Tensor Renormalization Group and its Application

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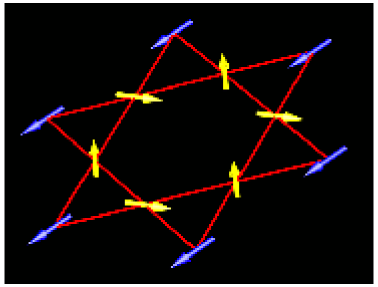


Motivation: Challenges in the study of strongly correlated systems

- ✓ **Non-perturbative: quantum field theory not always useful**
- ✓ **Exponential Wall: total degree of freedom grows exponentially with system size**

Wheat-chessboard problem

1st square:	1 grain
2nd square:	2 grains
3rd square:	4 grains
4th square:	8 grains
……	
64th square:	2^{63} grains

$$1 + 2 + 4 + 8 + \cdots\cdots + 2^{63} = 2^{64} - 1$$

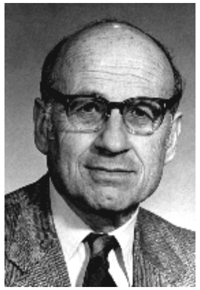
$$= 18446744073709551615 \text{ grains}$$

Weak Coupling Approach

Treat many-body interactions by certain mean-field approximation

$$2^{64} \rightarrow 64$$

Density Functional Theory(1960s)



Walter Kohn

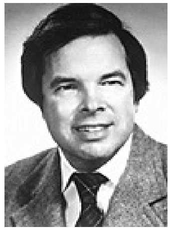
- **Most successful numerical method for treating weak coupling systems**
- **Based on LDA or similar approximation**

Strong Coupling Approach

$2^{64} \rightarrow$ a particularly selected set of basis states

Quantum Monte Carlo

Numerical Renormalization Group



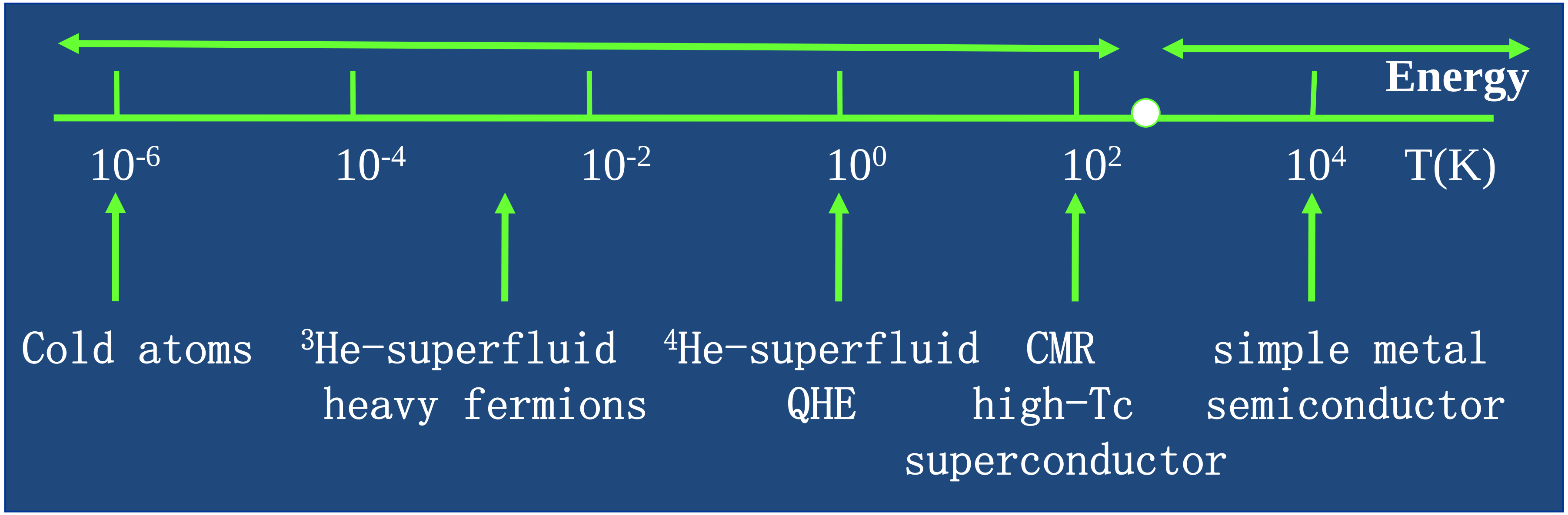
K. Wilson

- **Wilson NRG 1960s–1980s**
  - **Kondo problem**
- **Density-matrix renormalization group (White 1992)**
  - **Most accurate numerical method for studying 1D quatnum systems**
  - **Poor performance in 2D**

Characteristic Energy Scales

Numerical Renormalization Group
Quantum Monte Carlo

Density Functional Theory
Dynamical Mean Field

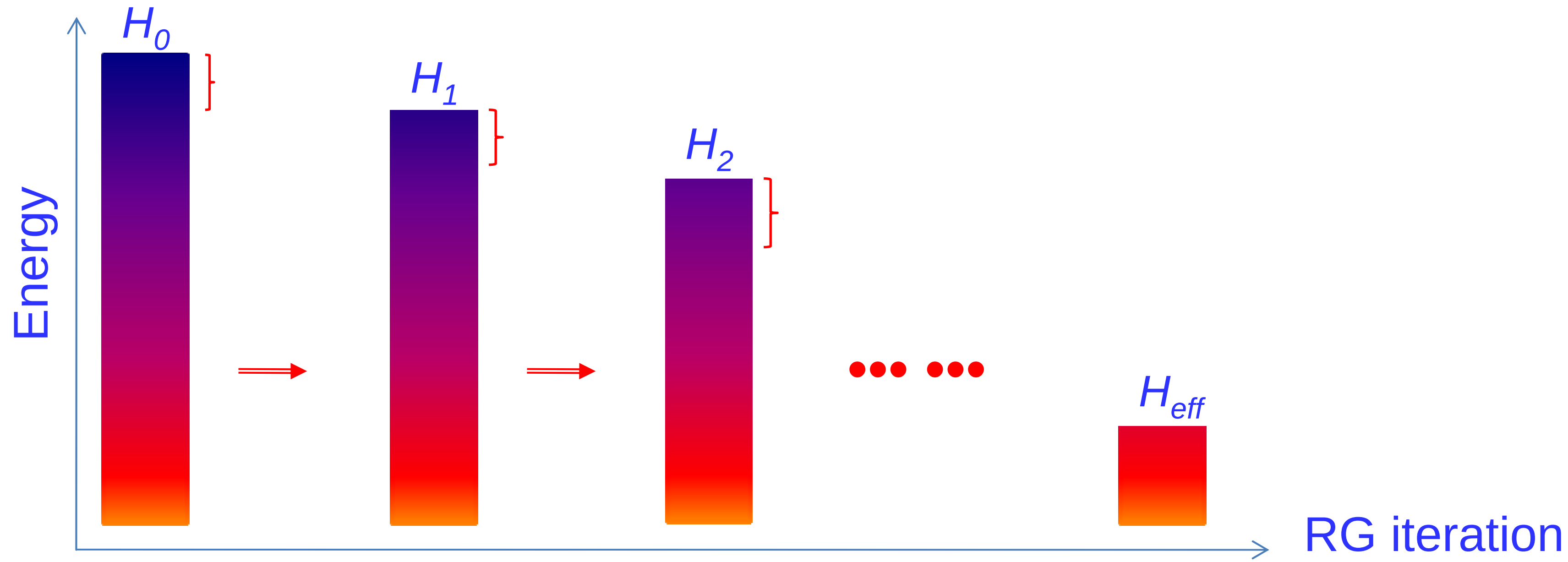


Strong coupling

Weak coupling

Strong coupling		Weak coupling
low	Dimensionality	high
strong	Quantum fluctuations	weak
weak	Coulomb screening	strong

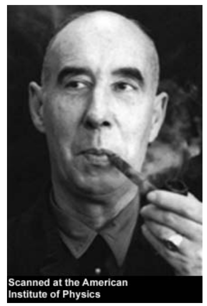
Concept of renormalization group



- 1943 Ernst Stueckelberg initialized a renormalization program to attack the problems of infinities in QED

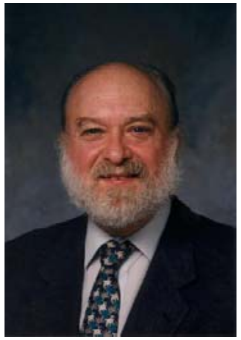
  but his paper was rejected by Physical Review.

- 1953 Ernst Stueckelberg and Andre Petermann opened the field of renormalization group

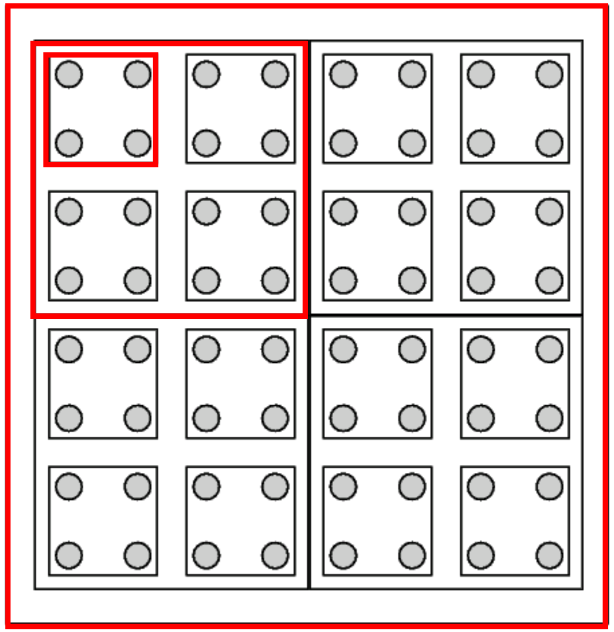


Ernst Stueckelberg

Block Spin Renormalization Group

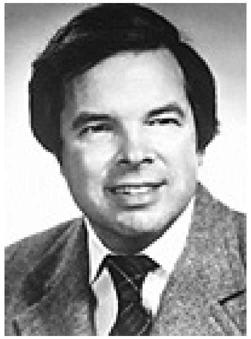


Leo P. Kadanoff



1966 Kadanoff introduced the block spin RG scheme in combine with the scaling invariance to solve the problem of phase transition and critical phenomena

Numerical Renormalization Group Method



Kenneth Wilson

- 1974 Wilson opened the field of numerical RG by combining the idea of renormalization group with numerical calculations.
- He solved the famous single-impurity Kondo model (Kondo effect).

Basic Idea of Numerical Renormalization Group

To represent a *targeted state*

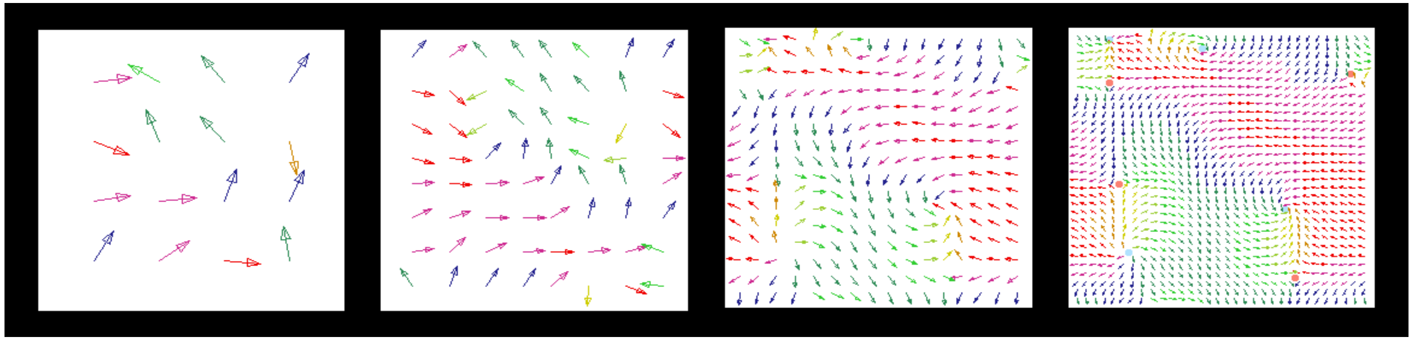
$$|\psi_0\rangle = \sum_{l=1}^{\infty} f_l |n_l\rangle$$

by an approximate wavefunction using a limited number of basis states

$$|\tilde{\psi}_0\rangle \approx \sum_{l=1}^{M} \tilde{f}_l |n_l\rangle$$

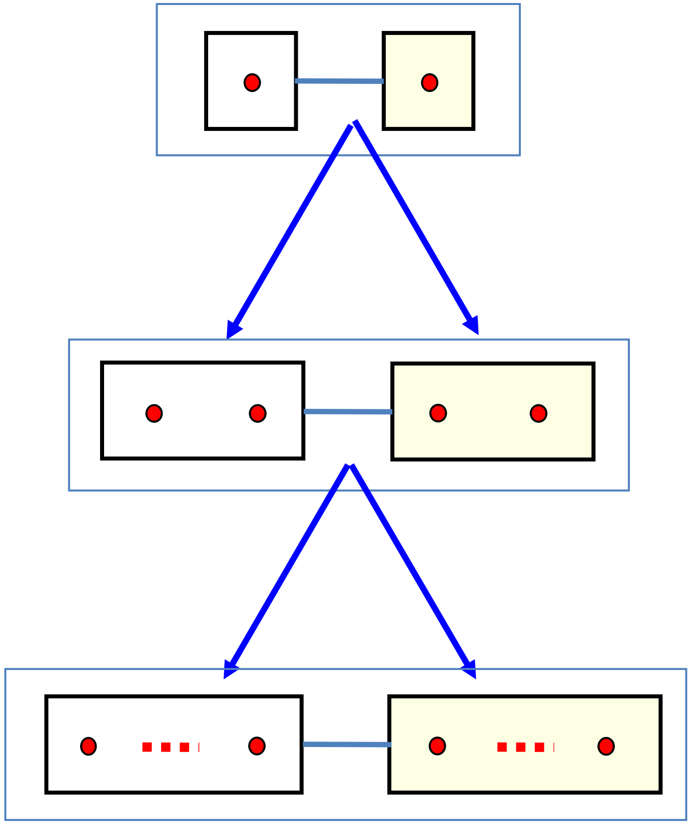
such that their overlap is maximized

$$\langle\tilde{\psi}_0|\psi_0\rangle = \sum_{l=1}^{M} \tilde{f}_l f_l$$



Refine a basis set by performing a series of basis transformations

Wilson block-spin NRG



$$H_2$$

keep the lowest *D* states of H_2

$$H_4 = H_2^L + H_2^R + H_4^{LR}$$

keep the lowest *D* states of H_4

$$H_{2n} = H_n^L + H_n^R + H_{2n}^{LR}$$

Diagonalize H, keep the states according to their energy

Reasons for the Failure of Wilson block-spin NRG

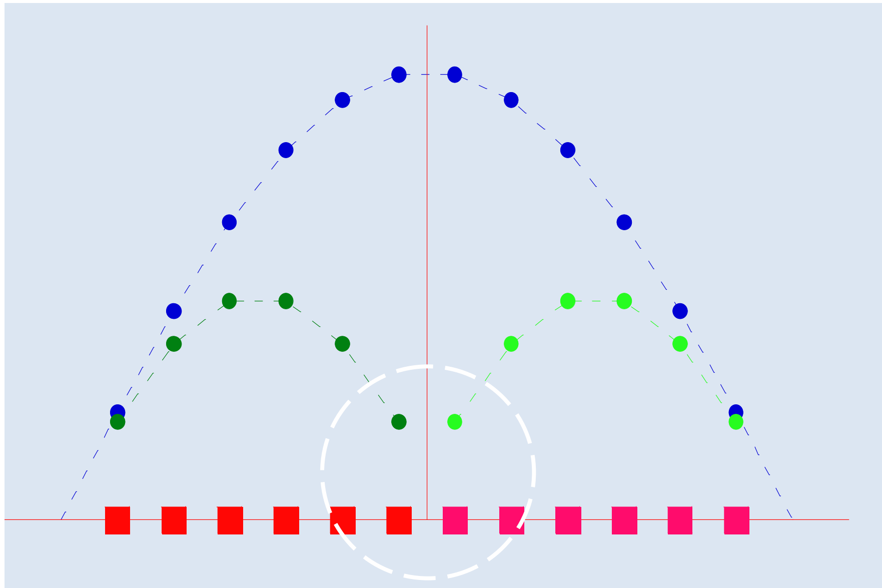
1. Interface effect is too big

2. Big truncation error:

   total D^2 states, but only D of them retained

3. Criterion of truncation:

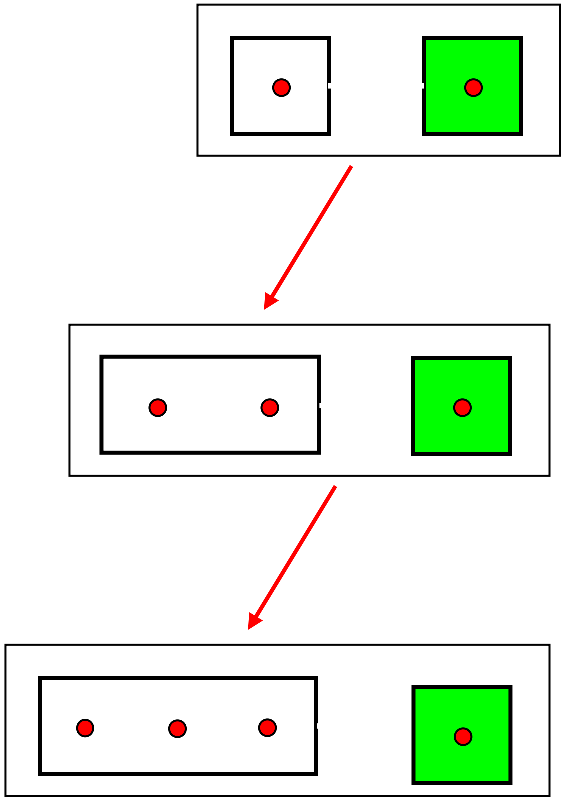
   energy is not a good indicator of basis states



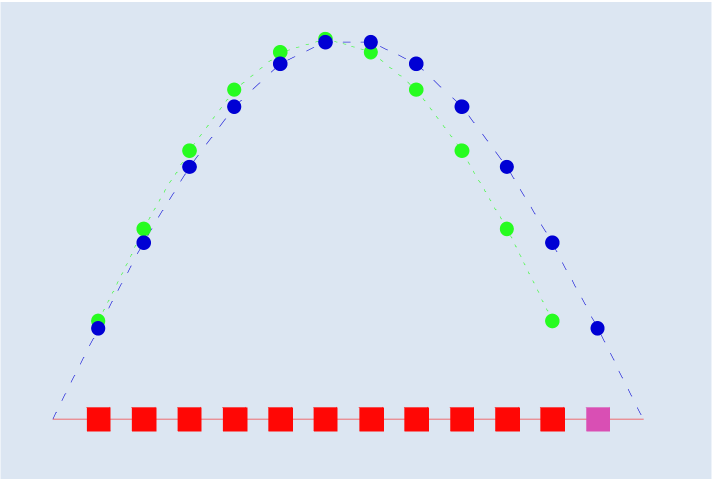
$$H = \sum_i \left(a_{i+1}^{+} a_i + h.c \right)$$

Example: Particle on a lattice

Improved NRG method



1. Boundary error is reduced



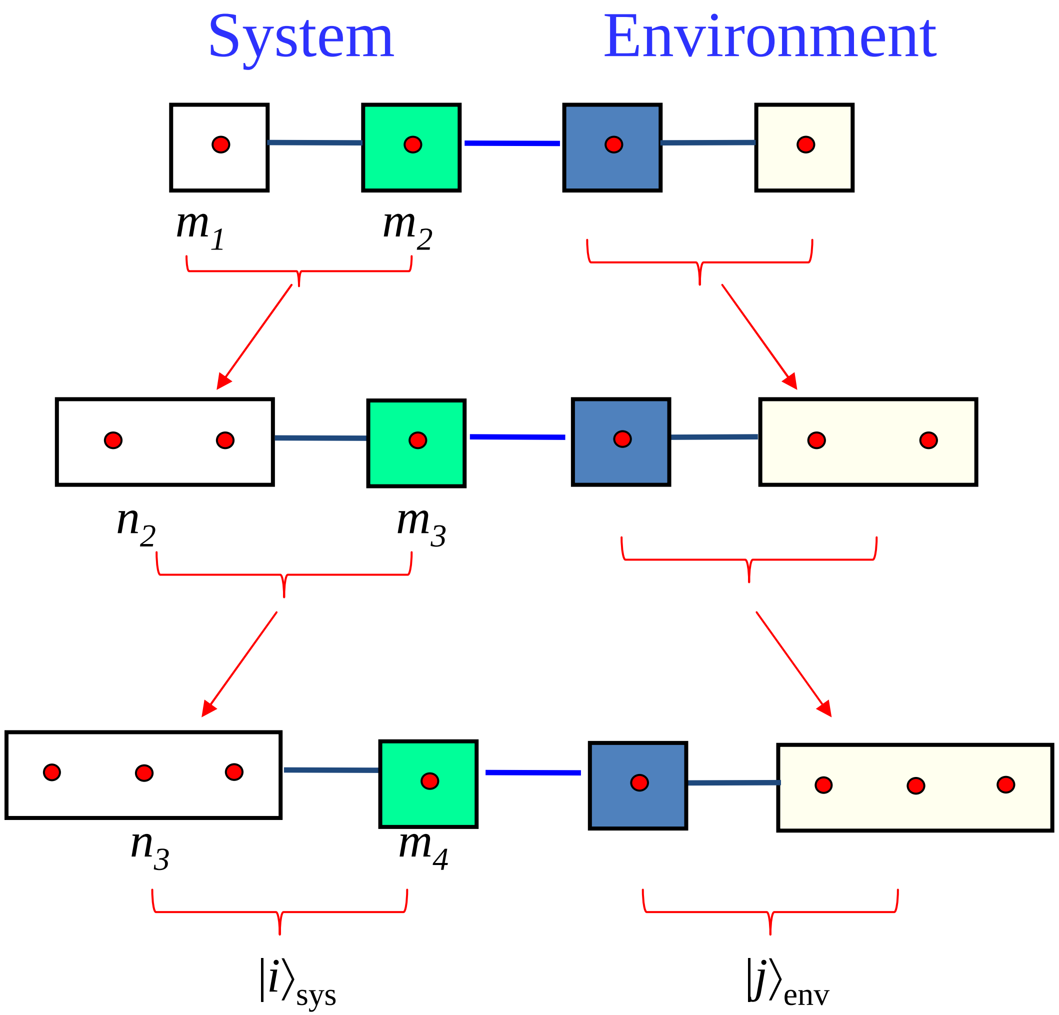
2. Truncation error is reduced

   Retain *D* states from *2D* states

3. Criterion of truncation: Energy

T. Xiang and G. A. Gehring, J. Mag. Mag. Mat. **104-107**, 861 (1992).

Density Matrix Renormalization Group (DMRG)



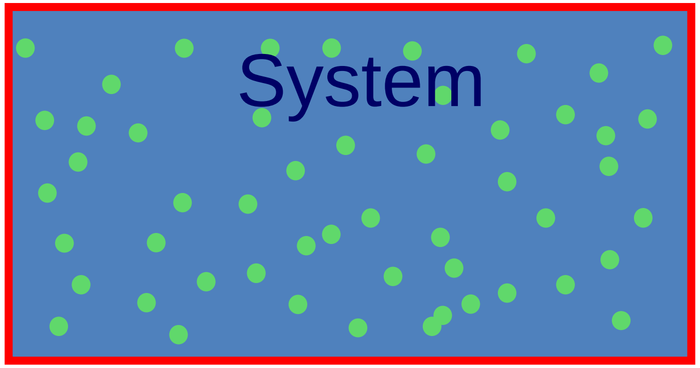
S. White, PRL (1992)

Use Environment as a pump to probe the basis states in System

$$|\psi\rangle = \sum_{i,j} f_{ij} \, |i\rangle_{sys} \, |j\rangle_{env}$$

NRG versus DMRG

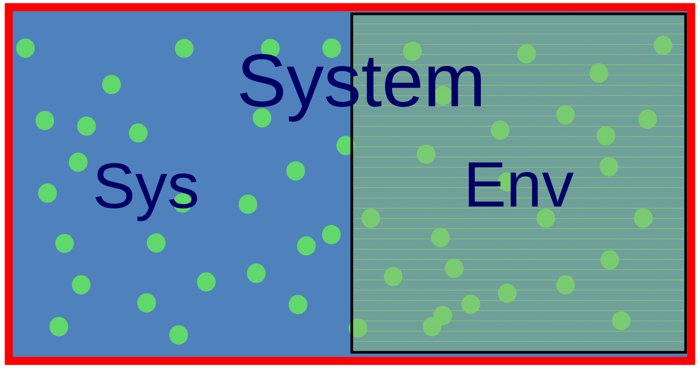
Wilson NRG



Energy is the only quantity that can be used to measure the weight of a basis state

$$\rho = e^{-\beta H}$$

DMRG

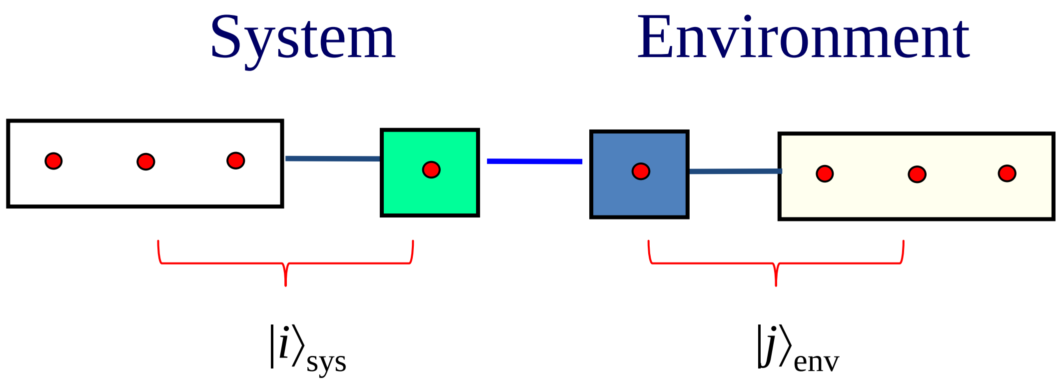


Use a sub-system as a pump to probe the other part of the system

$$\rho_{sys} = Tr_{env} e^{-\beta H}$$

The weight is measured by the entanglement between Sys and Env

What is a “Density Matrix” measurement?



$$|\psi\rangle = \sum_{i,j} f_{ij} \, |i\rangle_{sys} \, |j\rangle_{env}$$

Quantum Information:
Schmidt decomposition

$$|\psi\rangle = \sum_{n} \Lambda_n \, |n\rangle_{sys} \, |n\rangle_{env}$$

Λ_n^2 is the eigenvalue of reduced density matrix

Mathematician:
Singular value decomposition

$$f_{ij} = \sum_{n=1}^{N} U_{i,n} \Lambda_n V_{j,n}$$

$$\approx \sum_{n=1}^{D} U_{i,n} \Lambda_n V_{j,n}$$

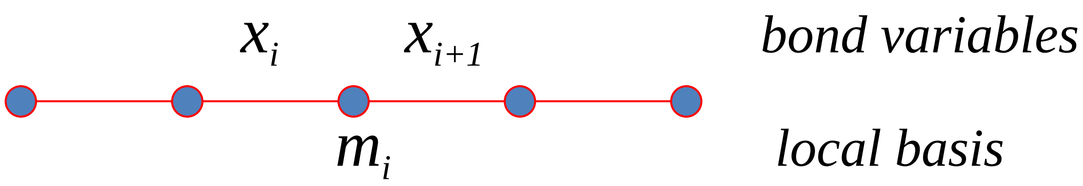
DMRG Wavefunction: Matrix Product State

S Ostlund, S Rommer, PRL 1995

- ✓ The wavefunction generated by the DMRG iteration is a matrix-product state
- ✓ It can be also regarded as a variational ansatz of many-body wavefunction

$$|\Psi\rangle = \sum_{m_1\cdots m_L} Tr\left(A[m_1]\ldots A[m_L]\right)|m_1\ldots m_L\rangle$$

$A_{x_1x_2}[m_1]$ ***D×D matrix***



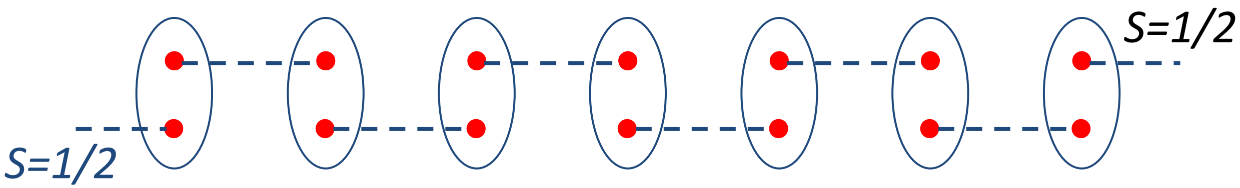
Valence bond solid state

S=1

$$H = \sum_i \frac{1}{2}\left[S_i \cdot S_{i+1} + \frac{1}{3}\left(S_i \cdot S_{i+1}\right)^2 + \frac{2}{3} \right]$$

$$\left|\Psi\right\rangle = \sum_{m_1 \cdots m_L} Tr\left(A[m_1]\ldots A[m_L]\right)\left|m_1 \ldots m_L\right\rangle$$

$$A[-1] = \begin{pmatrix} 0 & 0 \\ \sqrt{2} & 0 \end{pmatrix} \qquad A[0] = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A[1] = \begin{pmatrix} 0 & \sqrt{2} \\ 0 & 0 \end{pmatrix}$$

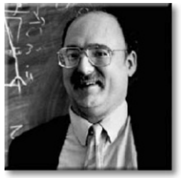


Affleck, Kennedy, Lieb, Tasaki, PRL 59, 799 (1988)

Haldane Conjecture

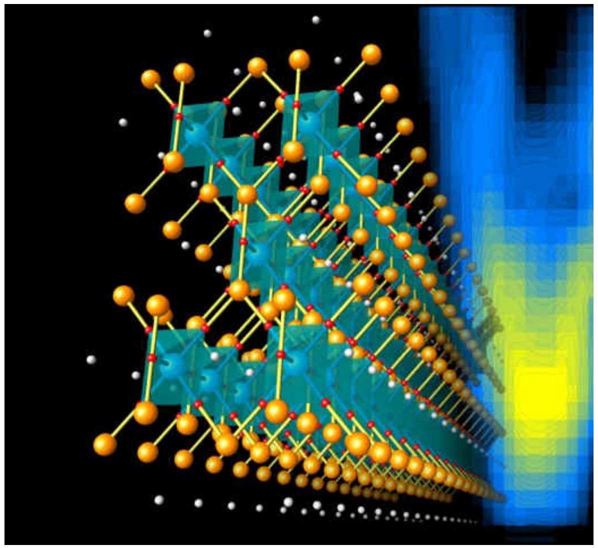
Integer Heisenberg spin chain has a finite excitation gap

$$H = \sum_i S_i \cdot S_{i+1}$$

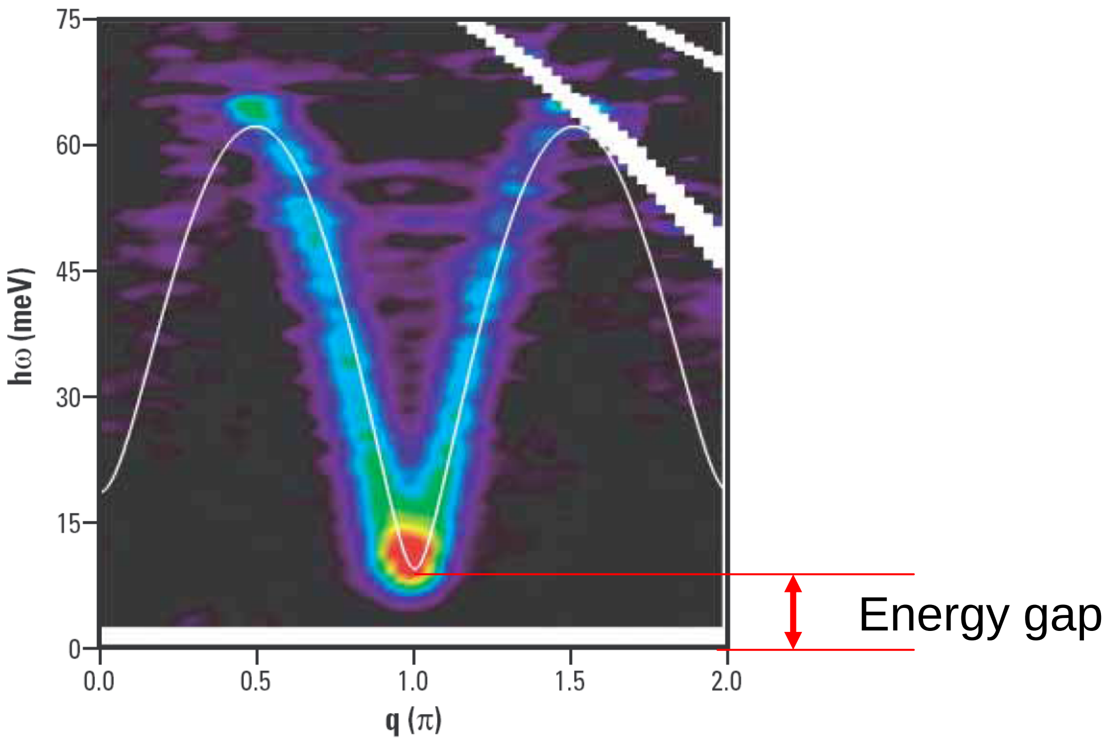


Haldane

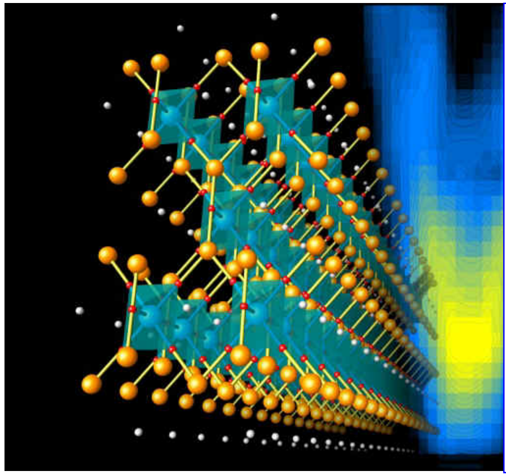
Ni^{2+} : S = 1



Y_2BaNiO_5



Hidden Order



Nd_2BaNiO_5

Hidden "antiferromagnetic" order

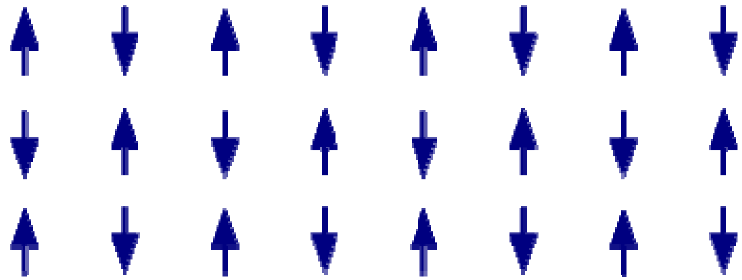
↑ 0 0 0 ↓ 0 ↑ 0 0 ↓ 0 ↑ 0 0 0 ↓ 0 ↑ 0 0 0 0 ↓

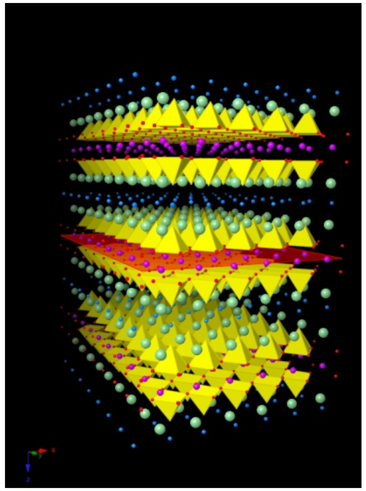
↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓

S = -1 (↑) , 0, 1 (↓)

Neel
Nobel 1970

Antiferromagneti Neel order





$YBa_2Cu_3O_6$

Accuracy of the DMRG in 1D

DMRG: Can calculate all static, thermodynamic, dynamic quantities

1D S=1 Heisenberg model

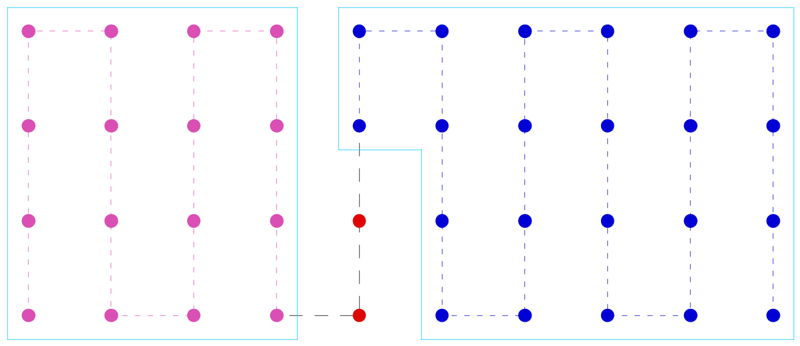
	Ground state energy
Quantum Monte Carlo	**-1.4015(5)**
DMRG	**-1.401484038971(4)** (keep D = 100 states)

Heisenberg

$$H = J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}$$

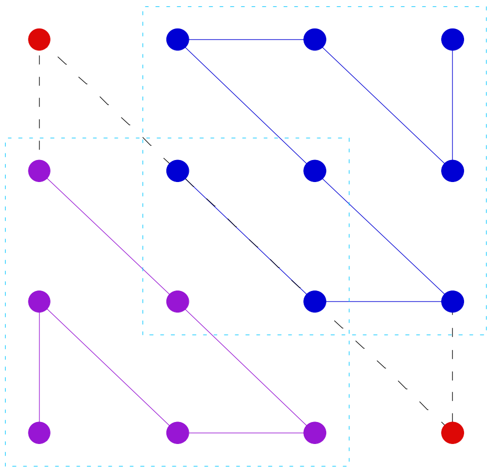
Extend DMRG to 2D: Map 2D lattice to 1D

DMRG is essentially a 1D method



Multi-chain mapping:

The width of the lattice is fixed

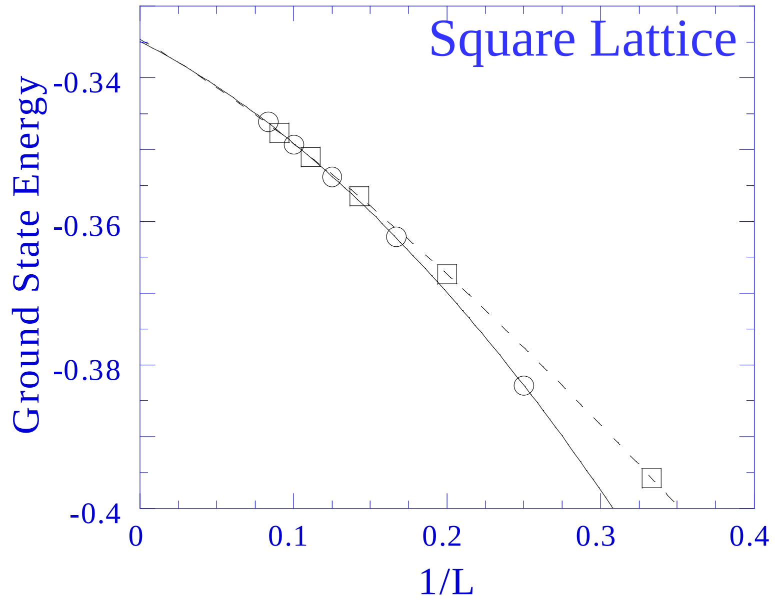


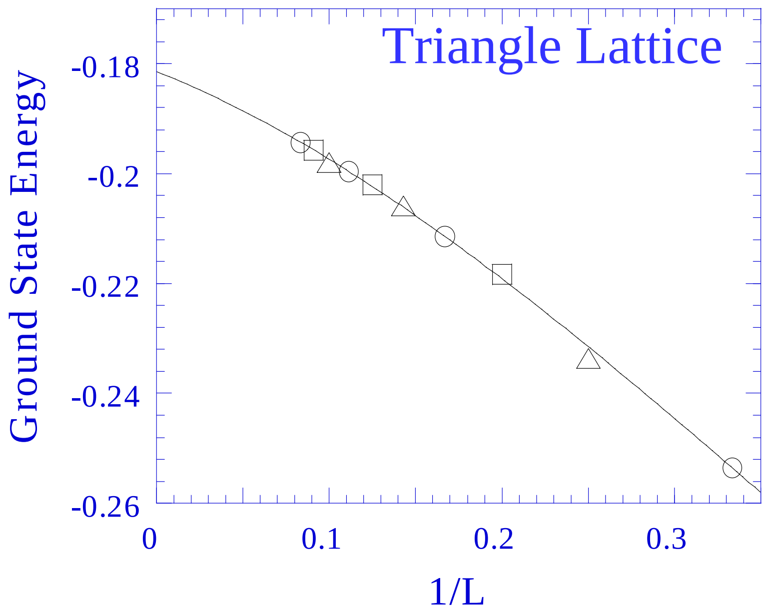
Diagonal-path:

Lattice grows in both directions

T Xiang, J Z Lou, Z B Su, PRB 64, 104414 (2001)

Ground state energy of the 2D Heisenberg model





	Square	Triangle
DMRG	-0.3346	-0.1814
MC	-0.334719	-0.1819
SW	-0.33475	-0.1822

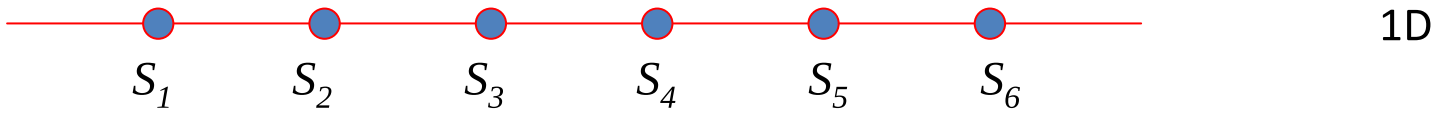
Free boundary conditions

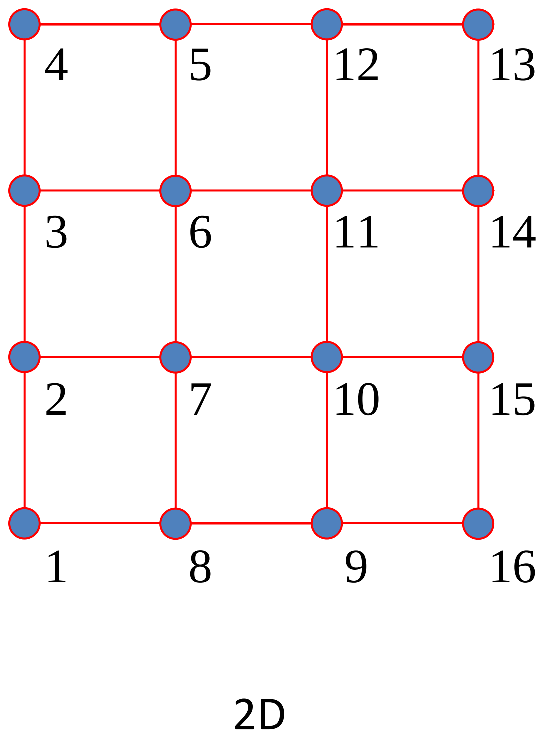
$\Delta E(L) \sim 1/L$

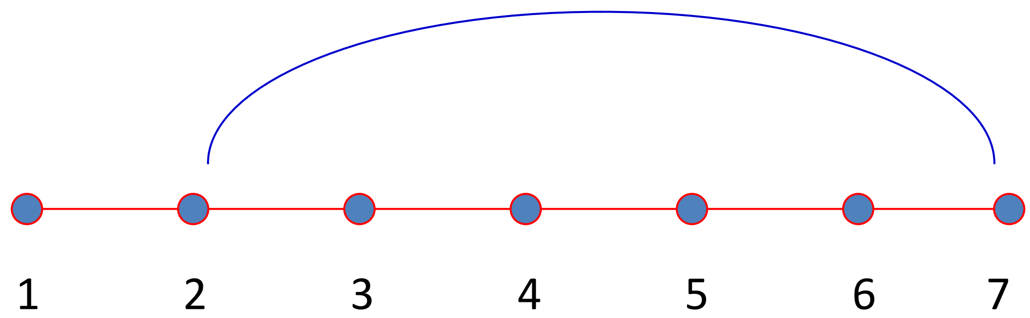
Periodic boundary conditions:

$\Delta E(L) \sim (1/L)^3$

Why is the performance of DMRG poor in 2D?







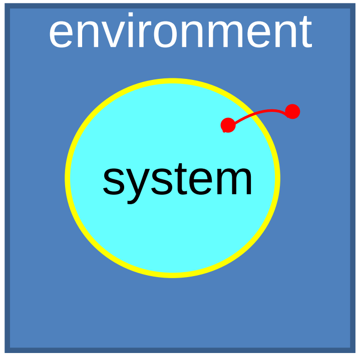
2D → 1D mapping

- Introduce long-range coupling
- Break the square lattice symmetry
- Demand grows exponentially with lattice size in order to satisfy the Area Law

Area Law of Entanglement Entropy

For a gapped system

$$S_{\mathrm{entanglement}} \sim L^{d-1} \sim \ln D_{\min}$$



$$\left|\Psi\right\rangle = \sum_{m_1 \cdots m_L} Tr\left(A[m_1]\ldots A[m_L]\right)\left|m_1 \ldots m_L\right\rangle$$

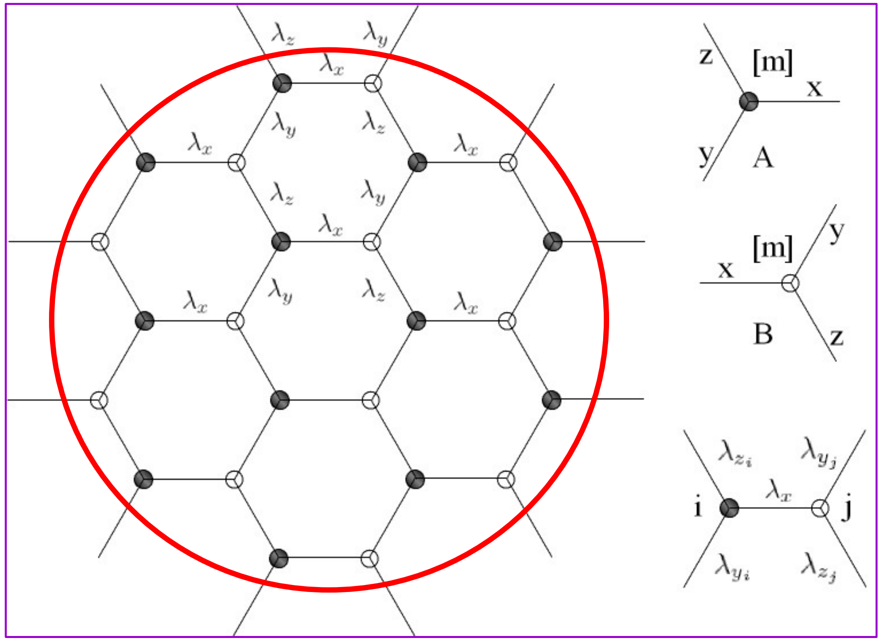
$A_{x_1 x_2}[m_1]$ ***D×D matrix***

- 1D (d=1) $D_{min} \sim L^0$
- 2D (d=2) $D_{min} \sim e^L$

D_{min} grows exponentially with the system size

Tensor-Network Wavefunction

$$\left|\Psi\right\rangle = Tr\prod_{\substack{i\in black\\ j\in white}} \lambda_{x_i}\lambda_{y_i}\lambda_{z_i} A_{x_i y_i y_i}[m_i] B_{x_j y_j y_j}[m_j]\left|m_i m_j\right\rangle$$



- ✓ keep the locality of local interactions
- ✓ satisfy the area law:

  The number of dangling bonds is proportional to the cross section

Tensor network state = tensor product state
: vertex state model — Niggemann, Zittartz, 96
: projected entangled-pair state (PEPS) — Cirac, Verstraete, 04

Two Problems Need To Be Solved

$$\left|\Psi\right\rangle = Tr \prod_{\substack{i \in black \\ j \in white}} \lambda_{x_i} \lambda_{y_i} \lambda_{z_i} A_{x_i y_i y_i}[m_i] B_{x_j y_j y_j}[m_j] \left| m_i m_j \right\rangle$$

1. How to determine the local tensor?
2. How to evaluate the expectation values, given a tensor-product wavefunction?

How to determine the local tensor?

$$\left|\Psi\right\rangle = Tr\prod_i T_{x_i y_i z_i}\left[m_i\right]\left|m_i\right\rangle$$

1. Variational approach

to minimize $\dfrac{\left\langle\Psi\right|H\left|\Psi\right\rangle}{\left\langle\Psi\,|\,\Psi\right\rangle}$

- Converging slowly
- The bond dimension that can be treated is small

$$D \le 5$$

Gu, Levin, Wen, PRB (2008)

How to determine the local tensor?

$$\left|\Psi\right\rangle = Tr \prod_{\substack{i\in black \\ j\in white}} \lambda_{x_i}\lambda_{y_i}\lambda_{z_i} A_{x_i y_i y_i}[m_i] B_{x_j y_j y_j}[m_j] \left| m_i m_j \right\rangle$$

2. Projection approach

$$\lim_{\beta\to\infty} e^{-\beta H}\left|\Psi\right\rangle = \text{ground state}$$

Projection Operator

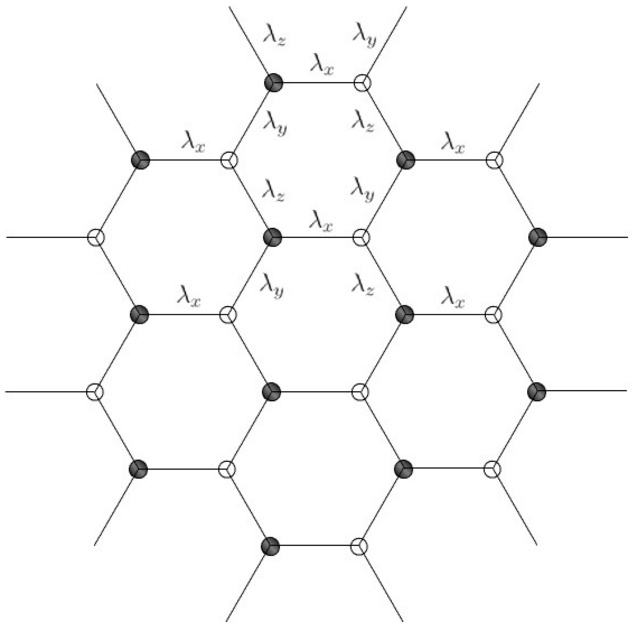
- Very accurate
- Fast converging
- Large bond dimension can be treated
  (more if symmetry is considered)

D ~ 70 (honeycomb lattice) ***D ~ 20*** (square or Kagome lattice)

Jiang, Weng, Xiang, PRL **101**, 090603 (2008)

1D: Vidal, PRL **98**, 070201 (2007)

Projection Approach



$$\lim_{\beta\to\infty} e^{-\beta H}|\Psi\rangle = \text{ground state}$$

$$\lim_{M\to\infty} \left(e^{-\tau H}\right)^{M}|\Psi\rangle = \text{ground state}$$

Heisenberg model

$$H = \sum_{\langle ij\rangle} H_{ij} = H_x + H_y + H_z$$

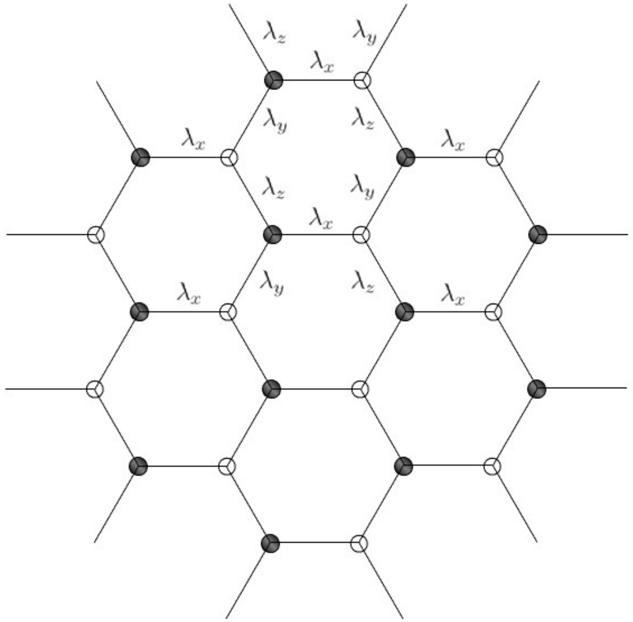
$$H_{ij} = J S_i \cdot S_j$$

Projection Iteration

$$e^{-\tau H} \approx e^{-\tau H_z} e^{-\tau H_y} e^{-\tau H_x} + o(\tau^2)$$

$$H_\alpha = \sum_{i \in black} H_{i,i+\alpha} \qquad (\alpha = x, y, z)$$

Trotter-Suzuki decomposition



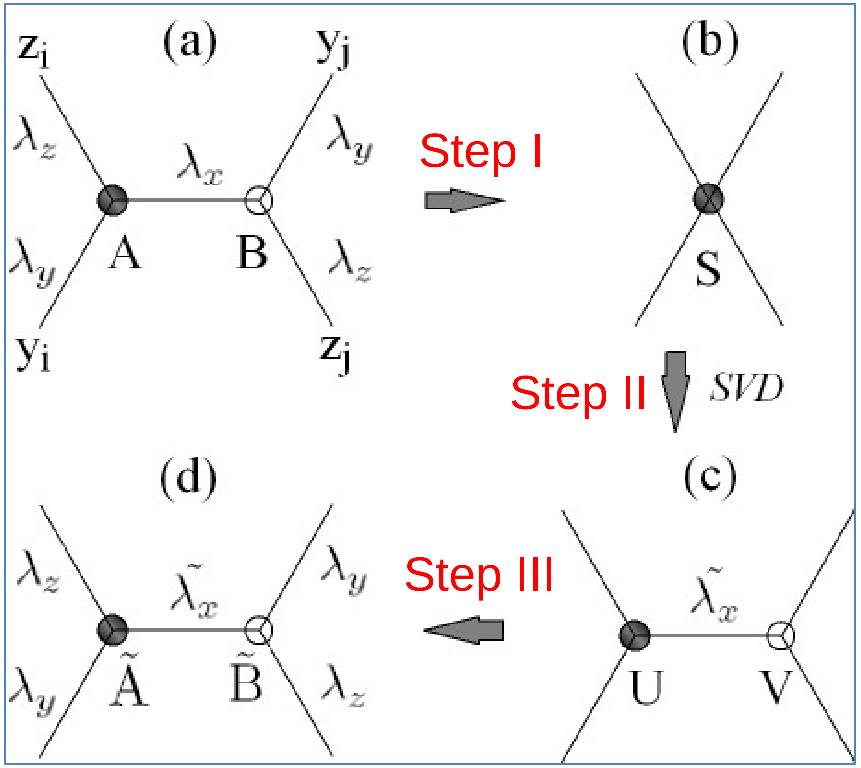
1. One iteration

$$|\Psi_1\rangle = e^{-\tau H_x} |\Psi_0\rangle$$
$$|\Psi_2\rangle = e^{-\tau H_y} |\Psi_1\rangle$$
$$|\tilde{\Psi}_0\rangle = e^{-\tau H_z} |\Psi_2\rangle$$

2. Repeat the above iteration until converged

Projection: x-bond

$$e^{-\tau H_x}\left|\Psi\right\rangle = Tr\prod_{\substack{i\in black\\ j=i+\hat{x}}}\left\langle m_i' m_j'\right|e^{-\tau H_{i,j}}\left|m_i m_j\right\rangle \lambda_{x_i}\lambda_{y_i}\lambda_{z_i} A_{x_i y_i y_i}[m_i] B_{x_j y_j y_j}[m_j]\left|m_i' m_j'\right\rangle$$



SVD: singular value decomposition

Step I

$$S_{y_i z_i m_i', y_j z_j m_j'} = \sum_{m_i m_j}\sum_{x}\langle m_i' m_j'|e^{-H_{ij}\tau}|m_i m_j\rangle \lambda_{y_i}\lambda_{z_i}A_{xy_iz_i}[m_i]\lambda_x B_{xy_jz_j}[m_j]\lambda_{y_j}\lambda_{z_j}$$

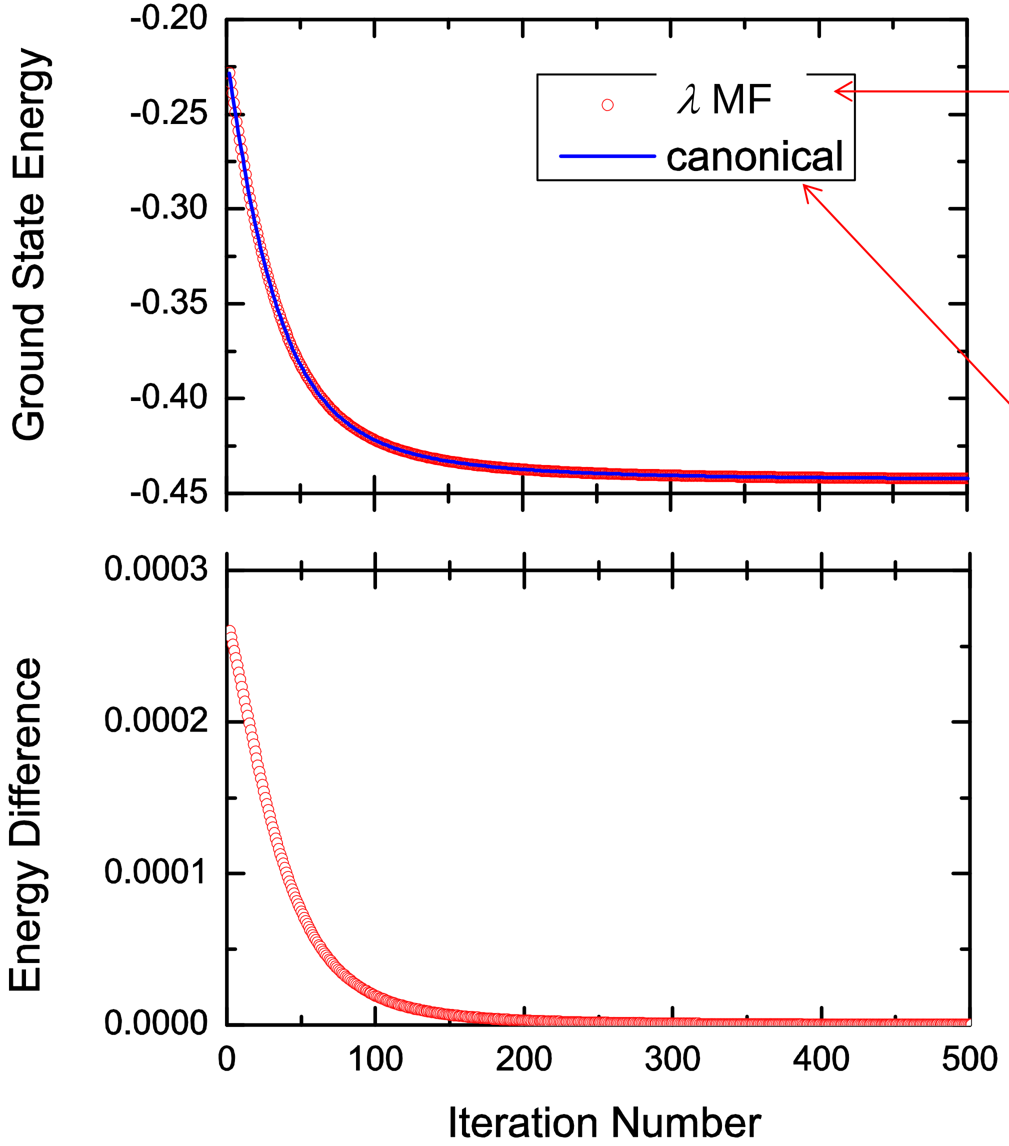
Step II

$$S_{y_i z_i m_i, y_j z_j m_j} = \sum_x U_{y_i z_i m_i, x}\tilde{\lambda}_x V^T_{x, y_j z_j m_j}$$

Step III — Truncate basis space

$$A_{xy_iz_i}[m_i] = \lambda_{y_i}^{-1}\lambda_{z_i}^{-1}U_{y_iz_im_i,x},$$
$$B_{xy_jz_j}[m_j] = \lambda_{y_j}^{-1}\lambda_{z_j}^{-1}V_{y_jz_jm_j',x}.$$

How accurate is this projection approach



Without performing the canonical transformation for the matrix product state

Using the canonical representation of the matrix product state:
λ is the eigenvalue of the density matrix

1D Heisenberg model

Expectation Value

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\left| \Psi \right\rangle = Tr \prod_i T_{x_i y_i y_i} [m_i] \left| m_i \right\rangle$$

$$\left\langle \Psi \middle| \Psi \right\rangle = Tr \prod_i A_{x_i x_i', y_i y_i', z_i z_i'}$$

$$A_{xx', yy', zz'} = \sum_m T_{xyz}[m] T_{x'y'z'}[m]$$

Bond dimension D^2

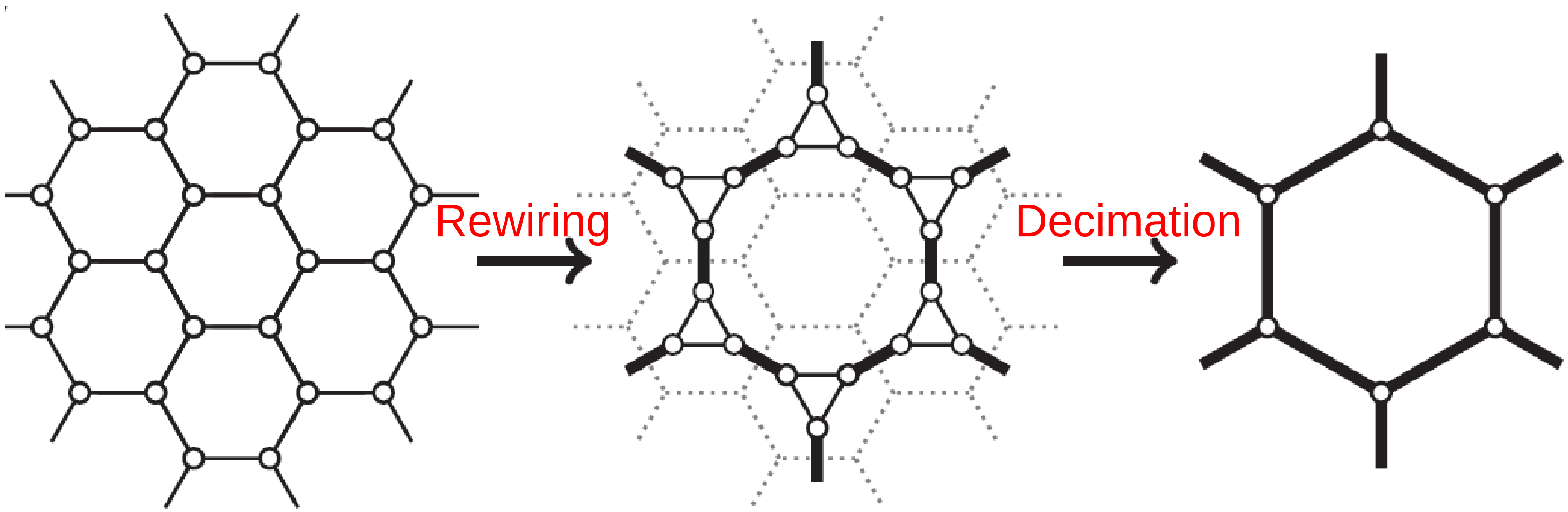
To evaluate

$\langle \Psi | \Psi \rangle$ and $\langle \Psi | O | \Psi \rangle$

is equivalent to evaluating the partition functions of classical statistical models, such as the S=1/2 Ising model

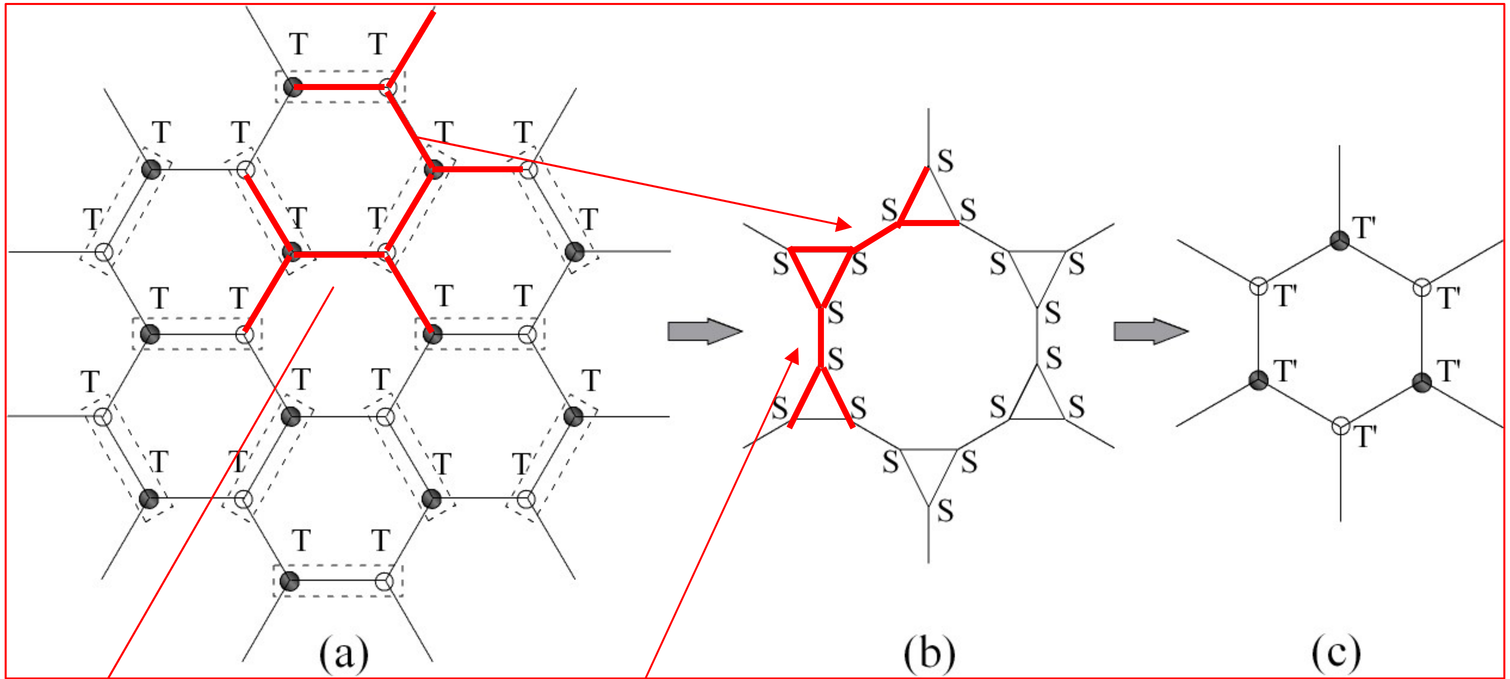
Coarse Grain Tensor Renormalization Group

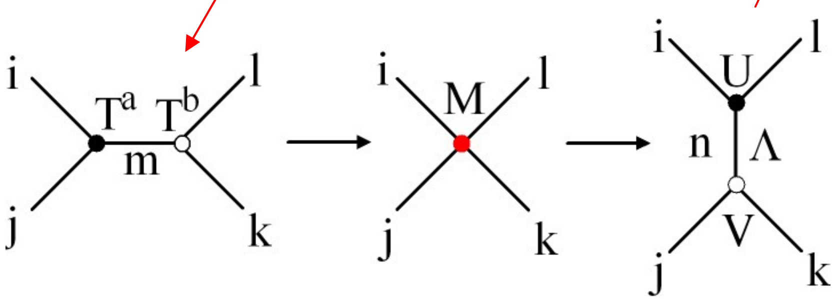
$$Z = Tr \prod_i T_{x_i y_i z_i}$$



Levin & Nave, PRL (2007)

Step I: Rewiring



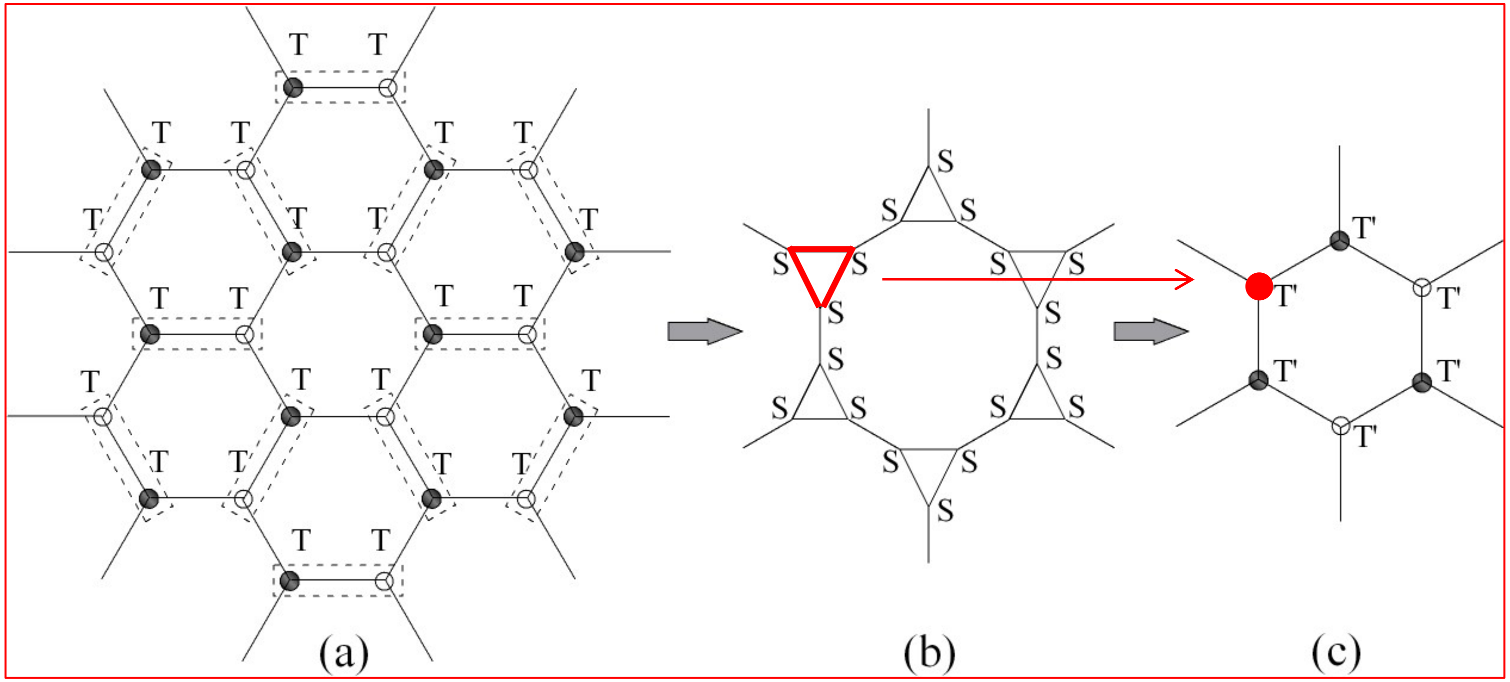


$$M_{kj,il} = \sum_m T_{mji} T_{mlk}$$

$$= \sum_{n=1}^{N} U_{kj,n} \Lambda_n V_{il,n}$$

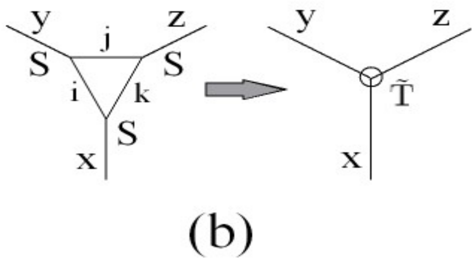
Bond field: measures the entanglement between U and V

Step II: Decimation

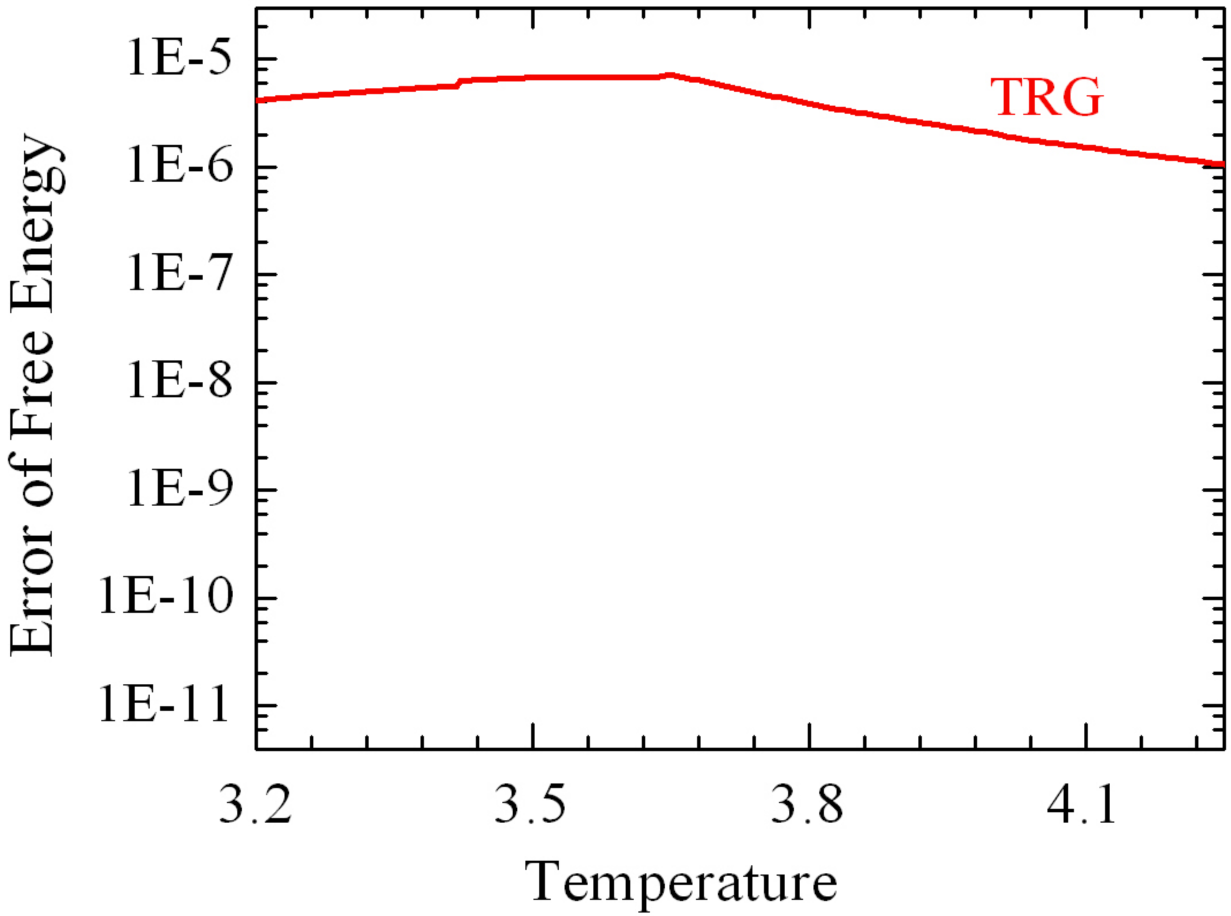


$$\tilde{T}^{a}_{xyz} = \sum_{ijk} S^{a}_{xik} S^{a}_{yji} S^{a}_{zkj}$$

$$\tilde{T}^{b}_{xyz} = \sum_{ijk} S^{b}_{xik} S^{b}_{yji} S^{b}_{zkj}$$



Accuracy of TRG



D = 24

Ising model on triangular lattice

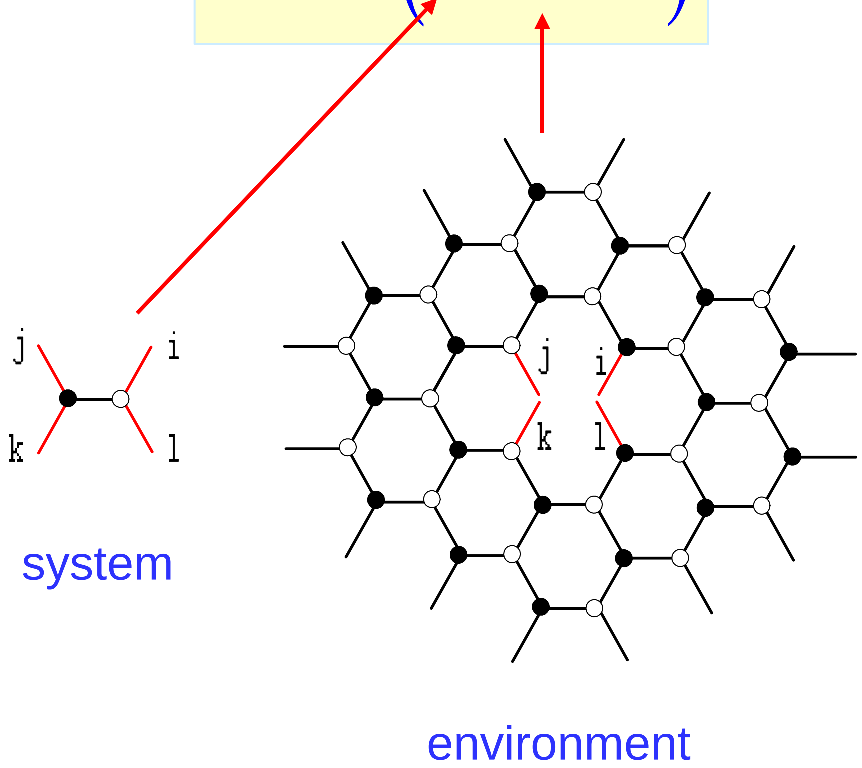
Second renormalization of tensor-network state (SRG)

- TRG:
  truncation error of M is minimized

  What needs to be minimized is the error of Z!

- SRG:
  The renormalization effect of M^{env} to M is considered

$$Z = Tr\left(MM^{env}\right)$$



Xie et al, PRL **103**, 160601 (2009)

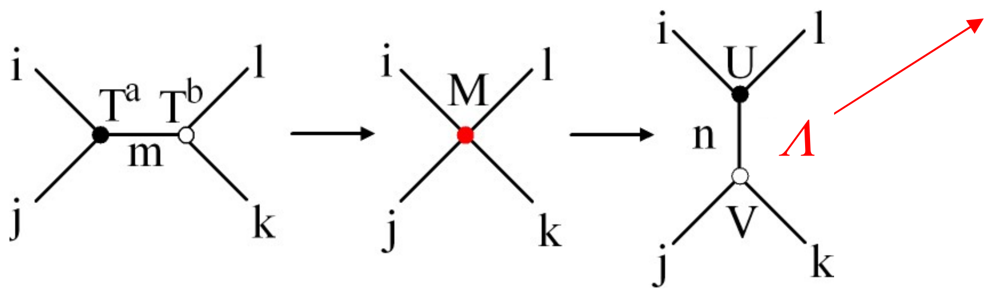
I. Poor Man's SRG: entanglement mean-field approach

$$Z = Tr\left(MM^{env}\right) = \sum_{ijkl} M_{ij,kl} M^{env}_{kl,ij}$$

$$M_{kj,il} = \sum_{n=1\ldots D^4} U_{kj,n} \Lambda_n V_{il,n}$$

$$M^{env}_{kl,ij} \approx \Lambda_k^{1/2} \Lambda_l^{1/2} \Lambda_i^{1/2} \Lambda_j^{1/2}$$

Mean field (or cavity) approximation



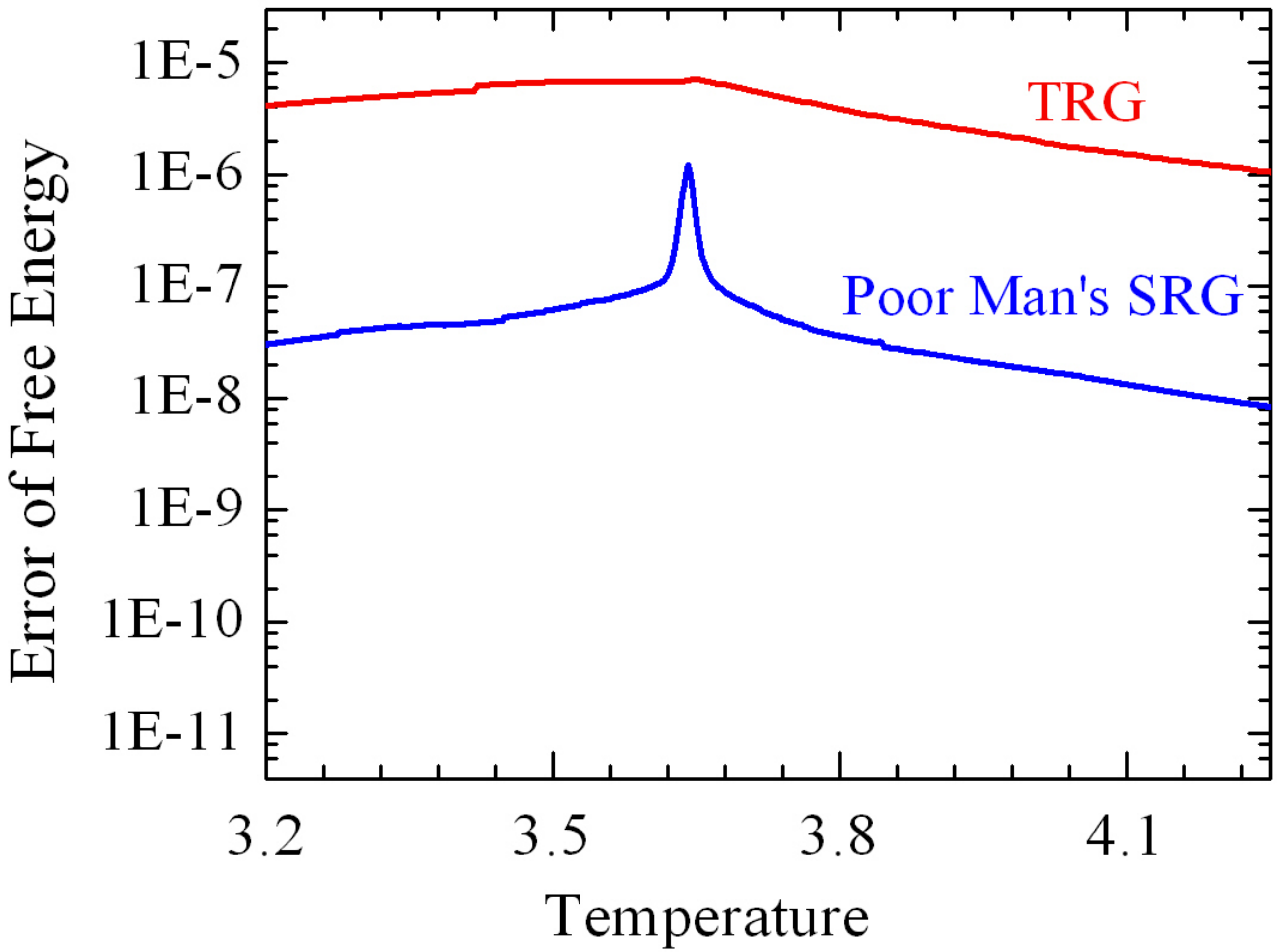
Bond field – mean field variable

$\Lambda = \Lambda^{1/2} \Lambda^{1/2}$

From environment

From system

Accuracy of Poor Man's SRG

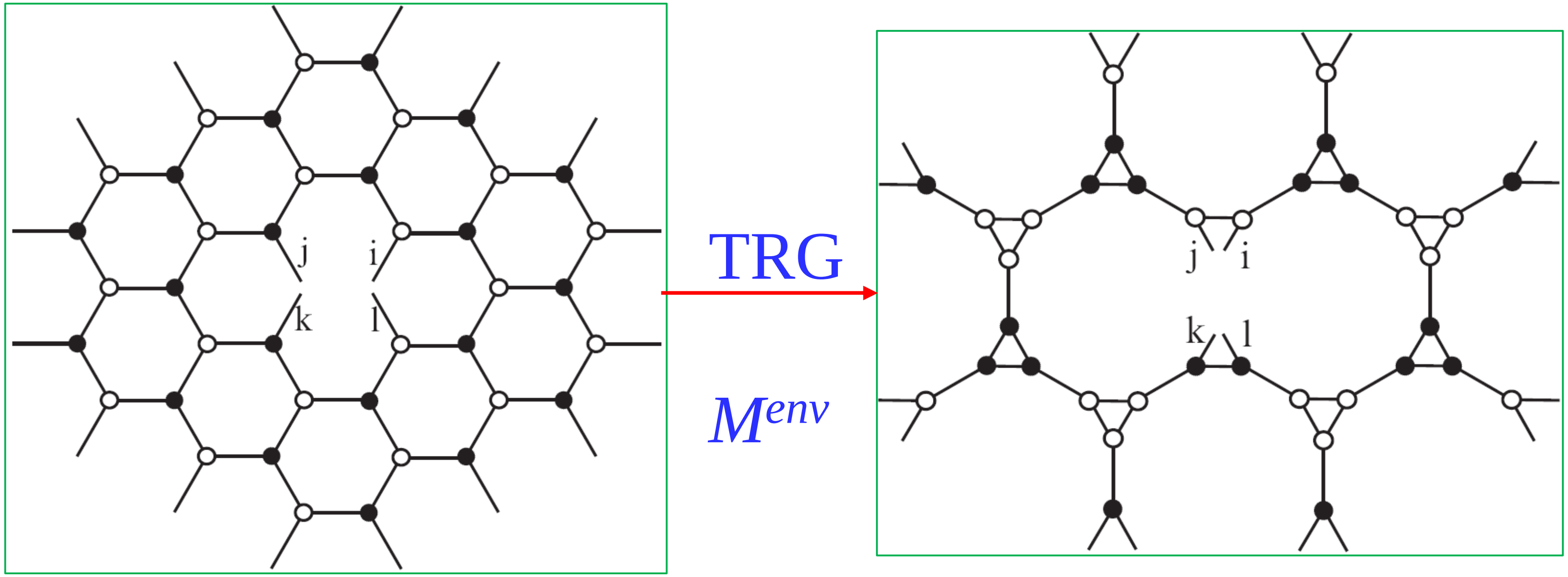


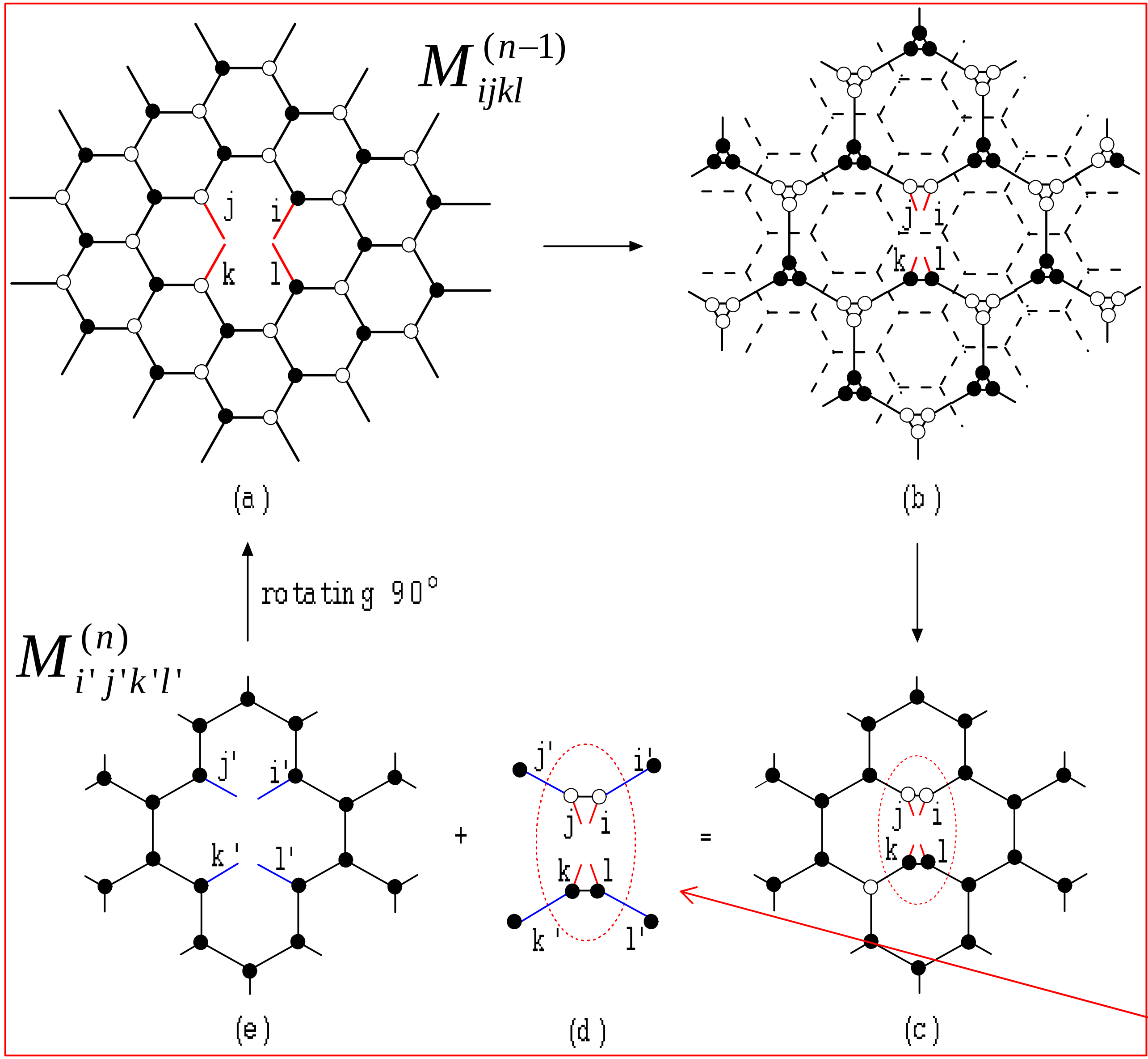
D = 24

Ising model on triangular lattice

II. More accurate treatment of SRG

Evaluate the environment contribution M^{env} using TRG





1. Forward iteration

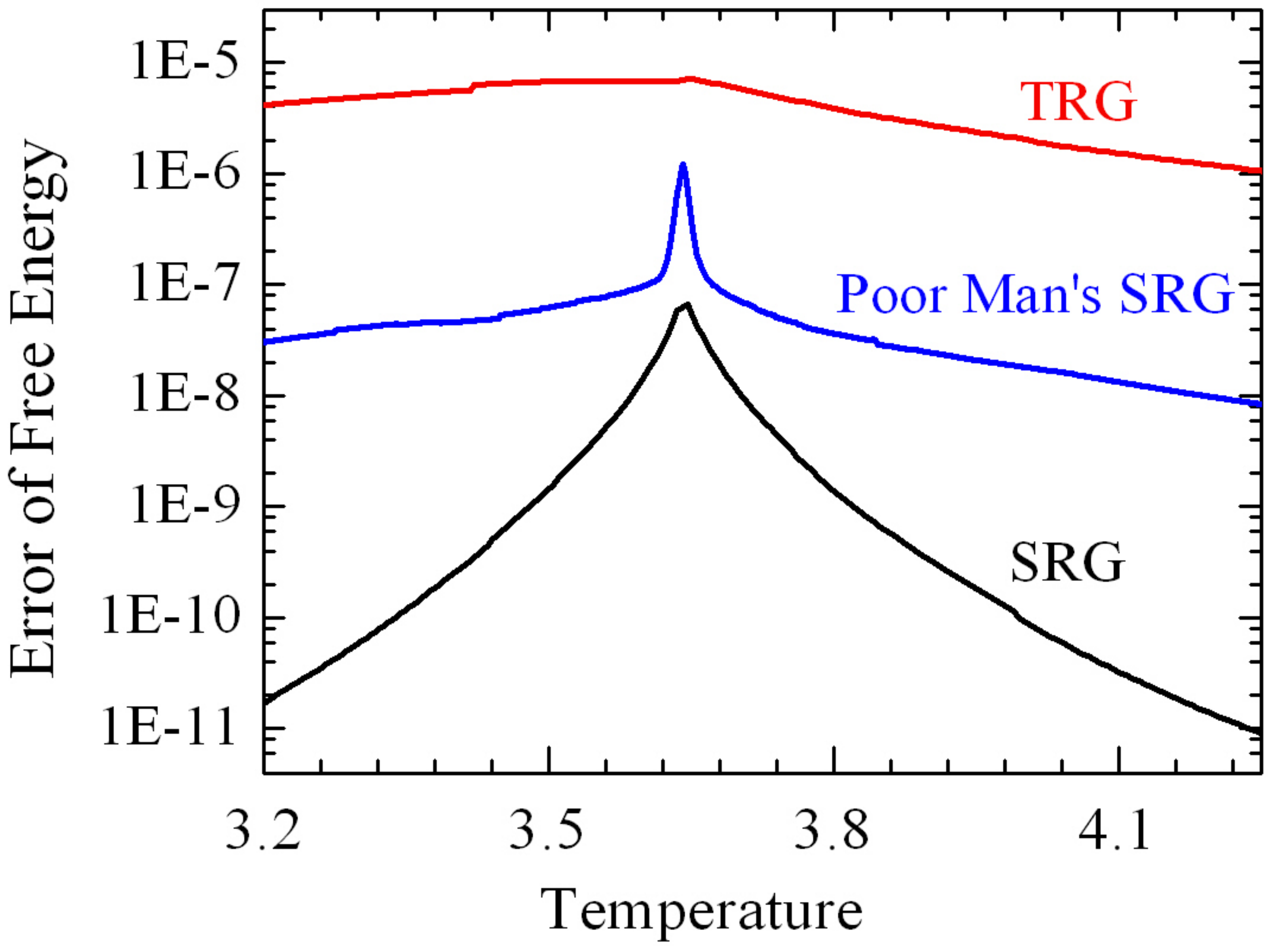
$$M^{(0)} \to M^{(1)} \to \cdots \to M^{(N)}$$

2. Backward iteration

$$M^{(N)} \to M^{(N-1)} \to \cdots \to M^{(0)} = M^{env}$$

$$M^{(n-1)}_{ijkl} = \sum_{i'j'k'l'} M^{(n)}_{i'j'k'l'} \sum_{pq} S_{k'jp} S_{j'pi} S_{i'lq} S_{l'qk}$$

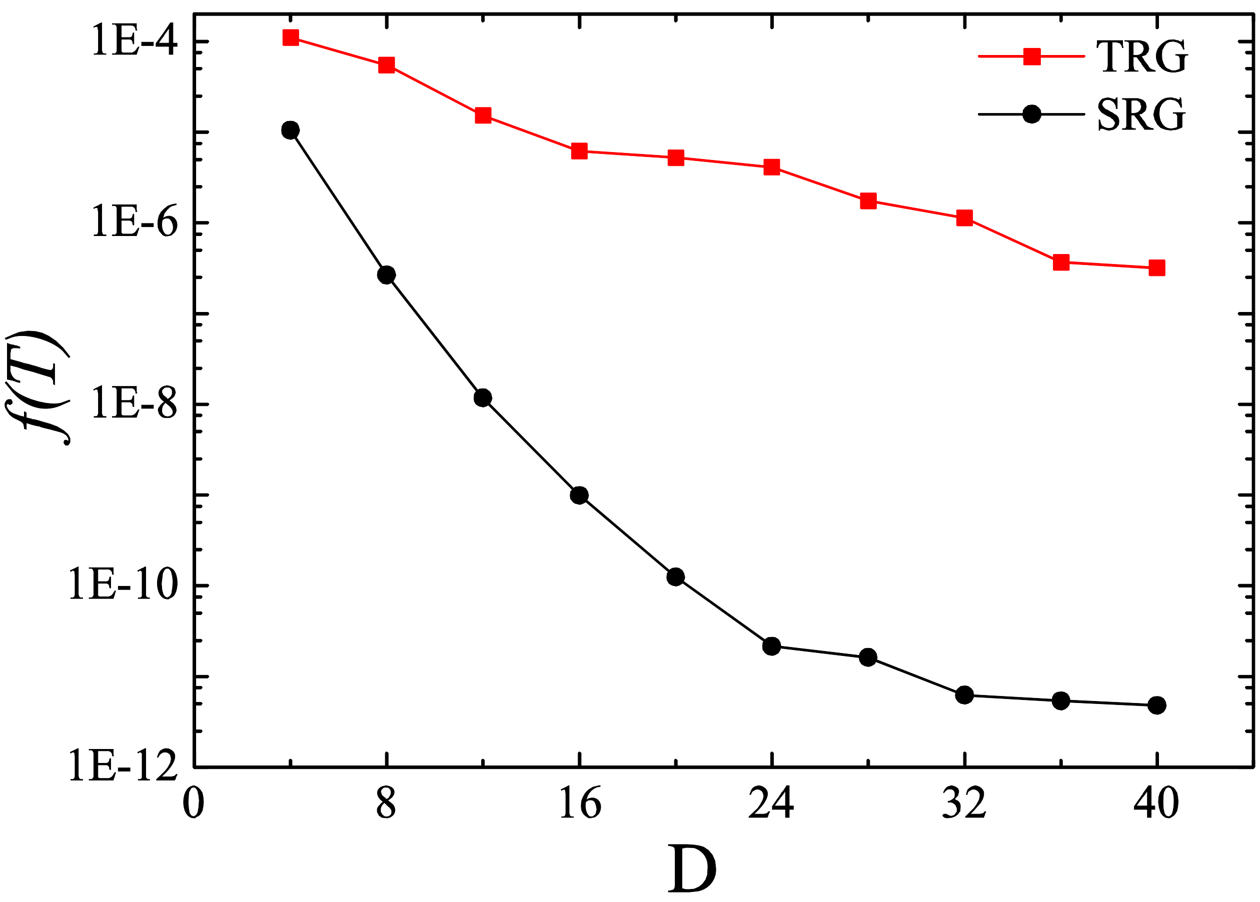
Accuracy of SRG



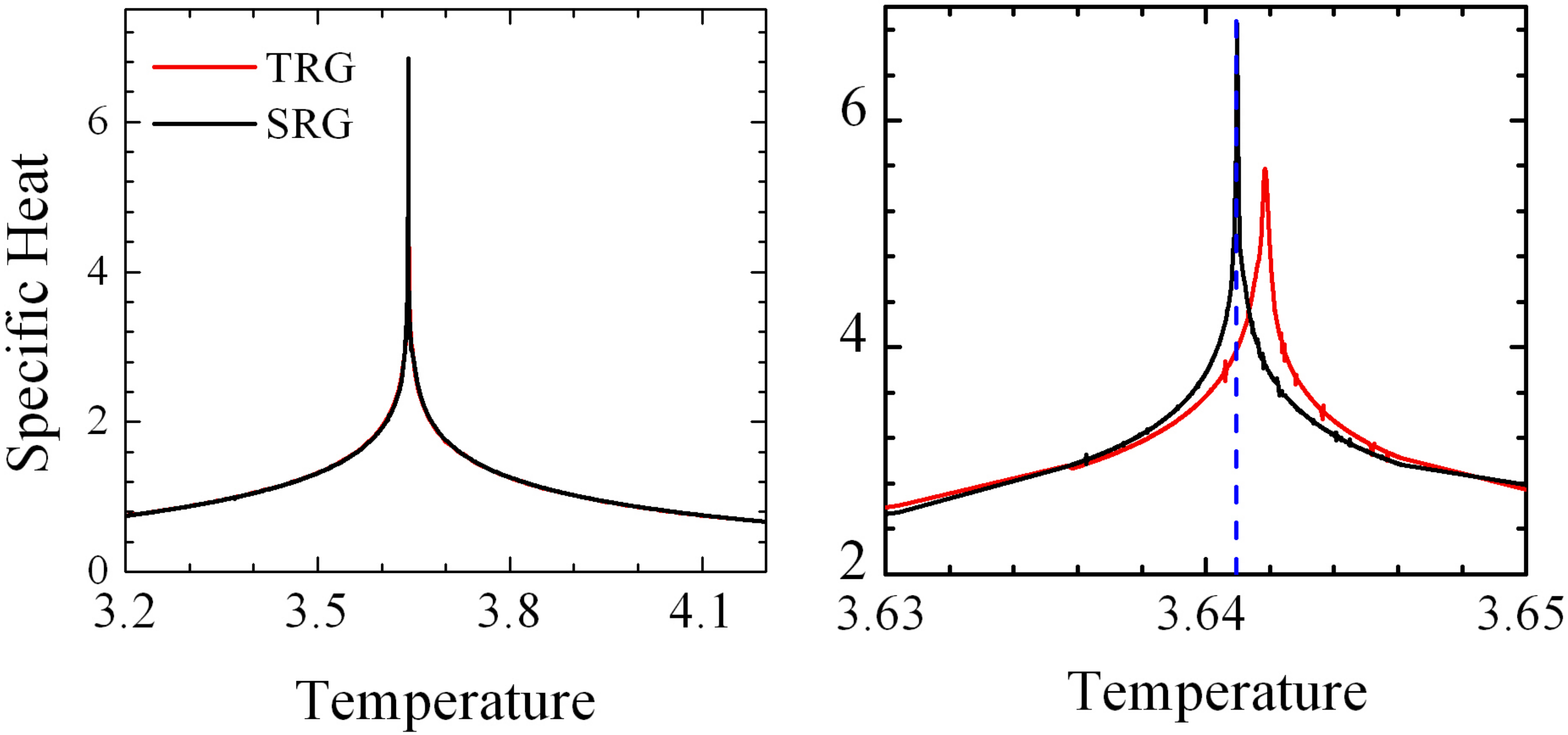
D = 24

Ising model on a triangular lattice

Error versus D



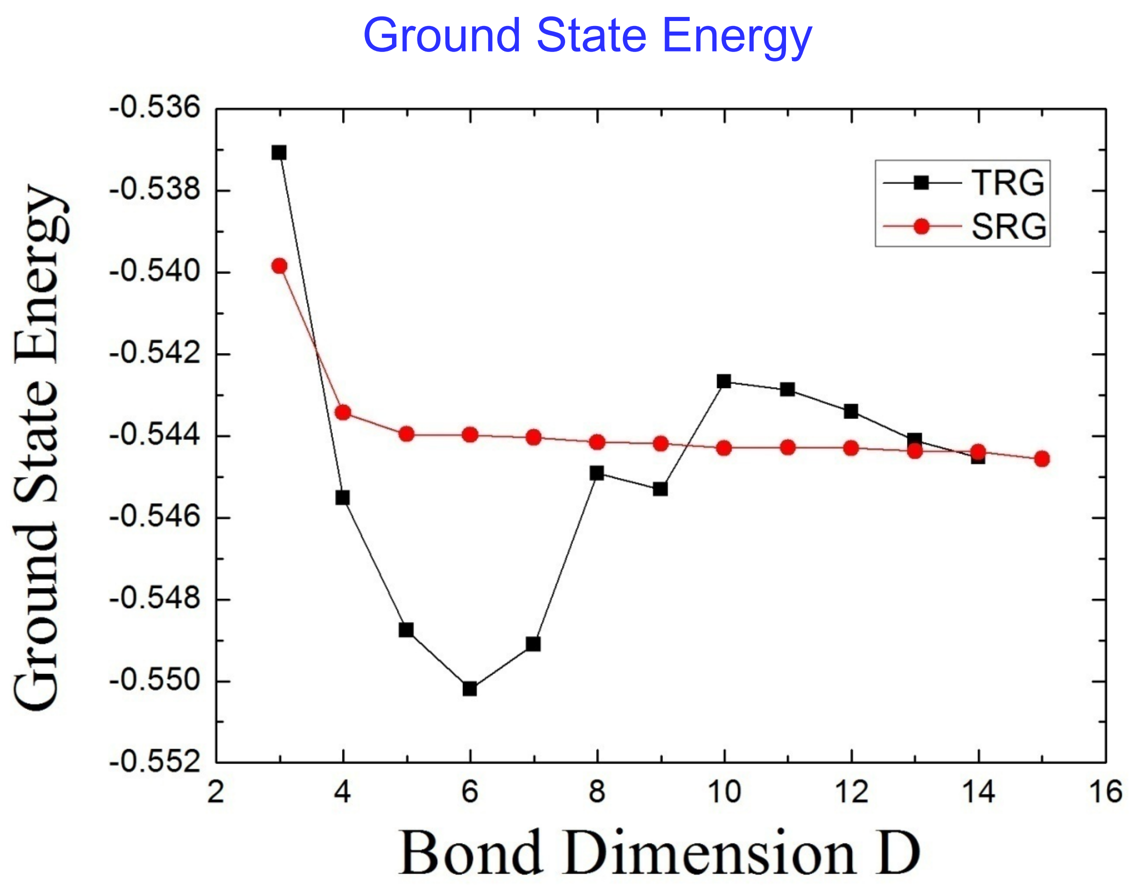
Specific Heat of the Ising model on Triangular Lattices



D = 24

Quantum Heisenberg Model on Honeycomb Lattice

$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$$



SRG D = 14
E = -0.54439

SRG D = 30
E = -0.54442

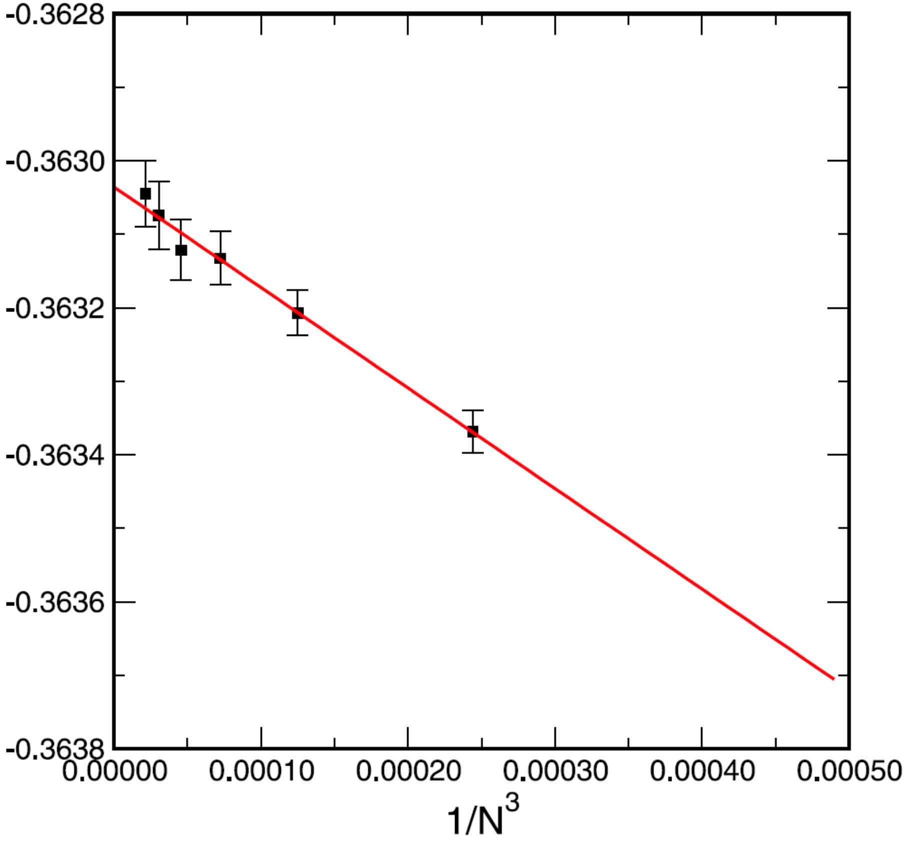
Monte Carlo:
E = -0.54454 (± 20)

U. Low, Condensed Matter Physics 2009 Vol 12, 497

Lattice size $N = 2\times 3^{30}$

Heisenberg Model on Honeycomb Lattice

Quantum Monte Carlo Result

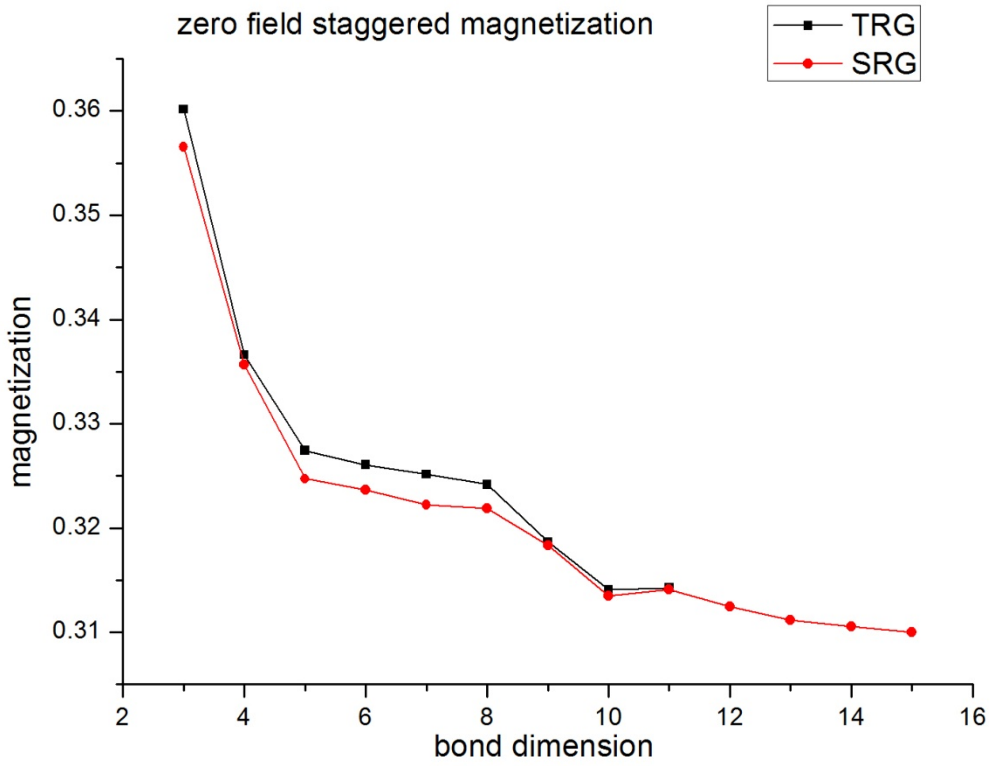


E = -0.36303 (± 13) per bond

= -0.54454 (± 20) per site

U. Low, Condensed Matter Physics 2009 Vol 12, 497

Staggered Magnetization



SRG D = 15
M = 0.31003

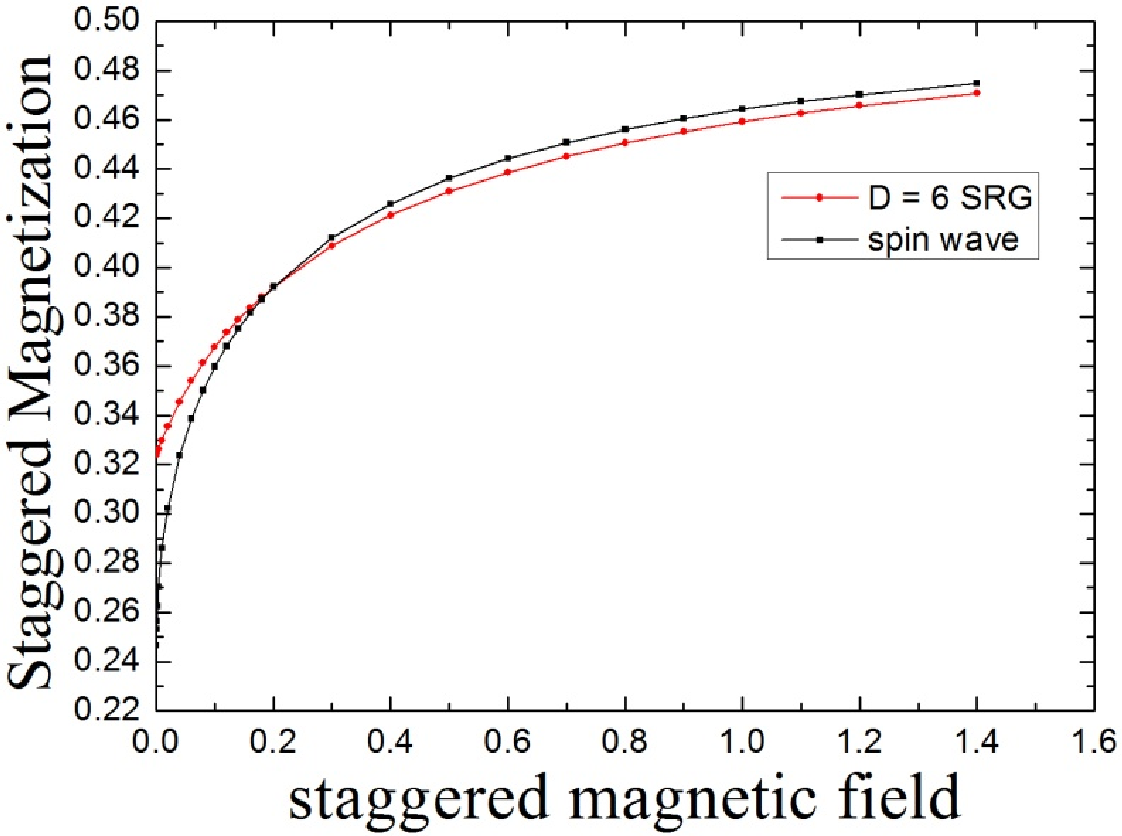
Monte Carlo:
M = 0.2681
U. Low, Condensed Matter Physics 2009 Vol 12, 497

M = 0.22
Reger, Riera, Young, JPC 1989

Spin Wave:
M = 0.24

Series expansion
M = 0.27

Staggered Magnetization

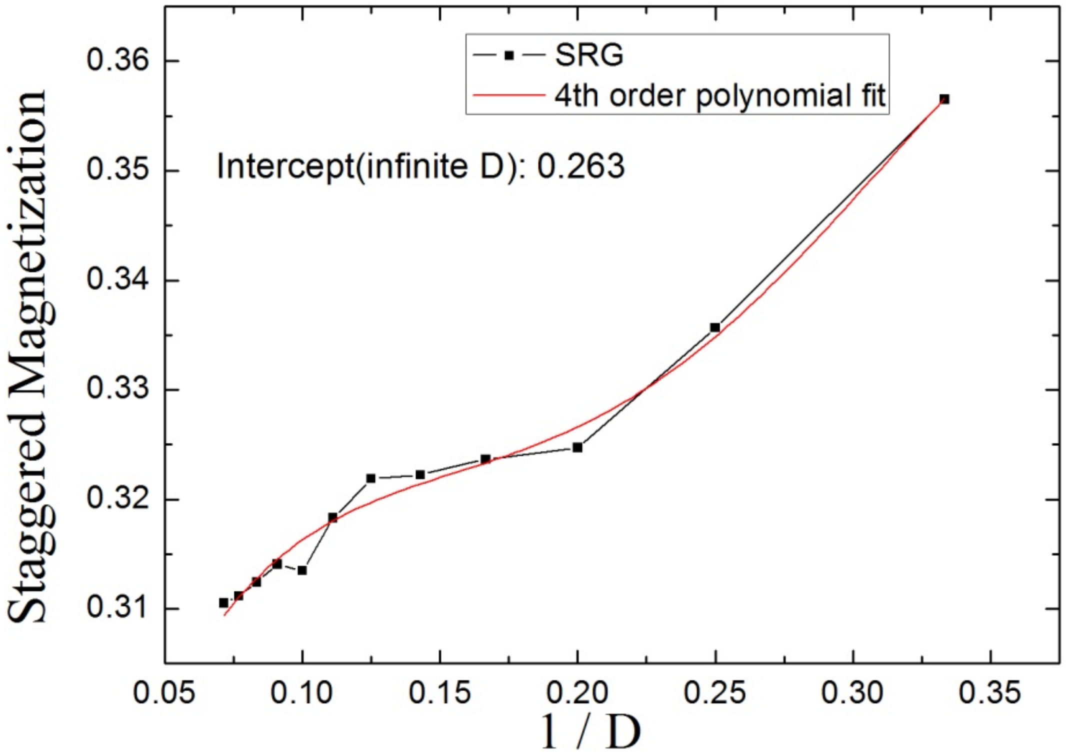


The tensor-network state cuts the long-range correlation

The bond dimension is roughly of the order of the correlation length of the tensor-network state

The logarithmic correction to the Area Law is important here

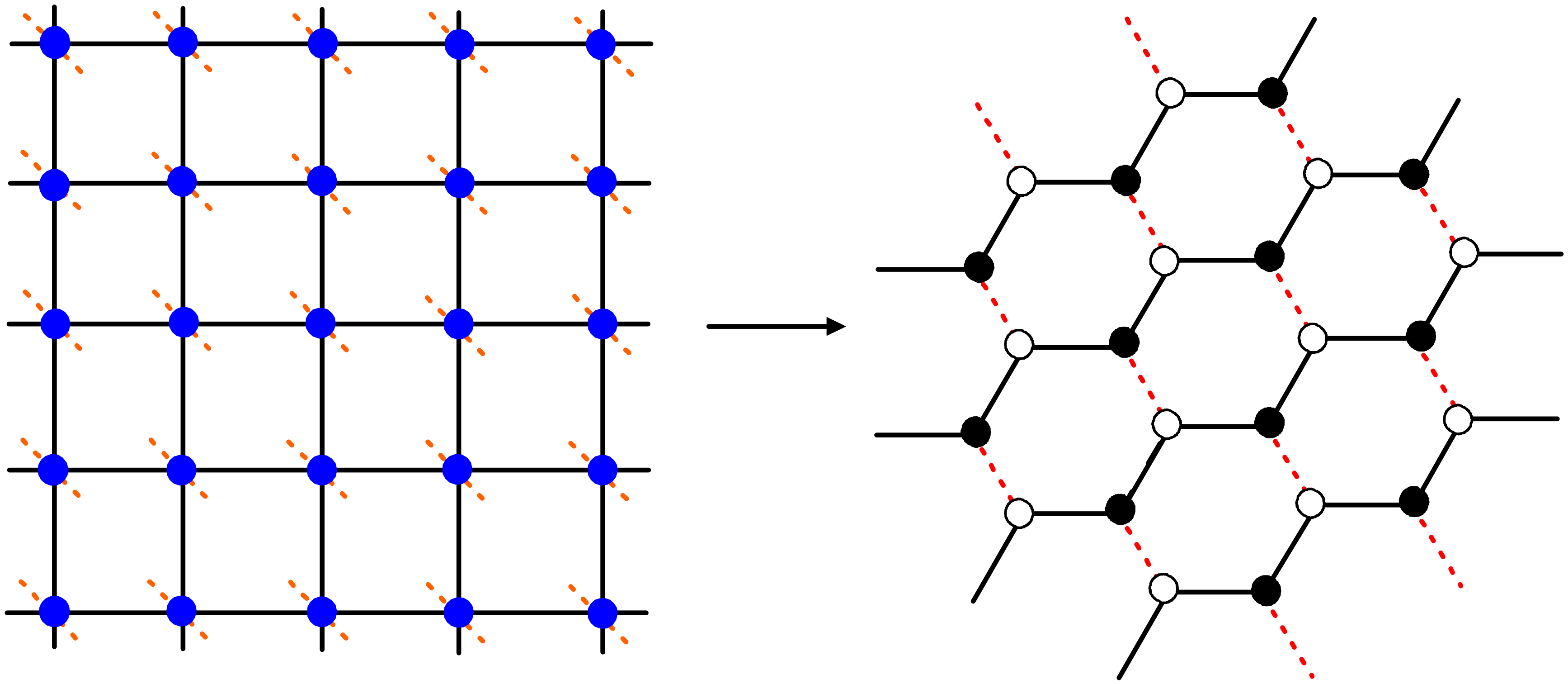
Staggered Magnetization



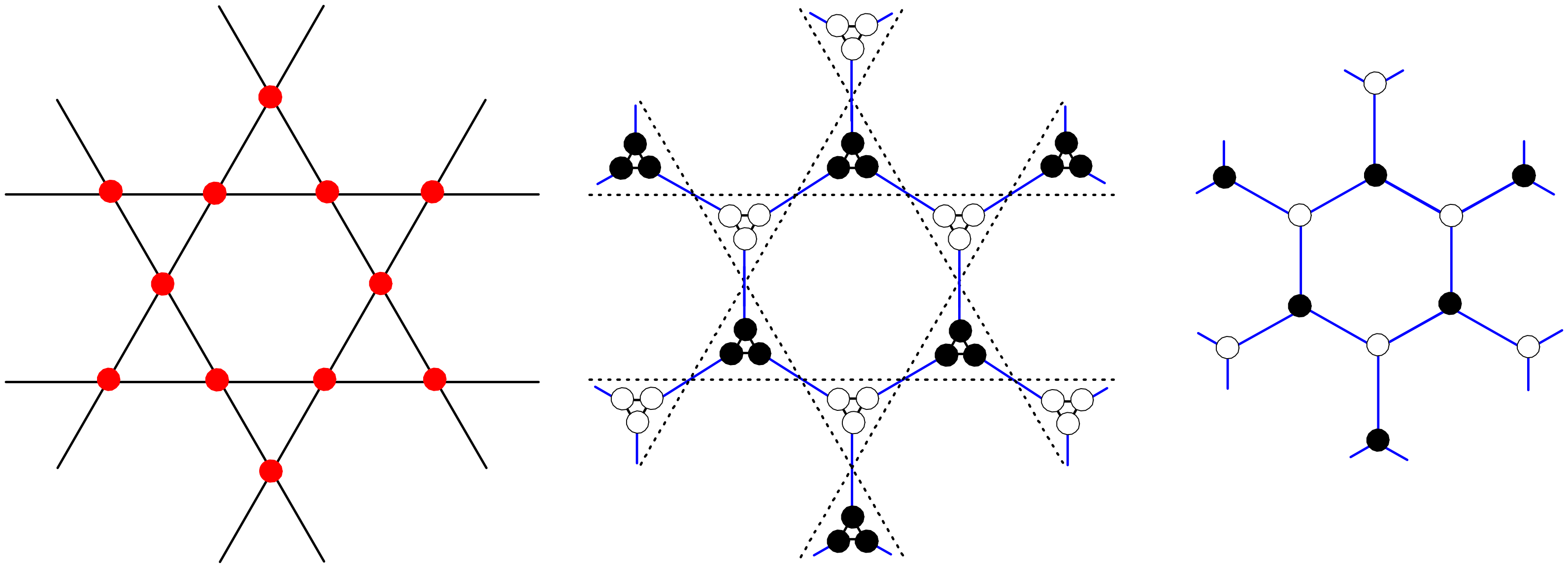
4^{th} order polynomial fit
M = 0.263

Monte Carlo:
M = 0.2681

Square Lattice



Kagome Lattice



(a) (b) (c)

Summary

- ✓ DMRG is an accurate numerical method for studying 1D quantum systems
- ✓ In 2D, the tensor-network representation of quantum many-body states is a good starting point
- ✓ The quantum tensor-network wavefunction can be accurately and efficiently evaluated by the projection method
- ✓ The partition function or expectation values of tensor-network model/state can be accurately determined by the SRG method

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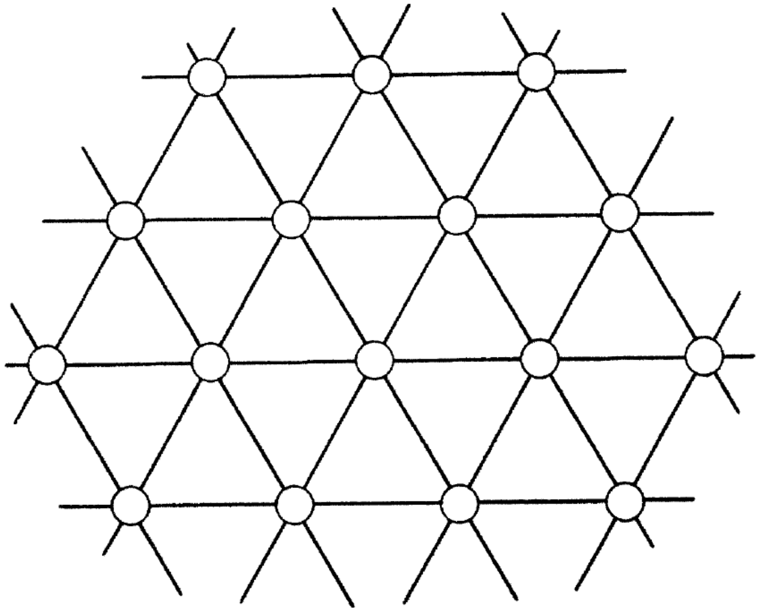
Zhengyu Weng, Hongchen Jiang Tsinghua University

Tensor-Network Representation of Classical Statistical Model

$$H = -J \sum_{\langle ij \rangle} S_i S_j$$

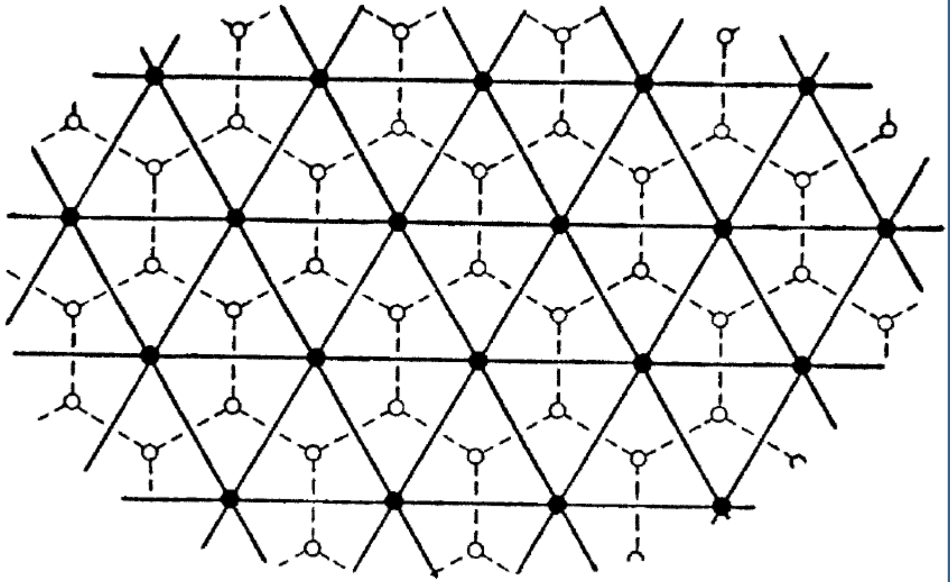
Ising model



Triangular lattice

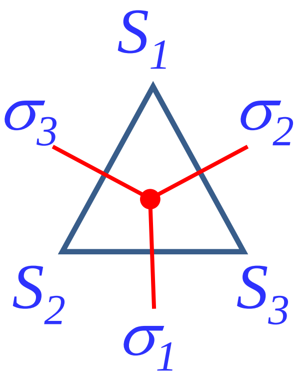
$$Z = Tr \prod_i T_{x_i y_i z_i}$$

Tensor-network model in dual lattice



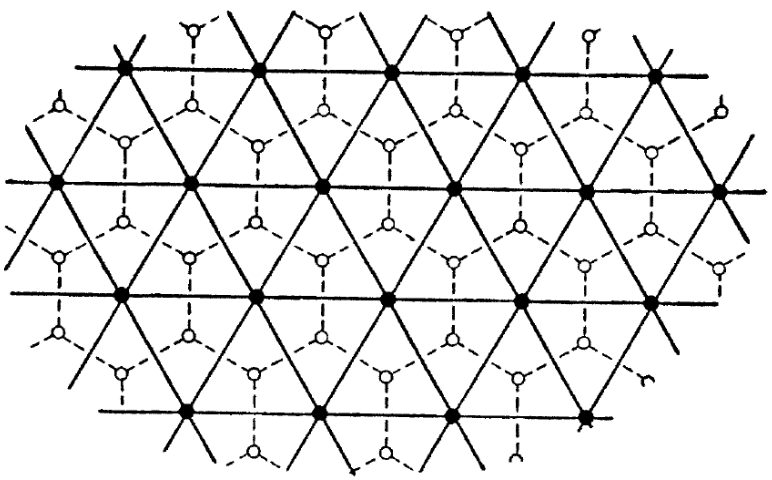
Dual lattice: honeycomb lattice

Tensor-network representation



$$H = -J\sum_{\langle ij\rangle} S_i S_j$$

$$Z = Tr\exp(-\beta H) = Tr\prod_{\Delta}\exp(-\beta H_{\Delta})$$



$$\sigma_1 = S_2 S_3$$

$$\sigma_2 = S_3 S_1$$

$$\sigma_3 = S_1 S_2$$

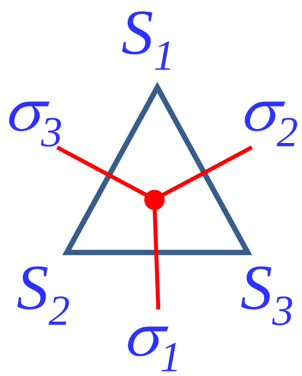
$$H_{\Delta} = -J(\sigma_1 + \sigma_2 + \sigma_3)/2$$

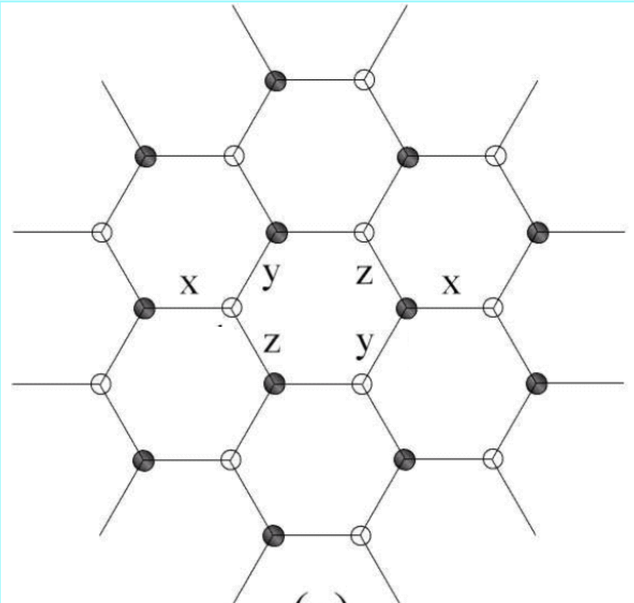
$$\sigma_1\sigma_2\sigma_3 = S_2 S_3 S_3 S_1 S_1 S_2 = 1$$

Tensor-network representation

$$Z = Tr\prod_i T_{x_i y_i z_i}$$

$$T_{\sigma_1\sigma_2\sigma_3} = e^{-J\beta(\sigma_1+\sigma_2+\sigma_3)/2}\,\delta(\sigma_1\sigma_2\sigma_3 - 1)$$





(a)