

ISSP workshop on 27/July/2006

# Is DMRG a renormalization group?



---unconventional introduction to DMRG---

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# outline

- transfer matrix in 2D classical system
- variational principle & matrix product
- connection to 1D quantum systems
- White's DMRG
- Is DMRG a renormalization group?
- Wilson's like NRG

# DMRG prehistory

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1941 Kramers-Wannier Approx.

1968 Wilson's RG

1968 Baxter's variational Approx

matrix product eigenvector  
corner transfer matrix

1971 Wilson's NRG

Kondo problem

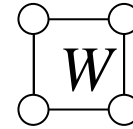
1987 VBS state/AKLT model

matrix product state

1992 White's DMRG

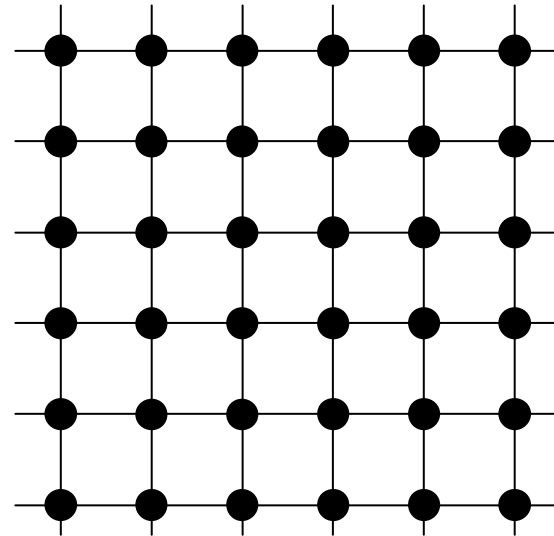
# Transfer matrix

$$W(s'_1 s'_2 s_1 s_2) = e^{-\frac{\beta}{2}(s_1 s_2 + s'_1 s'_2 + s_1 s'_1 + s_2 s'_2)}$$

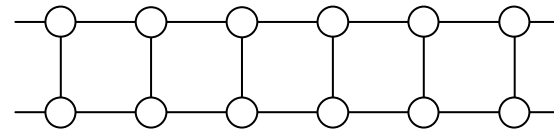


Boltzmann weight

$$Z = \sum_{all \bullet}$$



$$T =$$



row-to-row  
transfer matrix

Thermodynamic behaviors  $\Rightarrow$  the largest eigenvalue of  $T$

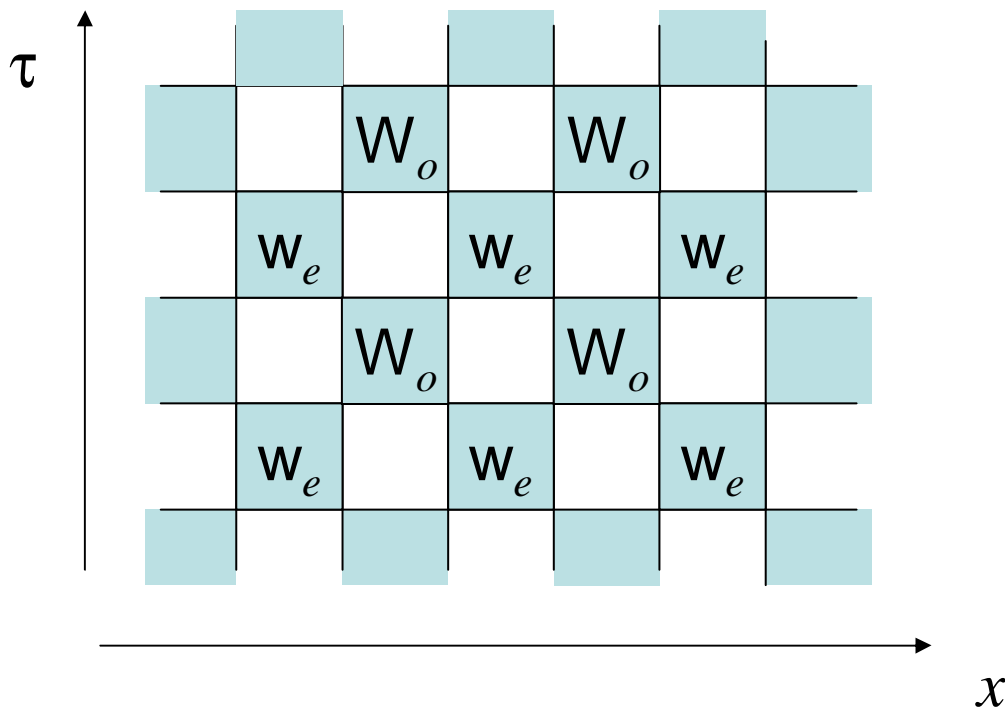
$$Z = \lim_{N \rightarrow \infty} Tr(T^N) \approx \Lambda^N$$

# 1D quantum and 2D classical

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Trotter formula — path integral(summation) representation---

$$e^{-\beta H} = \lim_{N \rightarrow \infty} \left[ e^{-\frac{\beta}{M} H_e} e^{-\frac{\beta}{M} H_o} \right]^M \quad [H_e, H_o] = 0$$



$$W_{e,o} = e^{-\frac{\beta}{M} H_{e,o,i,i+1}}$$

M.Suzuki,  
Prog.Theor.Phys.56.1454(1976)

# Kramers-Wannier Approx.

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Eigenvector of the transfer matrix can be approximated by the Ising model itself in an effective magnetic field.

$$\begin{aligned}\Psi(s_1, s_2 \dots) &= \text{const} \times e^{-\tilde{K}(s_1 s_2 + s_2 s_3 + \dots) + \tilde{h}(s_1 + s_2 + \dots)} \\ &= \phi(s_1, s_2) \phi(s_2, s_3) \dots \\ \phi(s, s') &= c e^{\tilde{K} s s' + \tilde{h}(s + s')/2}\end{aligned}$$

$\tilde{K}$ ,  $\tilde{h}$  : effective couplings maximizing  $\Lambda = \langle \Psi | T | \Psi \rangle / \langle \Psi | \Psi \rangle$

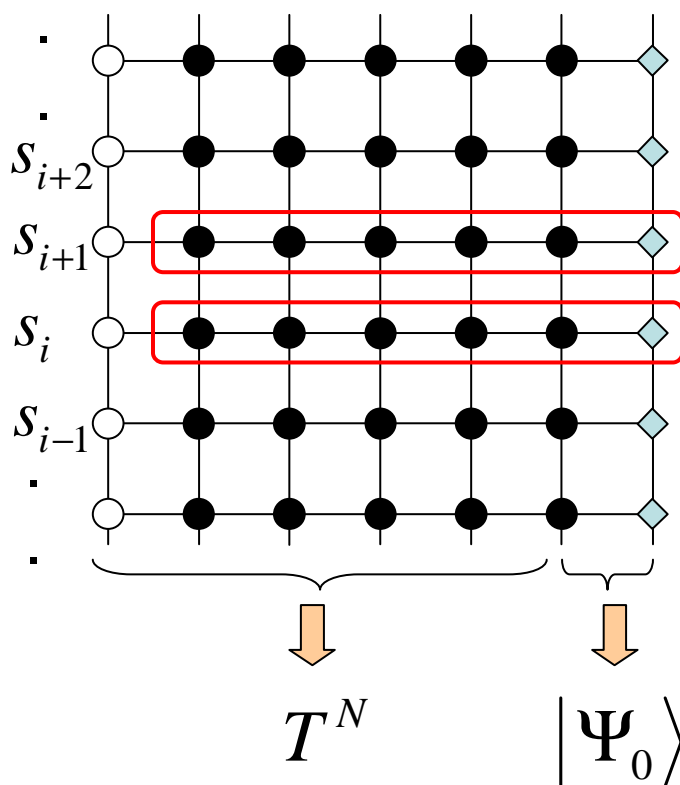
The result is much better than the well-known mean field approx, Bethe approx, etc...

eigenvector can be represented as a product of scalar function

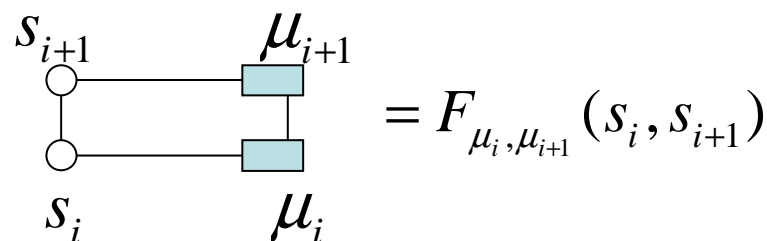
# Baxter's idea---matrix product form of the eigenvector---

$$|\Psi\rangle = \lim_{N \rightarrow \infty} T^N |\Psi_0\rangle$$

Max eigenvalue-eigenvector



block spin variables  $\mu$



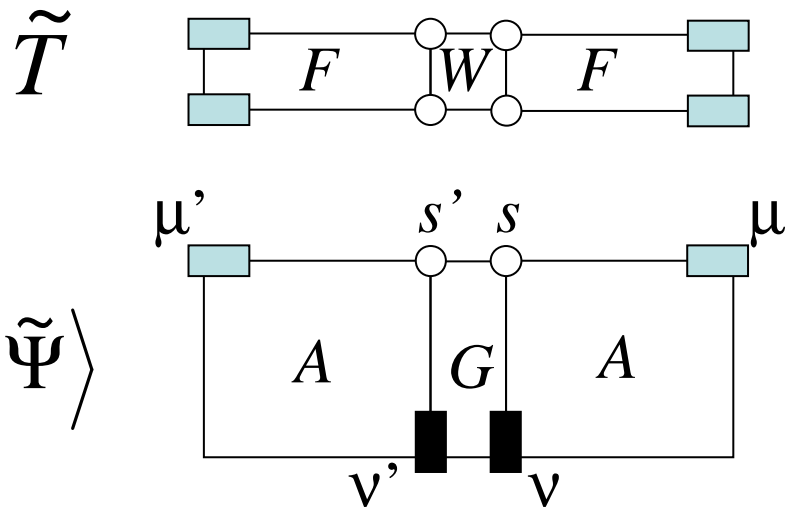
$$|\Psi\rangle = \sum_{\{\mu\}} \prod_{i=1}^N F_{\mu_i, \mu_{i+1}}(s_i, s_{i+1})$$

He write the eigenvector as a matrix product form.

# Corner transfer matrix ---variational approx. again---

$$\langle \Psi | T | \Psi \rangle = \sum_{\{\mu, \mu', s, s'\}} \prod_{i=1}^N [F_{\mu', \mu_{i+1}}(s'_i, s'_{i+1}) W(s'_i, s'_{i+1} | s_i, s_{i+1}) F_{\mu_i, \mu_{i+1}}(s_i, s_{i+1})]$$

➔ We can regard  $FWF$  as a renormalized transfer matrix  $\tilde{T}$  and use the variational approximation for  $\tilde{T}$  again.



$$\tilde{T} \equiv FWF$$

$$\tilde{T}|\tilde{\Psi}\rangle = \tilde{\Lambda}|\tilde{\Psi}\rangle$$

$$|\tilde{\Psi}\rangle = \sum_{v, v'} A_{\mu', v'}(s') G_{v', v}(s', s) A_{v, \mu}(s)$$

**A : corner transfer matrix(CTM)**

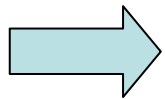
$$\tilde{\Lambda} = \langle \tilde{\Psi} | \tilde{T} | \tilde{\Psi} \rangle / \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$



# Reduced density matrix

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The previous “renormalized transfer matrix” is very similar to the block Hamiltonian in DMRG.



The connection in the eigenvector level

$A$

quadrant

$$\Psi \approx A^2$$

half infinite plane

$$\rho_{\text{DMRG}} \approx \Psi^2 \approx A^4$$

whole 2D plane with  
a half infinite cut

$$Z = \text{Tr} \rho_{\text{DMRG}} = \text{Tr} A^4$$

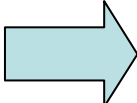
# Iterative method

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prepare initial matrices

extend size of CTM  diagonalize CTM  
 keep the larger eigenvalue eigenstates of CTM

result is very good and convergence is rapid

 Keeping larger  $\lambda$  gives a good approximation of the partition function.

$$Z \approx \left\langle \tilde{\Psi} \left\| \tilde{\Psi} \right\rangle_{\lambda} \approx \text{Tr} A^4 = \lambda_1^4 + \lambda_2^4 + \lambda_3^4 \dots$$

$\lambda$  : eigenvalues of CTM in decreasing order

keeping larger  $\lambda$ ,



variational principle

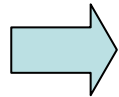
role of the renormalized transfer matrix is rather auxiliary.

# 2D classical v.s. 1D quantum

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## 2D classical

We can treat the two spatial dimension equivalently.



This is of great benefit in thinking in the 2D world

## 1D quantum

This is a kind of anisotropic limit of 2D classical case

Zero temperature & infinite trotter number limit  
in Suzuki-Trotter transformation

if the zero temp & Trotter limits is properly taken.  
the eigenvector of the transfer matrix in the mapped system  
becomes the groundstate wavefunction of the original system.

# How to approach 1D quantum systems?

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In principle, it would be possible to formulate a numerical algorithm to solve the 1D quantum system, based on the transfer matrix/corner transfer matrix approach.

But, the history did not go so. Why?

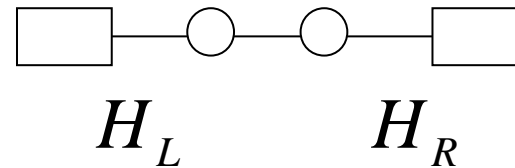
1. Boltzmann weight becomes singular as  $T \rightarrow 0$  !
2. We are not able to know the MP form of the groundstate wavefunction without the transfer matrix.
3. Timing! computer resources those days is insufficient for the transfer matrix computation.

**We need some breakthrough!**

# White's DMRG

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Hamiltonian formulation



1. The wavefunction is obtained by the direct diagonalization of super block Hamiltonian (full Hamiltonian including both left and right block)

lanczos diagonalization

2. maximize the norm of the wavefunction within the kept number of basis

$$|\Psi\rangle = \Psi_L \omega \Psi_R$$

singular value decomposition  
reduced density matrix

3. renormalization is performed for left/right block Hamiltonian

# How did he get such an idea?

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The answer is partly described by himself in “Density-matrix renormalization group”, eds. by Peschel et al, Springer (1999)

This question is just out of curiosity(^\_^)

NRG: particle in a box(Wilson’s approach)

QMC: for fermion(path integral)

Exact diagonalization

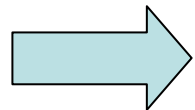
QMC: negative sign(block variables)

QMC: zero temp.

NRG: in momentum space

NRG: Wilson’s perturbative approach

NRG: boundary condition



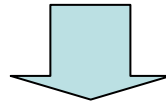
He got the idea of “projection of super block into a block” after a lot of trials and failures.

# Can I get such an idea?

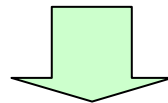
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This question is just for fun(^\_^), because DMRG had already been presented when I started my research in the graduate school.

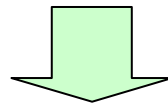
I started my research from the variational principle of the MP state and CTM.



In 2D classical lattice statistics, we can construct the eigenvector directly by using CTMs



I would try to a method which can directly manipulate the wavefunction in the 1D quantum case

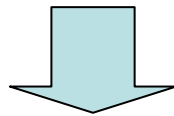


I would have never gotten the idea that I diagonalize the superblock to obtain the groundstate wavefunction.

# Matrix product & DMRG

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In contrast to 2D classical case, we can not decompose the wavefunction into a MP state directly.



Ostlund and Rommer reconstructed the wavefunction of DMRG, by analyzing the iteration process in DMRG.

$$\Psi(s_1, s_2, \dots) = \sum \prod A[s_i]_{\mu_i \mu_{i+1}}$$

$A[s]$  : projection(transformation) matrix in DMRG

In the bulk limit, the matrix in MP state should be uniform.  
For a finite size system, MP is position dependent.



# finite system size method

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finite system size method of DMRG is more useful.

- site resolved information: spin profile
- excitation, time evolution, etc..



Various improvements and applications of DMRG are based on the finite system size method, which were included in Prof. Jackelmann's talk

But, here...

In the context of statistical mechanics, infinite system size DMRG is more interesting.

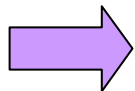
we are now interested in critical phenomena in DMRG.....

# Is DMRG a renormalization group?

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## questions

- How does DMRG behave in the critical limit?
  - What is a relevant/irrelevant operator in DMRG?
  - Can we extract a critical index through DMRG?
- What is the energy/length scale in DMRG?
- What is the meaning of eigenvalue spectrum of the reduced density matrix at critical point?

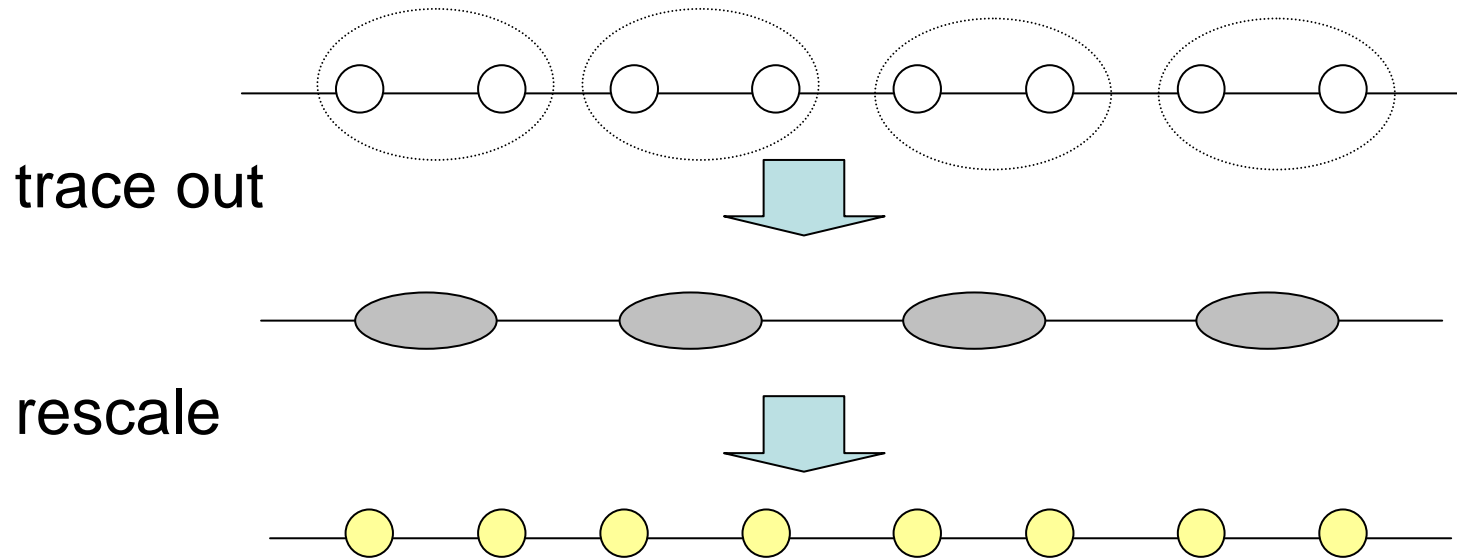


Comparison to Wilson's real space renormalization group

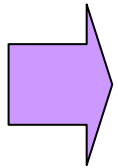
Wilson NRG for Kondo problem is only the method which can deal with critical properties of the 1D quantum system.

# block spin transformation RG

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

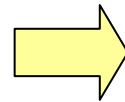
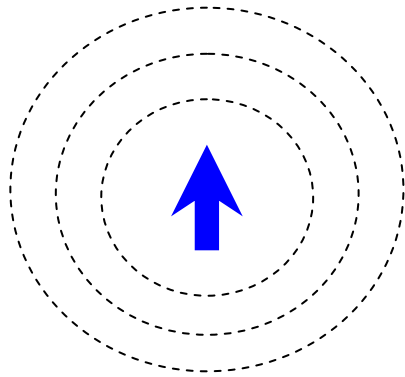


The “boundary” of the block spin is important.

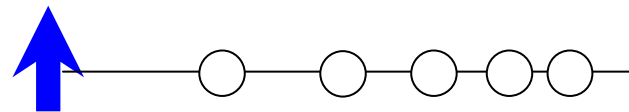
# Wilson's NRG

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Kondo impurity problem



1D quantum system  
with the boundary



Add free electrons and project out the higher energy states

$$H_{\Lambda}^{N+1} = H_{\Lambda}^N + \Lambda t (c_N^+ c_{N+1} + c_{N+1}^+ c_N)$$

$\Lambda(>1)$  is a cut off parameter, which controls the energy scale of the system.

$\Lambda$  itself comes from log-discretization of fermi sea

# Testing Wilson-like NRG

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$$H_{\Lambda}^{N+1} = H_{\Lambda}^N + \vec{S}_N \cdot \vec{S}_{N+1}$$

Free electrons  $\longrightarrow$  Interacting spins  $\vec{S} \cdot \vec{S}$

Cutoff  $\Lambda$   $\longrightarrow$   $\Lambda = 1$

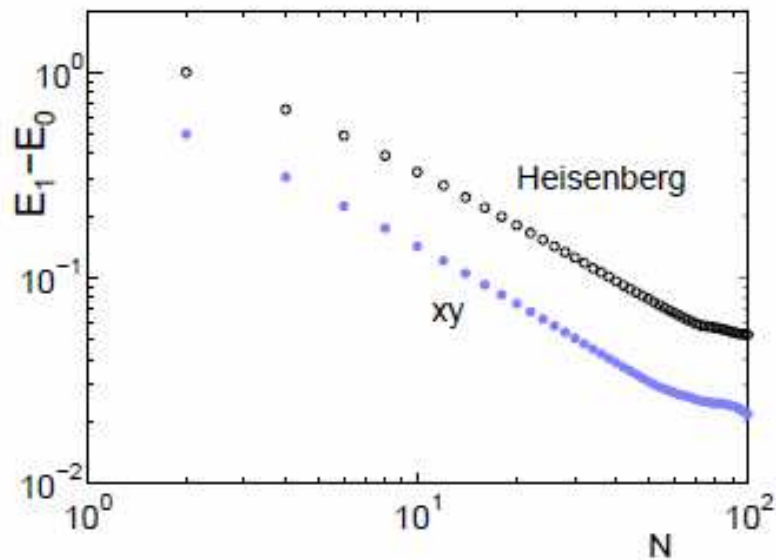
We do not touch the energy  
scale of the system

boundary  $\longrightarrow$  free boundary condition

cf. T. Xiang, (1991) PRB (almost the same timing as DMRG!)

# Results[excitation gap]

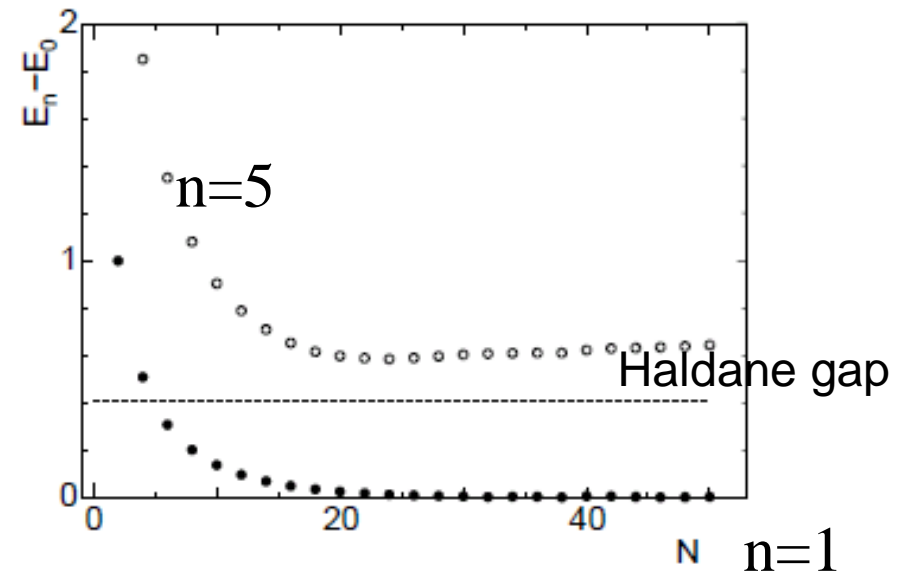
S=1/2 Heisenberg/XY



gapless;  $1/N$  dependence

$m=1600$

S=1 Heisenberg



4 fold degenerating ground state  
due to edge spins

$m=800$

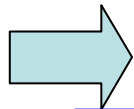
The ground state energy is consistent with the known value

## some implications

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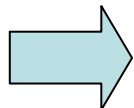
- The results are qualitatively reasonable, but the accuracy of DMRG is much better.

To improve the accuracy of NRG may be difficult.



The meaning of the density-matrix-based transformation in DMRG should be discussed again.

- The spectrum of Wilson-like NRG with  $\Lambda=1$  looks like the finite size scaling ( $S=1/2$  critical case)



The role of cutoff is significant in Wilson's NRG!

# Wilson and White

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**Wh**

reduced density matrix/larger eigenvalues  
angular quantization in 2D space-time

add the center sites

**Wi**

Hamiltonian/lower energy

add the boundary site  
(the other side of the impurity)

[cutoff parameter controlling the energy scale](#)



# conclusion at this stage

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Is DMRG a renormalization group? => No?

Renormalization group see a response of the system when changing cutoff parameter (energy scale/length scale)

(not only real space approaches

but also field theoretical renormalization group

In terms of “renormalization group”, the theory should have an actively controllable cutoff parameter.

Although the block spin transformation is used in DMRG, the theory has no explicit scale transformation.

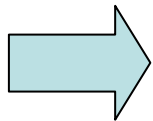
In order to see critical phenomena, a cutoff parameter controlling the energy scale should be implemented in DMRG

# corner Hamiltonian

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Is there any possible approach to transform DMRG into a Wilson-like NRG?

partially YES!



corner Hamiltonian approach

$$\rho \propto e^{-aH_{CTM}}$$

please see symposium

# Quantum information

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# Entanglement entropy

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$$S = -\rho \ln \rho$$

$$S = -k_B \left. \frac{\partial}{\partial n} \rho^n \right|_{n=1} = -k_B \rho \ln \rho$$