Magnetic impurities in metals: Kondo effect and the numerical renormalization group

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1. introduction to basic rg concepts

consider a model on a one-dimensional lattice, with operators $a_i$ ($i$: lattice site), parameters $J, h, \ldots$, and Hamiltonian $H(J, h, \ldots)$.

combine two sites to give (effectively) one site with operators $a'_i$ and parameters $J', h', \ldots$.

we assume that the Hamiltonian $H'$ of the effective model is of the same form, with renormalized parameters: $H' = H(J', h', \ldots)$.

then rescale the model to the original lattice spacing:
the mapping \( H \to H' \) is a renormalization group transformation

\[
H(J', h', \ldots) = R\{H(J, h, \ldots)\}
\]

with \( \vec{K} = (J, h, \ldots) \): \( R(\vec{K}) = \vec{K}' \)

now consider a sequence of transformations:

\[
\vec{K} \xrightarrow{R} \vec{K}' \xrightarrow{R} \vec{K}''
\]

this results in a trajectory in parameter space:

flow diagrams and fixed points

stable fixed point

all perturbations are irrelevant

unstable fixed point

at least one relevant perturbation
the central issue:

How does the behaviour of the system change under a scale transformation?

→ the physics of the problem described as a flow between fixed points.

- identify the fixed points of the model (and their physical meaning)
- identify the relevant/irrelevant perturbations
- if possible: describe the full flow from S to C

and finally: calculate physical properties
some technical issues:

- how to perform the mapping $H \rightarrow H'$ for a given model?
  - Ising model: (1d) in the partition function $Z$, sum over every second spin

- but: the whole strategy depends on the details of the model
  - spins/fermions/bosons
  - dimension, lattice structure, etc.

$\Rightarrow$ for a given model, it is a priori not clear whether a successful rg scheme can be developed at all

in the following:

- (numerical) renormalization group for quantum impurity models
  - Wilson’s NRG for the single-impurity Anderson model
- interpretation of fixed points and flow diagrams
2. Introduction to quantum impurity physics

The Kondo effect: magnetic impurities in metals

$T$-dependence of resistivity

$\rho$

$0$ $T$

Metal
2. introduction to quantum impurity physics

the Kondo effect: magnetic impurities in metals

$T$-dependence of resistivity

![Graph showing the $T$-dependence of resistivity with a curve indicating the transition from a metal to a non-metal phase.]

scattering processes of conduction electrons at magnetic impurities

- $\downarrow$ c
- $\uparrow$ f
- $\Rightarrow$
- $\downarrow$ c
- $\uparrow$ f
- $\Rightarrow$
- $\downarrow$ f
2. introduction to quantum impurity physics

the Kondo effect: magnetic impurities in metals

The $T$-dependence of resistivity, $\rho$, shows a sharp drop at $T_K$, indicating the formation of a singlet state due to magnetic moment screening.

Scattering processes of conduction electrons at magnetic impurities:

Screening of magnetic moments due to singlet formation:

\[
\frac{1}{\sqrt{2}} (|\uparrow_f\downarrow_c\rangle - |\downarrow_f\uparrow_c\rangle)
\]
modelling of magnetic impurities in metals

here: single-impurity Anderson model

[A.C. Hewson, *The Kondo Problem To Heavy Fermions*, CUP 1993]

\[
H = \varepsilon_f \sum_{\sigma} f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow \\
+ \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k\sigma} (f_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_\sigma)
\]

the model describes:

- formation of local moments: $|\uparrow\rangle_f, |\downarrow\rangle_f$
- scattering of conduction electrons
- screening of local moments below temperature scale $T_K$
3. the numerical renormalization group

K.G. Wilson, Rev. Mod. Phys. 47, 773 (1975) → Kondo problem

1. NRG-discretization parameter $\Lambda > 1$

$\Delta(\omega)$

$\omega$

$1$  $\Lambda^{-1} 1$  $\Lambda^{-2} 1$  $\Lambda^{-3} 1$

$E_{N+1}(r) E_N(r) E_N(r)$

$a)$ after truncation

$b)$

$c)$

$d)$

$0$
2. logarithmic discretization
3. mapping on semi-infinite chain
4. iterative diagonalization

\[ H_N : \]

\[ H_{N+1} : \]

\[ |r, s\rangle_{N+1} : \]

\[ |r\rangle_N \otimes |s\rangle_{(N+1)} \]
5. truncation
logarithmic discretization

starting point: siAm in the integral representation:

\[
H_{\text{imp}} = \sum_{\sigma} \varepsilon_{f} f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow} f_{\downarrow},
\]

\[
H_{\text{bath}} = \sum_{\sigma} \int_{-1}^{1} d\varepsilon \, g(\varepsilon) a_{\varepsilon\sigma}^{\dagger} a_{\varepsilon\sigma},
\]

\[
H_{\text{imp} - \text{bath}} = \sum_{\sigma} \int_{-1}^{1} d\varepsilon \, h(\varepsilon) \left( f_{\sigma}^{\dagger} a_{\varepsilon\sigma} + a_{\varepsilon\sigma}^{\dagger} f_{\sigma} \right).
\]

\(\Lambda > 1\) defines a set of intervals with discretization points

\[\pm x_n = \Lambda^{-n}, \quad n = 0, 1, 2, \ldots .\]
width of the intervals: \( d_n = \Lambda^{-n}(1 - \Lambda^{-1}) \)

within each interval: introduce a complete set of orthonormal functions

\[
\psi_{np}^{\pm}(\varepsilon) = \begin{cases} 
\frac{1}{\sqrt{d_n}} e^{\pm i \omega_n p \varepsilon} & \text{for } x_{n+1} < \pm \varepsilon < x_n \\
0 & \text{outside this interval .}
\end{cases}
\]

expand the conduction electron operators \( a_{\varepsilon \sigma} \) in this basis

\[
a_{\varepsilon \sigma} = \sum_{np} \left[ a_{np \sigma} \psi_{np}^+(\varepsilon) + b_{np \sigma} \psi_{np}^-(\varepsilon) \right],
\]

assumption:

\[
h(\varepsilon) = h_n^\pm, \quad x_{n+1} < \pm \varepsilon < x_n,
\]

the hybridization term then takes the form:

\[
\int_{-1}^{1} d\varepsilon \ h(\varepsilon) f^{\dagger}_{\sigma} a_{\varepsilon \sigma} = \frac{1}{\sqrt{\pi}} f^{\dagger}_{\sigma} \sum_{n} \left[ \gamma_n^+ a_{n0 \sigma} + \gamma_n^- b_{n0 \sigma} \right]
\]

the impurity couples only to the \( p = 0 \) components of the conduction band states!
the conduction electron term transforms to:

\[
\int_{-1}^{1} d\varepsilon \, g(\varepsilon) a_{\varepsilon\sigma}^\dagger a_{\varepsilon\sigma} = \sum_{np} \left( \xi_n^+ a_{np\sigma}^\dagger a_{np\sigma} + \xi_n^- b_{np\sigma}^\dagger b_{np\sigma} \right)
\]

\[
+ \sum_{n, p \neq p'} \left( \alpha_n^+ (p, p') a_{np\sigma}^\dagger a_{np'\sigma} - \alpha_n^- (p, p') b_{np\sigma}^\dagger b_{np'\sigma} \right).
\]

For a linear dispersion, \( g(\varepsilon) = \varepsilon \), one obtains:

\[
\xi_n^\pm = \pm \frac{1}{2} \Lambda^{-n} (1 + \Lambda^{-1}),
\]

\[
\alpha_n^\pm (p, p') = \frac{1 - \Lambda^{-1}}{2\pi i} \frac{\Lambda^{-n}}{p' - p} \exp \left[ \frac{2\pi i (p' - p)}{1 - \Lambda^{-1}} \right].
\]
structure of the Hamiltonian

\[ \varepsilon \]

impurity couples to \( p = 0 \) only

\[ \alpha (p, p') \]

\[ b_{02 \sigma} \]

discretization of the Hamiltonian:

drop the terms with \( p \neq 0 \) in the conduction band
now: relabel the operators $a_{n0\sigma} \equiv a_{n\sigma}$, etc.,
the discretized Hamiltonian takes the form:

$$H = H_{\text{imp}} + \sum_{n\sigma} \left[ \xi_n^+ a_{n\sigma}^\dagger a_{n\sigma} + \xi_n^- b_{n\sigma}^\dagger b_{n\sigma} \right]$$

$$+ \frac{1}{\sqrt{\pi}} \sum_{n\sigma} f_{\sigma}^\dagger \left[ \sum_n \left( \gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right) \right]$$

$$+ \frac{1}{\sqrt{\pi}} \sum_{n\sigma} \left[ \sum_n \left( \gamma_n^+ a_{n\sigma}^\dagger + \gamma_n^- b_{n\sigma}^\dagger \right) \right] f_{\sigma}$$
mapping on a semi-infinite chain

orthogonal transformation of the operators \( \{ a_{n\sigma}, b_{n\sigma} \} \) to a new set of operators \( \{ c_{n\sigma} \} \) such that the discretized Hamiltonian takes the form:

\[
H = H_{\text{imp}} + V \sum_\sigma \left[ f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right] \\
+ \sum_{\sigma n=0}^{\infty} \left[ \varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_n \left( c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \right]
\]

the mapping is equivalent to the tridiagonalization of a matrix
for a constant density of states

\[ t_n = \frac{(1 + \Lambda^{-1}) (1 - \Lambda^{-n-1})}{2\sqrt{1 - \Lambda^{-2n-1}} \sqrt{1 - \Lambda^{-2n-3}}} \Lambda^{-n/2}. \]

In the limit of large \( n \) this reduces to

\[ t_n \rightarrow \frac{1}{2} \left( 1 + \Lambda^{-1} \right) \Lambda^{-n/2}. \]

this means: in moving along the chain we start from high energies \((U, V, D)\) and go to arbitrary low energies.

in real space: double the system size by adding two sites to the chain (for \( \Lambda = 2 \))
iterative diagonalization

the chain Hamiltonian can be viewed as a series of Hamiltonians $H_N$ ($N = 0, 1, 2, \ldots$) which approaches $H$ in the limit $N \to \infty$:

$$H = \lim_{N \to \infty} \Lambda^{-(N-1)/2} H_N ,$$

with

$$H_N = \Lambda^{(N-1)/2} \left[ H_{\text{imp}} + \sqrt{\frac{\xi_0}{\pi}} \sum_{\sigma} \left( f_{\sigma}^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_{\sigma} \right) + \sum_{\sigma n=0}^N \varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + \sum_{\sigma n=0}^{N-1} t_n \left( c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \right].$$

two successive Hamiltonians are related by

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} \sum_{\sigma} \varepsilon_{N+1} c_{N+1\sigma}^\dagger c_{N+1\sigma}$$

$$+ \Lambda^{N/2} \sum_{\sigma} t_N \left( c_{N\sigma}^\dagger c_{N+1\sigma} + c_{N+1\sigma}^\dagger c_{N\sigma} \right) ,$$
starting point:

\[ H_0 = \Lambda^{-1/2} \left[ H_{\text{imp}} + \sum_{\sigma} \varepsilon_0 c_{0\sigma}^\dagger c_{0\sigma} + \sqrt{\xi_0} \pi \sum_{\sigma} \left( f_{\sigma}^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_{\sigma} \right) \right]. \]

renormalization group transformation:

\[ H_{N+1} = R(H_N) \]
set up an iterative scheme for the diagonalization of $H_N$
→ construct a basis for $H_{N+1}$

$$|r; s\rangle_{N+1} = |r\rangle_N \otimes |s(N + 1)\rangle.$$ 

diagonalization: new eigenenergies $E_{N+1}(w)$ and eigenstates $|w\rangle_{N+1}$

truncation:
renormalization group flow and fixed points

plot the rescaled many-particle energies $E_N(r)$ as a function of $N$ (odd $N$ only)

fixed points of the single-impurity Anderson model

FO: free orbital
LM: local moment
SC: strong coupling

parameters: $\varepsilon_f = -0.5 \cdot 10^{-3}$, $U = 10^{-3}$, $V = 0.004$, and $\Lambda = 2.5$
renormalization group flow and fixed points

plot the rescaled many-particle energies $E_N(r)$ as a function of $N$ (odd $N$ only)

fixed points of the single-impurity Anderson model

- **FO**: free orbital
- **LM**: local moment
- **SC**: strong coupling

parameters: $\varepsilon_f = -0.5 \cdot 10^{-3}$, $U = 10^{-3}$, $V = 0.004$, and $\Lambda = 2.5$
4. fixed points in quantum impurity models

quantum impurity models show a variety of different fixed points here:

- quantum critical point in the soft-gap Anderson model

  single-impurity Anderson model with hybridization function
  \[ \Delta(\omega) = \Delta|\omega|^r \]

  \( \rightarrow \) interacting fixed point

- non-Fermi liquid fixed point in the two-channel Kondo model

  \( \rightarrow \) Majorana fermions
soft-gap Anderson model

phase diagram

flow diagrams

quantum phase transition between SC and LM phases

non-trivial structure of the qcp

[H.-J. Lee, R. Bulla, M. Vojta
J. Phys.: Condens. Matter 17, 6935 (2005)]
two-channel Kondo model

\[ H = \sum_{k\sigma} \sum_{\alpha} \varepsilon_k c_{k\sigma\alpha}^\dagger c_{k\sigma\alpha} + J \sum_{\alpha} \vec{S} \cdot \vec{s}_\alpha \]

→ non-Fermi liquid fixed point with residual impurity entropy \( S_{\text{imp}} = \frac{1}{2} \ln 2 \)

NRG flow diagram

→ characteristic structure of the non-Fermi liquid fixed point
structure of the fixed point

the many-particle spectra of each sector can be constructed from single-particle spectra of Majorana fermions
single-particle spectra

[sector I]

\begin{align*}
E & \quad \text{level} \\
0 & : \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}
\end{align*}

[sector II]

\begin{align*}
E & \quad \text{level} \\
0 & : \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}
\end{align*}

where does this structure come from?

→ vector and scalar Majorana fermion chains with different boundary conditions

from the numerical analysis of the two-channel Anderson model we obtain

emergent fractionalized degrees of freedom (Majorana fermions) at the low-energy fixed point!

a quotation from:
Universality and Scaling in a Charge Two-Channel Kondo Device

Finally, we highlight a perspective on these results, connected with the ongoing search for Majorana fermions. The quantitative agreement between theory and experiment over 9 orders of magnitude in $T / T_K$ proves that this device realizes a non-Fermi liquid state involving a free Majorana localized on the dot, described by the 2CK critical fixed point. These results therefore unambiguously establish the existence of Majorana fermions in this frustrated strongly interacting system.
5. calculation of physical properties and applications

What can we do with the NRG?

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calculation of physical properties

A. thermodynamics

use the spectra of many-particle energies $E_N(r)$ at each iteration to calculate thermodynamic/static properties at a corresponding temperature

$$T_N \propto \Lambda^{-N/2}$$

→ specific heat $C(T)$, susceptibility $\chi(T)$, etc.

B. dynamic properties

example: single-particle Green function

$$G_\sigma(z) = \langle [f_\sigma, f_\sigma^\dagger] \rangle_z = i \int_0^\infty dt \ e^{izt} \langle [f_\sigma(t), f_\sigma^\dagger]_+ \rangle \quad (1)$$

spectral function:

$$A(\omega) = -\frac{1}{\pi} \text{Im } G(\omega + i\delta^+) \ , \quad (2)$$
In each iteration, calculate the spectral function for each cluster of size \( N \) via:

\[
A_{\sigma N}(\omega) = \frac{1}{Z_N} \sum_{nm} |n \langle f^\dagger_\sigma m \rangle_N|^2 \delta(\omega - (E_N^m - E_N^n)) \left( e^{-\beta E_N^m} + e^{-\beta E_N^n} \right) \tag{3}
\]
effect of the truncation on the spectral functions of each iteration:

\[ N = 14 \]
effect of the truncation on the spectral functions of each iteration:

\( N = 14 \)

\( N = 16 \)
effect of the truncation on the spectral functions of each iteration:

$N = 14$

$N = 16$

$N = 18$
effect of the truncation on the spectral functions of each iteration:

\[ N = 14 \]

\[ N = 16 \]

\[ N = 18 \]

this means:
final spectral function = superposition of the data from all iterations
superposition of δ-Peaks:

up to N

N+2

up to N+2
finally: broadening of the $\delta$-peaks $\rightarrow$ Gaussian on a logarithmic scale

$$
\delta(\omega - \omega_n) \rightarrow \frac{e^{-b^2/4}}{b \omega_n \sqrt{\pi}} \exp\left[-\frac{(\ln \omega - \ln \omega_n)^2}{b^2}\right]
$$

results for the single-impurity Anderson model:
finally: broadening of the $\delta$-peaks $\longrightarrow$ Gaussian on a logarithmic scale

$$\delta(\omega - \omega_n) \rightarrow \frac{e^{-b^2/4}}{b\omega_n\sqrt{\pi}} \exp \left[ -\frac{(\ln \omega - \ln \omega_n)^2}{b^2} \right]$$

(results for the single-impurity Anderson model:

![Graph showing $A(\omega)W$ vs $\omega/W$ for different values of $U/\Delta$](image-url)
finally: broadening of the δ-peaks $\rightarrow$ Gaussian on a logarithmic scale

$$
\delta(\omega - \omega_n) \rightarrow \frac{e^{-b^2/4}}{b \omega_n \sqrt{\pi}} \exp \left[ - \frac{(\ln \omega - \ln \omega_n)^2}{b^2} \right]
$$

results for the single-impurity Anderson model:
finally: broadening of the $\delta$-peaks $\rightarrow$ Gaussian on a logarithmic scale

$$\delta(\omega - \omega_n) \rightarrow \frac{e^{-b^2/4}}{b \omega_n \sqrt{\pi}} \exp \left[ -\frac{(\ln \omega - \ln \omega_n)^2}{b^2} \right]$$

(4)

results for the single-impurity Anderson model:
NRG for multi-channel models

Generalized Wilson chain for solving multichannel quantum impurity problems

a) standard approach

b) interleaved NRG
6. summary

in this talk:

- a short introduction to
  - the renormalization group concept
  - quantum impurity physics
  - the NRG method
    - flow diagrams and fixed points
    - calculation of physical properties

I did not discuss:

- quantum dots and Kondo physics
- non-equilibrium properties
- all the recent developments which considerably extended the power of the NRG method; see the work of
  - F. Anders, Th. Costi, J. von Delft, A. Mitchell, A. Weichselbaum, ...
- relation to other renormalization group methods
  - DMRG
  - fRG