,j>} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}
\]

\[
\equiv \sum_{\sigma} \vec{c}_{\sigma}^\dagger T \vec{c}_{\sigma}
\]

\[
\vec{c}_{\sigma}^\dagger = (c_{1\sigma}^\dagger, c_{2\sigma}^\dagger, c_{3\sigma}^\dagger, \ldots)
\]

\[
T = \begin{bmatrix}
    t_{11} & t_{12} & \cdots \\
    t_{12}^* & t_{22} & \\
    \vdots & \ddots & \ddots
\end{bmatrix}
\]
Host metal: 1d chain representation

\[ H_{\text{host}} = \sum_{\sigma} \vec{c}_\sigma^\dagger T \vec{c}_\sigma = \sum_{\sigma} \vec{f}_\sigma^\dagger W \vec{f}_\sigma \]

\[ = \sum_{\sigma} \sum_{n} e_n f_{n\sigma}^\dagger f_{n\sigma} + \left( h_n f_{n\sigma}^\dagger f_{(n+1)\sigma} + \text{H.c.} \right) \]

where,

\[ \vec{f}_\sigma = S \vec{c}_\sigma \quad \text{such that,} \quad W = S^\dagger T S \]
Tridiagonal

\[ H_{\text{host}} = \sum_{\sigma} \vec{c}_{\sigma}^\dagger T \vec{c}_{\sigma} = \sum_{\sigma} \vec{f}_{\sigma}^\dagger W \vec{f}_{\sigma} \]

\[ = \sum_{\sigma} \sum_{n} e_n f_{n\sigma}^\dagger f_{n\sigma} + \left( h_n f_{n\sigma}^\dagger f_{(n+1)\sigma} + \text{H.c.} \right) \]

\[
\begin{bmatrix}
  t_{11} & t_{12} & t_{13} & t_{14} \\
  t_{21} & t_{22} & t_{23} & t_{24} \\
  t_{31} & t_{32} & t_{33} & t_{34} \\
  t_{41} & t_{42} & t_{43} & t_{44} \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  e_1 & h_1 & 0 & 0 \\
  h_1 & e_2 & h_2 & 0 \\
  0 & h_2 & e_3 & h_3 \\
  0 & 0 & h_3 & e_4 \\
\end{bmatrix}
\]
Impurity problem as a 1d chain

- 1d chain representation of impurity problem

Choose ‘zero-orbital’ of the conduction electron chain to be the physical host orbital coupled to the impurity in real-space.

\[ f_0\sigma = c_0\sigma \quad \Rightarrow \quad \vec{s}_0 = \sum_{\sigma,\sigma'} f_0^\dagger \frac{\vec{\sigma}_{\sigma\sigma'}}{2} f_0\sigma' \]
Impurity problem as a 1d chain

\[ H_{Kondo} = H_{host} + H_{imp} \]

\[ H_{imp} = J \cdot \vec{S}_{imp} \cdot \vec{S}_0 \]

\[ H_{host} = \sum_{\sigma} \sum_n e_n f_{n\sigma}^{\dagger} f_{n\sigma} + \left( h_n f_{n\sigma}^{\dagger} f_{(n+1)\sigma} + \text{H.c.} \right) \]
Impurity problem as a 1d chain

- Idea: truncate chain?
  - Represent bath by the first N sites of the chain?
  - Then exact diagonalization of approximate model?
Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies

\[ t_i \equiv t = \frac{1}{2} \]
\[ \epsilon_i \equiv \epsilon = 0 \]
Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies

\[ t_i \equiv t = \frac{1}{2} \]
\[ \varepsilon_i \equiv \varepsilon = 0 \]

\[ N = 100 \]

\[ \rho_{0\sigma}(\omega) \]
Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies

\[ t_i \equiv t = \frac{1}{2} \]
\[ \varepsilon_i \equiv \varepsilon = 0 \]

\[ \rho_{0\sigma}(\omega) \]

\[ N = \infty \]
Impurity problem as a 1d chain

- **Problem!**
  - Continuum limit not well-described by finite chain!
  - Spectrum has $N$ poles for an $N$-site chain
  - Lowest energy scale resolved is of order $\sim t/N$
  - Unable to capture low-energy excitations around Fermi level, which are central to the Kondo effect
Impurity problem as a 1d chain

- Idea in NRG: diagonalize the chain iteratively
  - Throw away unimportant states at each step (successively truncate the Hilbert space)
  - Which states are unimportant?!

... more on that in next lecture!
Iterative diagonalization

- Take the ‘generic’ tight-binding 1d chain

\[ H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c_{i\sigma}^\dagger c_{(i+1)\sigma} + \text{H.c.} \]

+ \[ \varepsilon_i c_{i\sigma}^\dagger c_{i\sigma} \]

- Strategy: build up chain *successively* by adding on extra sites. Start by diagonalizing the dimer:

\[ H_1 = \sum_{\sigma} t_0 c_{0\sigma}^\dagger c_{1\sigma} + \text{H.c.} \]
Iterative diagonalization

- Take the ‘generic’ tight-binding 1d chain

\[ H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c_{i\sigma}^\dagger c_{(i+1)\sigma} + \text{H.c.} \]

- Strategy: build up chain \textit{successively} by adding on extra sites. Start by diagonalizing the dimer:

\[ H_2 = \sum_{\sigma} t_0 c_{0\sigma}^\dagger c_{1\sigma} + t_1 c_{1\sigma}^\dagger c_{2\sigma} + \text{H.c.} \]
Iterative diagonalization

- Take the ‘generic’ tight-binding 1d chain

\[ H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c_{i\sigma}^\dagger c_{(i+1)\sigma} + \text{H.c.} \]

- Strategy: build up chain *successively* by adding on extra sites. Start by diagonalizing the dimer:

\[ H_2 = H_1 + \sum_{\sigma} t_1 c_{1\sigma}^\dagger c_{2\sigma} + \text{H.c.} \]
Iterative diagonalization

Recursion:

\[ H_{N+1} = H_N + H_{N+1}^{\text{hop}} \]

\[ H_{N+1}^{\text{hop}} = \sum_{\sigma} t_N c_{N\sigma}^\dagger c_{(N+1)\sigma} + \text{H.c.} \]

... same transformation for any \( N \)!
Iterative diagonalization

- Use the **diagonal basis** of iteration $N$ and couple on an extra site. Then re-diagonalize.

- First, define matrix product states:

$$\left| N + 1; k, r \right\rangle_{bs} = \left| N + 1; k \right\rangle_a \otimes \left| N; r \right\rangle_d$$

Basis states for iteration $N+1$

Basis states for a single added site

Direct product

Diagonal states of previous iteration, $N$
Iterative diagonalization

- States of added site defined by:

\[
\begin{align*}
|N + 1; k = 0\rangle_a &= |\mp\rangle &= |\text{vac}\rangle \\
|N + 1; k = +1\rangle_a &= |\uparrow\rangle &= c^\dagger_{(N+1)\uparrow} |\text{vac}\rangle \\
|N + 1; k = -1\rangle_a &= |\downarrow\rangle &= c^\dagger_{(N+1)\downarrow} |\text{vac}\rangle \\
|N + 1; k = 2\rangle_a &= |\uparrow\downarrow\rangle &= c^\dagger_{(N+1)\uparrow} c^\dagger_{(N+1)\downarrow} |\text{vac}\rangle
\end{align*}
\]
Iterative diagonalization

- Diagonalized states expressed as a linear combination of basis states:

$$\left| N + 1; r \right\rangle_d = \sum_{k,r'} U_{N+1}^r (k, r') \left| N + 1; k, r' \right\rangle_{bs}$$

Coefficients obtained by diagonalizing matrix $H_{N+1}$
Iterative diagonalization

- **Construct Hamiltonian:**
  \[ H_{N+1} = H_N + H_{N+1}^{\text{hop}} \]

- **Matrix elements:**
  \[
  b_s \langle N+1; k, r | H_{N+1} | N+1; k', r' \rangle_{bs} \\
  = d \langle N; r | a \langle N+1; k | H_{N+1} | N+1; k' \rangle_a | N; r' \rangle_{d} \\
  = d \langle N; r | a \langle N+1; k | H_{N} | N+1; k' \rangle_a | N; r' \rangle_{d} \\
  + t_N \sum_{\sigma} d \langle N; r | a \langle N+1; k | c_{N\sigma}^\dagger c_{(N+1)\sigma} | N+1; k' \rangle_a | N; r' \rangle_{d}
  \]
Iterative diagonalization

\[
d\langle N; r | a \langle N + 1; k | H_N | N + 1; k' \rangle_a | N; r' \rangle_d = a \langle N + 1; k | N + 1; k' \rangle_a \times d \langle N; r | H_N | N; r' \rangle_d
\]

\[
\delta_{kk'}
\]

\[
E_N(r) \delta_{rr'}
\]
Iterative diagonalization

\[ t_N \sum_{\sigma} \sum_d \langle N; r \mid a \rangle \langle N + 1; k \mid c_{N\sigma}^{\dagger} \hat{1} c_{(N+1)\sigma} \mid N + 1; k' \rangle_a \mid N; r' \rangle_d \]

**insert complete set of basis states:**

\[ \hat{1} = \sum_{k'', r''} \langle N + 1; k'' \rangle_a \langle N; r'' \rangle_d \langle N; r'' \rangle_a \langle N + 1; k'' \rangle_d \]
Iterative diagonalization

\[ (-1)^{k''} a \langle N + 1; k | N + 1; k'' \rangle_a c_{N\sigma}^\dagger \]

\[ t_N \sum_{\sigma} \sum_{k'', r''} \langle N; r | a \langle N + 1; k | c_{N\sigma}^\dagger | N + 1; k'' \rangle_a | N; r'' \rangle_d \]

\[ \times \langle N; r'' | a \langle N + 1; k'' | c_{(N+1)\sigma} | N + 1; k' \rangle_a | N; r' \rangle_d \]
Iterative diagonalization

\[ \delta_{k,k''} (-1)^k c_{N\sigma} \]

\[ t_N \sum_{\sigma} \sum_{k'',r''} d \langle N; r | a \langle N + 1; k | c_{N\sigma}^\dagger | N + 1; k'' \rangle_a | N; r'' \rangle_d \]

\[ \times \langle N; r'' | a \langle N + 1; k'' | c_{(N+1)\sigma} | N + 1; k' \rangle_a | N; r' \rangle_d \]
Iterative diagonalization

\[ \delta_{k,k''} \ (-1)^k \times d \langle N;r \mid c_{N\sigma}^\dagger \mid N;r'' \rangle_d \]

\[ t_N \sum_\sigma \sum_{k'',r''} d \langle N;r \mid a \langle N + 1;k \mid c_{N\sigma}^\dagger \mid N + 1;k'' \rangle_a \mid N;r'' \rangle_d \]

\[ \times d \langle N;r'' \mid a \langle N + 1;k'' \mid c_{(N+1)\sigma} \mid N + 1;k' \rangle_a \mid N;r' \rangle_d \]
Iterative diagonalization

\[ \delta_{k,k''} (-1)^k \times \sum_d \langle N; r | c^\dagger_{N\sigma} | N; r'' \rangle_d \]

\[ t_N \sum_{\sigma} \sum_{k'', r''} \sum_d \langle N; r | \langle N + 1; k | c^\dagger_{N\sigma} | N + 1; k'' \rangle_a \rangle \sum_d \langle N; r'' | \langle N + 1; k'' | c_{(N+1)\sigma} | N + 1; k' \rangle_a \rangle \rangle \sum_d \langle N; r | \langle N; r' \rangle_d \]

\[ M^{\sigma}_{k'', k'} \]
Iterative diagonalization

\[ \delta_{k,k''} (-1)^k \times d \langle N; r | c_{N\sigma}^\dagger | N; r'' \rangle_d \]

\[ t_N \sum_{\sigma} \sum_{k'', r''} \left( d \langle N; r | a \langle N + 1; k | c_{N\sigma}^\dagger | N + 1; k'' \rangle_a | N; r'' \rangle_d \times d \langle N; r'' | a \langle N + 1; k'' | c_{(N+1)\sigma} | N + 1; k' \rangle_a | N; r' \rangle_d \right) \]

\[ d \langle N; r'' | N; r' \rangle_d M_{k'',k'}^\sigma \]
Iterative diagonalization

\[ \delta_{k,k''} \left(-1\right)^k \times \sum_d \left\langle N; r \left| c_{N\sigma}^\dagger \right| N; r'' \right\rangle \]

\[ t_N \sum_{\sigma} \sum_{k'', r''} \left( \begin{array}{c}
\sum_d \left\langle N; r \left| a \left\langle N + 1; k \left| c_{N\sigma}^\dagger \right| N + 1; k'' \right\rangle \right| N; r'' \right\rangle \\
\times \left\langle N; r'' \left| a \left\langle N + 1; k'' \left| c_{(N+1)\sigma} \right| N + 1; k \right\rangle \right| N; r' \right\rangle \end{array} \right) \]

\[ \delta_{r'', r'} M_{k'', k'}^{\sigma} \]
Iterative diagonalization

Putting it all together:

\[
bs \langle N + 1; k, r | H_{N+1} | N + 1; k', r' \rangle_{bs} = E_N(r) \delta_{rr} \delta_{kk'} + t_N \sum_{\sigma} (-1)^k M^{\sigma}_{k,k'} \times d \langle N; r | c_{N\sigma}^\dagger | N; r' \rangle_d
\]

So: iterative diagonalization requires only:

- Trivial matrix \( M^{\sigma}_{k,k'} \) which is independent of \( N \)
- Eigenenergies of previous iteration, \( E_N(r) \)
- Matrix elements \( d \langle N; r | c_{N\sigma}^\dagger | N; r' \rangle_d \)

between diagonal states of previous iteration
Iterative diagonalization

- Structure of Hamiltonian matrix:

```
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<th></th>
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<th></th>
<th>k = +1</th>
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<td>k = 2</td>
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<td></td>
</tr>
</tbody>
</table>
```
Iterative diagonalization

- How to calculate non-trivial matrix elements?

- First, diagonalize Hamiltonian numerically:

  \[ \langle N + 1; r \mid c^\dagger_{(N+1)\sigma} \mid N + 1; r' \rangle_d = \sum_{\tilde{k}, \tilde{r}} U^r_{N+1}(\tilde{k}, \tilde{r}) \langle N + 1; \tilde{k}, \tilde{r} \rangle_{bs} \]

- For the next iteration, we’ll need:

  \[ \langle N + 1; r \mid c^\dagger_{(N+1)\sigma} \mid N + 1; r' \rangle_d = \sum_{\tilde{r}, \tilde{k}} [U^r_{N+1}(\tilde{k}, \tilde{r})]^\dagger U^{r'}_{N+1}(\tilde{k}', \tilde{r}') \times \langle N + 1; \tilde{k}, \tilde{r} \mid c^\dagger_{(N+1)\sigma} \mid N + 1; \tilde{k}', \tilde{r}' \rangle_{bs} \]
Iterative diagonalization

\[
\begin{align*}
\langle N + 1; \tilde{k}, \tilde{r} | c^\dagger_{(N+1)\sigma} | N + 1; \tilde{k}', \tilde{r}' \rangle_{bs} \\
= d \langle N; \tilde{r} | a \langle N + 1; \tilde{k} | c^\dagger_{(N+1)\sigma} | N + 1; \tilde{k}' \rangle_a | N; \tilde{r}' \rangle_d \\
= \delta_{\tilde{r}, \tilde{r}'} \\
\left[ M^\sigma_{\tilde{k}, \tilde{k}'} \right]^\dagger
\end{align*}
\]
Starting at one end of the chain, we can couple on extra sites recursively, and iteratively diagonalize.
Obvious problem: Hilbert space grows by a factor of 4 at each iteration (fermionic sites)

- After only 10 sites have been added, Hamiltonian matrix in the many-particle basis is of dimension $10^6 \times 10^6$
- Diagonalization time scales as cube of matrix dimension
- Disaster!

Must stop after only a few steps: cannot access low-energy physics this way!
Truncation

- **Exploit RG concept**
  (which we know is at the heart of quantum impurity problems, from perturbative scaling)

- **Idea in NRG:** throw away *high-energy states* at each iteration, focusing on the low-energy physics at each step. Eventually determine ground state.

- **How do to this?**
  ... solution next lecture!