New Development of Numerical Simulation in Low-Dimensional Quantum Systems: From DMRG to Tensor Network Formulation

Scale Free Property of Wilson Numerical Renormalization Group

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Real Space RG for 1D Quantum systems

1975：　Wilson NRG for Kondo impurity problem

Magnetic impurity in a metallic system. **critical system**

Block spin transformation → Break down in1D quantum system

Wilson　NRG is an exception？

1992:　Density Matrix Renormalization Group（DMRG）

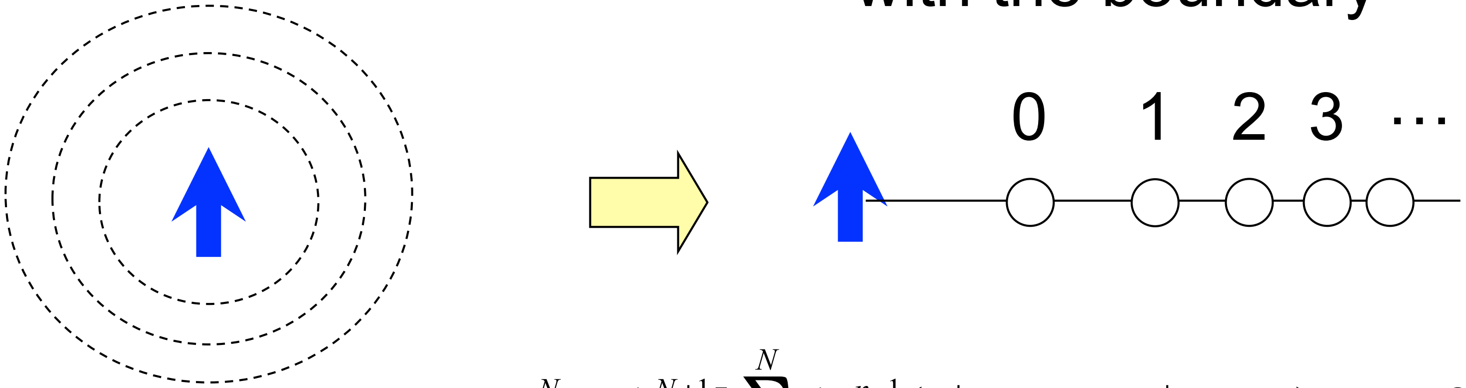
Very powerful for ground state problem of gapful 1D quantum systems

But　DMRG is hard to be considered as a conventional renormalization group

DMRG has no scale transformation

variation for the matrix product state

Wilson’s Numerical Renormalization Group(NRG)



Kondo impurity problem

1D quantum system
with the boundary

$$H_{\Lambda}^{N} = \Lambda^{N+1}\left[\sum_{n=0\sigma}^{N} \Lambda^{-n-1}\left(c_{n\sigma}^{+}c_{n+1\sigma} + c_{n+1\sigma}^{+}c_{n\sigma}\right) + \sigma_0 \cdot S_{imp}\right]$$

- $t_n \approx e^{-n\log\Lambda}$ effective 1D Hamiltonian is a tight-binding model with exponentially modulating hopping parameter
- effective system size $L \approx \dfrac{1}{\log\Lambda}$ → smooth cutoff of the infrared divergence

What is the role of cutoff beyond qualitative view?

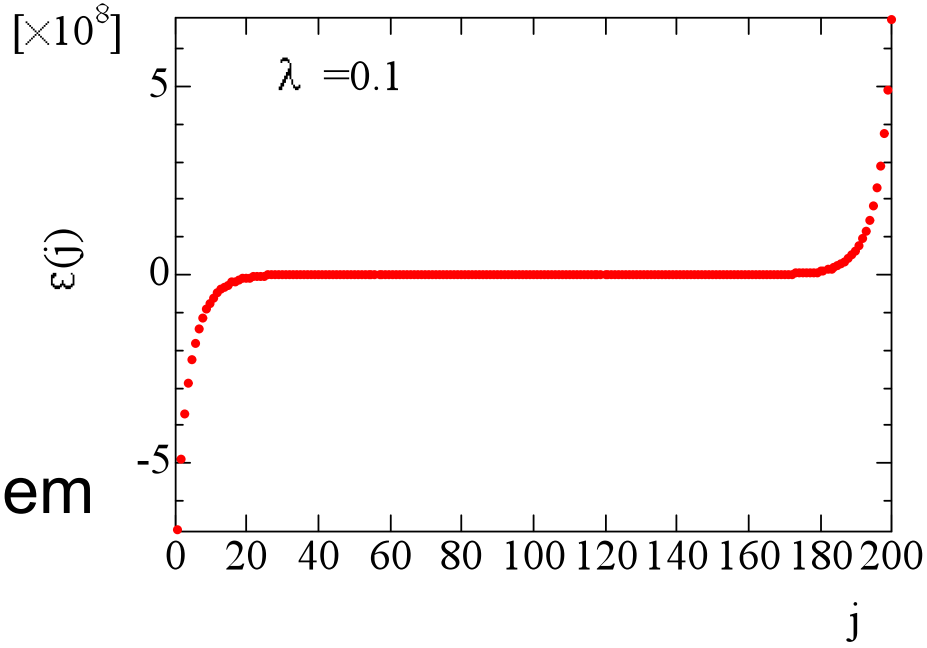
free fermion problem

essence of Wilson NRG => bulk fermion part

Free fermion with exponentially deformed interaction

$$H_\Lambda^N = \sum_{n=1}^{N} e^{\lambda n}(c_n^+ c_{n+1} + c_{n+1}^+ c_n)$$

$$\Lambda = e^{\lambda}$$



single particle eigenvalue problem

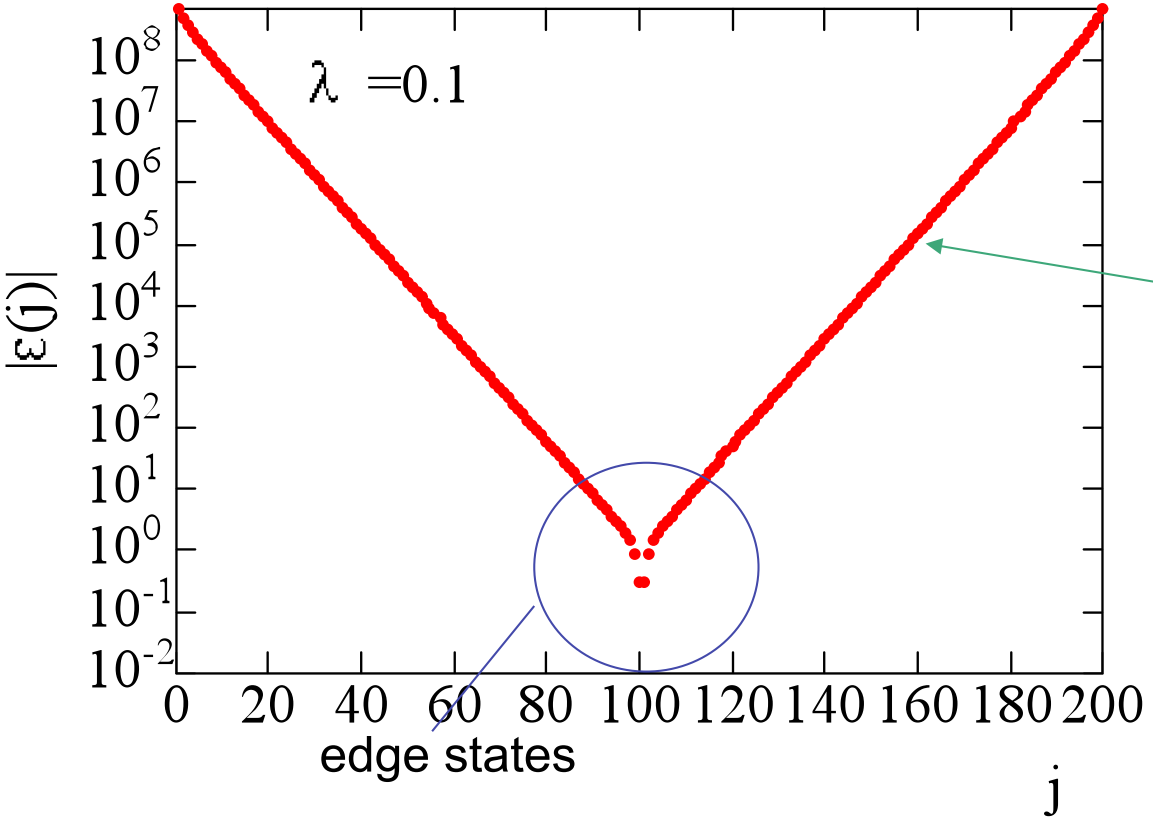
λ=0.1, N=200

cf. if λ=0, then $\varepsilon(j) = 2\cos(\frac{\pi j}{N+1})$

1-particle eigenvalue spectrum

N=200

log-scale plot



edge states

<u>bulk part</u>

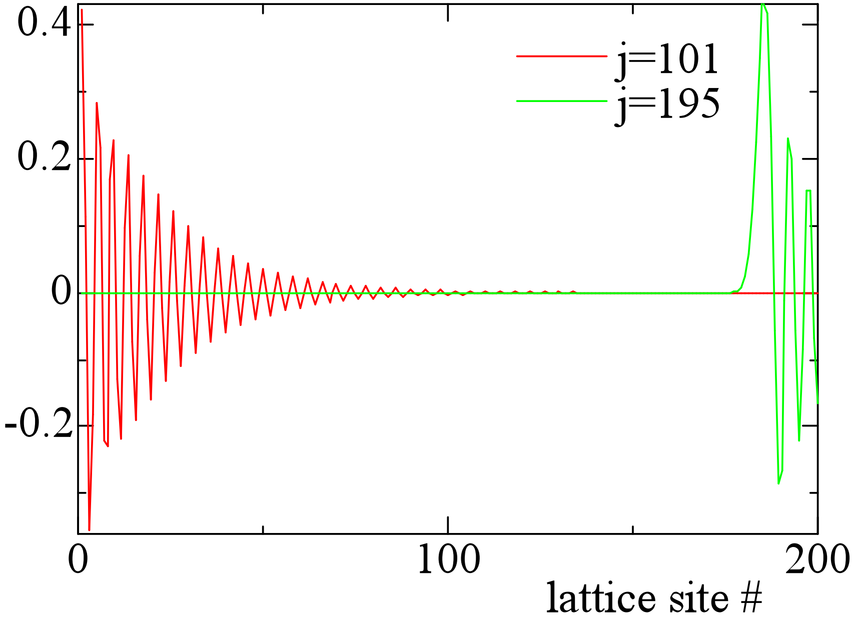
exponential dependence

j=100.5 corresponds to Fermi surface

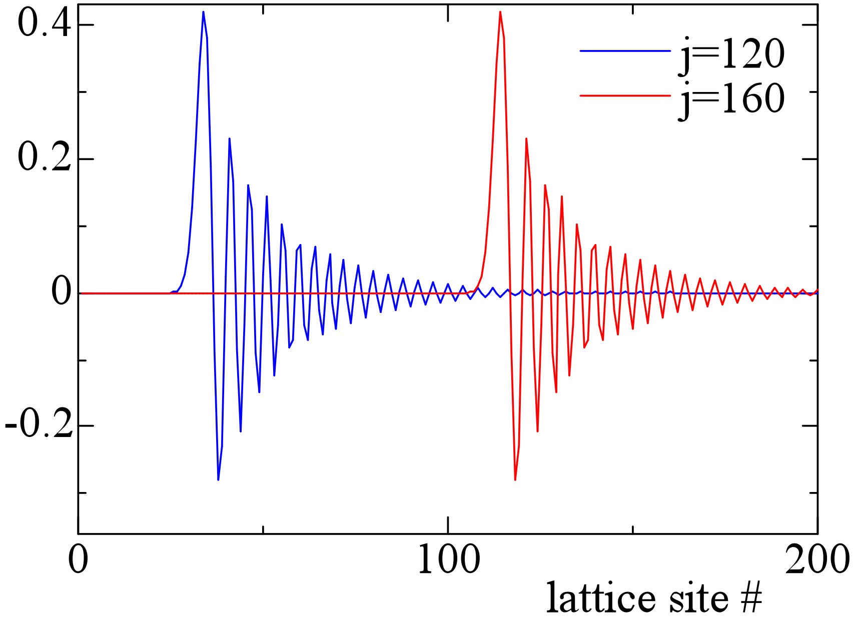
wavefunction

plane waves(uniform)

wave packets(exponential)



edge states



bulk states

translation = energy level shift

one-particle eigenvalue problem

1-body problem

$$|\psi\rangle = \sum \psi(n) c_n^{+} |0\rangle \quad \Rightarrow \quad e^{\lambda(n-1)}\psi(n-1) + e^{\lambda n}\psi(n+1) = E\psi(n)$$

$$\psi(n) = e^{-\lambda/2}\phi(n) \qquad \phi(n-1) + \phi(n+1) = e^{-\lambda n}\overline{E}\phi(n)$$

$$\phi(n) \to (-)^n \phi(n) \quad \Rightarrow \quad E \to -E$$ particle-hole

Lattice translation

$$n = n' + m \qquad E' = e^{-\lambda m}\overline{E}$$

$$\Rightarrow \qquad \phi(n'-1) + \phi(n'+1) = e^{-\lambda n'}E'\phi(n')$$

scale free theory! lattice translation = energy shift

All bulk wavefunctions have the same form!

wavepacket: “continuous” limit(λ→0)

$$x = n\lambda \qquad : \qquad \phi(x-\lambda)+\phi(x+\lambda)=e^{-x}\phi(x)$$

$$y=\exp(-x/2) \;\vdots \qquad \phi''(y)+\frac{1}{y}\phi''(y)+\frac{4}{\lambda^2}(\frac{2}{y^2}-1)\phi(x)=0$$

modified Bessel function with imaginary order

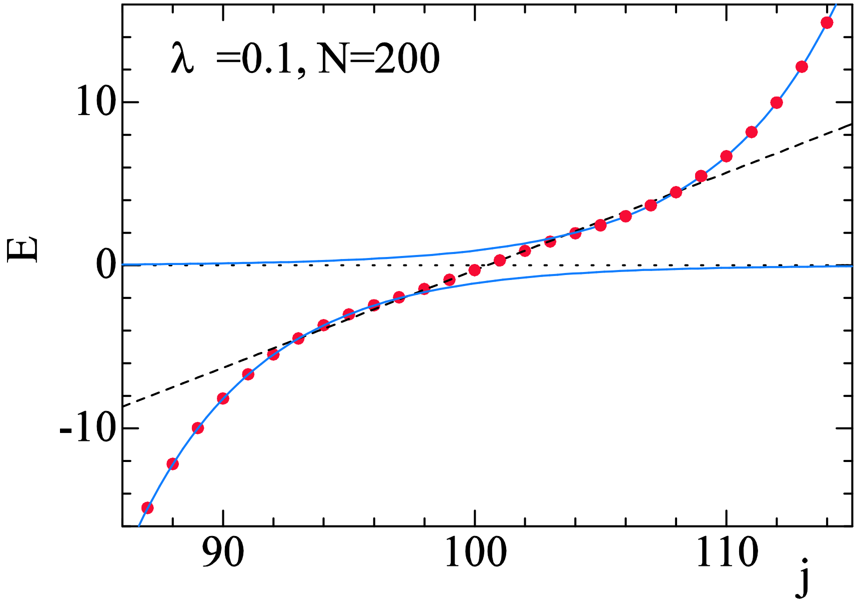
$$\phi(x)\sim K_{2ic}(ce^{-x/2}) \qquad c=2\sqrt{2}/\lambda$$

$$\text{x>>1} \quad \phi(x)\sim\exp(-icx)$$

$$\text{x<<-1} \quad \phi(x)\sim\sqrt{\frac{\pi}{2ce^{-x/2}}}\exp(-ce^{-x/2})$$

consistent with the wavepaket obtained by the numerical result

edge state



E shows linear dependence with respect to j
near the Fermi surcace.（$|E| \lesssim 2$）

edge state

$$\phi(n) = e^{\pm in\pi/2}\eta(n) \qquad \pm i[\eta(n-1)-\eta(n+1)] = e^{-\lambda n}\overline{E}\,\eta(n)$$

omit $O(\lambda^2)$:

$$i2\lambda\eta'(x) \mp Ee^{-x}\eta(x) = 0$$

⇒

$$\eta(x) \sim \exp(\pm i\frac{E}{2\lambda}e^{-x})$$

This wavefunction is not permitted as a bulk wavefunction

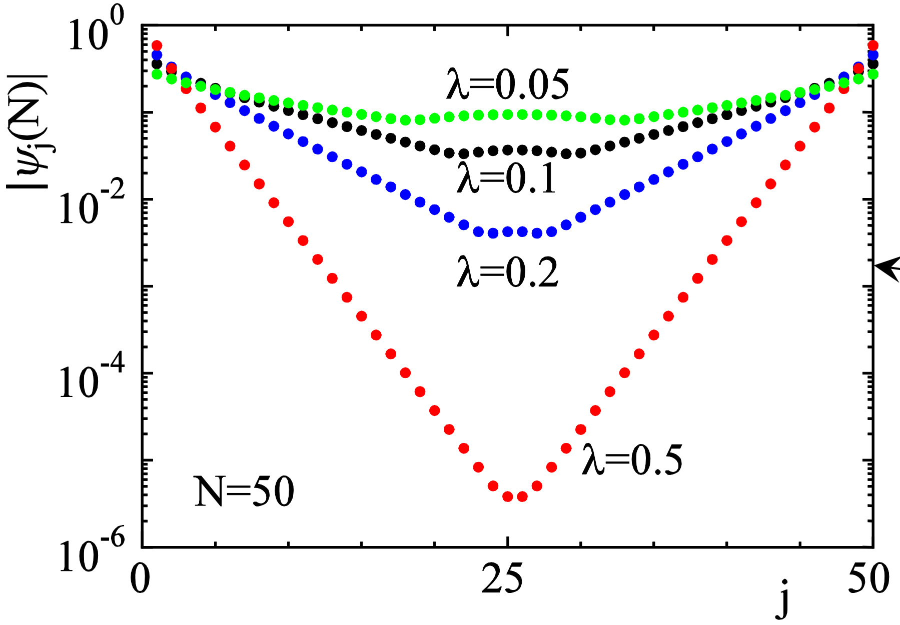
⇒ edge state of the lowest energy scale

$E = \pi\gamma e^{-\lambda/2}q$ with the boundary condition

$$q = \pm 1/2,\ \pm 3/2, \cdots \qquad \psi(0) = 0, \psi(N+1) = 0$$

This edge state is eventually invisible for a practical Λ~2

Amplitude at the Impurity site



N=50

edge state

$$\psi_j(N) = \begin{cases} a_j e^{-\lambda j} & 1 \le j \le N/2 \\ a_j e^{\lambda(j-N-1)} & N/2+1 \le j \le N \end{cases}$$

Kondo coupling

$$J_K e^{\lambda N}\psi^*{}_j(N)\psi_j(N)c^+_{j\sigma}[\sigma\cdot S]c_{j\sigma'}$$

$$\psi_j(N)=\begin{cases} a_j e^{-\lambda j} & 1\le j\le N/2 \\ a_j e^{\lambda(j-N-1)} & N/2+1\le j\le N \end{cases}$$

a is a constant of order unity

Lattice translation: $j\to j+2M$

$\Rightarrow$ $$\widetilde{J}_K e^{\lambda N}\psi^*{}_{j+M}(N)\psi_{j+M}(N)$$

Kondo Coupling scales with $\widetilde{J}_K = J_K e^{2\lambda M}$

canonical scale factor : $e^{2\lambda M}$

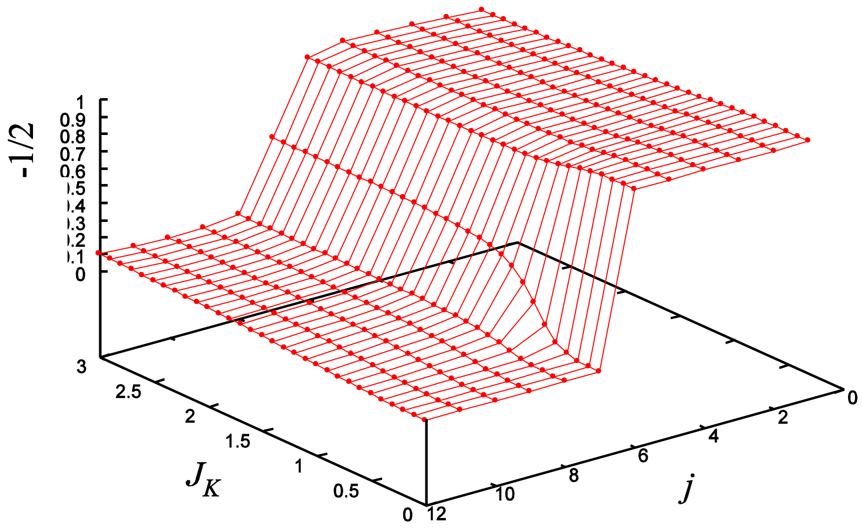
nontrivial competition

cf. Free fermion part $\widetilde{E} = E e^{2\lambda M}$

Diagonalization

distribution of ↑spin electron for each orbital

$$N = 12,\ N_e = 12,\ S^z = 1/2,\ \Lambda = \sqrt{2}$$



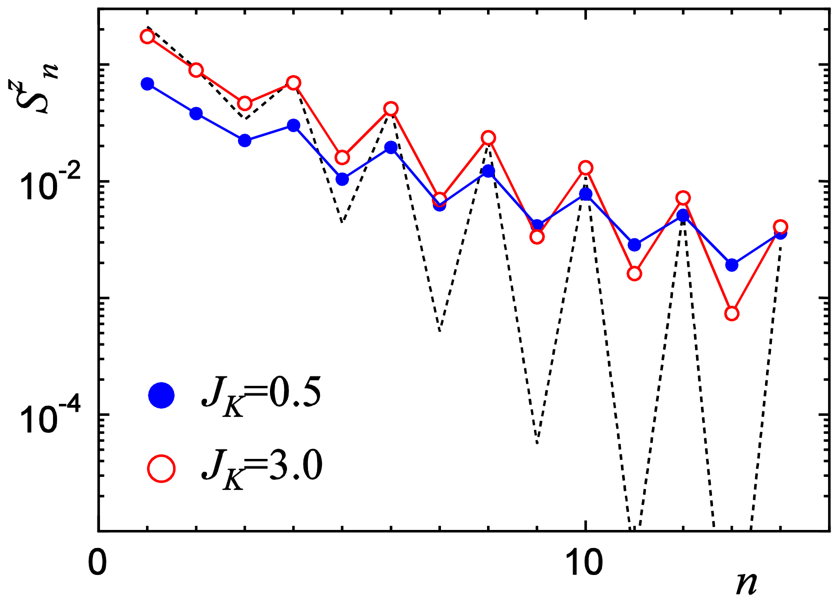
Kondo coupling

orbital index

j=6.5 corresponds to the Fermi surface

real-space spin distribution

N=14



impurity site

dotted line : free fermion at j=8(above fermi surface)

implication of N=14 results

decay rate of free fermion $\lambda = \ln 2 / 2 = 0.347$

renomralized decay rate of the groundstate spin density λ^*

$J_K = 3.0$ (strong coupling limit) $\lambda^* = 0.312 \approx 0.9\lambda$

$J_K = 0.5$ (crossorver region) $\lambda^* = 0.215 \cong 0.62\lambda$

The decay rate of the spin density is renormalied from the canonical scale factor $e^{2\lambda M} \Rightarrow e^{2\lambda^* M}$

Nontrivial correlation effect

summary

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essence of Wilson NRG

Scale free wavepacket basis

appearance of edge states

The edge states is less important in the practical region of cutoff Λ

Kondo coupling

The decay rate of the spin density is renormalized from the canonical scale factor

Kondo energy scale

$$e^{-1/2J_K} / \sqrt{2J_K}$$

⇐

$$\lambda^*(J_K;N)$$

further analysis for long chains

Lattice translation again

T is the lattice translation(n->n+1) operator
for fermion operators

$$THT^{-1} = \sum_n e^{n\lambda} T(c_n^+ c_{n+1} + c_{n+1}^+ c_n) T^{-1} = e^{-\lambda} H$$

[# infinite sum of "n" is assumed]

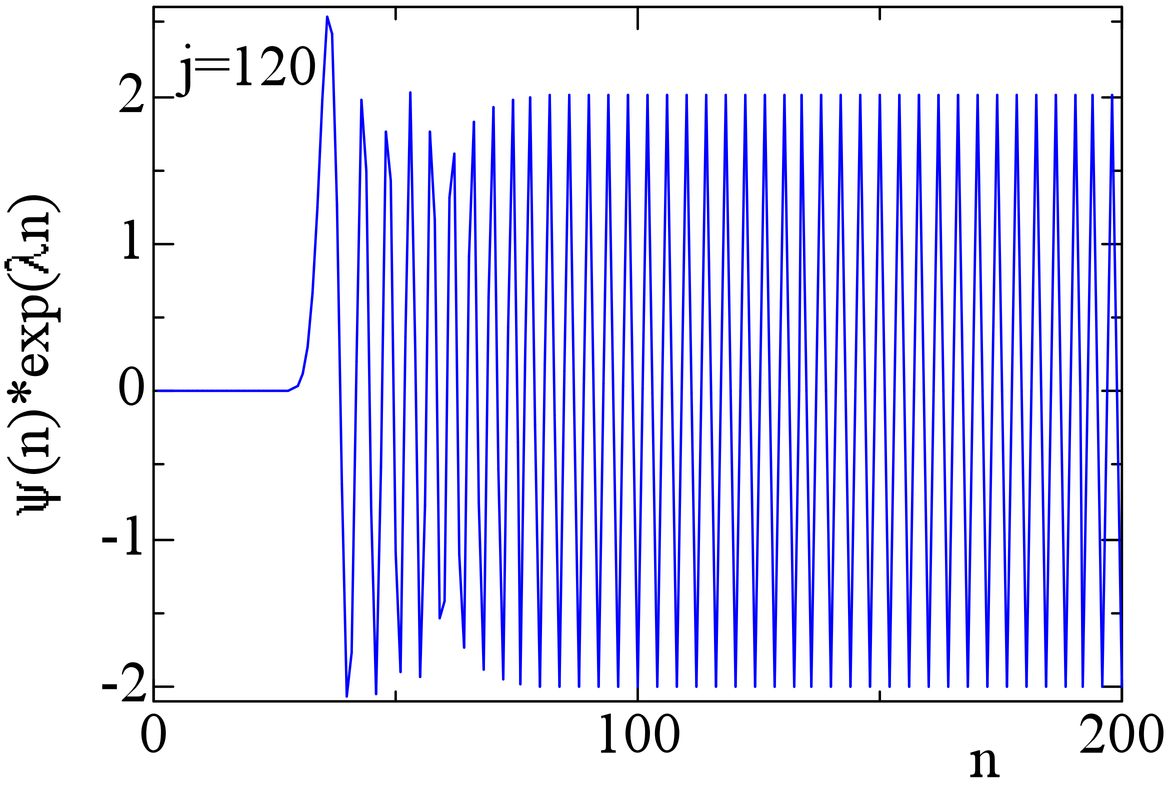
if $|\psi\rangle$ is an eigenstate of H $H|\psi\rangle = E|\psi\rangle$

$$TH|\psi\rangle = ET|\psi\rangle \Leftrightarrow THT^{-1}T|\psi\rangle = ET|\psi\rangle$$

$$\Leftrightarrow H(T|\psi\rangle) = e^{\lambda} E(T|\psi\rangle)$$

⇒ $E' = e^{-\lambda} E$ is also an eigenvalue

Energy-scale-free nature can be also seen.


j=120
ψ(n)*exp(λn)
2
1
0
-1
-2
0
100
200
n

Issue

What is the mechanism behind the success of Wilson NRG?

We want to understand the role of cutoff beyond qualitative understanding

- How can we understand the control of the energy scale in Wilson NRG?

  high-energy cutoff v.s. infra-red cut off

- Wilson NRG for a gapful system

  competition between the length scale of Λ and inherent energy scale of the system

Wilson like NRG for spin chain

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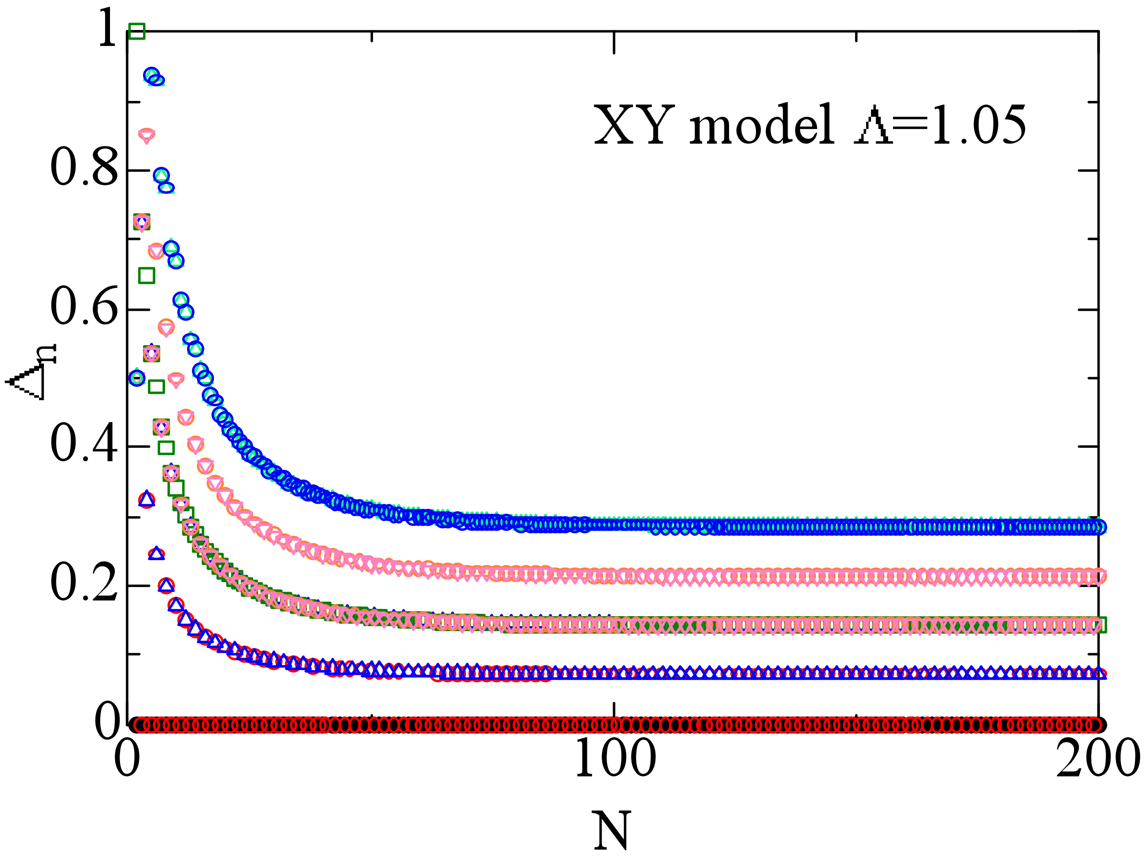
$$H_{\Lambda}^{N+1} = \Lambda H_{\Lambda}^{N} + h_{N,N+1}$$

$h_{N,N+1}$ two body interaction

The lowest energy scale is 1(new site)
The scale of the other part is multiplied by Λ



cut off

- converge for large N
- regular structure

low-energy spectrum of the XY model

$$H = \sum S_n^x S_{n+1}^x + S_n^y S_{n+1}^y$$

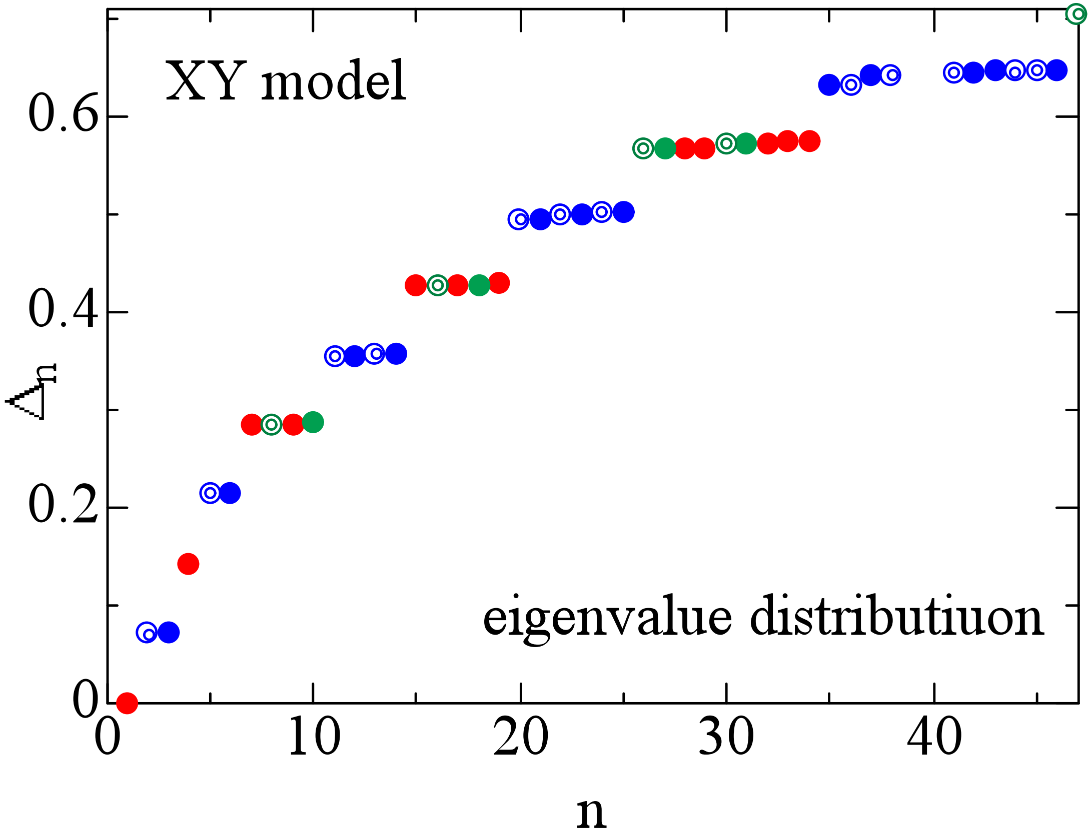
free fermion

invoke low-energy finite-size spectrum

$$H = e_0 L + f_0 - \frac{\pi v}{48L}$$

$$+ \frac{\pi v}{2L}\left[\sum_{m=0}\left(m+\frac{1}{2}\right)\xi_m^+\xi_m + \sum_{n=0}\left(n+\frac{1}{2}\right)\eta_n^+\eta_n\right]$$

excitatin spectrum is specified by two quantum numbers (m,n)
all of the level space isπv/2L.



color indicates M=total S^z

$$M = \eta^{+}\eta - \xi^{+}\xi$$

(m,n)=(0,0)
(1,0), (0,1)
(2,0), (0,2), (1,1)

level space is
determined by Λ

赤がM=0
青がM=±1
緑がM=±2

The correct spectrum of the XY model
can be reproduced!

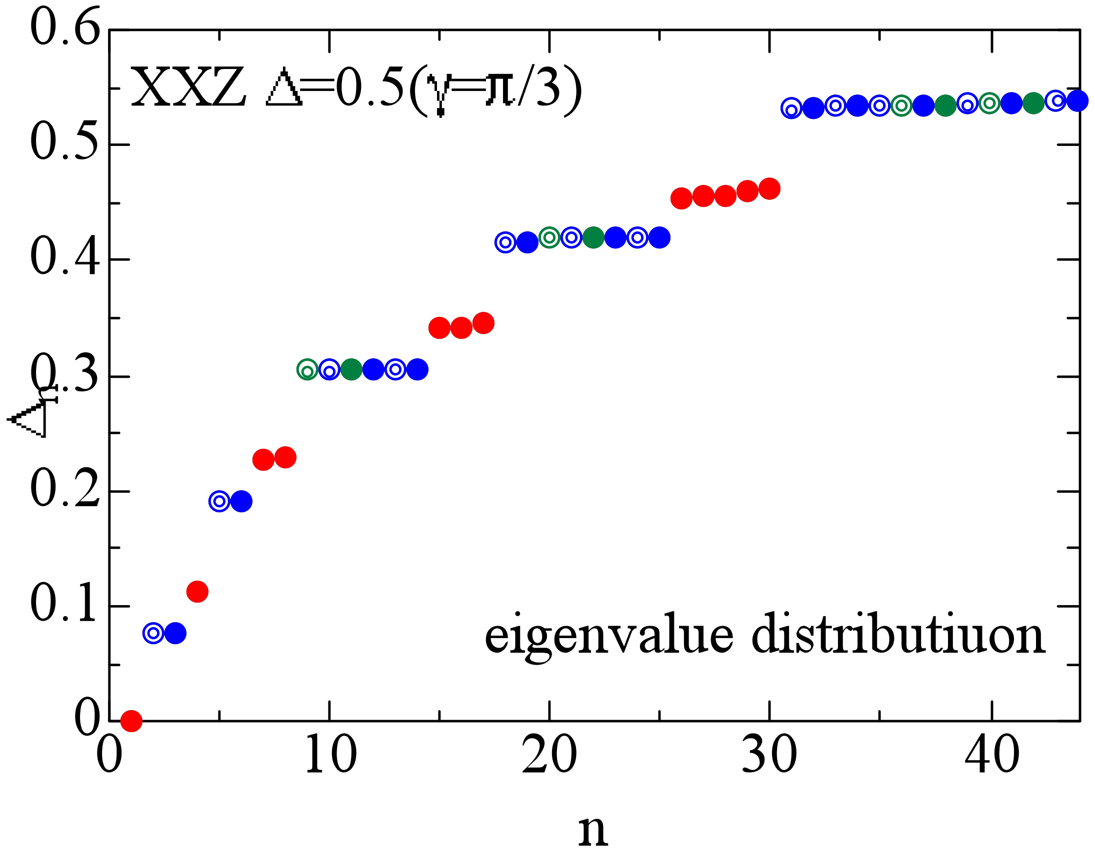
Wilson NRG works for a general model！

eigenvalue distribution of XXZ model

$$H = \sum S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z$$

$\gamma = \pi/3$ ⇨ $\xi = \sqrt{3}/2$

two quantum numbers (M, n)



red M=0

blue M=±1

green M=±2

（n quantum number increases for each M）

$$\prod_{n=1}^{\infty} (1-q^n)^{-1} = \sum_{n=0} P(n) q^n$$

P(n)=1,1,2,3,5…..
for n=0,1,2,3,4,…

finite size spectrum of XXZ model

$$H = \sum S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \cos\gamma S_n^z S_{n+1}^z$$

finite size spectrum obtained by Bethe ansaz

$$H = Le_0 + f_0 + \frac{\pi v}{2L}\left[\frac{1}{2}\frac{M^2}{\xi^2} + n - \frac{1}{24}\right]$$

$$\xi = 1/\sqrt{2(1-\gamma/\pi)}$$

n is the degeneracy defined by Euler's partition number $P(n)$

DMRGはRGか？

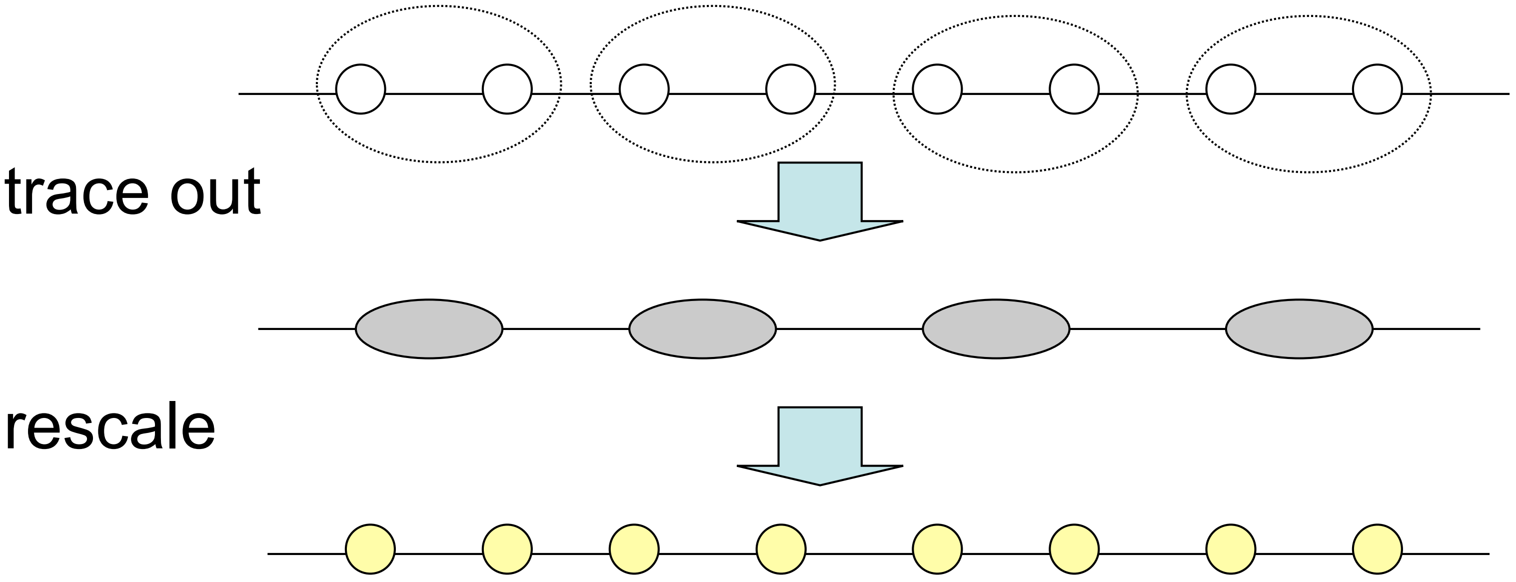
DMRG

- 密度行列経由で状態の削減
  （ハミルトニアンの低エネルギーかどうかは不明）
- 基底状態の情報は得られる
  （高エネルギー状態の部分和かどうかは不明）
- くりこみの流れが有るのか無い
  （結合定数はくりこまれているのか？）
- 相関長とくりこみ変換の関係が不明
  （ RG $\xi(u) \rightarrow b^{N}\xi(b^{xN}u)$ ）
- 臨界指数の計算は誰もやっていない！
  （できない？）

DMRGを“くりこみ群”と解釈するわけにはいかない

Wilsonのくりこみ群がなぜ臨界系の扱いに成功したのか？

block spin transformation RG



trace out

rescale

The reason for the failure of this procedure was analyzed by S.R.White

The role of “boundary” of the block spin is essential.

Wilson's NRG

Kondo model

linear dispersion

⇒ continuous model

s-wave+impurity

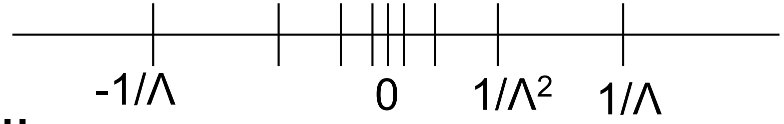
$$-i\sum \frac{\partial}{\partial x_i} + JS\cdot\sigma_i\delta(x_i)$$

1 Wave space $\int_{-1}^{1} k c^{+}_{k\sigma} c_{k\sigma}\, dk - J[S^{z}(A^{+}_{\uparrow}A_{\uparrow} - A^{+}_{\downarrow}A_{\downarrow}) + S^{-}A^{+}_{\uparrow}A_{\downarrow} + S^{+}A^{+}_{\downarrow}A_{\uparrow}]$

$$A_\sigma = \int_{-1}^{1} c_{k\sigma}\, dk$$

2 log-discritization

discritize wave space into shell

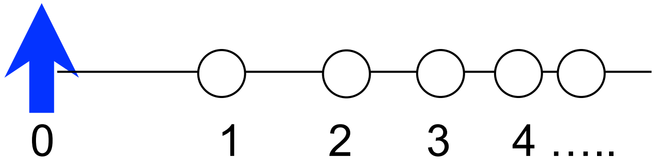


$$H_{\Lambda}^{N+1} = \Lambda H_{\Lambda}^{N} + t(c^{+}_{N\sigma}c_{N+1\sigma} + c^{+}_{N+1\sigma}c_{N\sigma})$$

cutoff Λ due to discritization

3

Numerical RG： add electrons on a 1D lattice step by step



Omit higher energy states and reduce the dimension of Hamiltonian matrix。

add an electron

diagonalize Hamiltonian

keep lower energy states

RG iteration