Numerical renormalization group
part 2

Rok Žitko

Jožef Stefan institute

and

Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

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- Basics of renormalization group
- NRG method
- Implementation
- Analysis of results

Effective hamiltonian

= description valid on a certain energy/length scale

Parameters can be extracted from the experiment.

What terms to retain:

- symmetry considerations
- energy considerations
- relevance of operators (renormalization group)

Example: from Hubbard model to Heisenberg model

$$H = -t \sum_{ij,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

large U, <n>=1

i.e., for Mott insulators

$$H = J \sum_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad J = \frac{4t^2}{U}$$

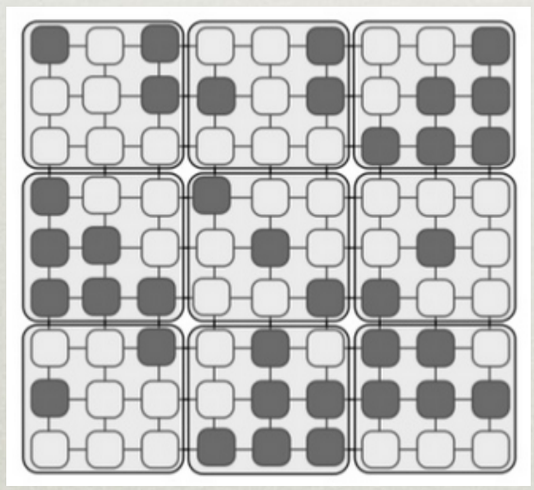
$$[S^x, S^y] = iS^z \quad \mathbf{S}^2 = S(S+1)$$

Renormalization group

1) procedure for finding relations between the effective descriptions of the same physical system on different energy scales

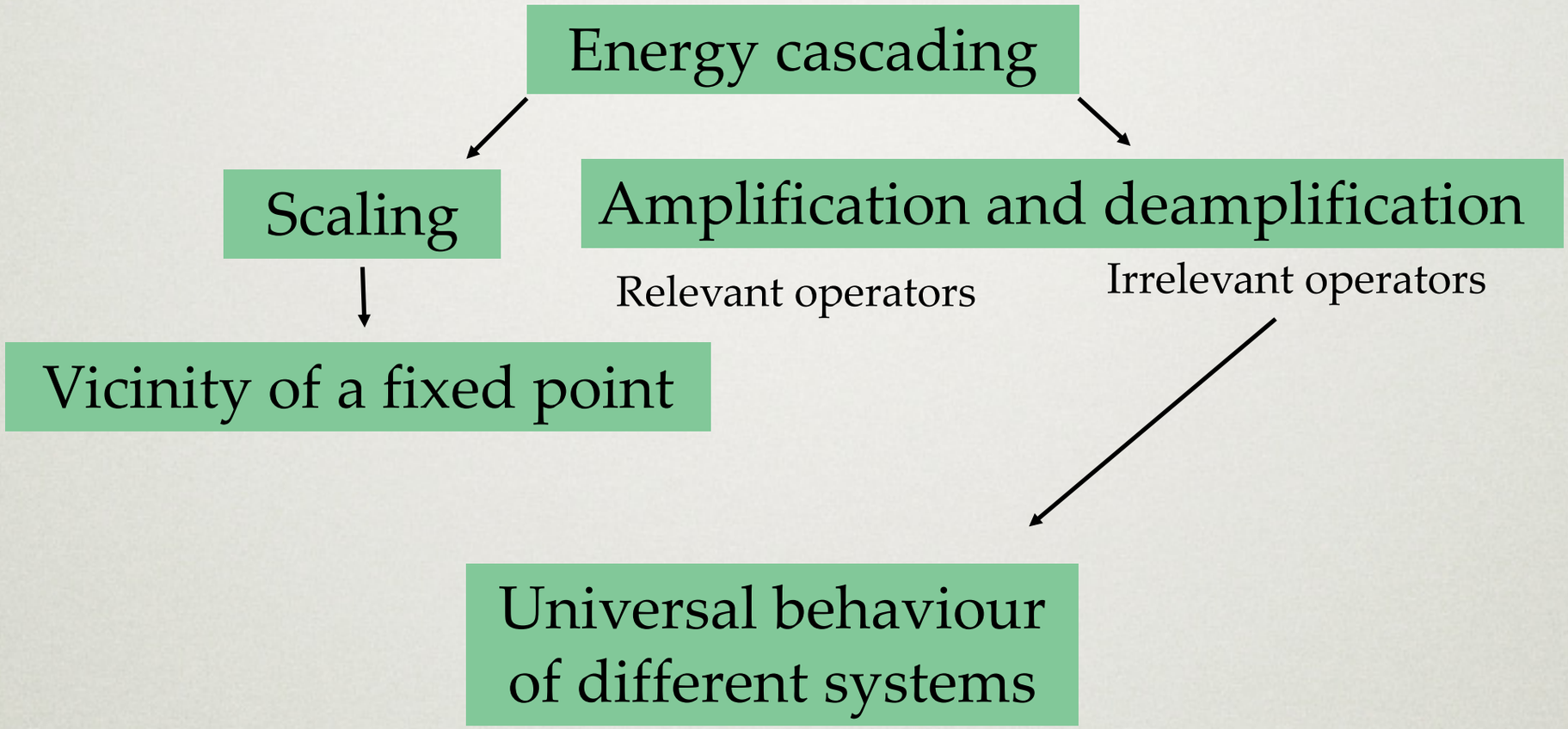
Approaches:

- by integrating out high-energy degrees of freedom by coarse graining
- unitary transformations and truncation



coarse graining

2) framework for discussing relations between physical theories


Energy cascading
Scaling
Amplification and deamplification
Relevant operators
Irrelevant operators
Vicinity of a fixed point
Universal behaviour
of different systems

Fixed points, (ir)relevant operators

$$H^* = T[H^*]$$

$$H_N = H^* + \delta H_N$$
$$H_{N+1} = T[H^* + \delta H] = H^* + L[H^*] \cdot \delta H + \mathcal{O}[\delta H_N^2]$$

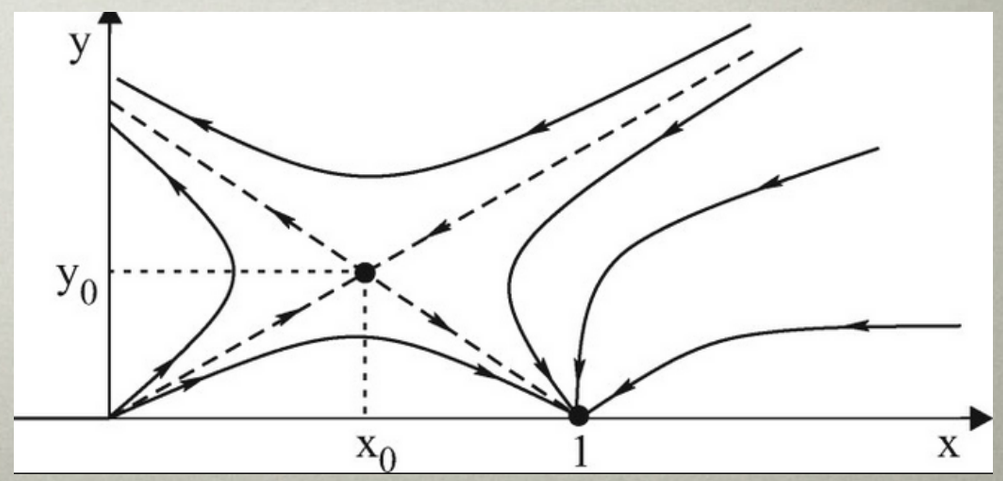
$$L[H^*] \cdot O = \lambda O$$

$$\delta H_N = \sum_m c_m \lambda_m^N O_m$$

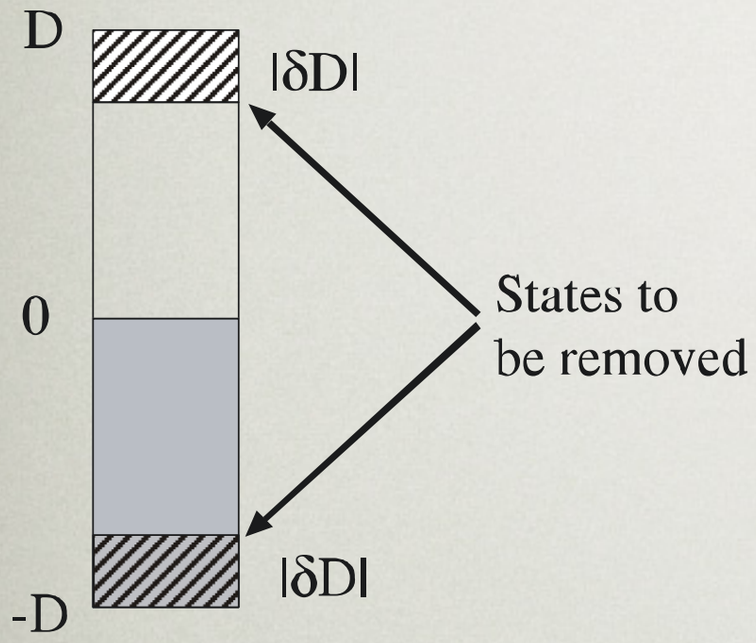
$\lambda > 1$ relevant operator

$\lambda < 1$ irrelevant operator (universality!)

$\lambda = 1$ marginal operator



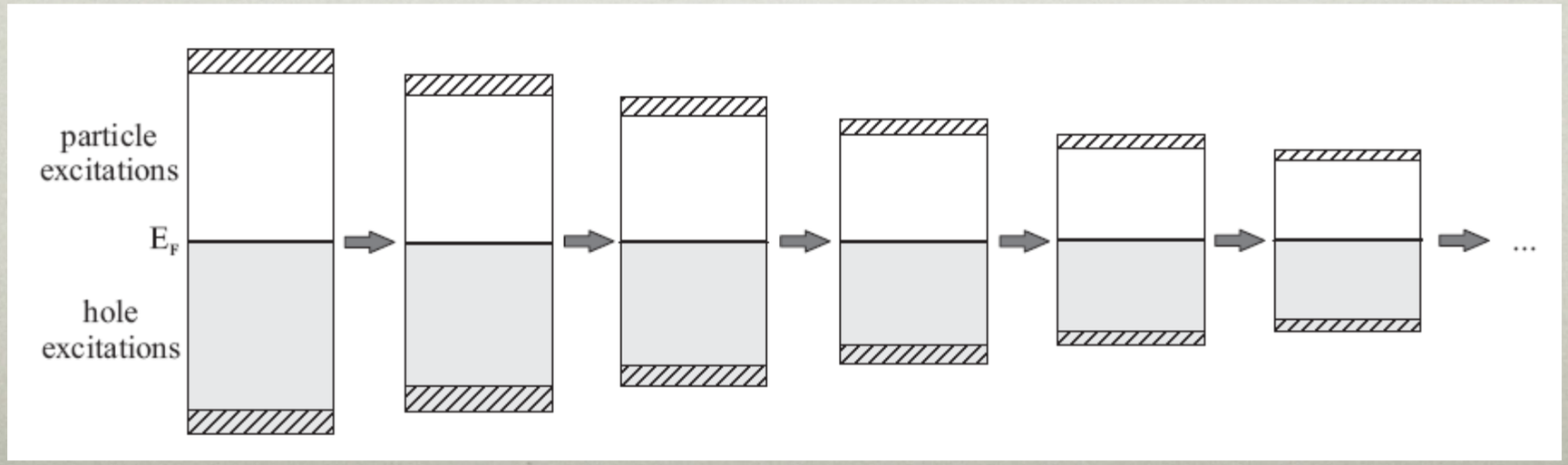
Cutoff renormalization



$$\frac{d\mathcal{J}}{d\ln\mathcal{D}} = -\rho\mathcal{J}^2$$

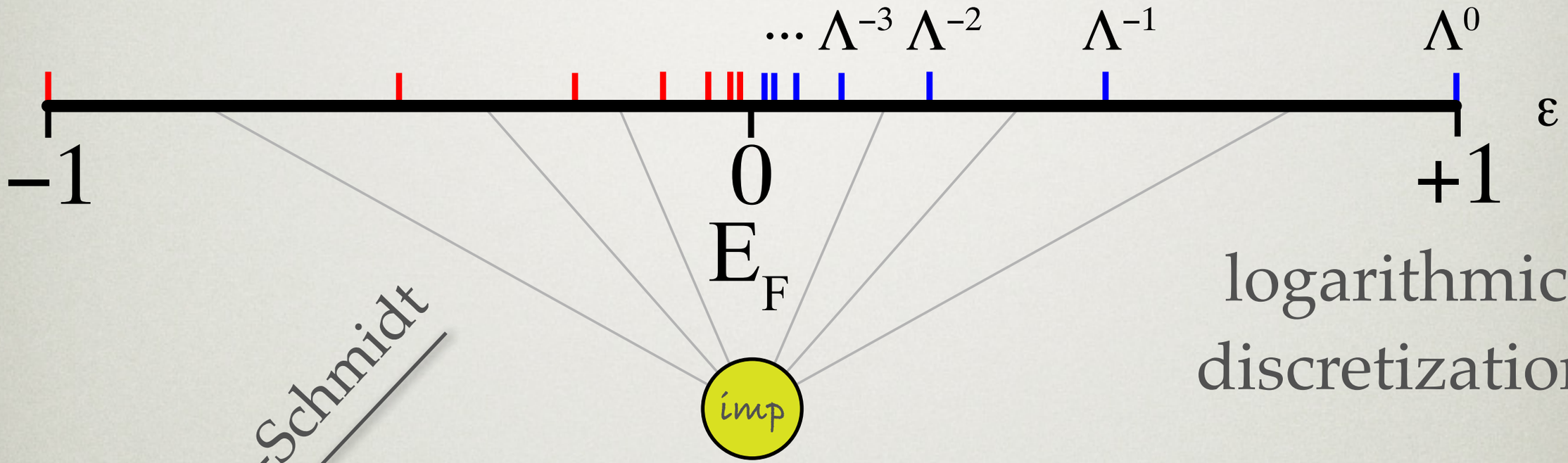
$$\mathcal{J}(D) = \frac{J}{1-\rho J\ln(\mathcal{D}/D)}$$

$$T_K \sim D\exp\left(-\frac{1}{\rho J}\right)$$



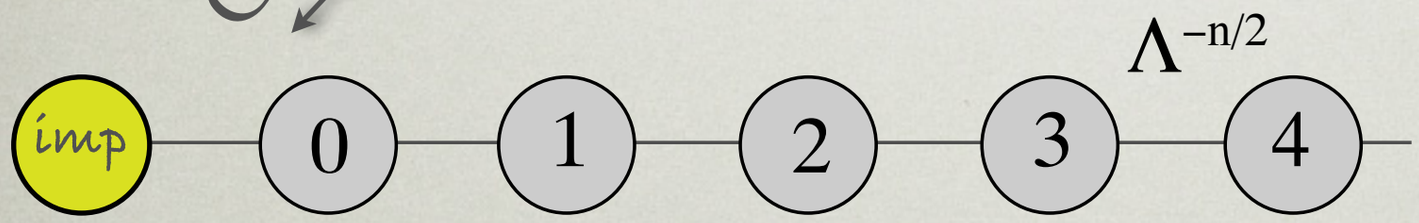
Numerical Renormalization Group

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



logarithmic discretization

$\Lambda > 1$

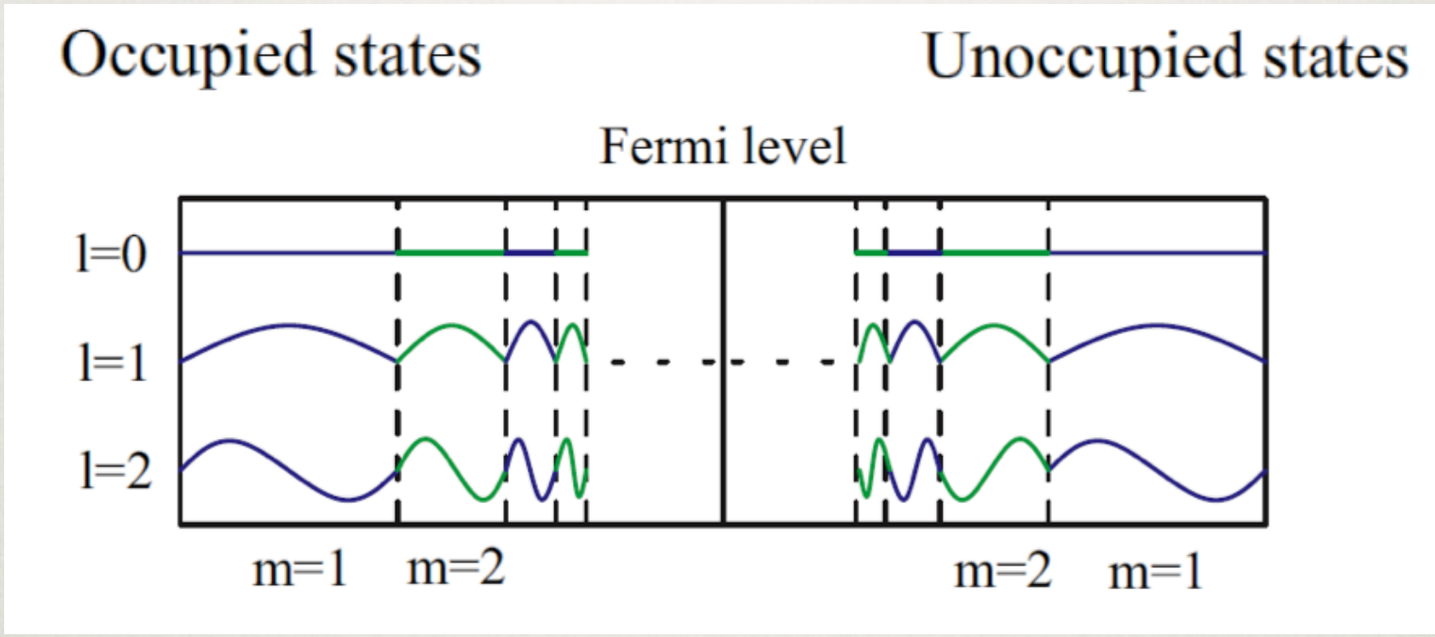


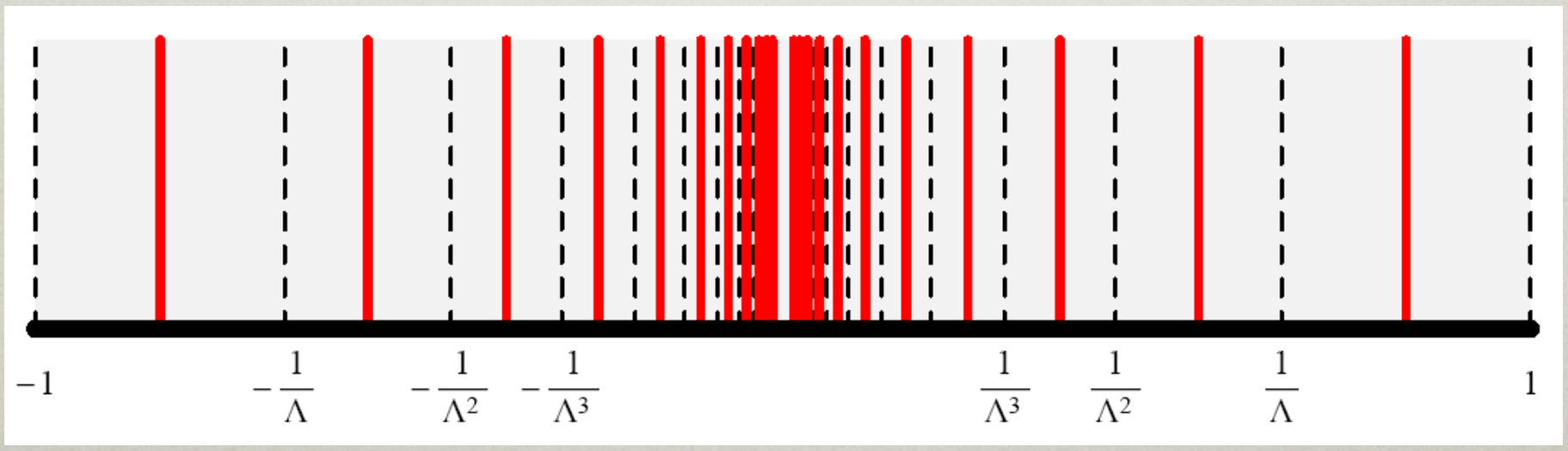
Wilson's chain

http://nrgljubljana.ijs.si/

METHOD

Logarithmic discretization





good sampling of the states near the Fermi energy

Zero-th site of the Wilson chain

$$f^\dagger_{0\mu} = \frac{1}{\sqrt{N_c}} \sum_k c^\dagger_{k\mu}$$

This is the conduction-band orbital at the position of the impurity.

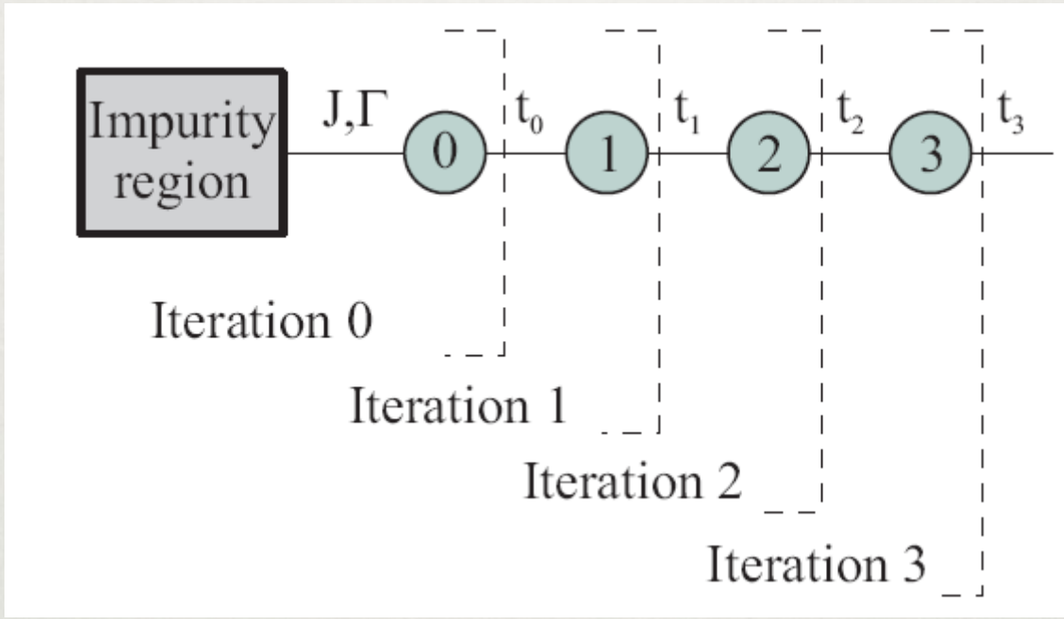
More generally:

$$V f^\dagger_{0\mu} = \frac{1}{\sqrt{N_c}} \sum_k V_k c^\dagger_{k\mu} \qquad |V|^2 = \frac{1}{N_c} \sum_k |V_k|^2$$

Characteristic energy scale

$$T_N \propto \frac{D}{k_B} \Lambda^{-N/2} / \bar{\beta} \qquad \bar{\beta} \sim 1$$

Iterative diagonalization



$$H_{N+1} = T\left[H_N\right]$$

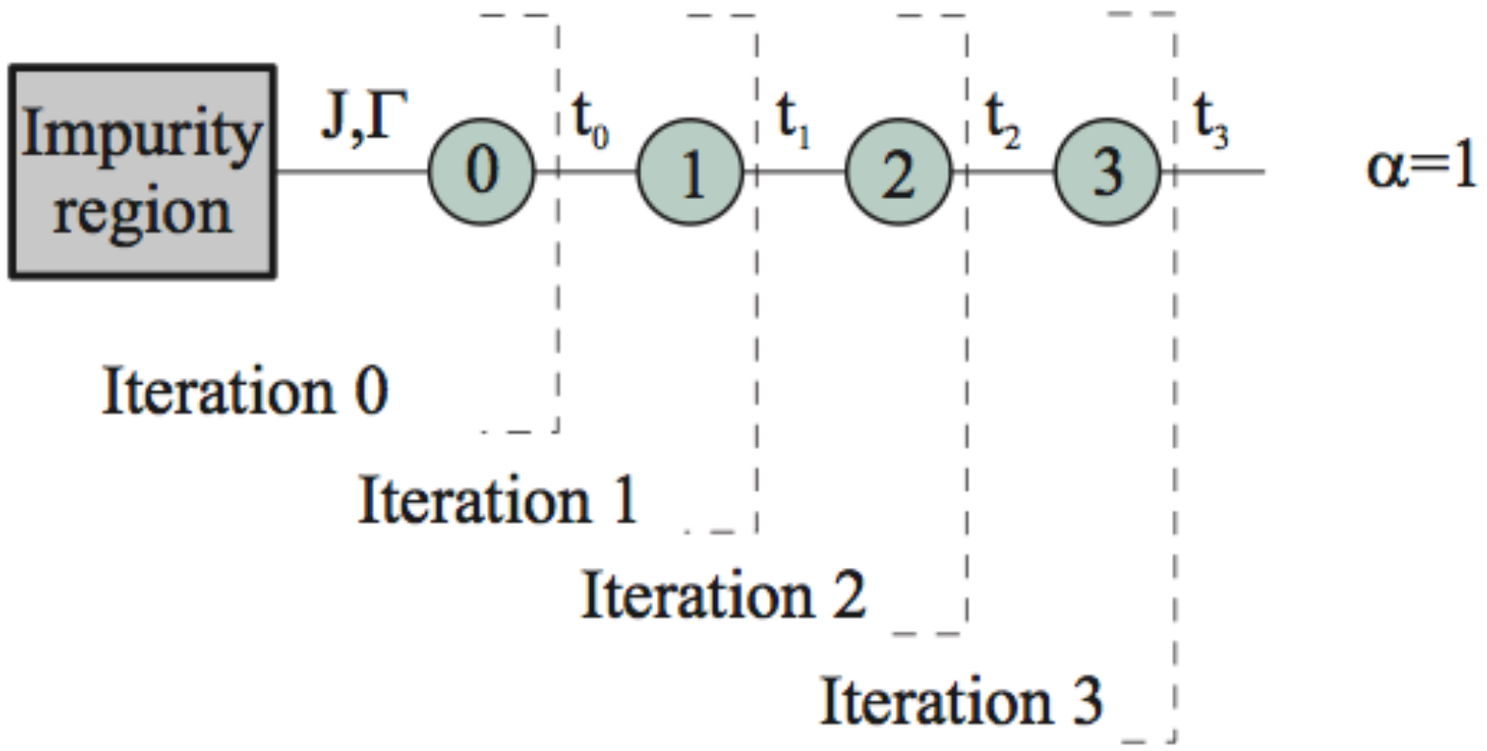
$$H_{N+1} = \Lambda^{-1/2} H_N + \xi_N (f^{\dagger}_{N+1,\sigma} f_{N,\sigma} + f^{\dagger}_{N,\sigma} f_{N+1,\sigma})$$

Initial Hamiltonian

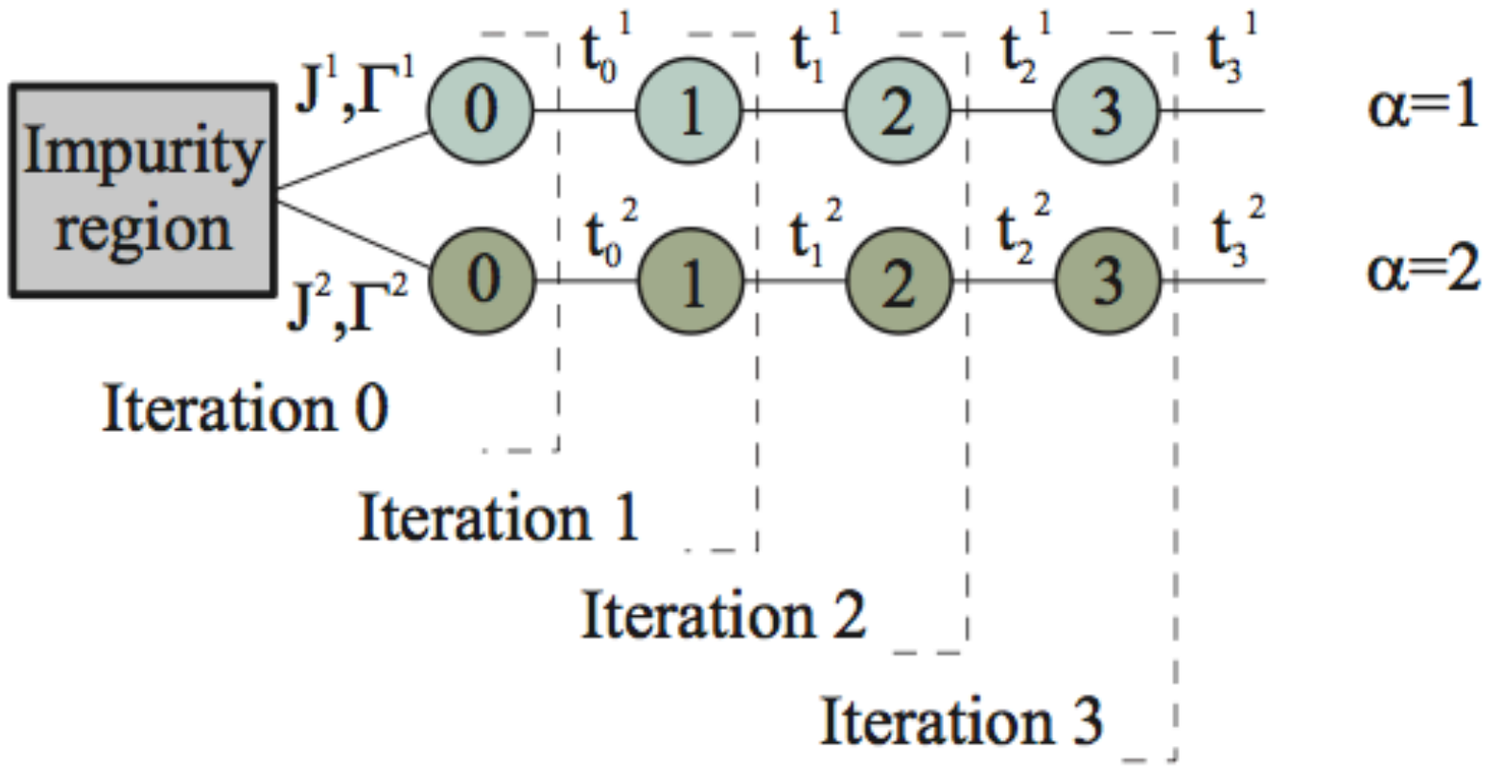
$$H_0 = H_{\text{imp}} + \sum_\sigma \epsilon_0 f_{0\sigma}^\dagger f_{0\sigma} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left(d_\sigma^\dagger f_{0\sigma} + f_{0\sigma}^\dagger d_\sigma \right)$$

$$H_0 |r\rangle_0 = E_0(r) |r\rangle_0$$

a) One-channel case



b) Two-channel case



Basis construction

$$|Q,S_z,r;1\rangle_{N+1} = |Q+1,S_z,r\rangle_N,$$

$$|Q,S_z,r;2\rangle_{N+1} = c^\dagger_{N+1\uparrow}\left|Q,S_z-\frac{1}{2},r\right\rangle_N,$$

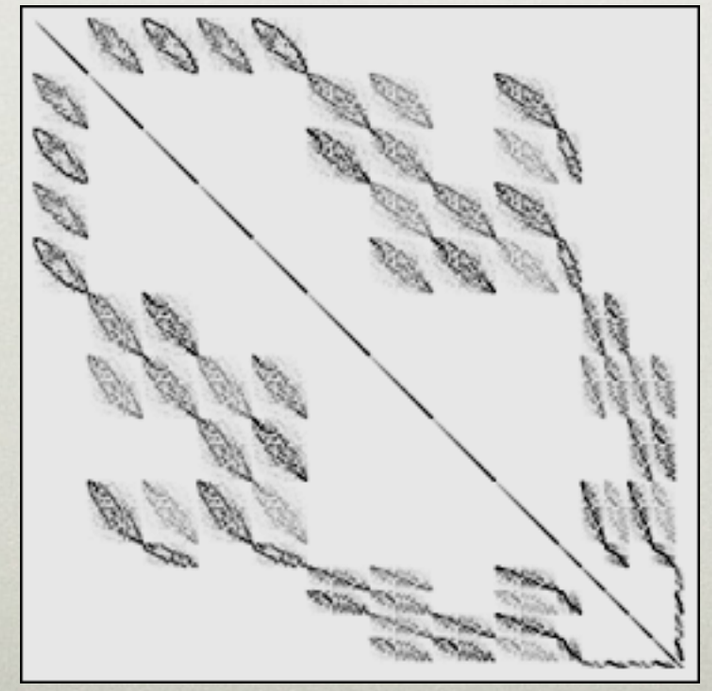
$$|Q,S_z,r;3\rangle_{N+1} = c^\dagger_{N+1\downarrow}\left|Q,S_z+\frac{1}{2},r\right\rangle_N,$$

$$|Q,S_z,r;4\rangle_{N+1} = c^\dagger_{N+1\uparrow}c^\dagger_{N+1\downarrow}|Q-1,S_z,r\rangle_N.$$

Hamiltonian matrix generation

$$H_{N+1}(rs, r's') = {}_{N+1}\langle r; s|H_{N+1}|r'; s'\rangle_{N+1}$$

$$H_{N+1} = \sqrt{\Lambda} H_N + X_{N,N+1} + Y_{N+1}$$



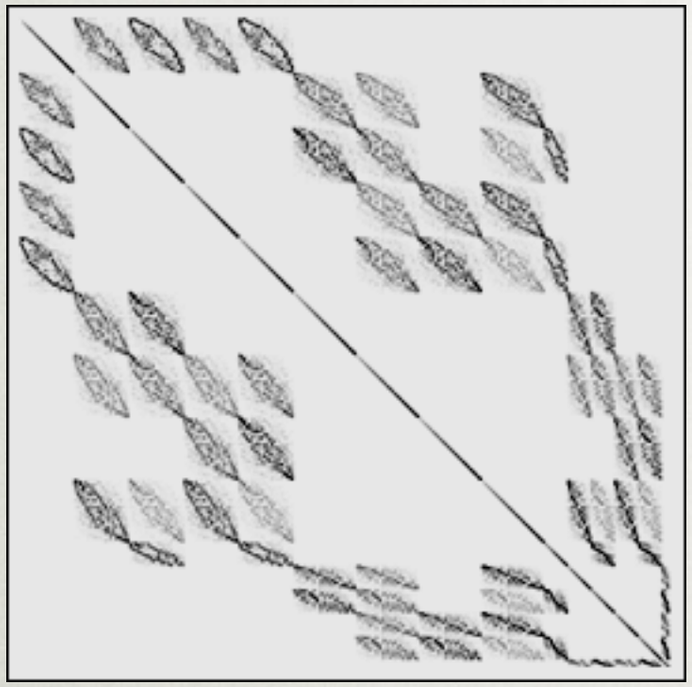
Matrix diagonalisation

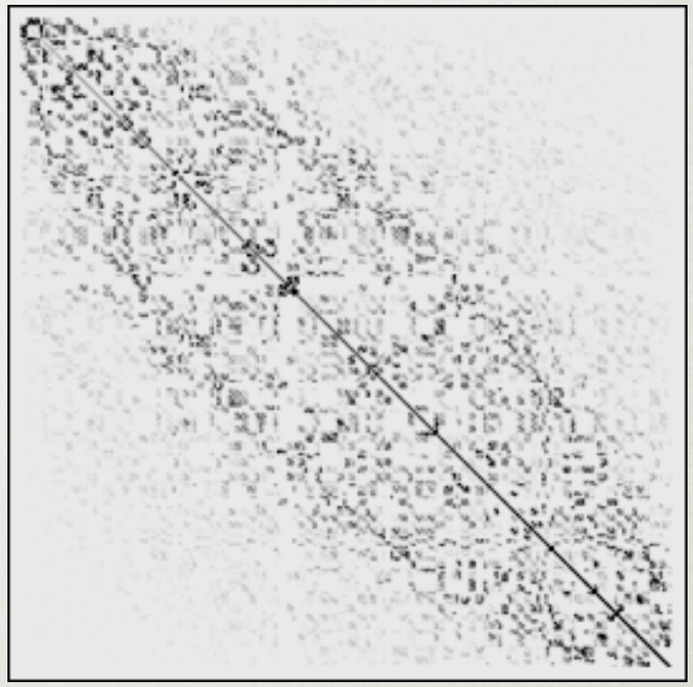
- Full diagonalisation with `dsyev/zheev`
- Partial diagonalisations with `dsyevr/zheevr`

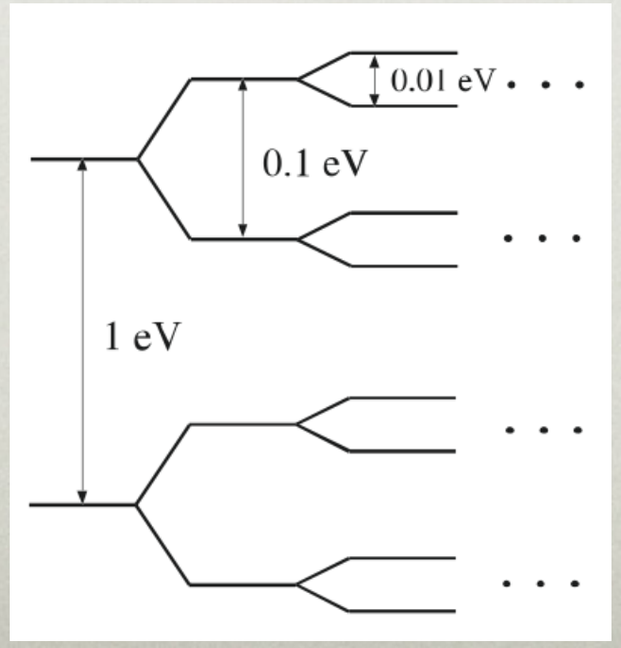
Largest amount of the processor time spent here!

$$|QS\omega\rangle = \sum_{ri} U_{QS}(\omega, ri)|QSri\rangle$$

Energy-scale separation

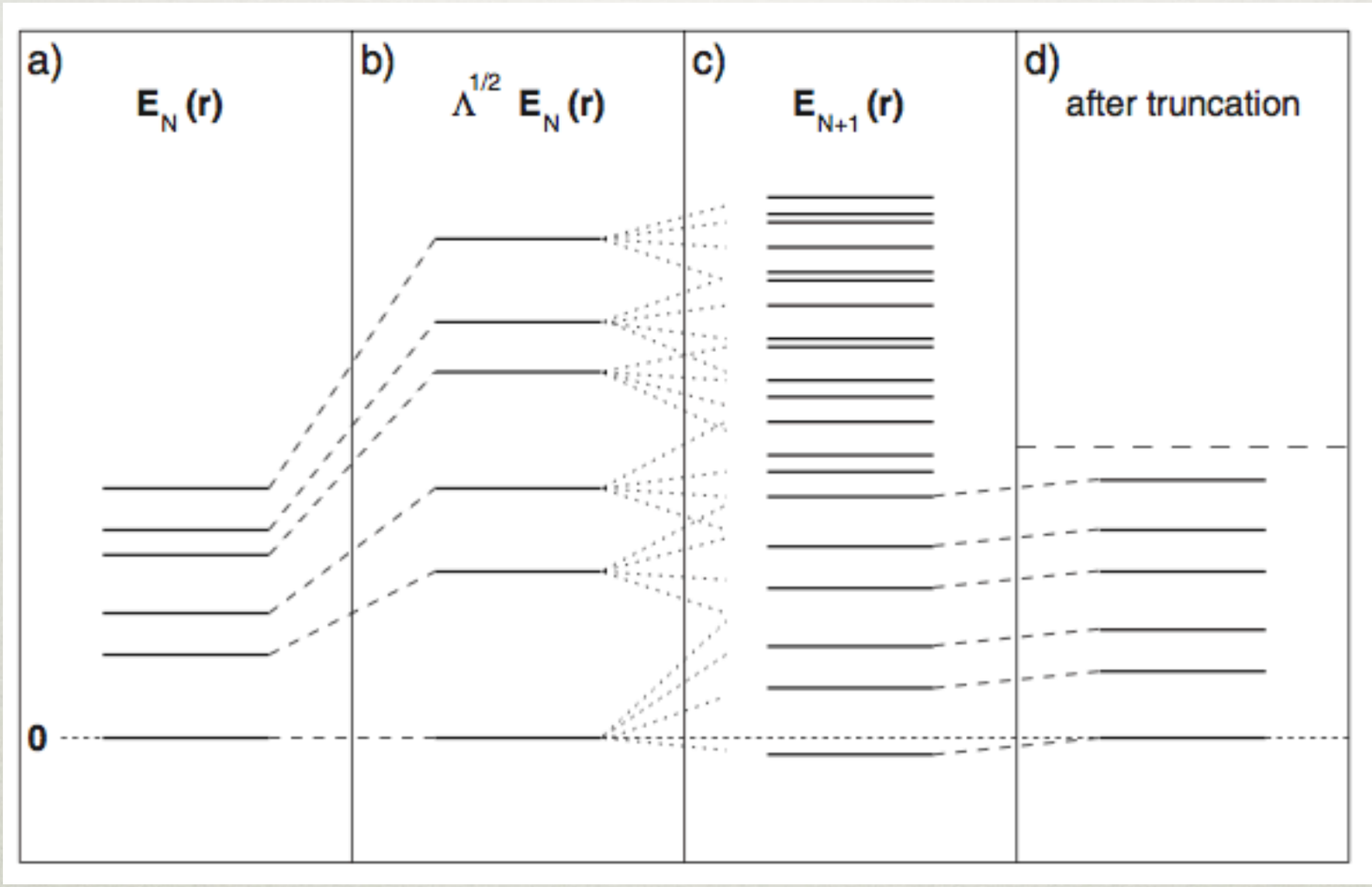






Energy scales are **locally** coupled

Truncation



Analysis

- Renormalization flow & analysis of fixed points and operators
- Thermodynamics properties
- Static quantities (expectation values)
- Dynamics properties (spectra, susceptibilities)
- Real-time evolution

IMPLEMENTATION

SNEG + NRG Ljubljana

Add-on package for the computer algebra system Mathematica for performing calculations involving non-commuting operators

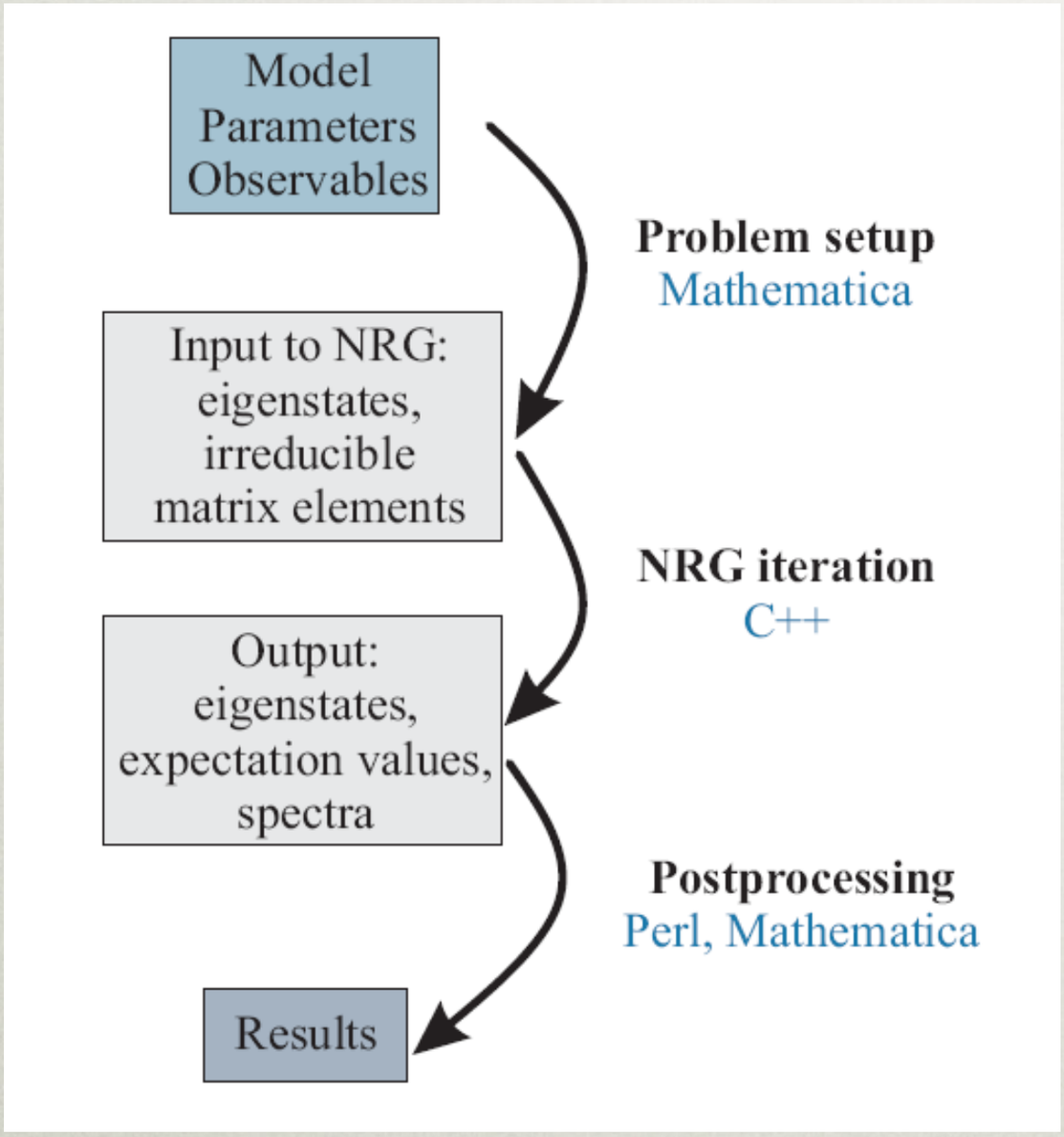
Efficient general purpose numerical renormalization group code

- flexible and adaptable
- highly optimized (partially parallelized)
- easy to use

http://nrgljubljana.ijs.si/

Design goals

- Flexibility (very few hard-coded limits) and adaptability (easy to extend)
- Implemented using modern high-level programming paradigms
  (pattern matching and functional programming in Mathematica, OOP in C++)
- Efficiency (LAPACK calls)



`nrginit`

`nrgrun`

various scripts

Example input files

param

```
[extra]
U=0.01
Gamma=0.0007
delta=0

[param]
symtype=QS
discretization=Z
Lambda=2
Tmin=1e-10
keepenergy=10
keep=5000

model=siam.m
```

siam.m

```
def1ch[1];

H1 = delta (number[d]-1) +
     U/2 pow[number[d]-1, 2];
Hc = gammaPol hop[f[0], d[]];

H = H0 + H1 + Hc;
```

Symmetries

$\mathrm{SU}(2)_{\mathrm{spin}}$

$$\mathbf{S} = \sum_{\mu\mu'} d^\dagger_\mu \left(\frac{1}{2} \boldsymbol{\sigma}_{\mu\mu'} \right) d_{\mu'}$$

$$\boldsymbol{\sigma} = \{\sigma^x, \sigma^y, \sigma^z\}$$

$$S^z = \frac{1}{2}\left(d^\dagger_\uparrow d_\uparrow - d^\dagger_\downarrow d_\downarrow \right)$$

$$S^+ = S^x + iS^y = d^\dagger_\uparrow d_\downarrow$$

$$S^- = S^x - iS^y = d^\dagger_\downarrow d_\uparrow$$

Total spin: $\mathbf{S}_{\mathrm{total}} = \sum_i \mathbf{S}_i$

Wigner-Eckart theorem

O is a **spherical tensor operator** of rank M if:

$$\begin{aligned}\left[J_z, O_\mu^M\right] &= \mu O_\mu^M \\ \left[J_+, O_\mu^M\right] &= A(M,\mu) O_{\mu+1}^M \\ \left[J_-, O_\mu^M\right] &= A(M,-\mu) O_{\mu-1}^M\end{aligned}$$

$$A(M,\mu) = \sqrt{(M-\mu)(M+\mu+1)}$$

$$\langle \alpha, j, j_z | O_\mu^M | \alpha', j', j_z' \rangle = \left\langle j' j_z'; M\mu | j j_z \right\rangle \langle \alpha, j \| O^M \| \alpha', j' \rangle$$

For a more general treatment of non-Abelian symmetries in NRG, see
A. I. Toth, C. P. Moca, O. Legeza, G. Zarand, PRB 78, 245109 (2008),
A. Weichselbaum, Annals of Physics 327, 2972-3047 (2012).

Basis construction

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

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-1,0)$	1
$(0,\frac{1}{2})$	$a^\dagger_\uparrow$
$(1,0)$	$a^\dagger_\downarrow a^\dagger_\uparrow$

(a) One channel

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-2,0)$	1
$(-1,\frac{1}{2})$	$b^\dagger_\uparrow,\ a^\dagger_\uparrow$
$(0,0)$	$b^\dagger_\downarrow b^\dagger_\uparrow,\ \frac{1}{\sqrt{2}}\left(a^\dagger_\downarrow b^\dagger_\uparrow - a^\dagger_\uparrow b^\dagger_\downarrow\right),\ a^\dagger_\downarrow a^\dagger_\uparrow$
$(0,1)$	$b^\dagger_\uparrow a^\dagger_\uparrow$
$(1,\frac{1}{2})$	$a^\dagger_\uparrow b^\dagger_\downarrow b^\dagger_\uparrow,\ b^\dagger_\uparrow a^\dagger_\downarrow a^\dagger_\uparrow$
$(2,0)$	$a^\dagger_\uparrow a^\dagger_\downarrow b^\dagger_\uparrow b^\dagger_\downarrow$

(b) Two channels

$$|QSS_z ri\rangle_{N+1} = \sum_{\mu=-S(i)}^{S(i)} \left\langle g_i^\mu(SS_z);S(i),\mu|SS_z\right\rangle \ |F_i(QS)f_i^\mu(S_z)r\rangle_N \otimes |i,\mu\rangle$$

Recalculation of operators

$$\langle QS\omega \| \hat{O} \| Q'S'\omega' \rangle_{N+1} = \frac{\langle QSS_z\omega | \hat{O}_\mu | Q'S'S'_z\omega' \rangle_{N+1}}{\langle S'S'_z; M\mu | SS_z \rangle}$$

$$\langle QS\omega \| \hat{O} \| Q'S'\omega' \rangle_{N+1} = \sum_{ii'} C(QS, Q'S', ii') \sum_{rr'} U_{QS}(\omega, ri) U_{Q'S'}(\omega', r'i') \langle F_i(QS)r \| \hat{O} \| F_{i'}(Q'S')r' \rangle_N$$

Important to be efficiently implemented! We use BLAS routine **GEMM** (general matrix multiply). (GEMM from Intel MKL library has >80% efficiency on Xeon processors.)

Level	Data Movement	Floating-Point Operations	Example
Level 1 BLAS	O(N)	O(N)	DDOT
Level 2 BLAS	$O(N^2)$	$O(N^2)$	DGEMV
Level 3 BLAS	$O(N^2)$	$O(N^3)$	DGEMM

Common symtype settings

- **QS**: conservation of charge and full invariance in spin space
- **QSZ**: external magnetic field (axial spin symmetry)
- **U1**: no spin symmetry
- **SPSU2**, **SPU1**: superconducting case (with full and axial spin symmetry)
- **NONE**: no symmetry at all

Real vs. complex numerics

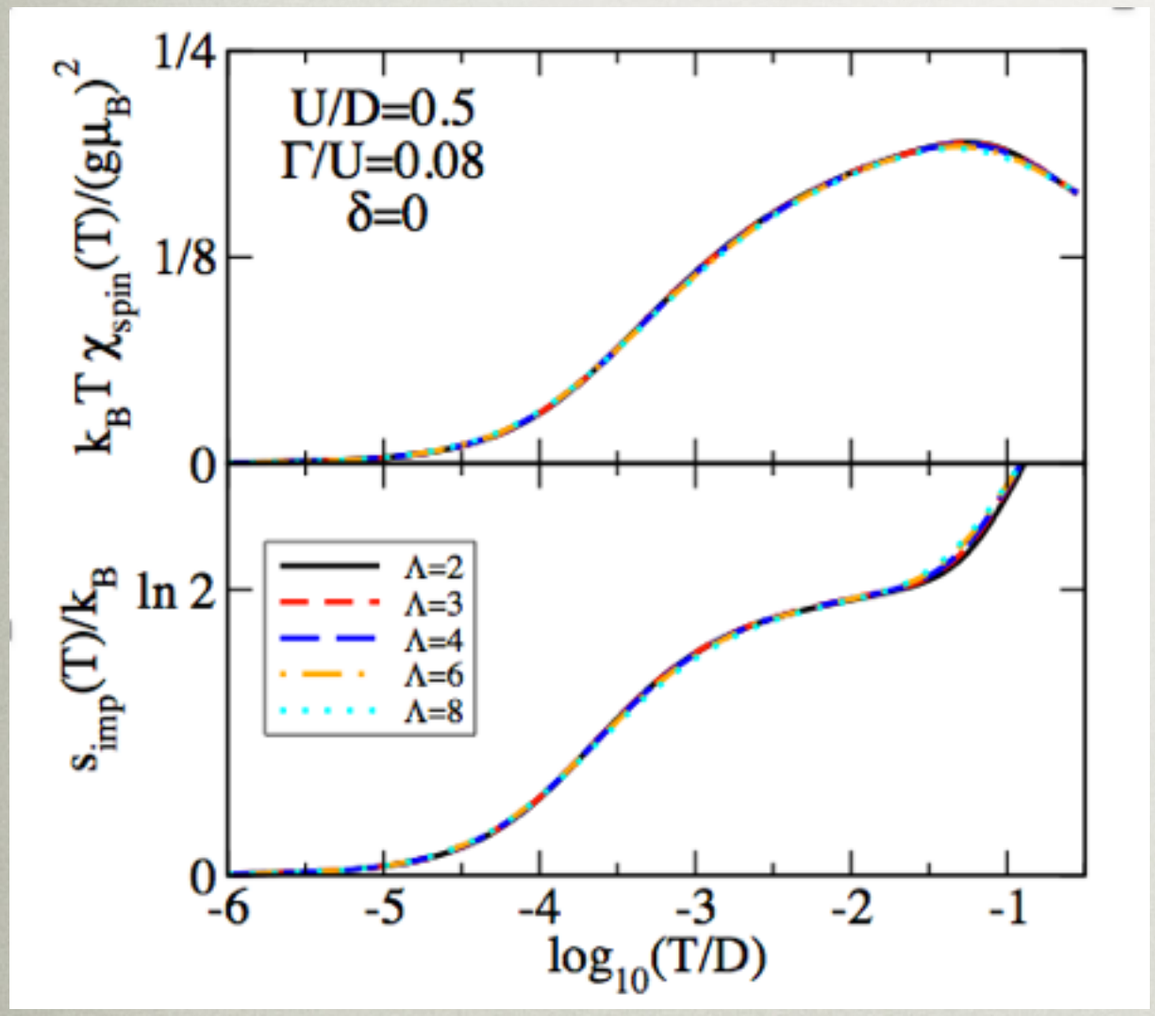
Choice depends on the Hamiltonian
and all operators of interest.

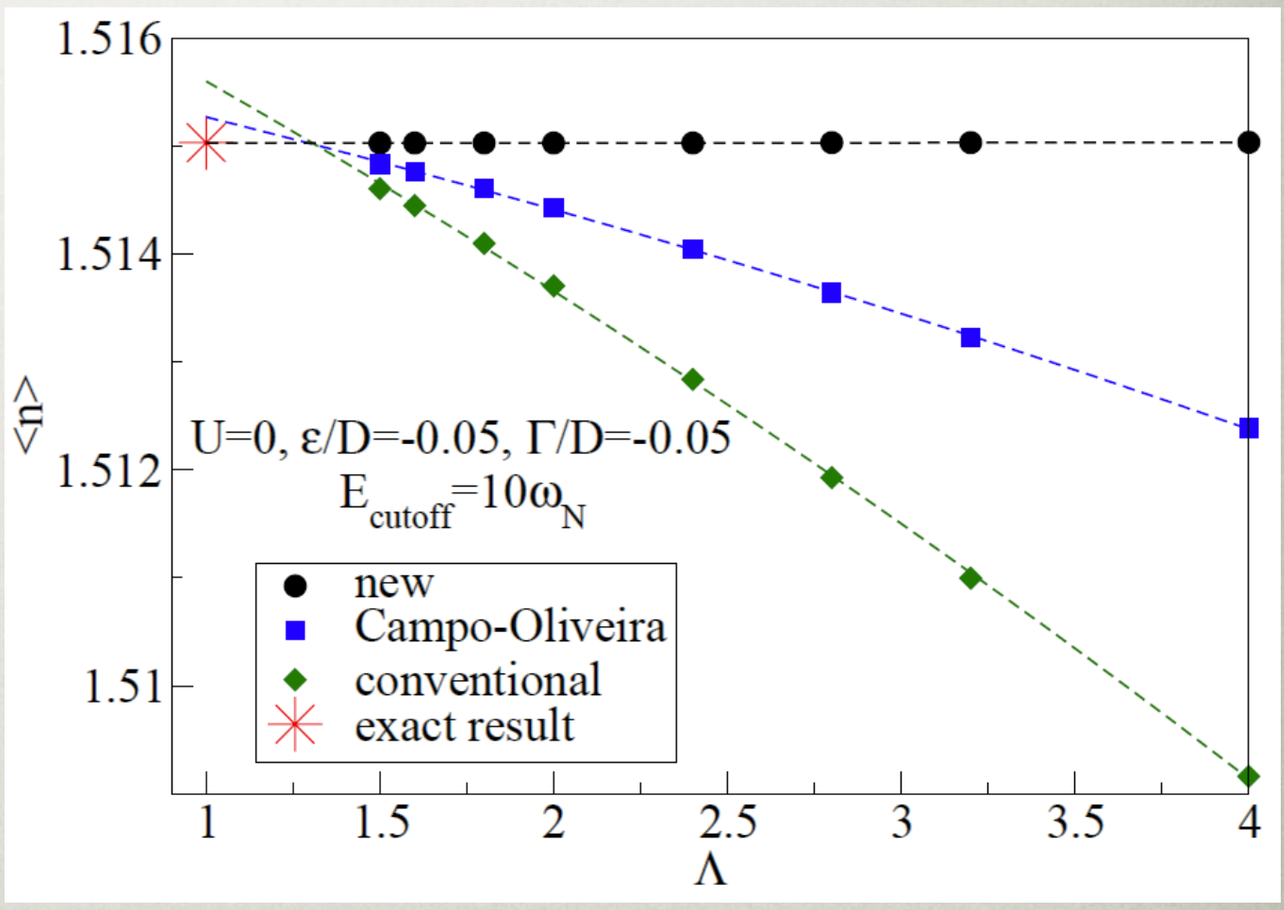
Examples:
- magnetic field along the y-axis
- two superconducting leads with phase difference
- calculations of transverse magnetic susceptibility

Two executables: `nrg2_4` and `nrgcmpl2_4`

`(nrgrun and nrgcmplrun)`

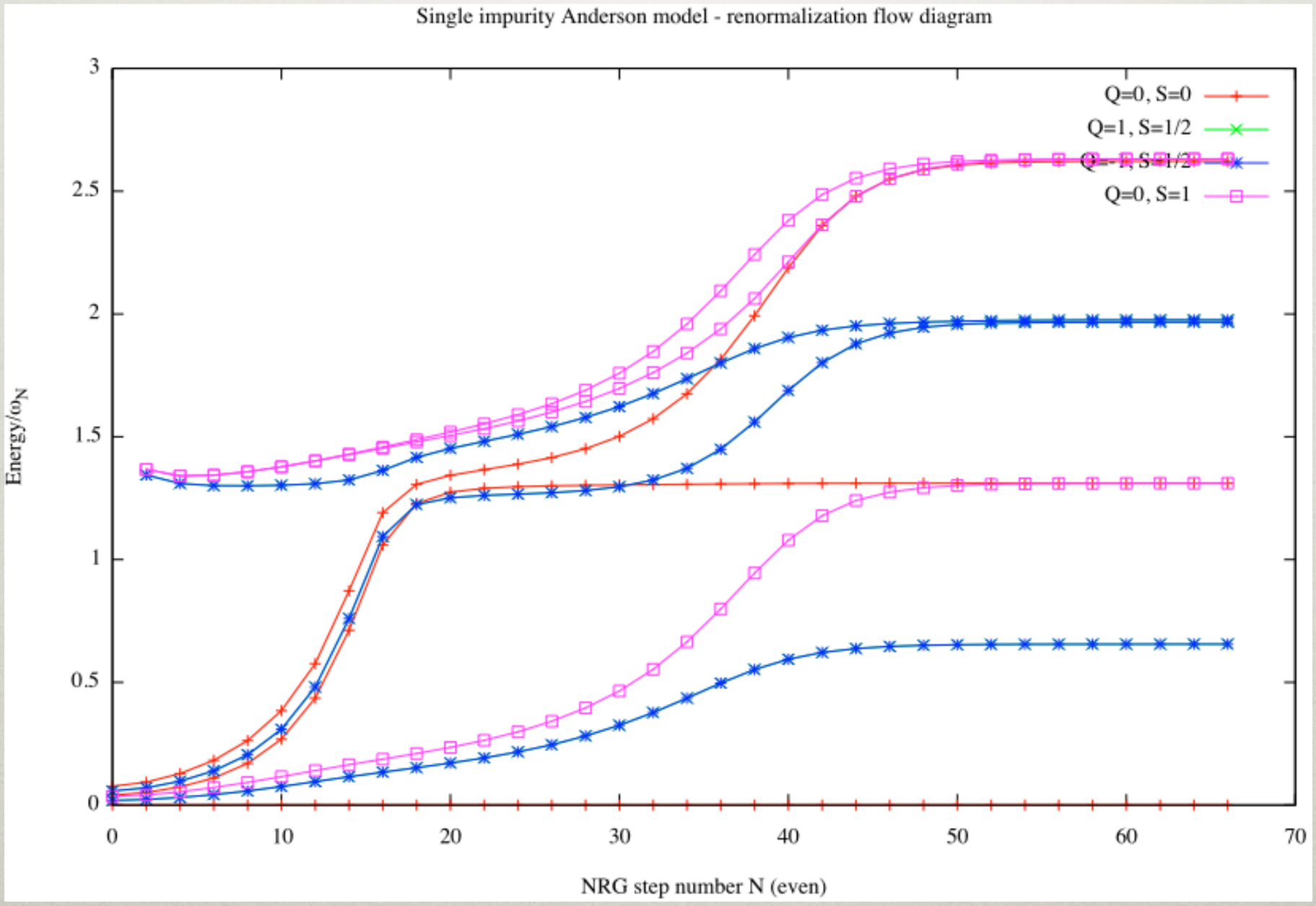
Choice of Λ


U/D=0.5
Γ/U=0.08
δ=0
1/4
1/8
0
$k_B T \chi_{spin}(T)/(g\mu_B)^2$
ln 2
0
$s_{imp}(T)/k_B$
Λ=2
Λ=3
Λ=4
Λ=6
Λ=8
-6
-5
-4
-3
-2
-1
$\log_{10}(T/D)$


1.516
1.514
1.512
1.51
<n>
U=0, ε/D=-0.05, Γ/D=-0.05
$E_{cutoff}=10\omega_N$
new
Campo-Oliveira
conventional
exact result
1
1.5
2
2.5
3
3.5
4
Λ

ANALYSIS

RG flow diagrams (spaghetti plots)



Calculation of thermodynamic quantities

$$\rho = \frac{1}{Z} e^{-\beta H} \qquad Z = \mathrm{Tr}[e^{-\beta H}]$$

$$E = \langle H \rangle = \mathrm{Tr}[\rho H] = \frac{\mathrm{Tr}[H e^{-\beta H}]}{\mathrm{Tr}[e^{-\beta H}]}$$

$$F = -k_B T \ln Z$$

$$S = -\frac{\partial F}{\partial T} \qquad C = \frac{\partial E}{\partial T}$$

Trick: avoid numerical differentiation!

ISOTHERMAL SUSCEPTIBILITY

$$H' = BS_z$$

$$\chi(T) = \frac{\partial \langle S_z \rangle}{\partial B}$$

Kubo, linear response theory:

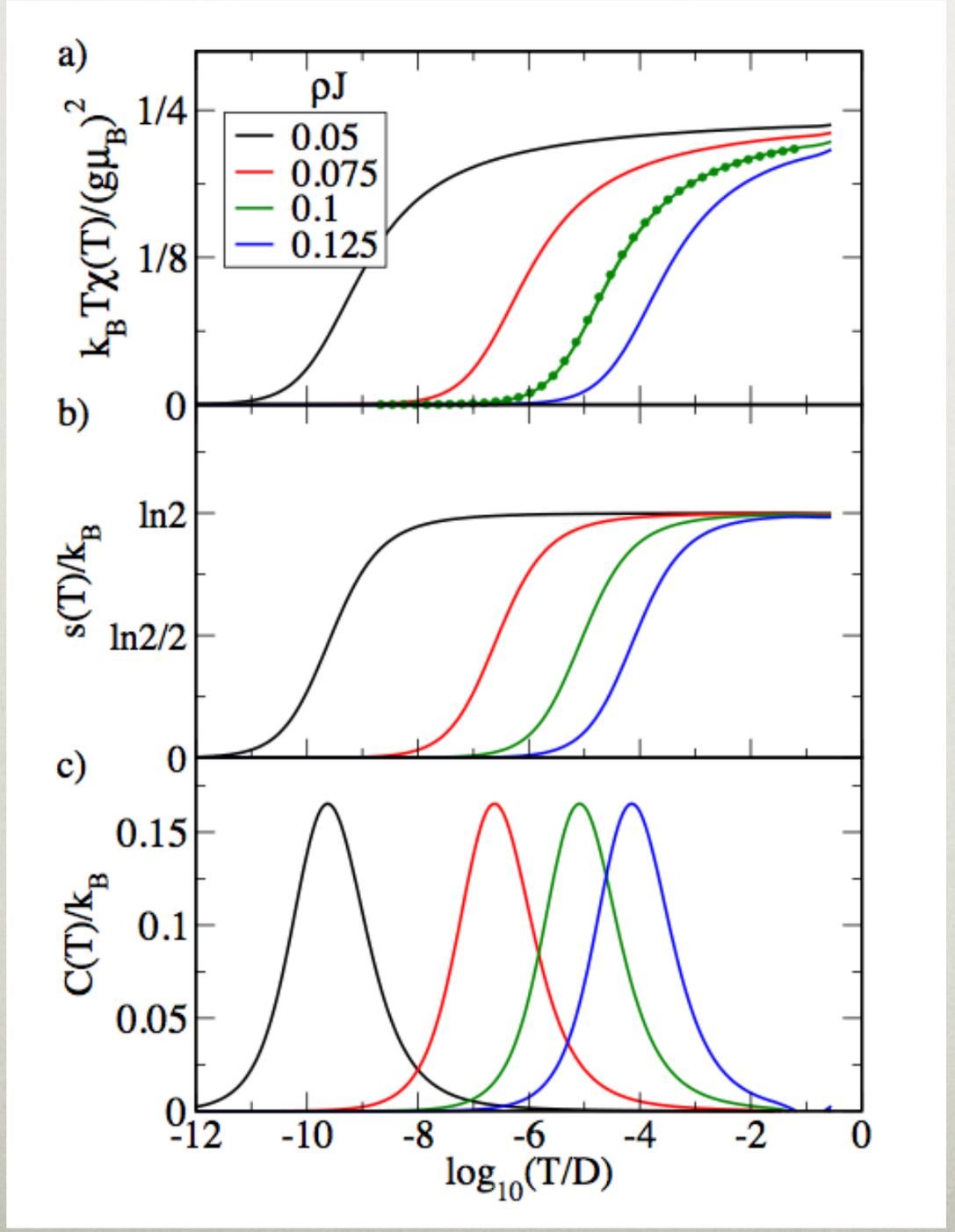
$$\chi(T) = \int_0^\beta \mathrm{d}\tau \, \langle S_z(\tau) S_z \rangle - \beta \langle S_z \rangle^2$$

Impurity contribution to...

$$S_{\mathrm{imp}}(T) = \frac{(E-F)}{T} - \frac{(E-F)_0}{T}$$

$$\chi_{\mathrm{imp}}(T) = \frac{(g\mu_B)^2}{k_B T}\Big(\langle S_z^2\rangle - \langle S_z^2\rangle_0\Big)$$

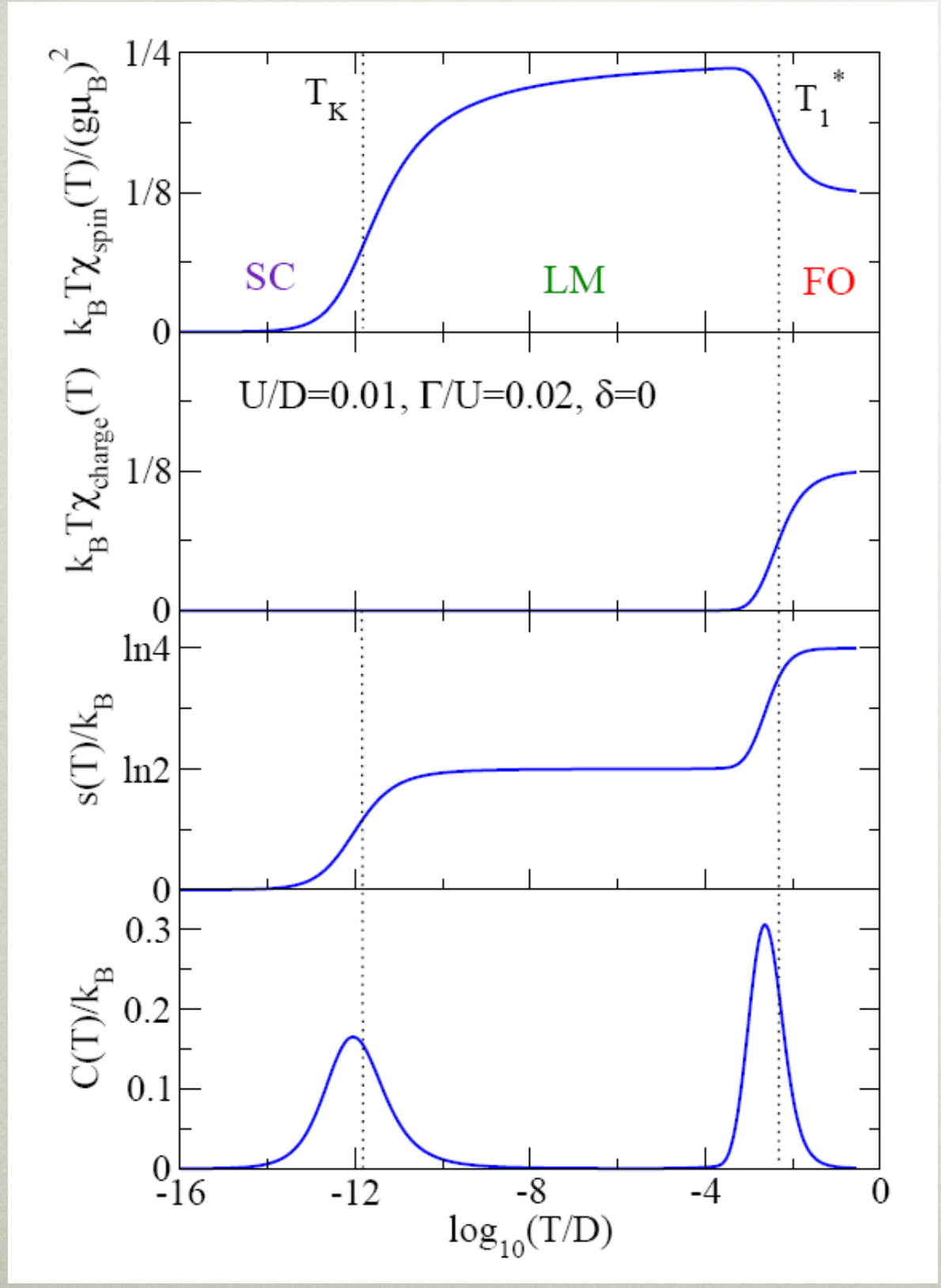
Thermodynamics of the Kondo model



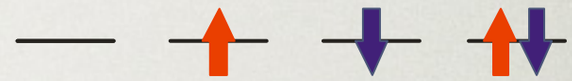
$$T_K\,\chi(T_K) = 0.07$$

Wilson's definition of the Kondo temperature

Single impurity Anderson model



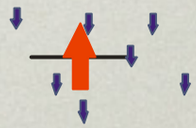
FO: free orbital



LM: local moment



SC: strong coupling



Phase diagram of SIAM

