Introduction to Density Matrix Renormalization Group（DMRG）and Matrix Product States（MPS）

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Shanghai Jiao Tong University

Refs:

1. Steven R. White, Phys. Rev. Lett. 69, 2863 (1992)
2. Steven R. White, Phys. Rev. B 48, 10345 (1993)
3. Ulrich Schollwöck, Annals of Physics 326, 96 (2011))

Beijing Computational Science Research Center, June 13, 2024

Outline

- Introduction to Numerical Renormalization Group
- Density Matrix Renormalization Group
- Matrix Product States

Resistance minimum in dilute Magnetic Alloys

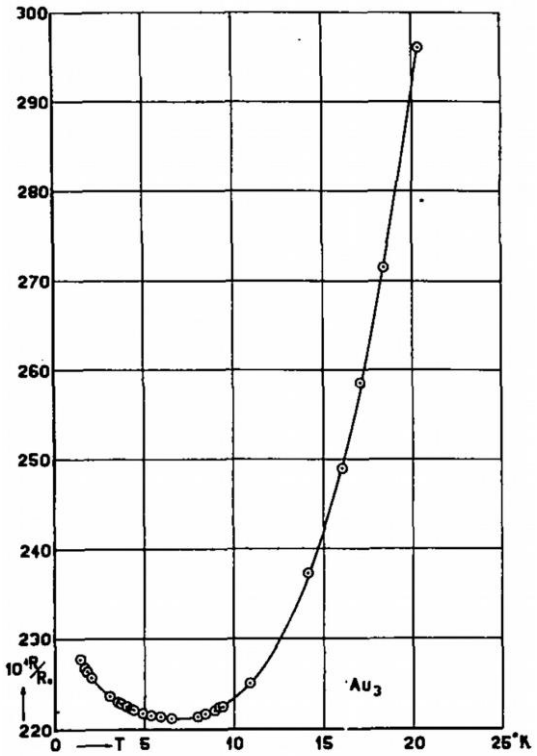

Fig. 1. Electrical resistance of Au_3.

Physica III, no. 6 Juni 1936

THE ELECTRICAL RESISTANCE
OF GOLD AND SILVER AT LOW TEMPERATURES

by W. J. DE HAAS and G. J. VAN DEN BERG

- For metal, resistivity ~ T^2 at low T (electron contribution), ~ T^5 at high T (phonon contribution).
- With magnetic impurity, it has a minimum.

Resistance minimum in dilute Magnetic Alloys

Jun Kondo (近藤 淳 *Kondō Jun*, born on February 6, 1930) is a theoretical physicist from Japan.

Progress of Theoretical Physics, Vol. 32, No. 1, July 1964

Resistance Minimum in Dilute Magnetic Alloys

Jun KONDO

Electro-technical Laboratory
Nagatacho, Chiyodaku, Tokyo

(Received March 19, 1964)

Kondo model

Kondo model (sd model)

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + 2J\mathbf{s}\cdot\mathbf{S}$$

In momentum space

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}'\sigma'}\, \boldsymbol{\sigma}_{\sigma'\sigma}\, c_{\mathbf{k}\sigma} \cdot \mathbf{S}$$

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Second order perturbation

$$R = R_0 \left[1 - 4J\rho \ln\left(\frac{k_B T}{D}\right) + \ldots \right]$$

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Problem: resistivity diverges when T goes to 0 !!!

Numerical Renormalization Group (NRG)

The Kondo problem was solved by Wilson with numerical renormalization group method (in **1975**).

Kenneth Geddes "Ken" Wilson (June 8, 1936 – June 15, 2013) was an American theoretical physicist and a pioneer in leveraging computers for studying particle physics. He was awarded the 1982 Nobel Prize in Physics for his work on phase transitions—illuminating the subtle essence of phenomena like melting ice and emerging magnetism. It was embodied in his fundamental work on the renormalization group.

He earned his PhD from Caltech in 1961, studying under Murray Gell-Mann (September 15, 1929 – May 24, 2019)

Numerical Renormalization Group (NRG)

By linearize the dispersion and replaced it with a spectrum of discrete levels equally distributed on logarithm scale as

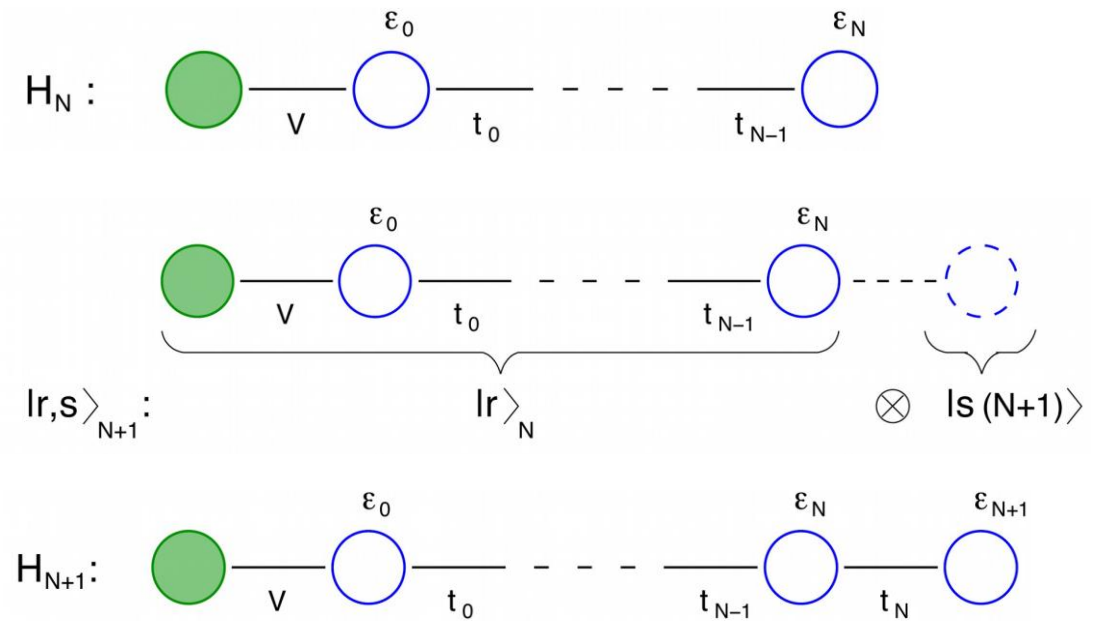
$$\varepsilon_n = \Lambda^{-n}$$

The Kondo model is transformed to

$$\mathcal{H}_N = \Lambda^{(N-1)/2} \left\{ \sum_{n=0}^{N-1} \Lambda^{-\frac{n}{2}} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \tilde{J} c_0^\dagger \boldsymbol{\sigma} c_0 \cdot \mathbf{S} \right\}$$

$$\hat{H} = \lim_{N\to\infty} \Lambda^{-(N-1)/2} \mathcal{H}_N$$

Numerical Renormalization Group (NRG)



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

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

Numerical Renormalization Group (NRG)

Truncation criteria: energy

$$H = UEU^{\dagger}$$

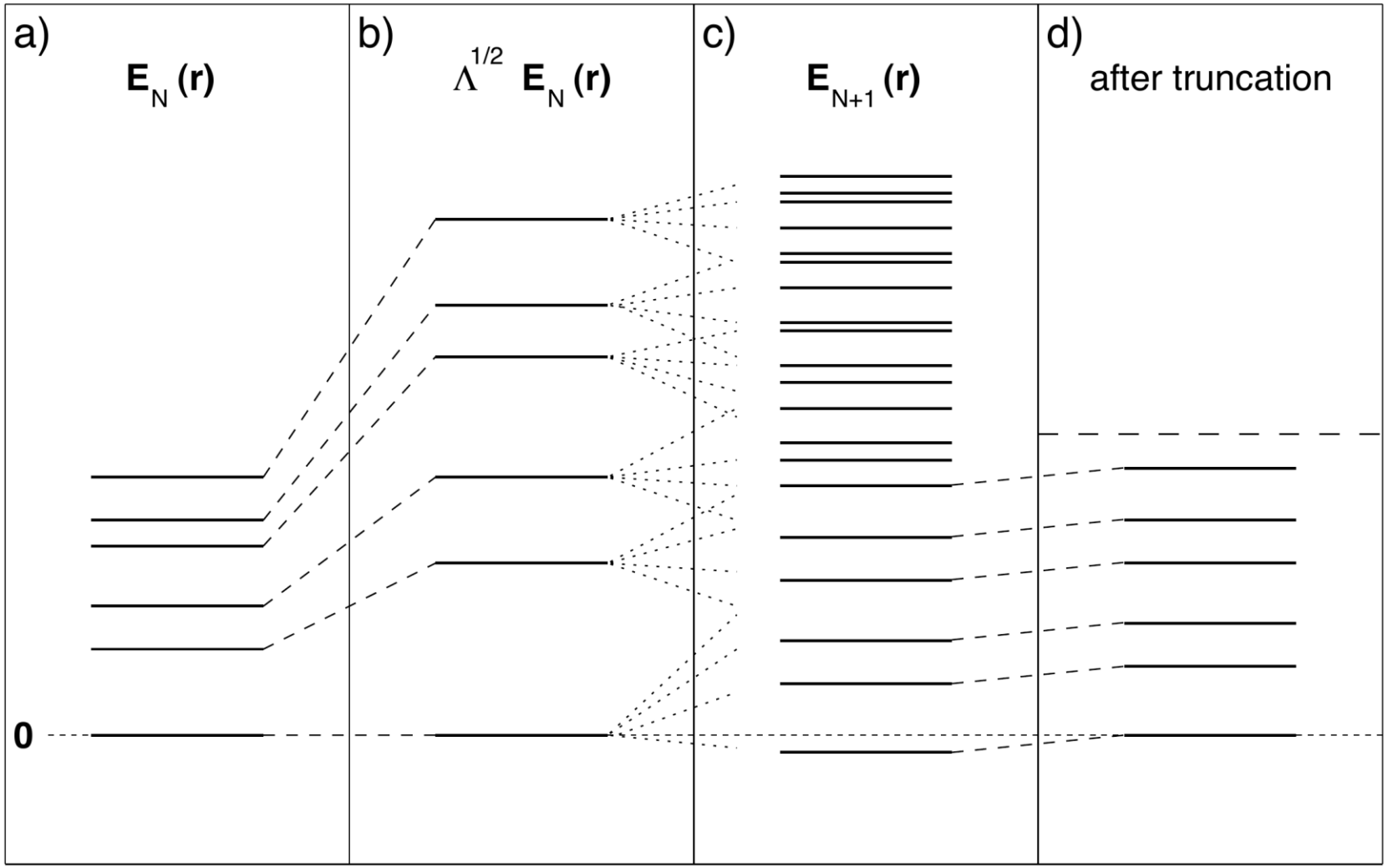
$$H = \sum_{i=1}^{N} \epsilon_i u_i u_i^{\dagger} \approx \sum_{i=1}^{N_{cut}} \epsilon_i u_i u_i^{\dagger}$$

In NRG, that is:

$$|w\rangle_{N+1} = \sum_{rs} U(w, rs)|r; s\rangle_{N+1}$$

U is the unitary matrix to diagonalize H. In order to truncate the basis, we truncate the row index of U, which means the dimension of w is less than the multiply of the dimension of r and s.

Numerical Renormalization Group (NRG)



Application of NRG to lattice models

(1) Describe interactions on an initial sublattice ("block") A of length ℓ by a block Hamiltonian $\hat{H}_{\mathrm{A}}$ acting on an M-dimensional Hilbert space.

(2) Form a compound block AA of length 2ℓ and the Hamiltonian $\hat{H}_{\mathrm{AA}}$, consisting of two block Hamiltonians and interblock interactions. $\hat{H}_{\mathrm{AA}}$ has dimension M^2.

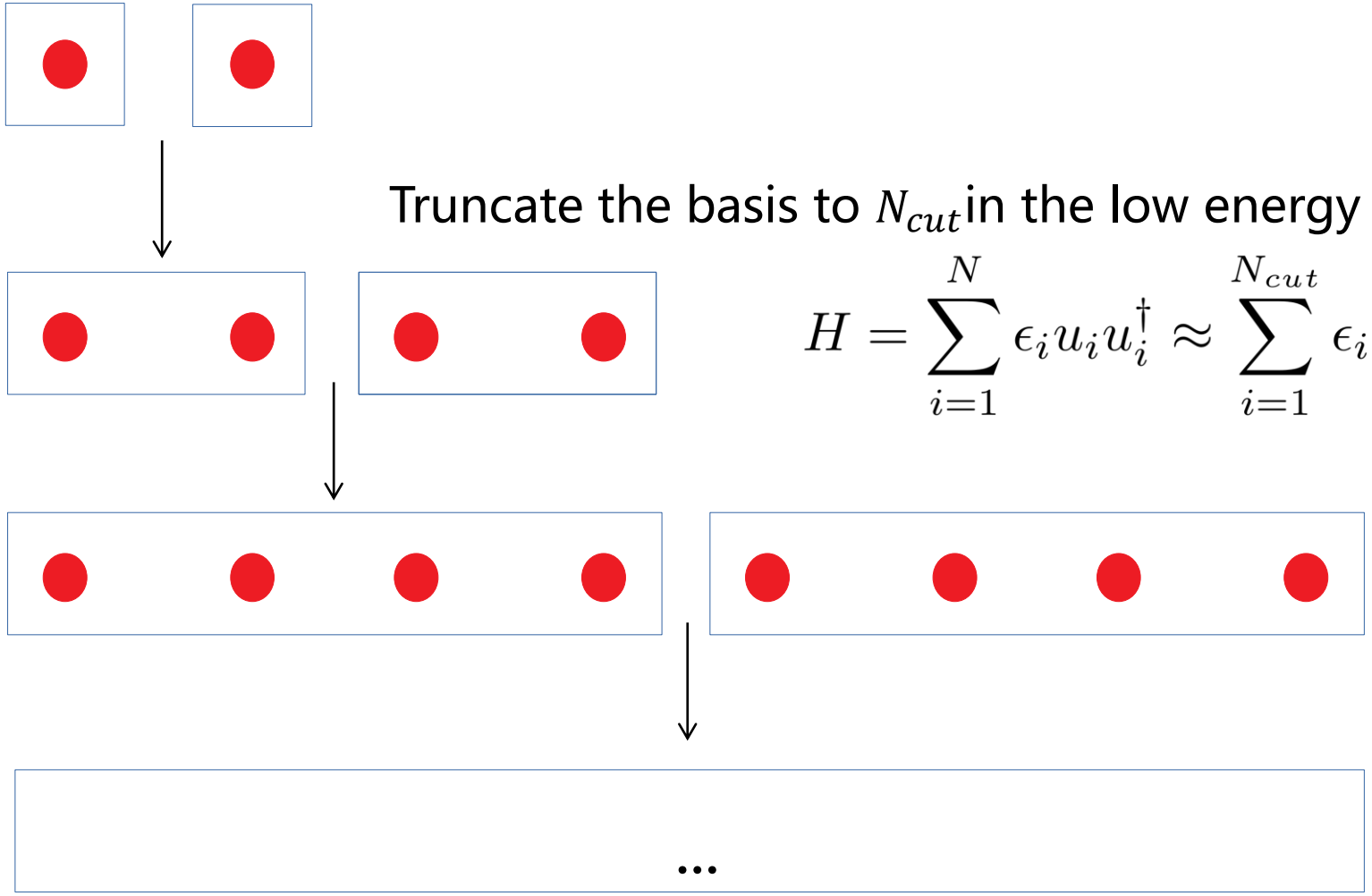
(3) Diagonalize $\hat{H}_{\mathrm{AA}}$ to find the M lowest-lying eigenstates.

(4) Project $\hat{H}_{\mathrm{AA}}$ onto the truncated space spanned by the M lowest-lying eigenstates, $\hat{H}_{\mathrm{AA}} \rightarrow \hat{H}^{\mathrm{tr}}_{\mathrm{AA}}$.

(5) Restart from step (2), with doubled block size: $2\ell \rightarrow \ell$, $\mathrm{AA} \rightarrow \mathrm{A}$, and $\hat{H}^{\mathrm{tr}}_{\mathrm{AA}} \rightarrow \hat{H}_{\mathrm{A}}$, until the box size is reached.

This idea was proposed in **Mitchel D. Kovarik, Phys. Rev. B 41, 6889 (1990)**

Application of NRG to lattice models



Truncate the basis to N_{cut} in the low energy space

$$H = \sum_{i=1}^{N} \epsilon_i u_i u_i^\dagger \approx \sum_{i=1}^{N_{cut}} \epsilon_i u_i u_i^\dagger$$

Application of NRG to lattice models

TABLE III. E_0, E_1, and ΔE at indicated maximum value of N_b, corrected values at the indicated maximum value of N_b (corr.), linear extrapolations (lin. ext.), corrected linear extrapolations (corr. lin. ext.), and the results of Nightengale and Blöte (NB) for $s=1$. The values for E_0 and E_1 obtained at $N_b=300$ are the best upper bounds for these eigenvalues.

	E_0	E_1	ΔE
	$N=16$		
$N_b=195$	−22.440 275 72	−21.991 180 77	0.449 014 95
Lin. ext.	−22.446±0.005	−22.005±0.005	0.441±0.005
NB	−22.4463±0.005	−22.0049±0.005	0.4414±0.007
	$N=32$		
$N_b=300$	−44.761 730 76	−44.313 232 95	0.447 497 81
$N_b=300$ corr.	−44.7867	−44.3452	0.4415
Lin. ext.	−44.820±0.005	−44.391±0.005	0.429±0.005
Corr. lin. ext.	−44.845±0.005	−44.424±0.005	0.421±0.005
NB	−44.8497±0.015	−44.4364±0.015	0.4133±0.02

Gap for spin-1 chain ~ 0.4105

NRG "failed" in lattice models

PHYSICAL REVIEW
LETTERS

VOLUME 68 | 15 JUNE 1992 | NUMBER 24

Real-Space Quantum Renormalization Groups

S. R. White and R. M. Noack
Department of Physics, University of California, Irvine, California 92717
(Received 20 January 1992; revised manuscript received 27 April 1992)

Although originally thought to show great promise in solving quantum many-body problems on a lattice, numerical real-space renormalization-group techniques have had little success for such problems. We explore the nature of the difficulties involved by studying the application of the method to the simple tight-binding model in one dimension. The standard approach fails dramatically for this model. We show that the key to successfully applying the renormalization-group technique lies in applying a variety of boundary conditions to a block in order to simulate the effect of neighboring blocks.

S. R. White and R. M. Noack, Phys. Rev. Lett. 68, 3487 (1992)

NRG "failed" in lattice models

It is easy to see in this simple example, however, that this procedure is quite *poor* in describing large-scale, low-energy behavior. The Hamiltonian in this example is just a finite-difference discretization of the kinetic energy of a 1D particle, and in the limit of large block size, the eigenstates are just particle-in-a-box eigenstates. The boundary condition of ignoring the connections T to neighboring blocks corresponds to setting the wave function to 0 at the sites just outside the block. Figure 1 illustrates the difficulty. Any state made only of low-lying states from the previous iteration must have a "kink" in the middle. In order to accurately represent states in the larger block, one must make use of nearly all the states in the smaller block: Any truncation leads to large errors.

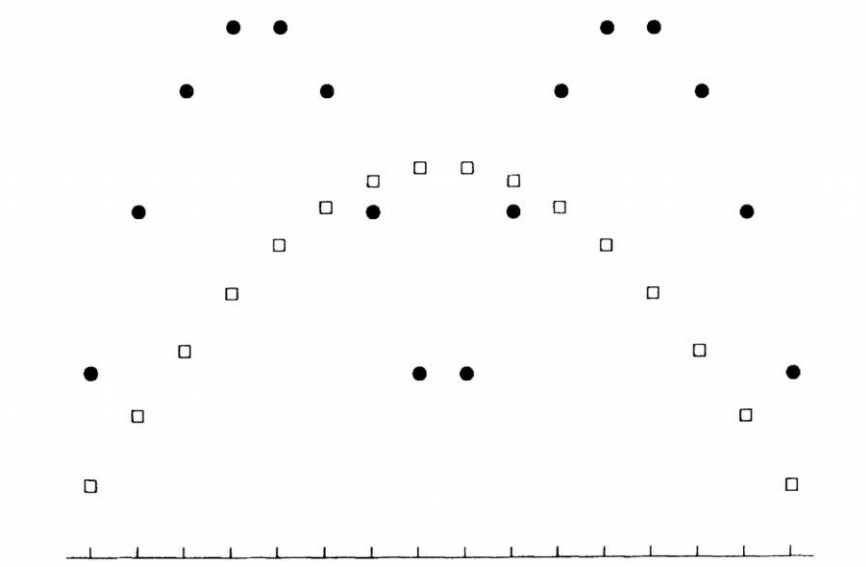


FIG. 1. Lowest eigenstates of two 8-site blocks (solid circles) and a 16-site block (open squares) for the one-dimensional tight-binding model with fixed boundary conditions.

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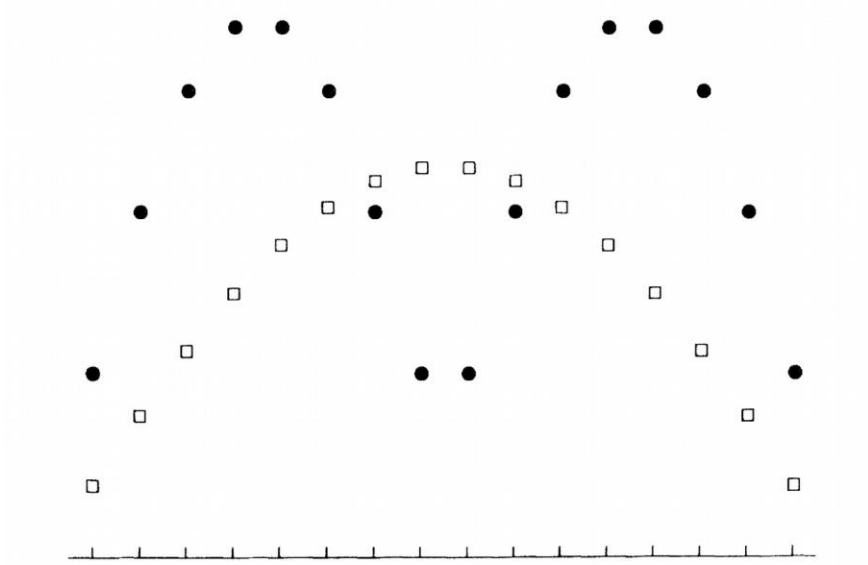


FIG. 1. Lowest eigenstates of two 8-site blocks (solid circles) and a 16-site block (open squares) for the one-dimensional tight-binding model with fixed boundary conditions.

TABLE I. Lowest energies after ten blocking transformations for the noninteracting single particle on a 1D chain with fixed boundary conditions.

	Exact	Standard	Fixed free
E_0	2.3508×10^{-6}	1.9207×10^{-2}	2.3508×10^{-6}
E_1	9.4032×10^{-6}	1.9209×10^{-2}	9.4032×10^{-6}
E_2	2.1157×10^{-5}	1.9214×10^{-2}	2.1157×10^{-5}
E_3	3.7613×10^{-5}	1.9217×10^{-2}	3.7613×10^{-5}

An attempt to cure the failure of NRG in lattice model

Journal of Magnetism and Magnetic Materials 104–107 (1992) 861–862
North-Holland

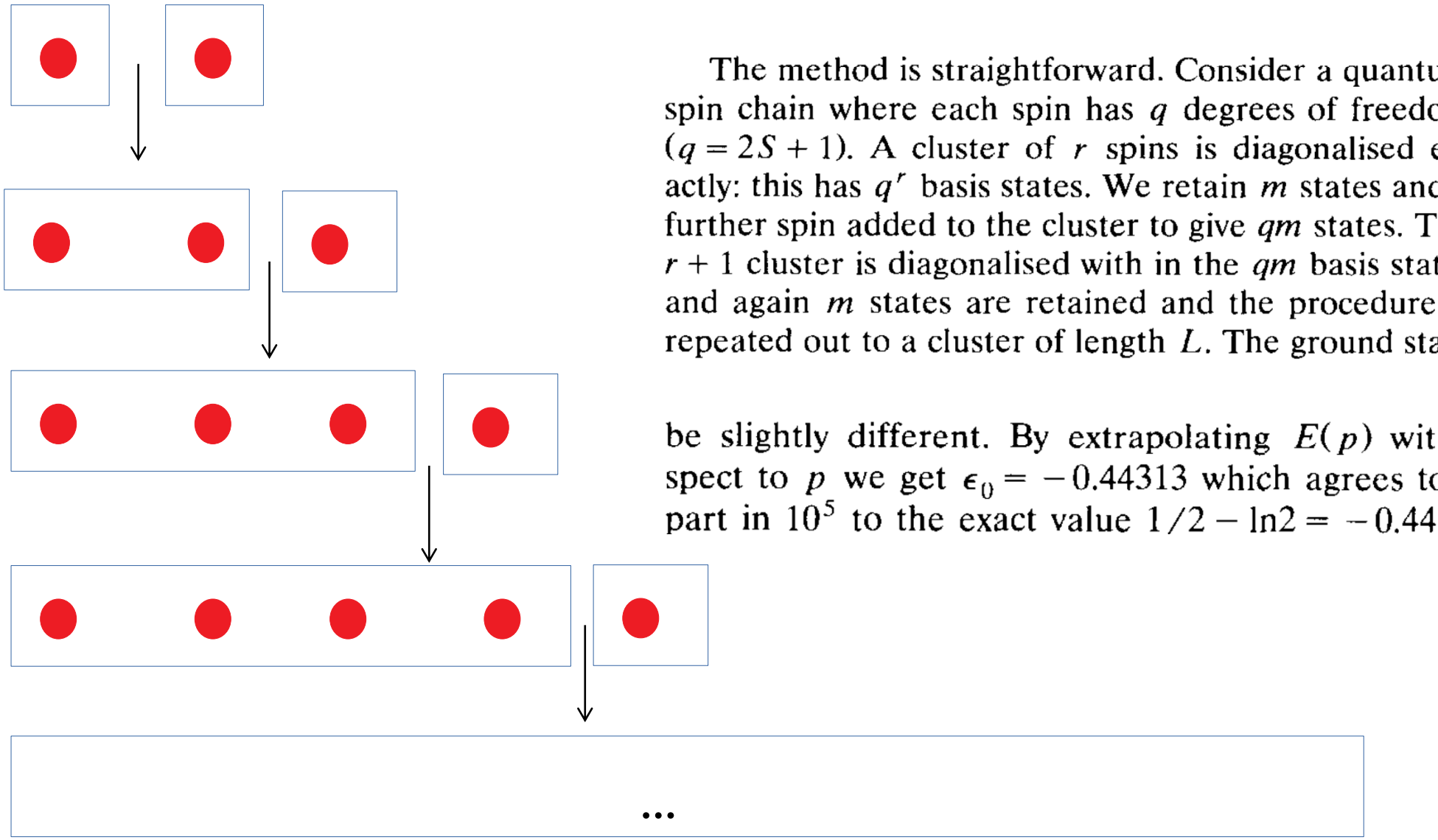
Real space renormalisation group study of Heisenberg spin chain

Tao Xiang [a,1] and G.A. Gehring [b]

[a] *Department of Theoretical Physics, University of Oxford, UK*
[b] *Department of Physics, University of Sheffield, Sheffield S3 7RH, UK*

A new method for determining the ground state and first excitation state energy of a one-dimensional quantum Hamiltonian with short range interaction is proposed. This method, based on the Wilson renormalisation group technique, is illustrated by applying it to the one-dimensional quantum antiferromagnetic systems. Long spin chain calculations are performed iteratively by diagonalising a smaller system, retaining the lowest m states, and constructing from these a longer spin chain basis and corresponding Hamiltonian matrices. The computation can be easily and quickly done for spin $S = 1/2$ and 1 system on a chain up to 60 sites. By extraploting with respect to both m and the chain length L, the ground state energy of the spin 1/2 Heisenberg model is estimated to be -0.44313. It agrees to one part in 10^5 to the exact result. The energy gap between the first excitation state and the ground state for the spin 1 Heisenberg model with both open and closed boundary conditions is calculated. As m increases, it converges to the exact result rapidly.

An attempt to cure the failure of NRG in lattice model



The method is straightforward. Consider a quantum spin chain where each spin has q degrees of freedom ($q = 2S + 1$). A cluster of r spins is diagonalised exactly: this has q^r basis states. We retain m states and a further spin added to the cluster to give qm states. The $r + 1$ cluster is diagonalised with in the qm basis states and again m states are retained and the procedure is repeated out to a cluster of length L. The ground state

be slightly different. By extrapolating $E(p)$ with respect to p we get $\epsilon_0 = -0.44313$ which agrees to one part in 10^5 to the exact value $1/2 - \ln 2 = -0.443147$.

The birth of Density Matrix Renormalization Group (DMRG)

VOLUME 69, NUMBER 19 PHYSICAL REVIEW LETTERS 9 NOVEMBER 1992

Density Matrix Formulation for Quantum Renormalization Groups

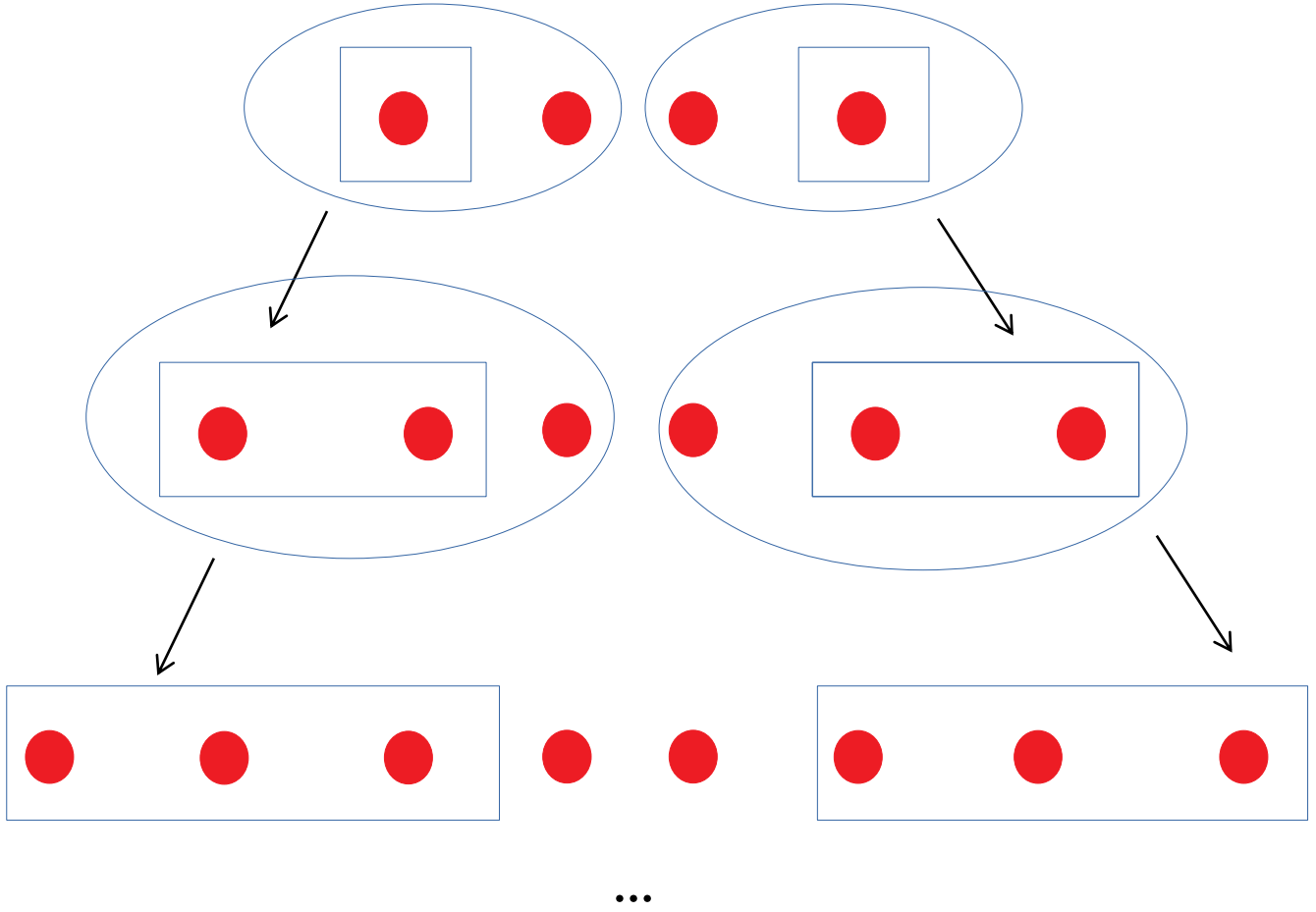
Steven R. White
Department of Physics, University of California, Irvine, California 92717
(Received 22 May 1992)

A generalization of the numerical renormalization-group procedure used first by Wilson for the Kondo problem is presented. It is shown that this formulation is optimal in a certain sense. As a demonstration of the effectiveness of this approach, results from numerical real-space renormalization-group calculations for Heisenberg chains are presented.

Results from DMRG

m	$S=\frac{1}{2}$ $E_0-E_0^{\text{exact}}$	$S=\frac{1}{2}$ $1-P_m$	$S=1$ $-E_0$	$S=1$ $1-P_m$
16	5.8×10^{-5}	8.0×10^{-6}	1.401 089	4.8×10^{-5}
24	1.7×10^{-5}	1.9×10^{-6}	1.401 380	1.6×10^{-5}
36	7.8×10^{-6}	9.0×10^{-7}	1.401 437	6.6×10^{-6}
44	3.2×10^{-6}	3.6×10^{-7}	1.401 476	1.1×10^{-6}
∞	1.9×10^{-7}		1.401 484(2)	
MC	$\sigma=5\times10^{-4}$		1.401 5(5)	

The birth of Density Matrix Renormalization Group (DMRG)



Truncation scheme in DMRG

Suppose we have a wave-function as

$$|\psi\rangle = \sum_{m,n}^{D_s D_e} \psi_{mn} |s_m\rangle |e_n\rangle$$

We need to truncate it to a new wave-function

$$|\psi'\rangle = \sum_{m,n}^{D_{cut} D_{cut}} \psi'_{mn} |s'_m\rangle |e'_n\rangle$$

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The reasonable criteria is to minimize the difference

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In the original paper of Steven R White, the answer is to truncate according to the reduced density matrix.

Truncation scheme in DMRG

Density matrix:

$$\rho = |\psi\rangle\langle\psi| = \sum_{m,n,m',n'} \psi_{mn}|s_m\rangle|e_n\rangle\psi^*_{m'n'}\langle s_{m'}|\langle e_{n'}|$$

Reduced density matrix:

$$\rho_s = Tr_e(\rho) = \sum_{n''}\langle e_{n''}|\rho|e_{n''}\rangle = \sum_{m,n,m'} \psi_{mn}\psi^*_{m'n}|s_m\rangle\langle s_{m'}|$$

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In matrix form:

$$(\rho_s)_{mm'} = \sum_n \psi_{mn}\psi^*_{m'n} = \psi\psi^\dagger$$

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$$(\rho_s)_{mm'} = (U\Omega U^\dagger)_{mm'} = \sum_r \omega_r u_r u_r^\dagger$$

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For *e*, we also have

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and

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Why can we use the same Ω here?

Truncation scheme in DMRG

We have

$$|\psi\rangle = \sum_{m,n}^{D_s D_e} \psi_{mn}|s_m\rangle|e_n\rangle$$

$$= \sum_{mm'm'',n,n'n''} U_{mm''}U^{\dagger}{}_{m''m'}\psi_{m'n'}V_{n'n''}V^{\dagger}_{n''n}|s_m\rangle|e_n\rangle$$

$$= \sum_{m'',n''} \widetilde{\psi}_{m''n''}|s'_{m''}\rangle|e'_{n''}\rangle$$

with

$$\widetilde{\psi}_{m''n''} = U^{\dagger}_{m''m'}\psi_{m'n'}V_{n'n''}$$

$$|s'_{m''}\rangle = U_{mm''}|s_m\rangle \qquad |e'_{n''}\rangle = V^{\dagger}_{n''n}|e_n\rangle = V^{*}_{nn''}|e_n\rangle$$

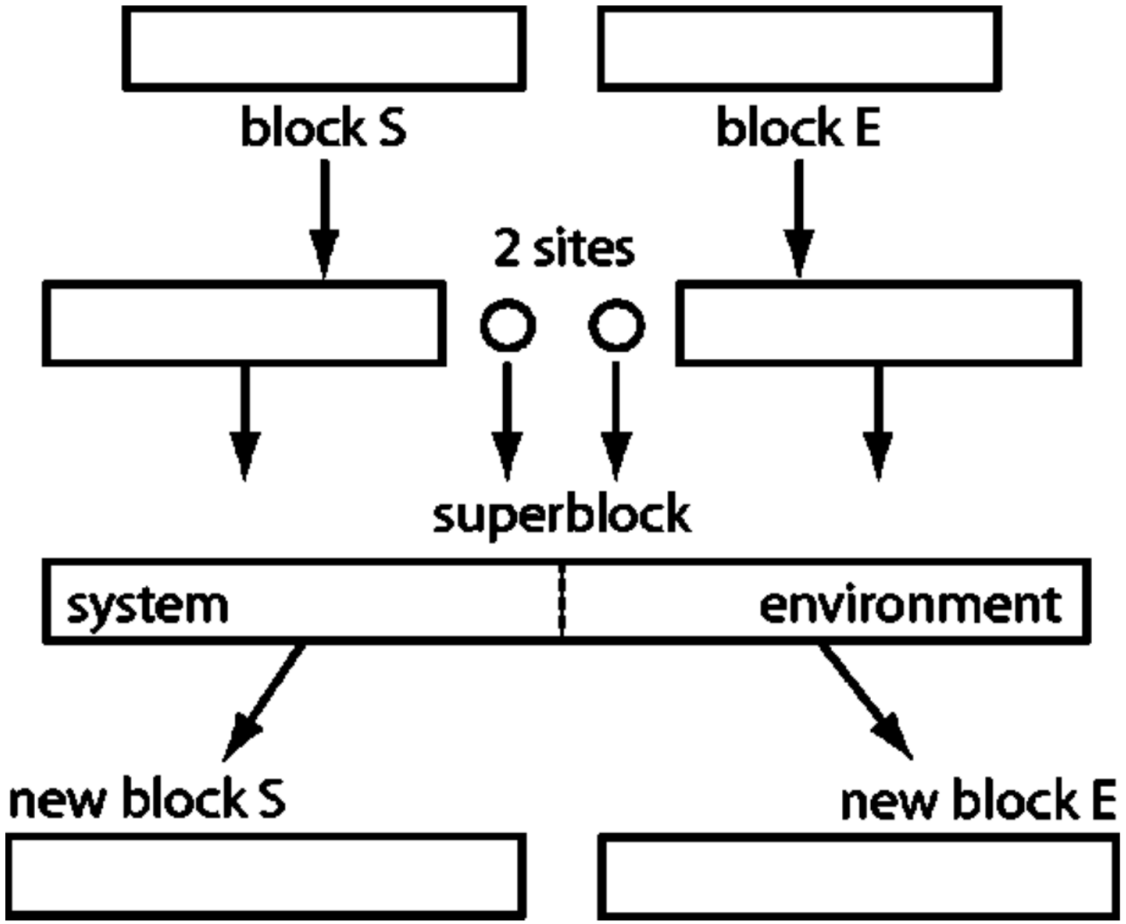
$\widetilde{\psi}_{m''n''}$ is a diagonal matrix. Why?

Then we can truncate the new basis $|s'_{m''}\rangle$ and $|e'_{n''}\rangle$

Truncation scheme in DMRG

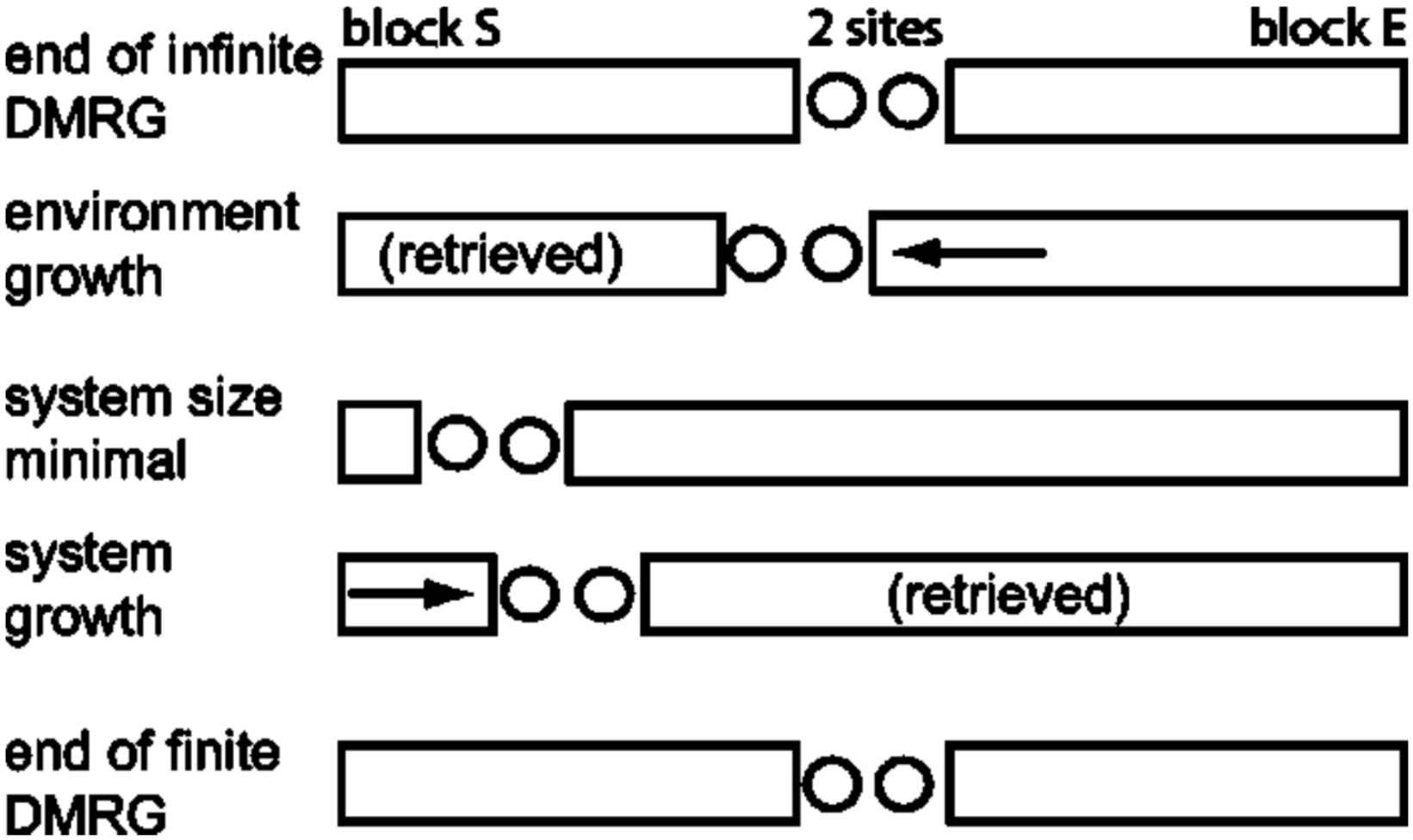
- The essence of DMRG is to truncate the reduced density matrix instead of the energy as in NRG.
- DMRG is a variational method.
- DMRG is very accurate for 1D system.

Infinite algorithm



U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005)

Finite algorithm



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Extrapolation to infinite M (kept states)

Suppose wave-function has error λ

$$|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle$$

Energy is

$$\begin{aligned}
E &= \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \\
&= \frac{(\langle\psi_0| + \lambda\langle\psi_1|)H(|\psi_0\rangle + \lambda|\psi_1\rangle)}{(\langle\psi_0| + \lambda\langle\psi_1|)(|\psi_0\rangle + \lambda|\psi_1\rangle)} \\
&= \frac{E_0 + \lambda^2 E_1}{1 + \lambda^2} \\
&= (1 - \lambda^2)(E_0 + \lambda^2 E_1) + O(\lambda^4) \\
&= E_0 + \lambda^2(E_1 - E_0) + O(\lambda^4)
\end{aligned}$$

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\end{aligned}$$

Truncation error δ: the total truncation error in reduced density matrix.

$$\delta \sim \lambda^2$$

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$$|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle$$

Energy is

$$\begin{aligned} E &= \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{(\langle\psi_0| + \lambda\langle\psi_1|)H(|\psi_0\rangle + \lambda|\psi_1\rangle)}{(\langle\psi_0| + \lambda\langle\psi_1|)(|\psi_0\rangle + \lambda|\psi_1\rangle)} \\ &= \frac{E_0 + \lambda^2 E_1}{1 + \lambda^2} \\ &= (1-\lambda^2)(E_0 + \lambda^2 E_1) + O(\lambda^4) \\ &= E_0 + \lambda^2(E_1 - E_0) + O(\lambda^4) \end{aligned}$$

Truncation error δ: the total truncation error in reduced density matrix.

$$\delta \sim \lambda^2$$

Linear extrapolation with δ gives the exact energy $E = E_0 + C\delta$

Extrapolation to infinite M (kept states)

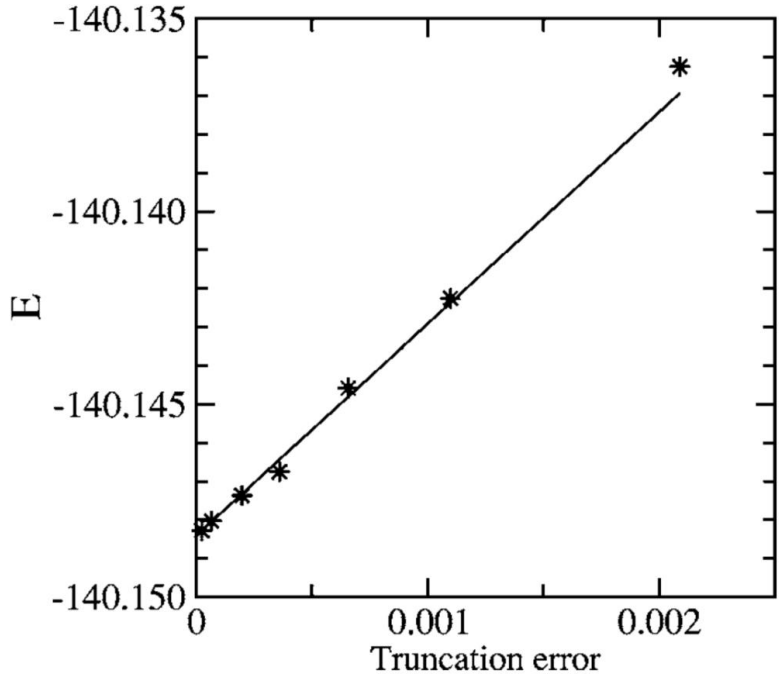


FIG. 4. Error in the total energy for the system of Fig. 3 versus the truncation error, with $a=10^{-2}$. In this run two sweeps for each value of m were made. The points shown are for $m=80$, 100, 120, 160, 200, 260, and 340. The line is a linear extrapolation, weighted with a standard deviation for each point assumed to be proportional to the truncation error at that point.

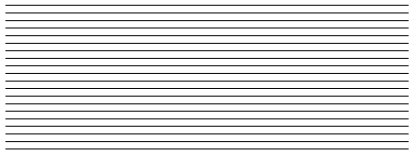
100 site spin-1 chain, PBC

S. R. White, PRB, **72**, 180403 (2005)

Haldane conjecture

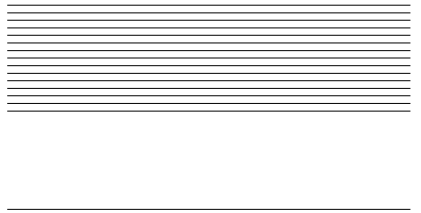
S = half odd integer spin chain, S=1/2, 3/2, ...

gapless

Energy levels: 

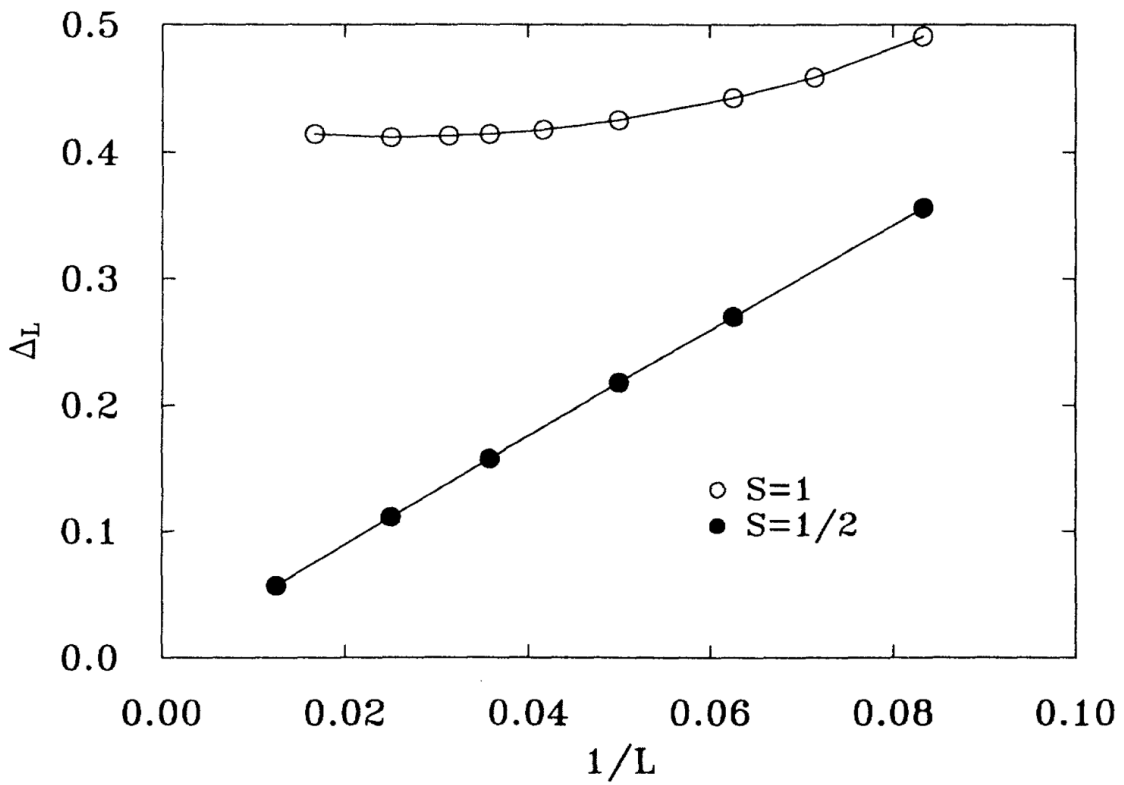
S = integer spin chain, S=1, 2, ...

gapped



F.D.M. HALDANE, PHYSICS LETTERS, **93**, 464 (1983); PRL, **50**, 1153 (1983)

Haldane conjecture



S. R. White, PRB, 48, 10345 (1993)

V. CONCLUSIONS

Using density-matrix numerical renormalization-group techniques, we have calculated a variety of properties of the Heisenberg chain with unprecedented reliability and accuracy. The results we have obtained largely support conclusions obtained from a variety of other methods over the last decade. In the case of the Haldane gap Δ, previous numerical work had established with reasonable certainty the existence of a gap, in agreement with Haldane's conjecture, with $\Delta \cong 0.41$. Our results must remove all remaining doubt, and provide an accurate value for the gap, $\Delta = 0.41050(2)$. We were able to determine the ground-state energy per site of the infinite chain to especially high accuracy, $e_0 \cong -1.401484038971(4)$. The correlation length was found to be identical to the decay length of the local spin moment away from the effective $S = 1/2$ spins on the ends of open $S = 1$ chains, with $\xi \cong 6.03(1)$.

S. R. White & D. A. Huse, PRB, 48 , 3844 (1993)

Generalization of DMRG and its applications

- Finite T
- Real time evolution (out of Equilibrium)
- Dynamic properties
- Quantum Chemistry
- Nuclear Physics
- ……

Matrix Product States

The wave-function in DMRG is Matrix Product States

VOLUME 75, NUMBER 19 PHYSICAL REVIEW LETTERS 6 NOVEMBER 1995

Thermodynamic Limit of Density Matrix Renormalization

Stellan Östlund and Stefan Rommer
Institute of Theoretical Physics, Chalmers University of Technology, S-41296 Göteborg, Sweden
(Received 20 March 1995)

The density matrix renormalization group discovered by White is investigated. In the case where renormalization eventually converges to a fixed point we show that quantum states in the thermodynamic limit with periodic boundary conditions can be simply represented by a "matrix product ground state" with a natural description of Bloch states of elementary excitations. We then observe that these states can be rederived through a simple variational ansatz making no reference to a renormalization construction. The method is tested on the spin-1 Heisenberg model.

Any state can be transformed to an MPS

For an arbitrary wave-function

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1,\ldots,\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle$$

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Reshape the wave-function

$$\Psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} = c_{\sigma_1,\ldots,\sigma_L}$$

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Perform a SVD decomposition

$$c_{\sigma_1,\ldots,\sigma_L} = \Psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2,\ldots,\sigma_L)}$$

$$\equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2,\ldots,\sigma_L}$$

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$$\equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2,\ldots,\sigma_L}$$

Rewrite U

$$A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1} \qquad c_{a_1\sigma_2,\ldots,\sigma_L} = \Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$$

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$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1,\ldots,\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$$

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$$\Psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} = c_{\sigma_1,\ldots,\sigma_L}$$

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$$A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1} \qquad c_{a_1\sigma_2,\ldots,\sigma_L} = \Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$$

The wave-function is now

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$$

Any state can be transformed to an MPS

Perform a SVD decomposition of $\Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3,\ldots,\sigma_L)} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4,\ldots,\sigma_L)}$$

Where we define:

$$A^{\sigma_2}_{a_1,a_2} = U_{(a_1\sigma_2),a_2} \qquad \Psi_{(a_2\sigma_3),(\sigma_4,\ldots,\sigma_L)} = S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3,\ldots,\sigma_L)}$$

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Repeat the above procedure to site *L-1*, we have

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}} \qquad \text{or:} \qquad c_{\sigma_1,\ldots,\sigma_L} = A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L}$$

Any state can be transformed to an MPS

Perform a SVD decomposition of $\Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3,\ldots,\sigma_L)} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4,\ldots,\sigma_L)}$$

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The wave-function is now in a MPS form

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$$

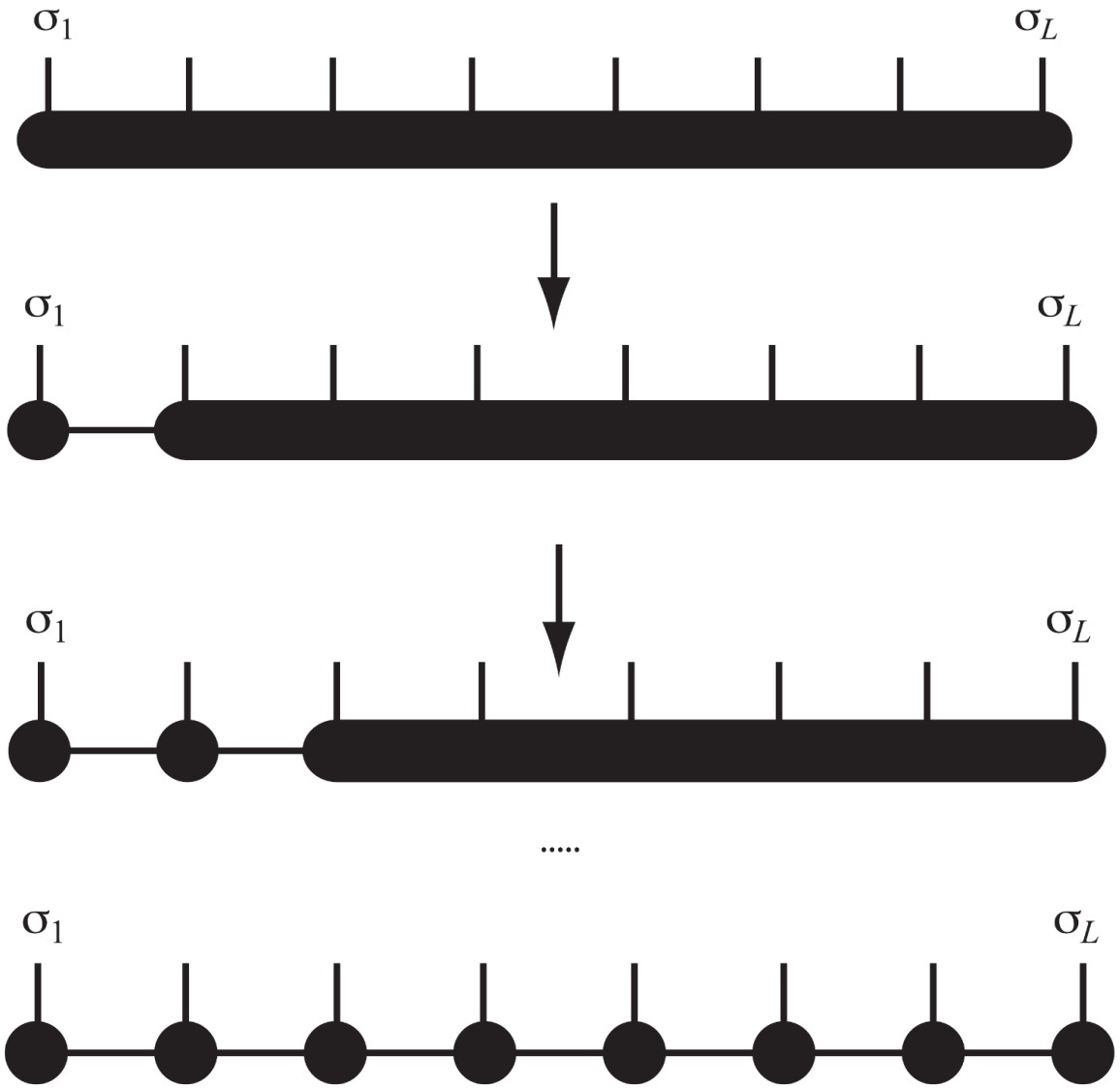
Any state can be transformed to an MPS

The number of parameters in wave-function is d^L $c_{\sigma_1,\ldots,\sigma_L}$

The number of parameters in MPS ~ L $c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}}$

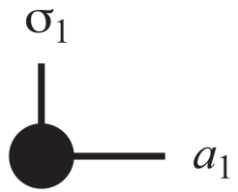
A^{σ_1}	$(1 \times d)$
A^{σ_2}	$(d \times d^2)$
$\cdots$	$\cdots$
$A^{\sigma_{L/2-1}}$	$(d^{L/2-1} \times d^{L/2})$
$A^{\sigma_{L/2}}$	$(d^{L/2} \times d^{L/2-1})$
$\cdots$	$\cdots$
$A^{\sigma_{L-1}}$	$(d^2 \times d)$
A^{σ_L}	$(d \times 1)$

Graphical representation of MPS

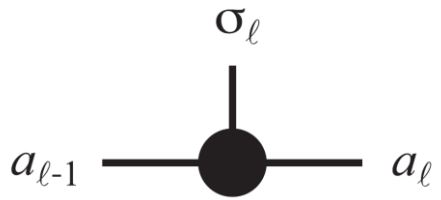


Graphical representation of MPS

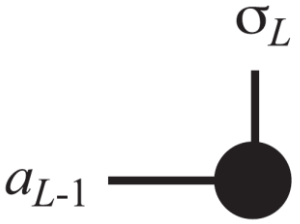
$A^{\sigma_1}_{1,a_1}$



$A^{\sigma_\ell}_{a_{\ell-1},a_\ell}$



$A^{\sigma_L}_{a_L,1}$



Gauge degree freedom of MPS

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle$$

$$A^{\sigma_i} \to A^{\sigma_i} X$$

$$A^{\sigma_{i+1}} \to X^{-1} A^{\sigma_{i+1}}$$

Entanglement entropy

For any state written in basis of two parts $|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$

Reduced density matrix: $\rho_A = \Psi\Psi^\dagger \quad \rho_B = \Psi^\dagger\Psi$

Entanglement entropy

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Reduced density matrix: $\rho_{\mathrm{A}} = \Psi \Psi^{\dagger} \quad \rho_{\mathrm{B}} = \Psi^{\dagger} \Psi$

Entanglement entropy defined as: $S_{\mathrm{A|B}} = -\mathrm{Tr}\, \rho_{\mathrm{A}} \log_2 \rho_{\mathrm{A}} = -\sum_{\alpha} w_a \log_2 w_a$

Entanglement entropy

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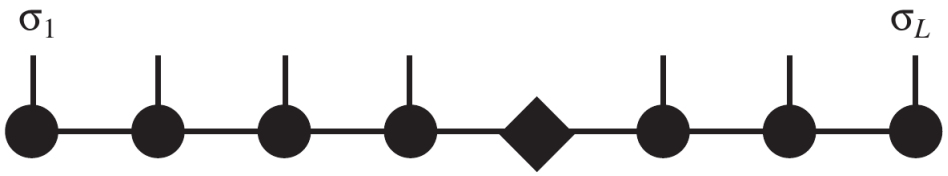
Entanglement entropy defined as: $S_{A|B} = -\mathrm{Tr}\,\rho_A \log_2 \rho_A = -\sum_\alpha w_a \log_2 w_a$

Renyi entropy $\mathcal{S}_\alpha(\rho_A) = \frac{1}{1-\alpha} \log \mathrm{tr}(\rho_A^\alpha) = \mathcal{S}_\alpha(\rho_B)$

Question 1: prove when α→1, Renyi entropy → Entanglement entropy

Question 2: What if α→ ∞?

Entanglement Entropy vs bond dimension



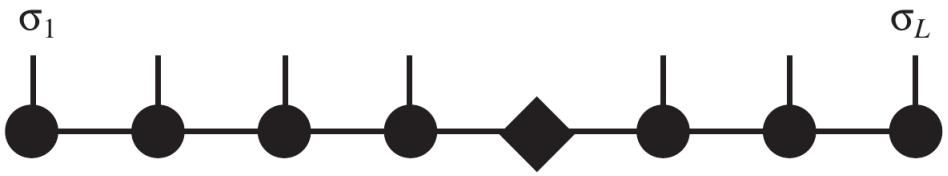
$$c_{\sigma_1,\ldots,\sigma_L} = A^{\sigma_1}\cdots A^{\sigma_\ell} S B^{\sigma_{\ell+1}}\cdots B^{\sigma_L}$$

$$|a_\ell\rangle_{\mathrm{A}} = \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1}\cdots A^{\sigma_\ell})_{1,a_\ell} |\sigma_1,\ldots,\sigma_\ell\rangle$$

$$|a_\ell\rangle_{\mathrm{B}} = \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (B^{\sigma_{\ell+1}}\cdots B^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1},\ldots,\sigma_L\rangle$$

$$|\psi\rangle = \sum_{a_\ell} s_a |a_\ell\rangle_{\mathrm{A}} |a_\ell\rangle_{\mathrm{B}}$$

Entanglement Entropy vs bond dimension



$$c_{\sigma_1,\ldots,\sigma_L} = A^{\sigma_1}\cdots A^{\sigma_\ell} S B^{\sigma_{\ell+1}}\cdots B^{\sigma_L}$$

$$|a_\ell\rangle_{\mathrm{A}} = \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1}\cdots A^{\sigma_\ell})_{1,a_\ell} |\sigma_1,\ldots,\sigma_\ell\rangle$$

$$|a_\ell\rangle_{\mathrm{B}} = \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (B^{\sigma_{\ell+1}}\cdots B^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1},\ldots,\sigma_L\rangle$$

$$|\psi\rangle = \sum_{a_\ell} s_a |a_\ell\rangle_{\mathrm{A}} |a_\ell\rangle_{\mathrm{B}}$$

Suppose the bond dimension of MPS is *M*, what is the largest entanglement entropy this state can support?

$$S_{max} = \sum_{i=1}^{M} \frac{1}{M} \log(\frac{1}{M}) = \log M$$

Volume law for a random state

The number of parameters in wave-function is d^L $\quad c_{\sigma_1,\ldots,\sigma_L}$

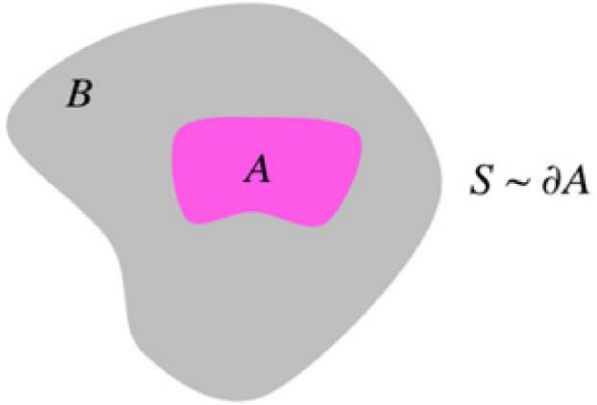
The number of parameters in MPS ~ L $\quad c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}}$

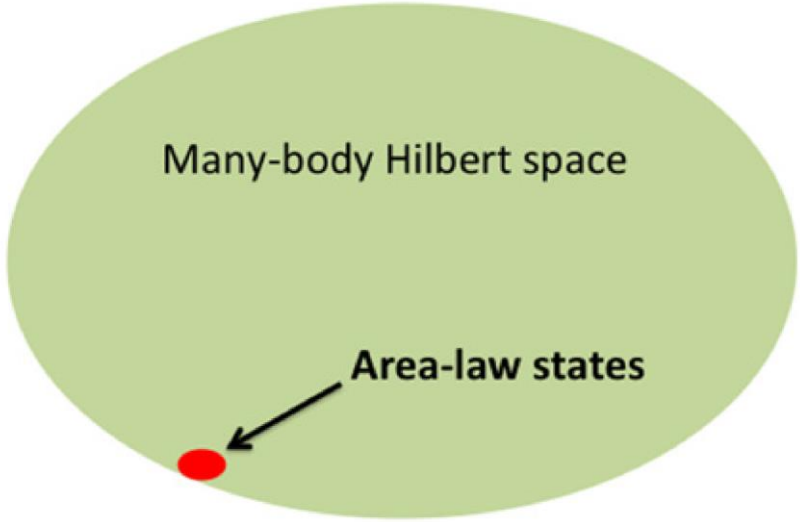
A^{σ_1}	$(1 \times d)$
A^{σ_2}	$(d \times d^2)$
$\cdots$	$\cdots$
$A^{\sigma_{L/2-1}}$	$(d^{L/2-1} \times d^{L/2})$
$A^{\sigma_{L/2}}$	$(d^{L/2} \times d^{L/2-1})$
$\cdots$	$\cdots$
$A^{\sigma_{L-1}}$	$(d^2 \times d)$
A^{σ_L}	$(d \times 1)$

$$S \sim \log(d^{L/2}) = \frac{L}{2} \log d$$

Volume law!!

Area law for low energy states





For one dimension system $S \sim C$ ⟶ Can be described by MPS with finite bond dimension M

For n-D system (L^n) $S \sim L^{n-1}$

In DMRG, PBC needs more kept states than OBC, why?

Area law for low energy states

An area law for one-dimensional quantum systems

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Received 16 May 2007
Accepted 27 July 2007
Published 20 August 2007

Online at stacks.iop.org/JSTAT/2007/P08024
doi:10.1088/1742-5468/2007/08/P08024

Abstract. We prove an area law for the entanglement entropy in gapped one-dimensional quantum systems. The bound on the entropy grows surprisingly rapidly with the correlation length; we discuss this in terms of properties of quantum expanders and present a conjecture on matrix product states which may provide an alternate way of arriving at an area law. We also show that, for gapped, local systems, the bound on Von Neumann entropy implies a bound on Rényi entropy for sufficiently large $\alpha < 1$ and implies the ability to approximate the ground state by a matrix product state.

Keywords: rigorous results in statistical mechanics, entanglement in extended quantum systems (theory)

ArXiv ePrint: 0705.2024

J. Stat. Mech. (2007) P08024

Area law for low energy states

We now introduce some notation. We let $X_{j,k}$ denote the set of sites i with $j \leq i \leq k$. We let Ψ_0 denote the ground state of the Hamiltonian H and we let $\rho^0_{1,N} = \Psi_0\rangle\langle\Psi_0$ be the ground state density matrix. We let $\rho^0_{j,k}$ denote the reduced ground state density matrix on the interval $X_{j,k}$. That is, $\rho^0_{j,k} = \mathrm{tr}_{i \notin X_{j,k}}(\rho^0_{1,N})$, where the partial trace is over sites not in $X_{j,k}$. We define the entropy of any density matrix $\rho_{j,k}$ by $S(\rho_{j,k}) = -\mathrm{tr}_{i \in X_{j,k}}(\rho_{j,k} \ln(\rho_{j,k}))$.

Theorem 1. *Consider a Hamiltonian on a finite lattice as above satisfying the finite range and finite interaction strength conditions above. Suppose H has a unique ground state with a gap ΔE to the first excited state. Then, for any i,*

$$S(\rho^0_{1,i}) \leq S_{\max} \tag{2}$$

where we define

$$S_{\max} = c_0 \xi' \ln(\xi') \ln(D) 2^{\xi' \ln(D)}, \tag{3}$$

for some numerical constant c_0 of order unity, and where we define

$$\begin{aligned} \xi &= \min(2v/\Delta E, \xi_C), \\ \xi' &= 6\xi. \end{aligned} \tag{4}$$

1D critical chain

In 1D, criticality means:

- The spectral is gapless.
- correlation function decay algebraically.

1D critical chain

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- The spectral is gapless.
- correlation function decay algebraically.

For 1D critical chain, logarithm correction to area law (cut the chain in the middle):

$$S = c \log L$$

c is related to the central charge in the underlying conformal field theory (CFT).

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- The spectral is gapless.
- correlation function decay algebraically.

For 1D critical chain, logarithm correction to area law (cut the chain in the middle):

$$S = c \log L$$

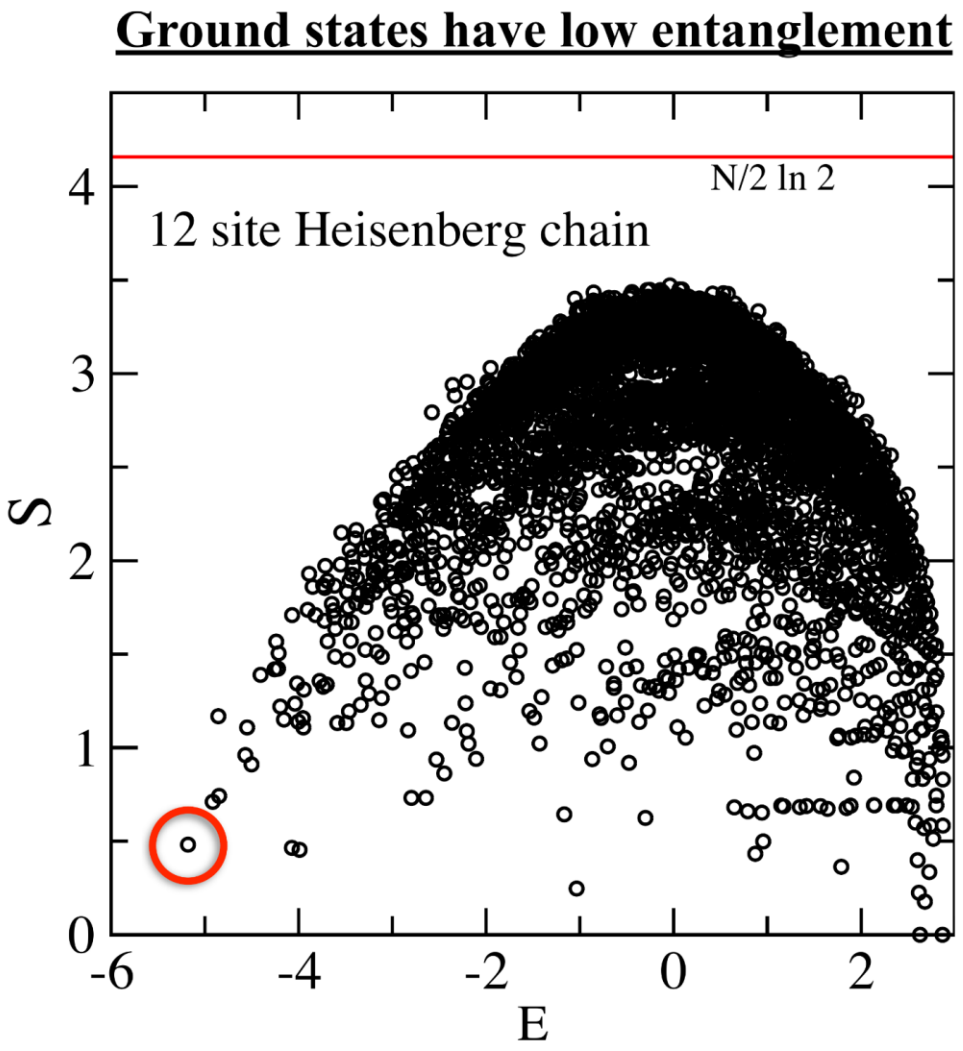
c is related to the central charge in the underlying conformal field theory (CFT).

Recall that for MPS with bond dimension *M*, we have

$$S_{max} = \sum_{i=1}^{M} \frac{1}{M} \log(\frac{1}{M}) = \log M \qquad \log M = c \log L \Rightarrow M = L^c$$

So to capture the EE of a critical chain, *M* needs to increase algebraically with the length of the chain.

The ground state of spin ½ chain?



From Steven R White' s talk

Question: what are the states with S = 0?

AKLT state

Spin-1 Chain:

$$H_{AKLT} = \sum_{ij} (\frac{1}{2} S_i S_j + \frac{1}{6} (S_i S_j)^2 + \frac{1}{3})$$

AKLT state

Spin-1 Chain:

$$H_{AKLT} = \sum_{ij} (\frac{1}{2} S_i S_j + \frac{1}{6} (S_i S_j)^2 + \frac{1}{3})$$

$$1 \otimes 1 = 0 \oplus 1 \oplus 2$$

Consider 2 sites:

$$S_1 S_2 = \frac{1}{2}((S_1 + S_2)^2 - S_1^2 - S_2^2) = \frac{1}{2} S(S+1) - 2$$

$$S_1 S_2 |0_{12}\rangle = -2, S_1 S_2 |1_{12}\rangle = -1, S_1 S_2 |2_{12}\rangle = 1$$

AKLT state

Spin-1 Chain:

$$H_{AKLT} = \sum_{ij} (\frac{1}{2} S_i S_j + \frac{1}{6} (S_i S_j)^2 + \frac{1}{3})$$

$$1 \otimes 1 = 0 \oplus 1 \oplus 2$$

Consider 2 sites:

$$S_1 S_2 = \frac{1}{2}((S_1 + S_2)^2 - S_1^2 - S_2^2) = \frac{1}{2} S(S+1) - 2$$

$$S_1 S_2 |0_{12}\rangle = -2, S_1 S_2 |1_{12}\rangle = -1, S_1 S_2 |2_{12}\rangle = 1$$

$$P_2 = a + b S_1 S_2 + c (S_1 S_2)^2$$

Projection operator:

$$P_2 |0_{12}\rangle = a - 2b + 4c = 0$$

$$P_2 |1_{12}\rangle = a - b + c = 0$$

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So P_{ij} is a projection operator, which project the two sites into the S=2 sector

AKLT state

The Hamiltonian is non-negative, why?

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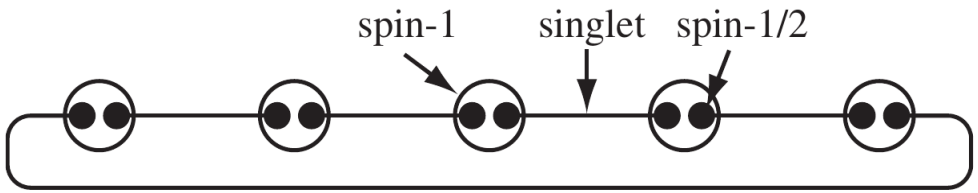

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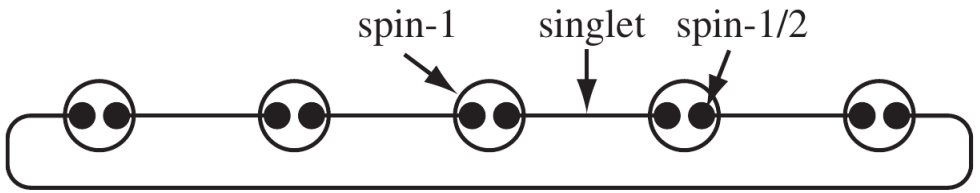
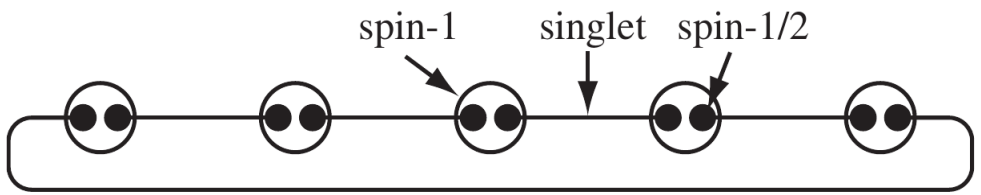


Why?

$$\frac{1}{2} \otimes 0 \otimes \frac{1}{2} = 0 \oplus 1$$

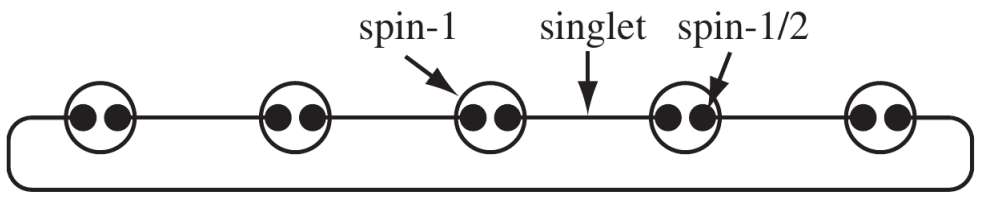
AKLT state



$|\mathbf{a}\rangle = |a_1, \ldots, a_L\rangle$ and $|\mathbf{b}\rangle = |b_1, \ldots, b_L\rangle$ representing the first and second spin-$\frac{1}{2}$ on each site

The singlet state is $|\Sigma^{[i]}\rangle = \sum_{b_i a_{i+1}} \Sigma_{ba} |b_i\rangle |a_{i+1}\rangle$ with $\Sigma = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$

AKLT state



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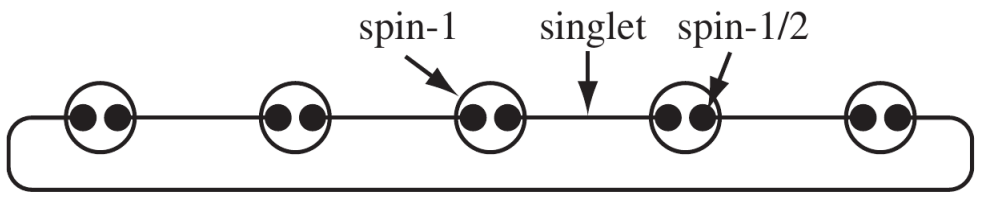
The product of all singlet states $|\psi_\Sigma\rangle = \sum_{\mathbf{a}} \sum_{\mathbf{b}} \Sigma_{b_1 a_2} \Sigma_{b_2 a_3}, \ldots, \Sigma_{b_{L-1} a_L} \Sigma_{b_L a_1} |\mathbf{ab}\rangle$

AKLT state



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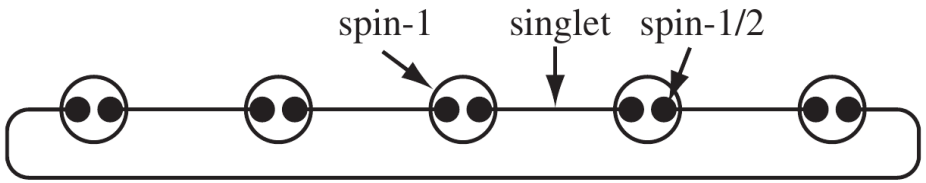
Map the two S = ½ spins into a S = 1 spin (why?) $\sum_{\boldsymbol{\sigma}} \sum_{\mathbf{ab}} M^{\sigma_1}_{a_1 b_1} M^{\sigma_2}_{a_2 b_2} \cdots M^{\sigma_L}_{a_L b_L} |\boldsymbol{\sigma}\rangle\langle\mathbf{ab}|$

With the mapping matrix $M^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ $M^0 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$ $M^- = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

AKLT state



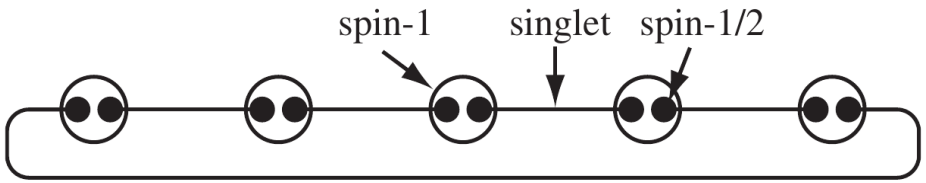
Now the wave-function is

$$\sum_{\boldsymbol{\sigma}} \sum_{\mathbf{ab}} M^{\sigma_1}_{a_1 b_1} \Sigma_{b_1 a_2} M^{\sigma_2}_{a_2 b_2} \Sigma_{b_2 a_3}, \ldots, \Sigma_{b_{L-1} a_L} M^{\sigma_L}_{a_L b_L} \Sigma_{b_L a_1} |\boldsymbol{\sigma}\rangle$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(M^{\sigma_1} \Sigma M^{\sigma_2} \Sigma \cdots M^{\sigma_L} \Sigma]) |\boldsymbol{\sigma}\rangle$$

Define:

AKLT state



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Define:

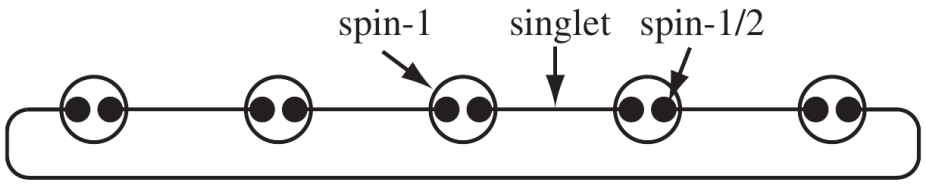
$$\widetilde{A}^{\sigma} = M^{\sigma} \Sigma$$

$$\widetilde{A}^{+} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \quad \widetilde{A}^{0} = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & +\frac{1}{2} \end{bmatrix} \quad \widetilde{A}^{-} = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

AKLT state in MPS form:

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(\widetilde{A}^{\sigma_1} \widetilde{A}^{\sigma_2} \cdots \widetilde{A}^{\sigma_L}) |\boldsymbol{\sigma}\rangle$$

AKLT state



- Spectral is gapped with PBC (4-fold degeneracy with OBC)
- Spin correlation function decays exponentially
- Hidden order: $\left\langle S_i^z e^{i\pi \sum_{i<k<j} S_k^z} S_j^z \right\rangle = -4/9 \text{ for } j-i>2$
- In the same phase with isotropic spin-1 chain: Haldane conjecture