Dynamical properties of quantum impurity systems in and out of equilibrium: a numerical renormalization group approach

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Collaborators

NRG Review
R. Bulla, T. Costi and Th. Pruschke
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Introduction

1. Kondo effect in bulk materials
2. Kondo effect in nano-devices

The Numerical Renormalization Group

2. Discretization of the bath continuum
3. Fixed points

Spectral functions at finite temperatures

4. Complete basis set of the Wilson chain

Real-time dynamics out of equilibrium

4. Time-dependent numerical renormalization group
5. Spin decay in the anisotropic Kondo model

Conclusion
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   - Kondo effect in nano-devices

2 The Numerical Renormalization Group
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   - Fixed points

3 Spectral functions at finite temperatures
   - Complete basis set of the Wilson chain

4 Real-time dynamics out of equilibrium
   - Time-dependent numerical renormalization group
   - Spin decay in the anisotropic Kondo model

5 Conclusion
scattering increases for $T \to 0$!
dehaas, de Boer, van den Berg, Physica 1,1115 (1934)
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de Haas, de Boer, van den Berg, Physica 1,1115 (1934)

but: saturation $T < T_K$

Onuki et al 1987
Zero bias anomaly

\[ G(0) \propto \ln(T) \text{ for } T \to 0! \]
Wyatt, PRL 13,401 (1964)

\[ G(V) \text{ in Ta-I-Al} \]
Wyatt, PRL 13,401 (1964)

Kondo 1964
- single spin + metal
- AF coupling: \( H_K = J \vec{S} \vec{s}_{\text{band}} \)
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Kondo effect in a single electron transistor (SET)

D. Goldhaber-Gordon, Nature 98

M. Kastner RMP 1992
Kondo effect in nano-devices

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D. Goldhaber-Gordon, Nature 98

Kondo effect in nano-devices

lattice problem

- Mapping the lattice problem onto an effective site problem (quantum impurity problem) plus dynamical bath (DMFT).
  Kuramoto 85; Grewe 87; Metzner, Volhardt; Müller-Hartmann, Brand, Mielsch 89;
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5. **Conclusion**
Quantum Impurity Problems

Quantum Impurity

- finite number of localized DOF
- interacting with a bath continuum
- bosonic bath: see Ingersent

Problem:

- infrared divergence in perturbation theory
- indicator for a change of ground state
- Kondo singlet vs free moment

quantum impurity
metallic host
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Discretization of the bath continuum

**Numerical Renormalization Group**

Wilson 1975, Krishnamurthy et al. 1980

- discretization of the bath continuum on a logarithmic grid:
  \( I_n^+ = D[\Lambda^{-n-1}, \Lambda^{-n}] \)

- Mapping onto a semi-finite chain for an arbitrary bath coupling function \( \Delta(\omega), J(\omega) \)
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quantum impurity 
\[ |\alpha\rangle \]
\[ |\gamma\rangle \]
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Wilson’s NRG (1975)

- switching on iteratively the couplings $\xi_m \propto \Lambda^{-m/2}$
- recursion relation (RG transformation)

$$H_{N+1} = \sqrt{\Lambda} H_N + \sum_{\sigma} \xi_N \left( f_{N\sigma}^\dagger f_{N+1\sigma} + f_{N+1\sigma}^\dagger f_{N\sigma} \right)$$

iteratively diagonalize the series of Hamiltonians $H_m$
- RG: elimination of the high energy states, rescaling by $\sqrt{\Lambda}$
- temperature: $T_m \propto \Lambda^{-m/2}$
- stop at chain length $N$, when desired $T_N \propto \Lambda^{-N/2}$ is reached
Wilson’s NRG (1975)

- Impurity
- 1
- 2
- 3
- N

\[ \xi_1, \xi_2, \xi_3, \xi_N \sim \Lambda^{-N/2} \]

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CEF Splitting in the SU(4) SIAM

NRG not only a numerical tool! Wilson 1975, Krishnamurty et al. 1980

- analysis of the fixed points $H^* = T_{RG}^2[H^*]$: deep insight into the physics of a model, crossover scales $T^*$
Numerical Renormalization Group

NRG Review: R. Bulla, T. Costi and Th. Pruschke, cond-mat/0701105

Extensions of Wilson’s method in recent years

- **bosonic baths**: Tong, Bulla, Vojta 2003
- bosonic and fermionic baths: Glossop, Ingersent 2005
- non-equilibrium: Costi, 1997, Anders, Schiller 2005

Calculation of spectral functions

- Frota, Olivera 1986
- Sakai et al 1989
- Costi, Hewson 1992, 1994
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Problem:

- dynamical properties unsystematic:
  - how are different energy scale connected?
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Spectral functions at finite temperatures

- Assumption: solve the Wilson chain exactly, i.e. $H_N|n\rangle = E_n|n\rangle$
- Then: Lehmann representation of $\rho(\omega)$ (text book)

$$\rho_{A,B}(\omega) = \sum_{n,m} \frac{(e^{-\beta E_n} + e^{-\beta E_m})}{Z} A_{nm}B_{mn} \delta(\omega + E_n - E_m)$$

The challenge:

- discrete spectrum $\rightarrow$ continuous $\rho(\omega)$, broading of $\delta(\omega)$
- how do we gather the information from different iterations?
- how do we guarantee the sum-rule

$$\int_{-\infty}^{\infty} d\omega \rho(\omega) = 1 \ ?$$
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\]
All discarded states: a complete basis set for Wilson chain

Anders, Schiller PRL 95, 196801 (2005), PRB 74,245113 (2006)

complete basis: \{\ket{e}\} = \{\ket{\alpha_{imp}, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \cdots, \alpha_N}\}
Complete basis set of the Wilson chain

All discarded states: a complete basis set for Wilson chain

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\[
\begin{align*}
|k',e,1> & \quad |e> \\
|e> & \quad |k,e,1>
\end{align*}
\]

complete basis: \( \{|e\rangle\} = \{|k, e; 1\rangle\} \)
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\[
|l,e,2\rangle = |k,e,2\rangle + |l,e,3\rangle
\]

complete basis: \( \{|e\rangle\} = \{|k, e; 2\rangle\} + \{|l, e; 2\rangle\} \)
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Complete basis: \[ |e\rangle = \{|k, e; 3\rangle \} + \sum_{m=2}^{3} \{|l, e; m\rangle \} \]
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\[
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Complete basis set of the Wilson chain

**Sum-rule conserving NRG Green functions**

\[ G_{A,B}(z) = \sum_{m=m_{\text{min}}}^{N} \sum_{l} \sum_{k,k'} A_{l,k'}(m) \rho_{k',k}^{\text{red}}(m) B_{k,l}(m) \]

\[ + \sum_{m=m_{\text{min}}}^{N} \sum_{l} \sum_{k,k'} B_{l,k'}(m) \rho_{k',k}^{\text{red}}(m) A_{k,l}(m) \]

\[ \frac{z + E_l - E_k}{z + E_k - E_l} \]

- **reduced density matrix** (Feynman 72, White 92, Hofstetter 2000)

\[ \rho_{k,k'}^{\text{red}}(m) = \sum_{\text{e}} \langle k, e; m | \hat{\rho} | k', e; m \rangle , \]

- Weichelbaum, von Delft: cond-mat/0607497

- extension to NEQ GF \( G(t, t') \) possible (Anders 2007)
Complete basis set of the Wilson chain

**Sum-rule conserving NRG Green functions**

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Spectral function in the presents of CEF splitting

\[ \Sigma_\alpha(z) \text{ causal} \]

\[ G_\alpha^{-1}(z) = z - E_\alpha - \Gamma_\alpha(z) - \Sigma_\alpha(z) \]

\[ \text{NCA: } \Sigma_\alpha(z) \text{ violates causality already for } T \gg T_K \]
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Real-time dynamics of an observable

\[ \langle \hat{O} \rangle(t) = \text{Tr} \left[ \hat{O} \hat{\rho}(t) \right] \]

- Equilibrium: single condition \( \hat{\rho}(t) = \hat{\rho}_0 = \exp(-\beta \mathcal{H}^f) / \mathcal{Z} \)
- Non-equilibrium: two conditions: \( \hat{\rho}_0 \) and \( \mathcal{H}^f \)

\[ \hat{\rho}(t) = e^{-i\mathcal{H}^f t} \hat{\rho}_0 e^{i\mathcal{H}^f t} \]

- Calculation of the trace using an energy eigenbasis of \( \mathcal{H}^f \)

\[ \langle \hat{O} \rangle(t) = \sum_{n,m} \langle E_n|\hat{O}|E_m \rangle \langle E_m|\hat{\rho}_0|E_n \rangle e^{-i(E_m-E_n)t} \]
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The challenge

Non-equilibrium dynamics in quantum impurity systems

The problem

- evaluation of all energy scales
- avoid overcounting
- relaxation into the new thermodynamic ground state?

The solution

complete NRG basis set of the Wilson chain
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The solution

complete NRG basis set of the Wilson chain
New method: time-dependent NRG

\[ \langle \hat{O} \rangle(t) = \sum_{n,m} \langle E_n | \hat{O} | E_m \rangle \langle E_m | \hat{\rho}_0 | E_n \rangle e^{-i(E_m-E_n)t} \]

- \( \hat{O} \): local operator, diagonal in \( \epsilon \)
- reduced density matrix

\[ \rho^{\text{red}}_{ll'}(m) = \sum_{l, e; m} \langle l, e; m | \hat{\rho}_0 | l', e; m \rangle \]

- RG upside down: eliminated states contain the information on the time evolution
- discretization averaging simulates continuum

New method: time-dependent NRG

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\langle \hat{O}(t) \rangle = \sum_m \sum_{l,l'} \langle l | \hat{O} | l' \rangle e^{i(E_l - E_{l'})t} \rho^{\text{red}}_{l' l}(m)
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\[ \langle \hat{O} \rangle (t) = \sum_m \sum_{l,l'} \langle l | \hat{O} | l' \rangle e^{i(E_l - E_{l'})t} \rho_{l' l}(m) \]

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- RG upside down: eliminated states contain the information on the time evolution
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Discussion of the method

- resolving the contradiction: RG and including all energy scale
- no accumulated error in time in contrary to td-DMRG
- exponentially long time scales accessible (up to $t \ast T \approx 1$)
- calculation of time-dependent NEQ Green functions $G(t, t')$ for steplike Hamiltonians possible
Spin decay in the anisotropic Kondo model

Benchmark: decoherence of a pure state

\[ |s\rangle = \left( |\uparrow\rangle + |\downarrow\rangle \right) / \sqrt{2} \]

TD-NRG

analytical exact solution and TD-NRG: excellent agreement
Spin decay in the anisotropic Kondo model

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TD-NRG plus analytic solution PRB 74,245113 (2006)

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Spin decay in the anisotropic Kondo model

**short-time dynamics:** perturbative in $J_\perp$

- AFM regime: infrared divergence
  - exponentially long time-scale $1/T_K$
Spin decay in the anisotropic Kondo model

- **short-time dynamics**: perturbative in $J_{\perp}$
- **AFM regime**: infrared divergence
- Exponentially long time-scale $1/T_K$
Spin decay in the anisotropic Kondo model

- long time relaxation: $t_{spin} \propto 1/T_K$
- conformal field theory and flow equation
  - exponential decay only for $t \gg 1/T_K$

Flow equation solution: Kehrein 2005

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Conclusion

The numerical renormalization group

- accurate, non-perturbative solution to any QIP
- fixed points: insight into the physics of a model
- thermodynamics and quantum phase transitions
- equilibrium spectral function
- extendable to non-equilibrium
- TD-NRG: no accumulated error in time

Applications

- one, two-site, multi-channel impurity models
- zoo of coupled quantum dot models
- impurity solver for DMFT calculations
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