Renormalization of Tensor-Network States

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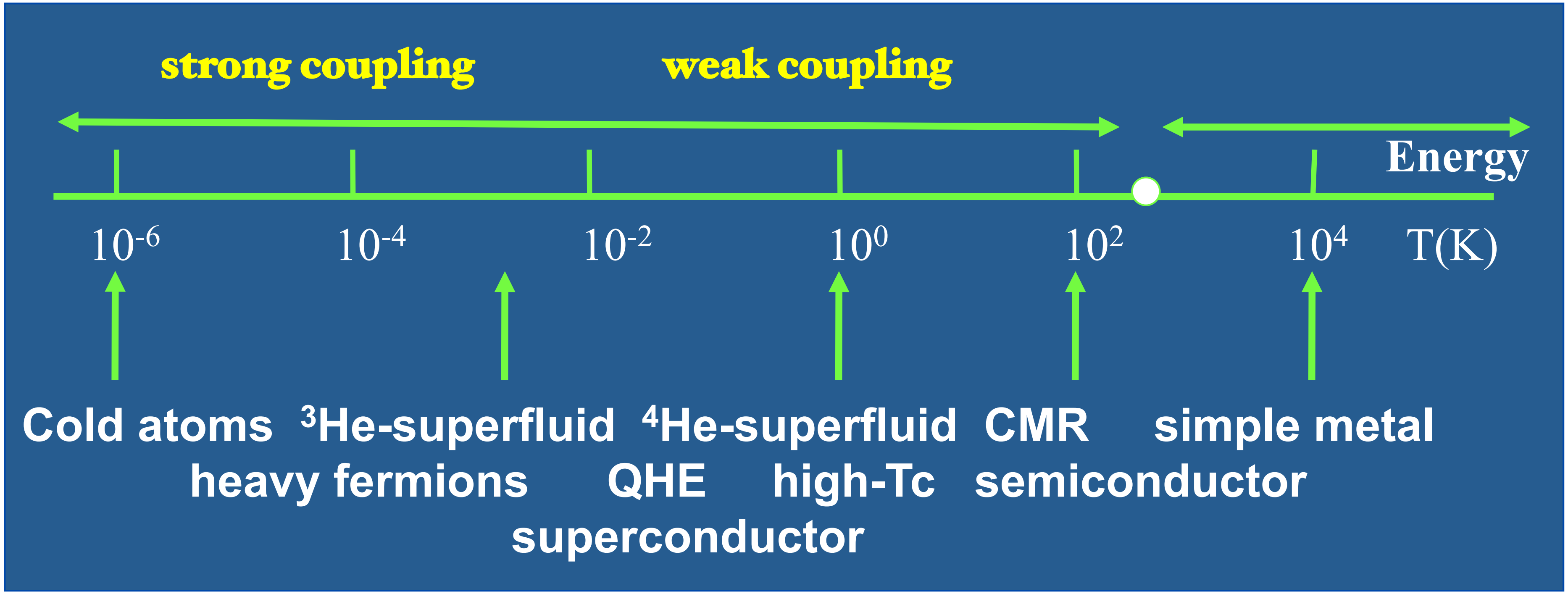
Physical Background:

characteristic energy scales of correlated quantum phenomena



To understand the physical mechanism of correlation effects, we need a theoretical probe which can resolve the fine structures below the characteristic energy scale!

Weak Coupling Approach

Convert a many-body problem into a one-body problem

✓ **Hartree-Fock self-consistent mean field theory**

✓ **Density Functional Theory**

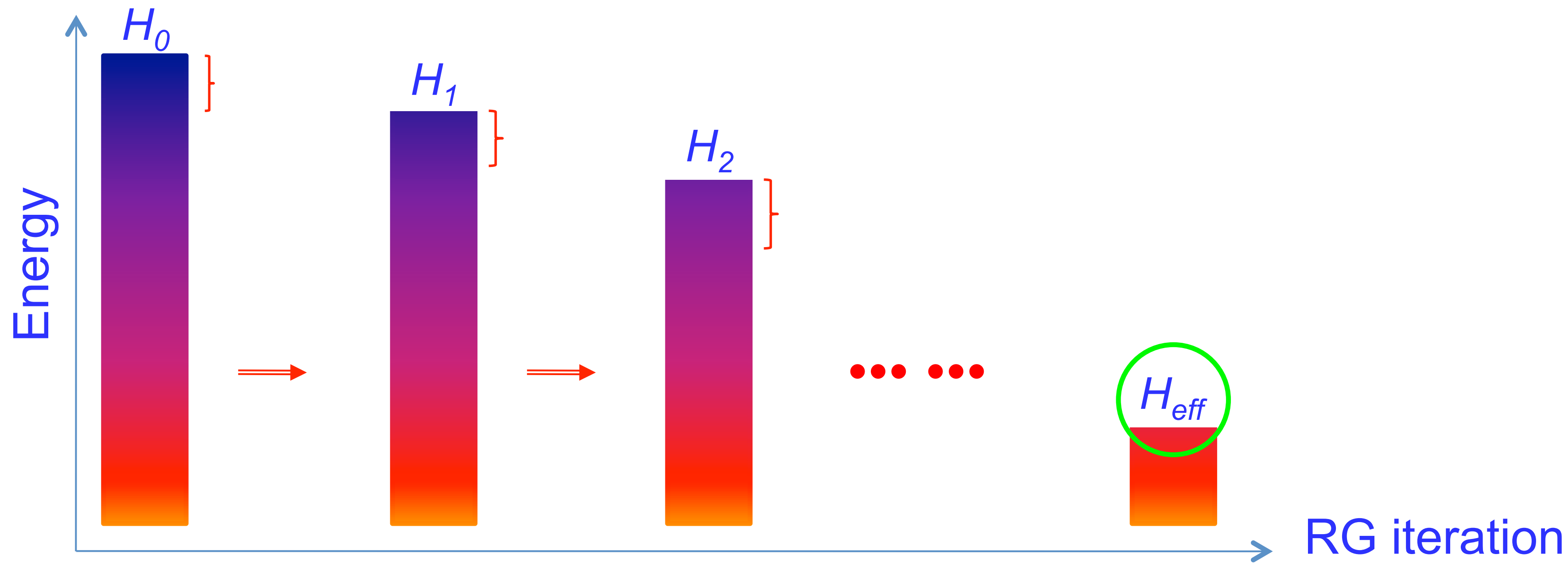
- **Most successful numerical method for treating weak coupling systems**
- **Based on LDA or other approximations, less accurate**

Strong Coupling Approach

Use a finite set of many-body basis states to treat a correlated system

- ✓ **Configuration Interactions (CI)**
  - **Conceptually simple, but can only deal a small number of orbitals**
- ✓ **Coupled Cluster Expansion (CC)**
  - **Perturbative**
- ✓ **Quantum Monte Carlo**
  - **Suffer from the "minus-sign" problem**
- ✓ **Numerical renormalization group**
  - **Variational, accurate and highly controllable,**

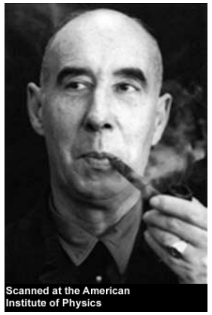
Concept of renormalization group



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

  but his paper was rejected by Physical Review.

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



Ernst Stueckelberg

Basic Idea of Numerical Renormalization Group

To represent a *targeted state*

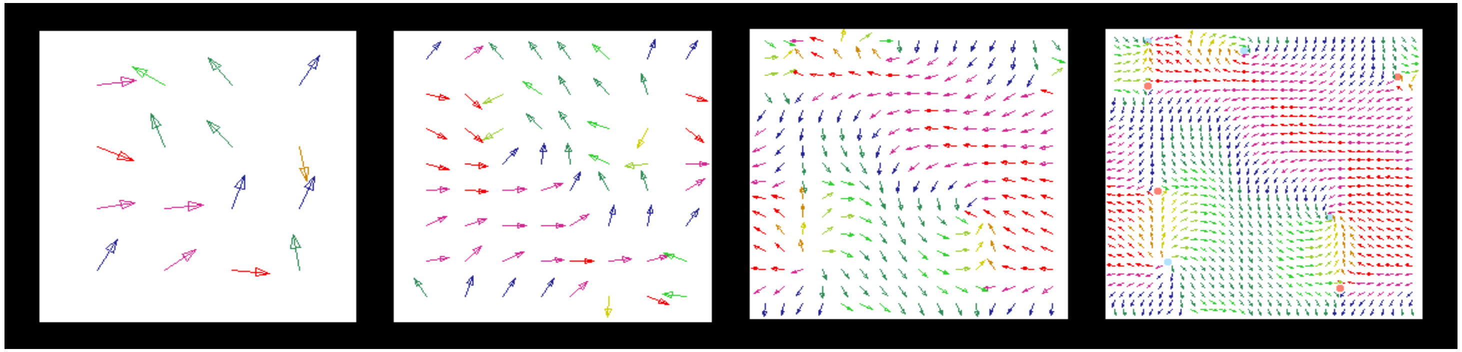
$$|\psi_0\rangle = \sum_{l=1}^{\infty} f_l |n_l\rangle$$

by an approximate wavefunction using a limited number of many-body basis states

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

such that their overlap is maximized

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



Refine a basis set by performing a series of basis transformations

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 many-body basis states

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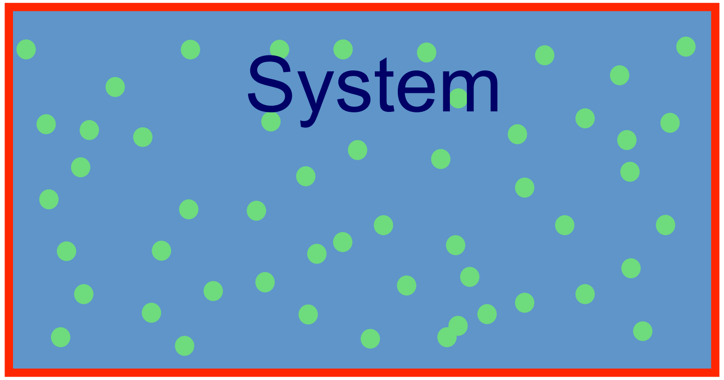
$$\langle\tilde{\psi}_0|\psi_0\rangle = \sum_{l=1}^{D} \tilde{f}_l f_l$$

Key issue:

How to determine these optimal basis states?

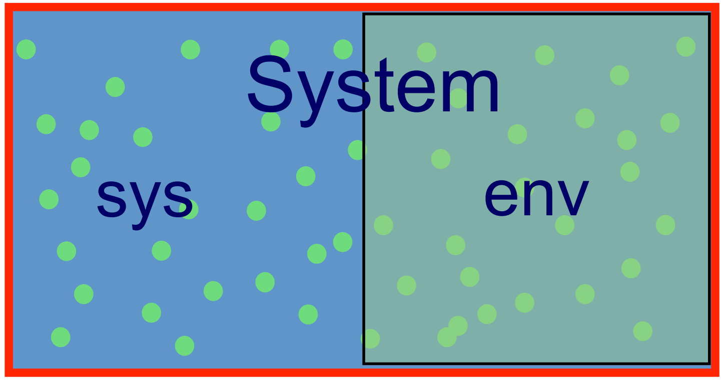
Wilson NRG



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

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

DMRG

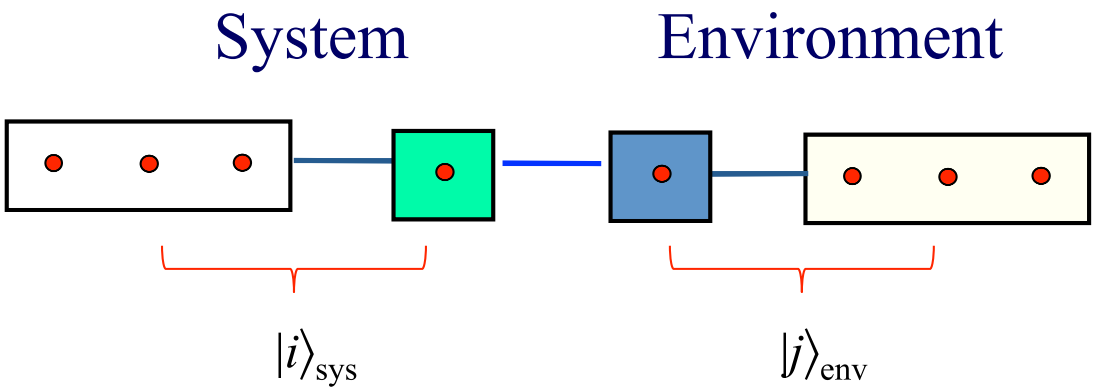


Use a sub-system as a pump to probe the other part of the system

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

The weight is measured by the entanglement between sys and env

DMRG 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

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

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

What is a tensor-network state?

- **Classical model of statistical physics:**

  all statistical models with local interactions can be represented as tensor-network states

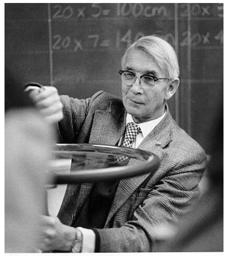
- **Quantum lattice models:**

  Tensor network state is a faithful representation of the ground state wavefunction of quantum lattice model that satisfies the area law of entanglement

Classical Statistical Physics

Tensor-network representation of the partition function

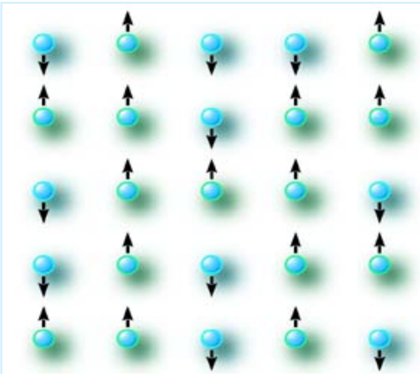
- Example: Ising model



Ernst Ising

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

$$S_i^z = -1,\ 1$$



1D: partition function is a matrix product

$$Z = \sum_{S_1 \ldots S_N} \exp\left(\beta \sum_i S_i S_{i+1}\right)$$
$$= Tr\left(A \cdots A\right)$$
$$= \lambda_{\max}^N \qquad N \to \infty$$

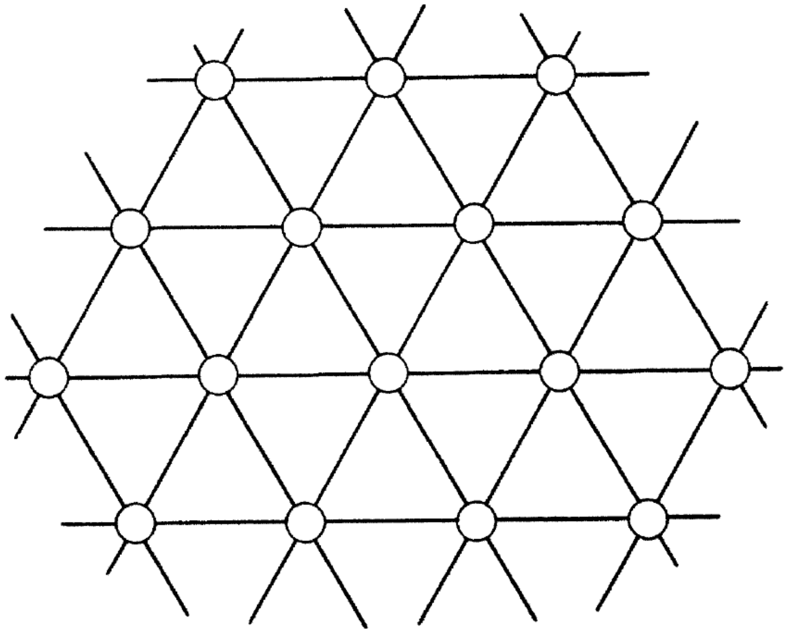
$$A = \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix}$$

matrix is a 2-index tensor

Tensor-Network Representation of Classical Statistical Model

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

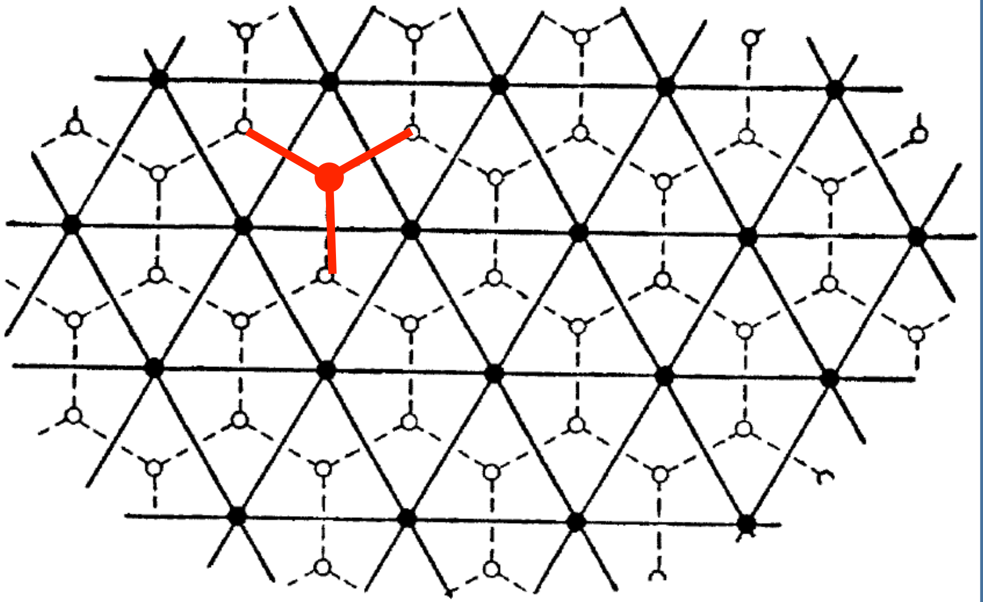
Ising model



Triangular lattice

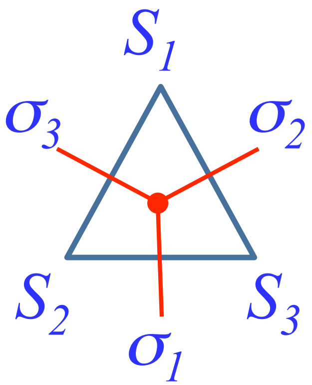
$$Z = Tr \prod_i T_{x_i y_i z_i}$$

Tensor-network model in dual lattice



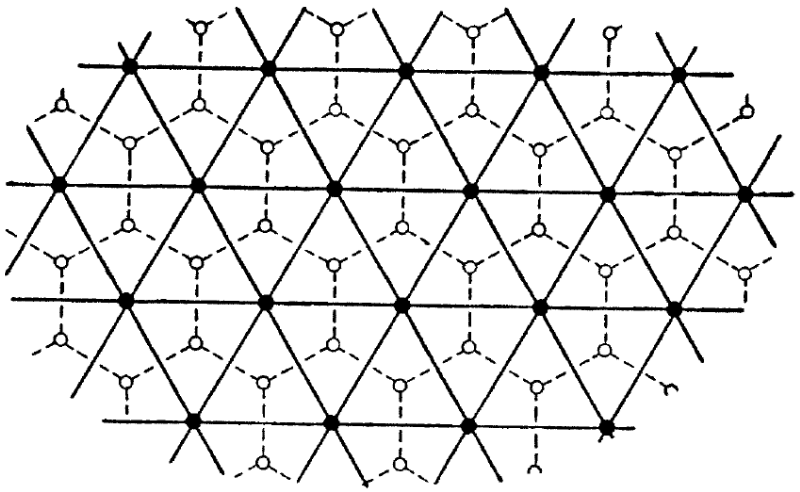
Dual lattice: honeycomb lattice

Tensor-Network Model in the Dual Lattice



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

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



$$\sigma_1 = S_2 S_3$$

$$\sigma_2 = S_3 S_1$$

$$\sigma_3 = S_1 S_2$$

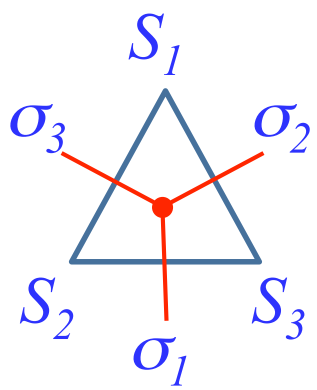
$$H_{\Delta} = -J\left(\sigma_1 + \sigma_2 + \sigma_3\right)/\,2$$

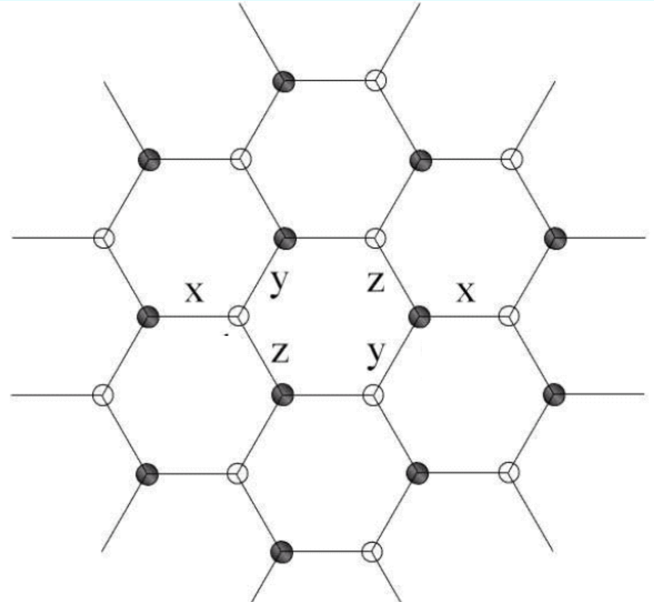
$$\sigma_1 \sigma_2 \sigma_3 = S_2 S_3 S_3 S_1 S_1 S_2 = 1$$

Tensor-network representation

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

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





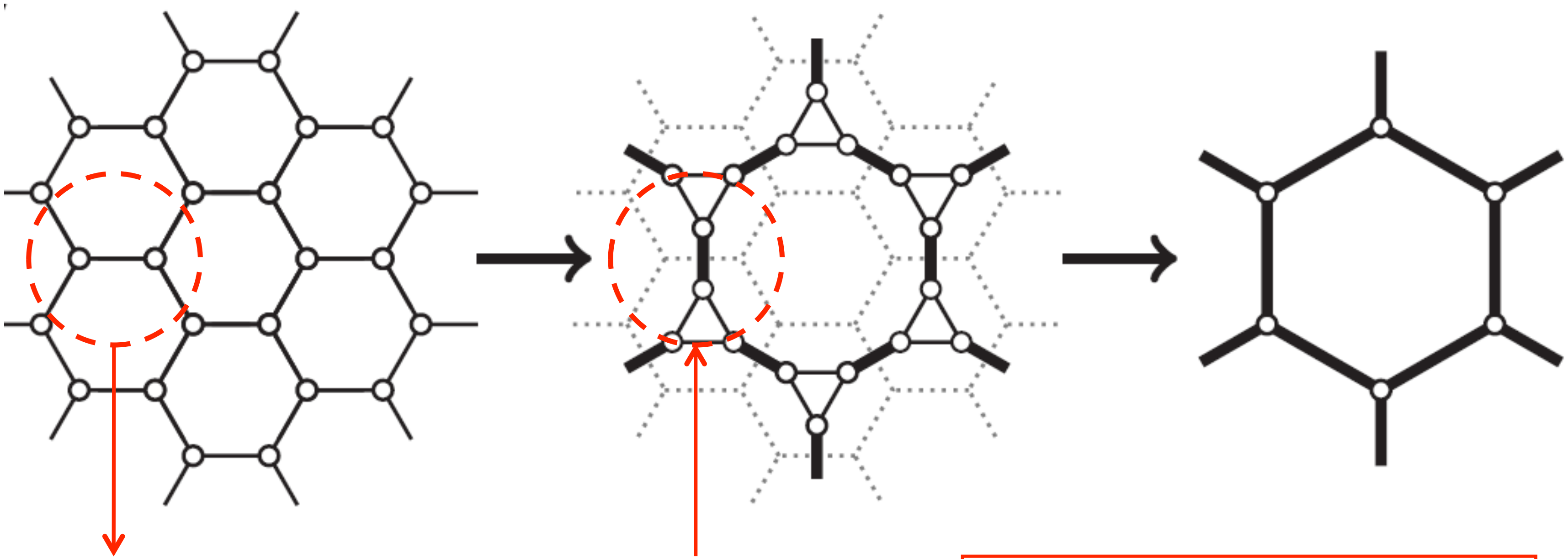
(a)

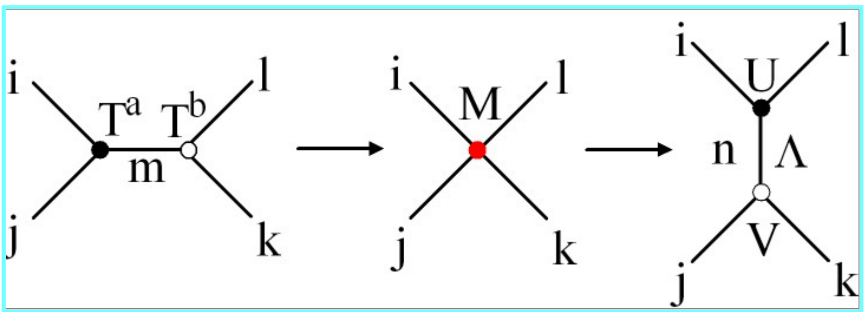
Coarse Grain Tensor Renormalization Group

Levin, Nave, PRL 99 (2007) 120601

Step I: Rewiring

Step II: decimation





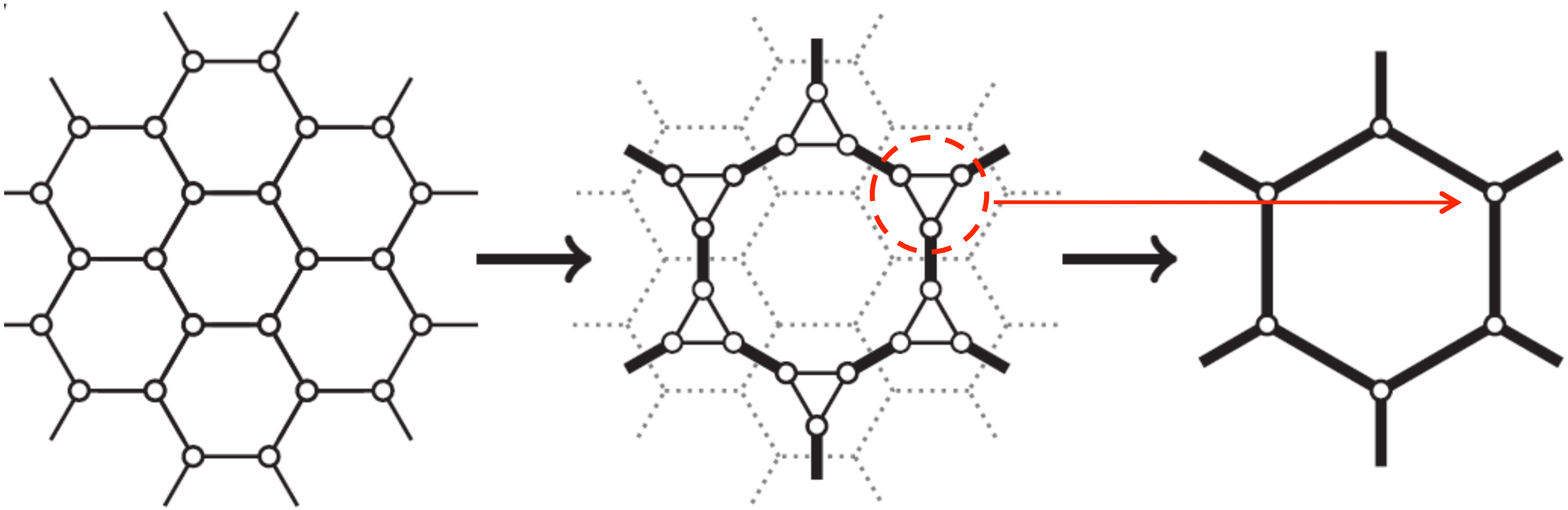
$$M_{kj,il} = \sum_{m} T_{mji} T_{mlk}$$

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

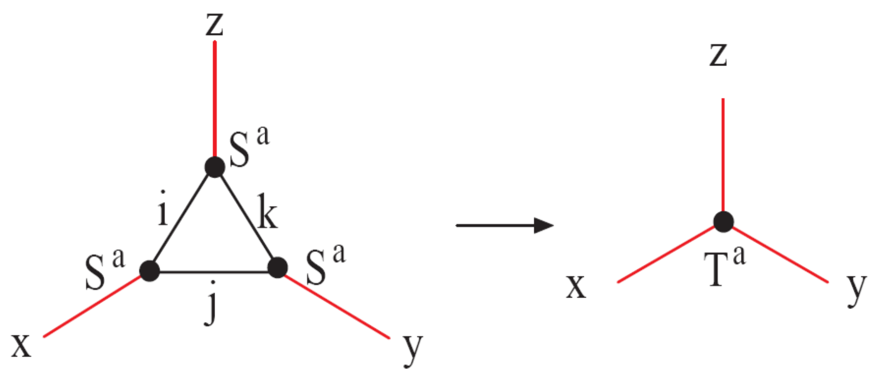
Singular value decomposition

Coarse Grain Tensor Renormalization Group

Step II: decimation

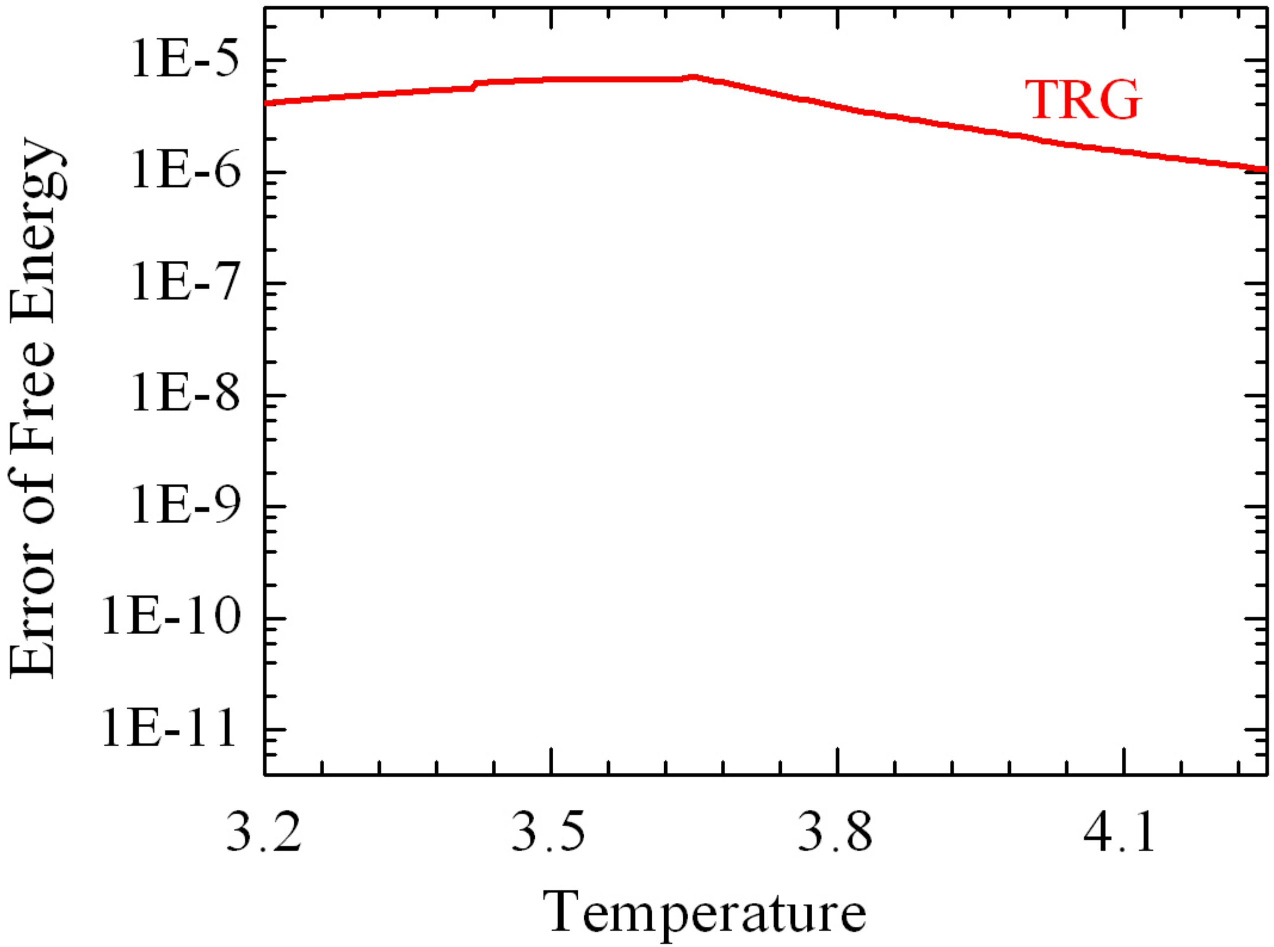


$$T_{xyz} = \sum_{ijk} S_{xik} S_{yji} S_{zkj}$$



Accuracy of TRG

TRG is a good method, but it is still not good enough



D = 24

Ising model on a triangular lattice

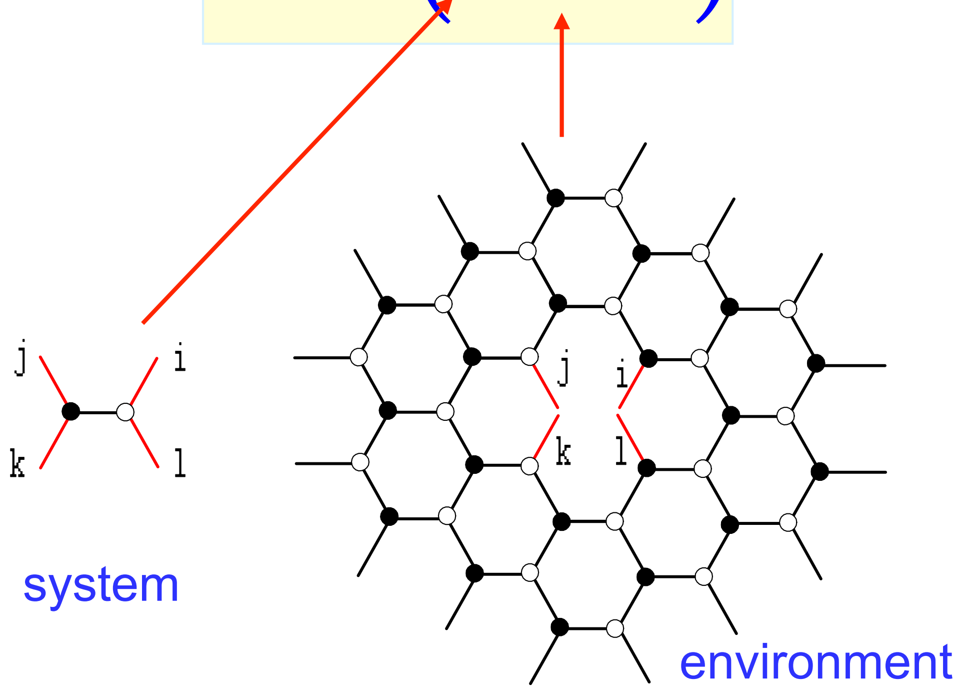
Second renormalization of tensor-network state (SRG)

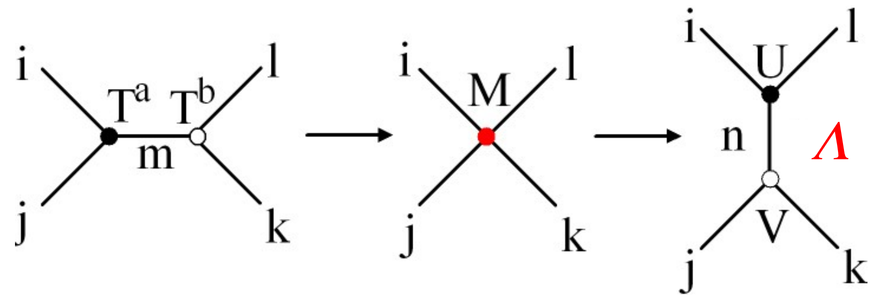
- **TRG:**
  truncation error of M is minimized by the singular value decomposition

But, <u>what really needs to be minimized is the error of Z!</u>

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

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





Xie et al, PRL **103**, 160601 (2009)
Zhao, et al, PRB **81**, 174411 (2010)

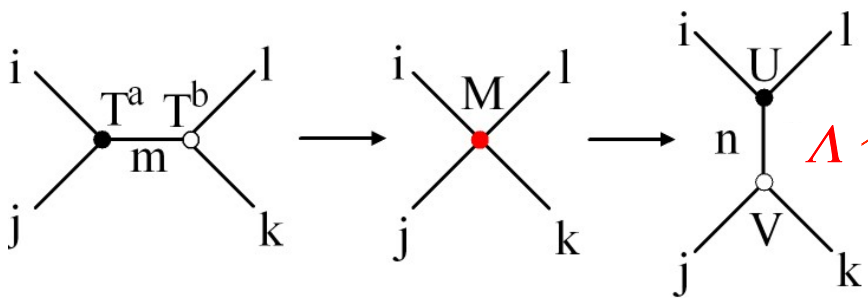
I. Poor Man's SRG: entanglement mean-field approach

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

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

Mean field (or cavity) approximation

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



Λ

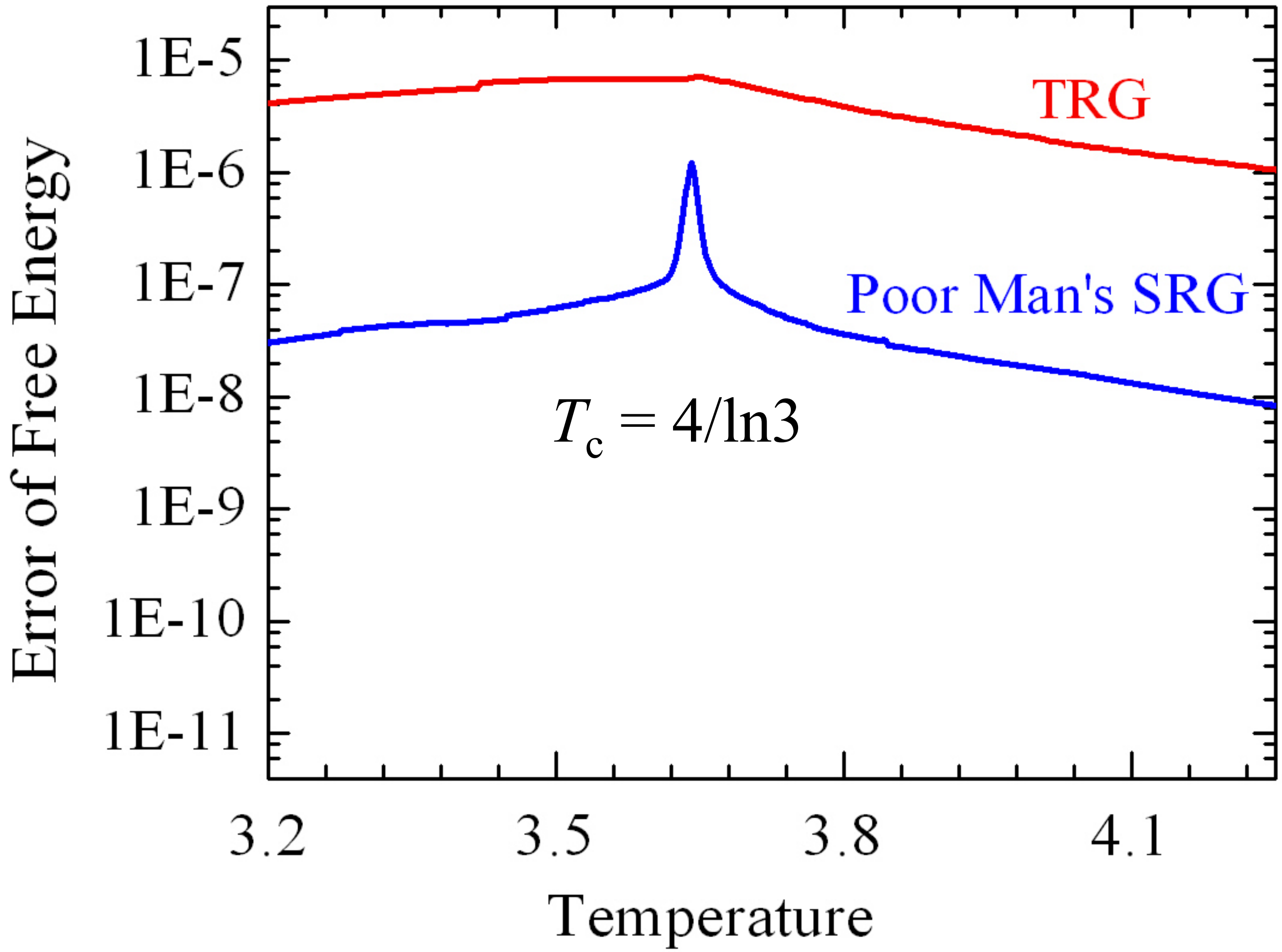
Bond field – measures the entanglement between *U* and *V*

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

From environment

From system

Accuracy of Poor Man's SRG

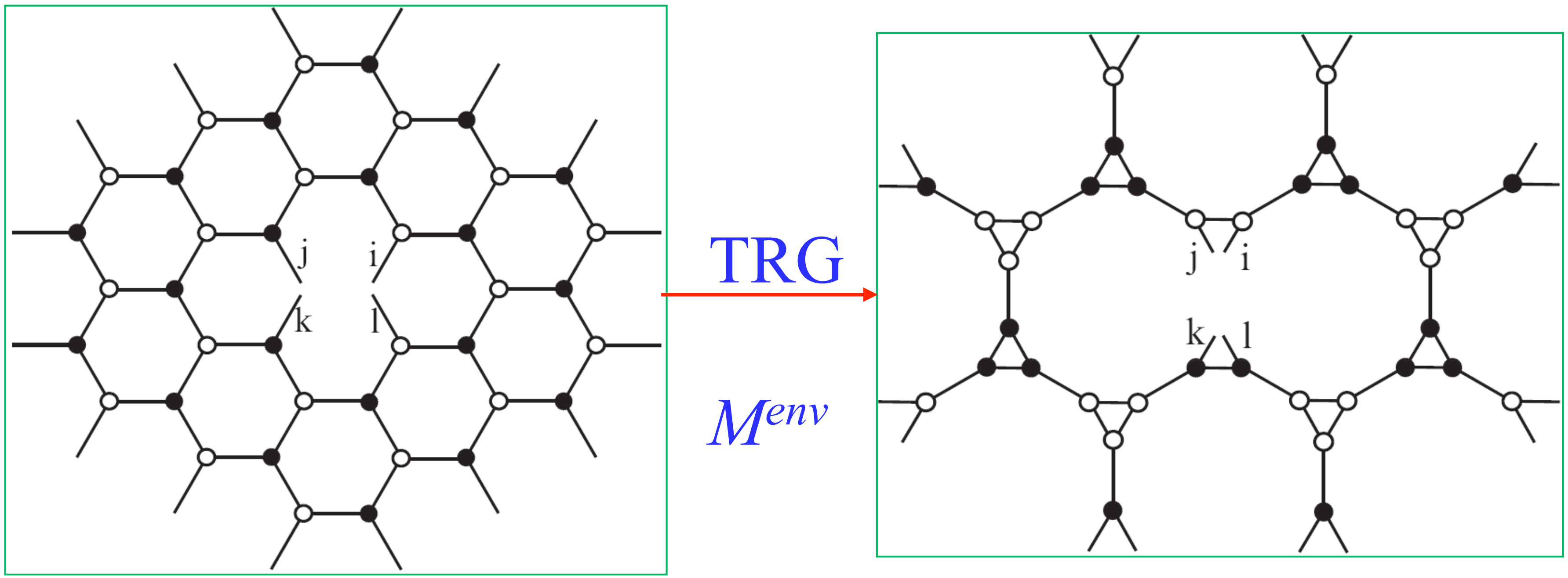


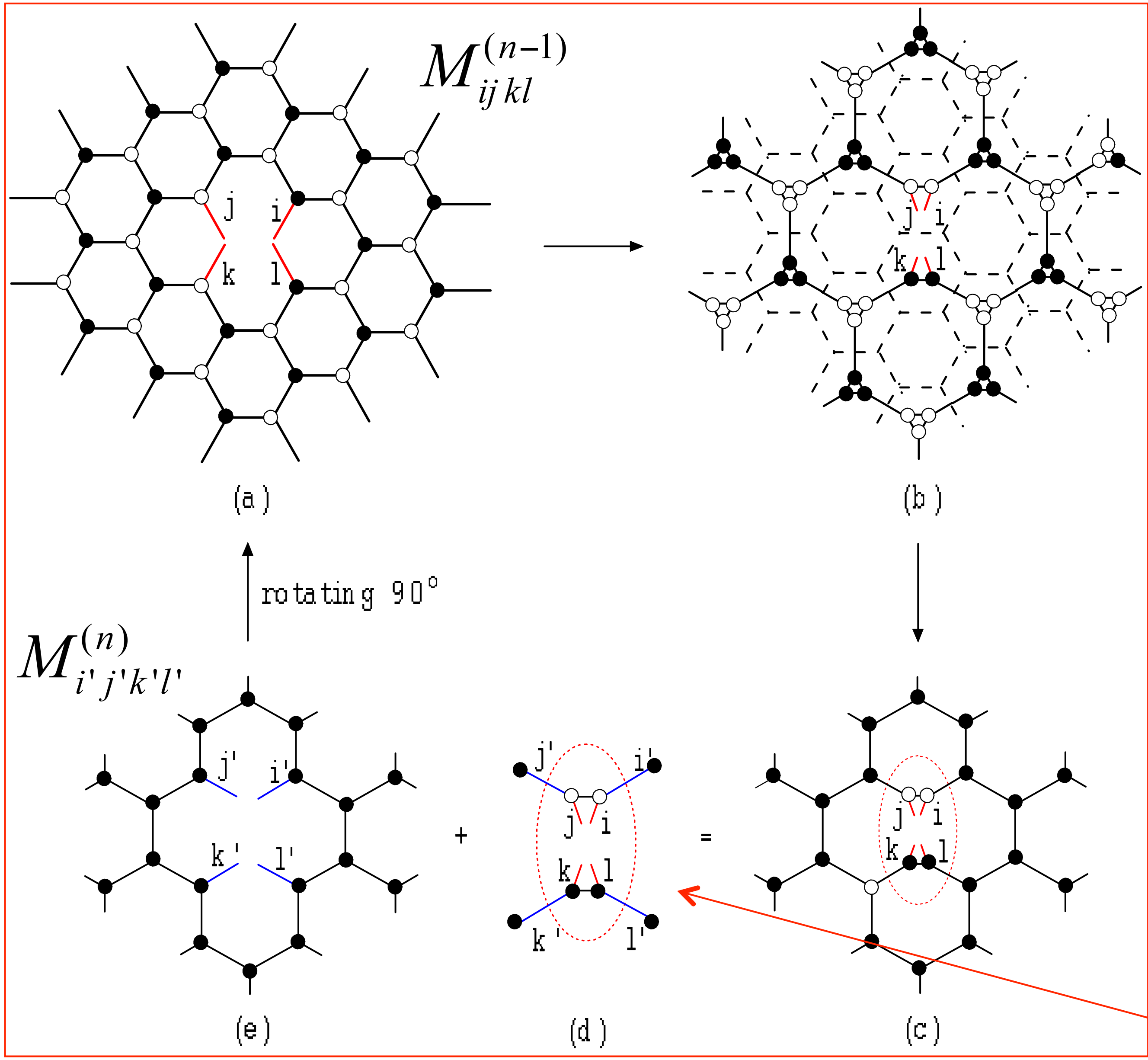
D = 24

Ising model on a triangular lattice

II. More accurate treatment of SRG

Evaluate the environment contribution M^{env} using TRG





1. Forward iteration

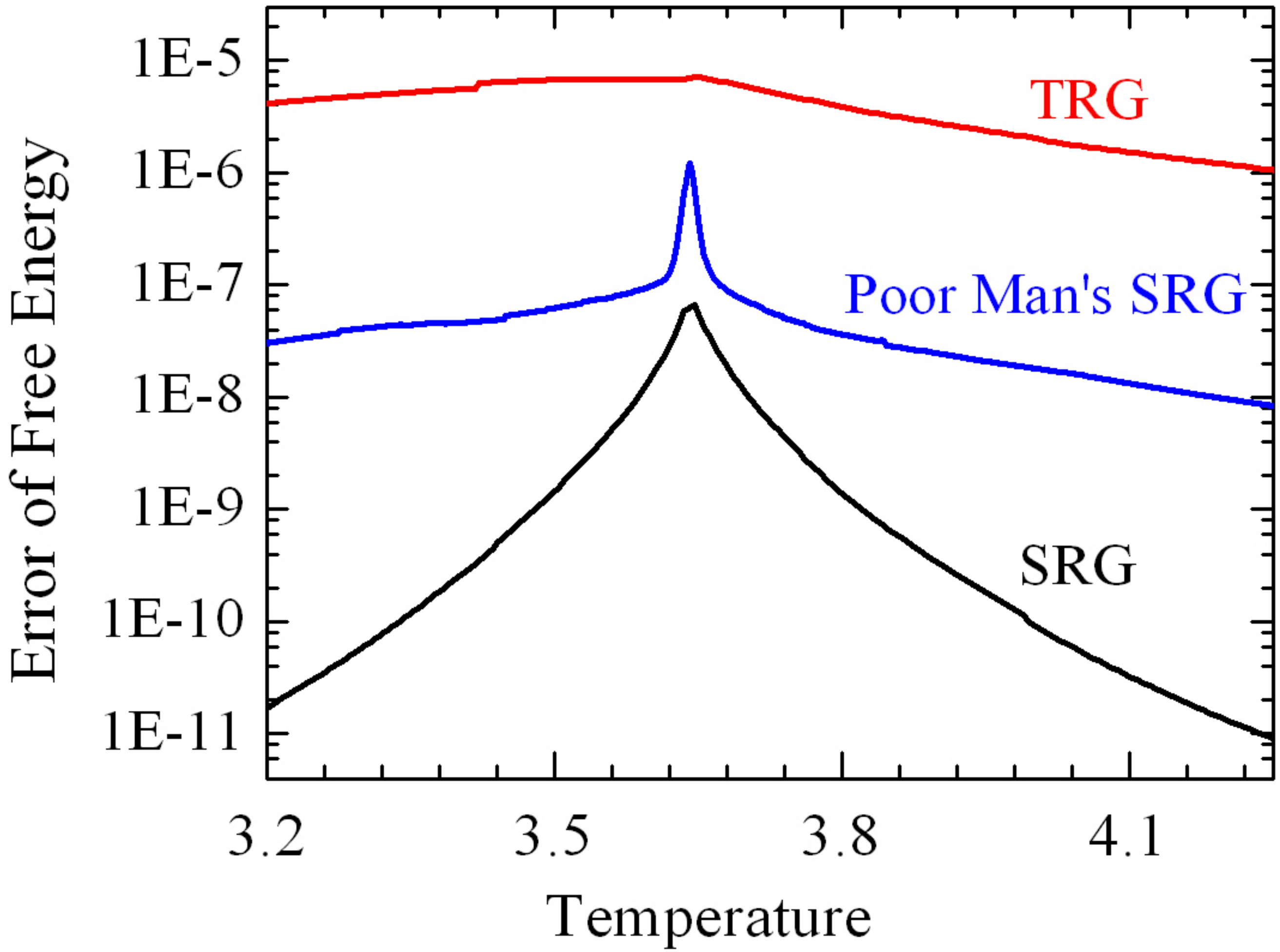
$$M^{(0)} \rightarrow M^{(1)} \rightarrow \cdots \rightarrow M^{(N)}$$

2. Backward iteration

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

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

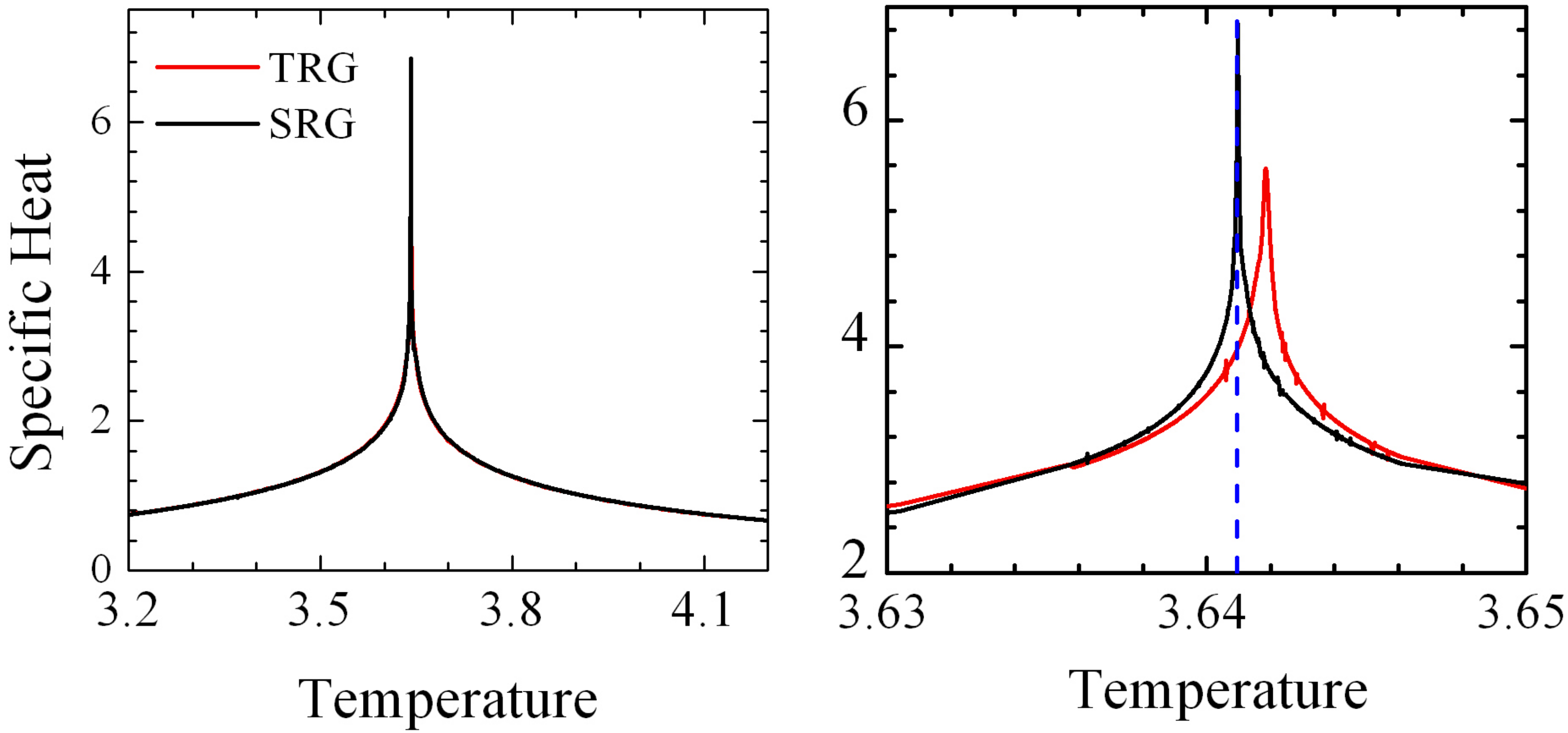
Accuracy of SRG



D = 24

Ising model on a triangular lattice

Specific Heat of the Ising model on Triangular Lattices



D = 24

Quantum Lattice Models

- Tensor-network state is a wavefunction of the ground state wavefunction satisfying the area law of entanglemnt
- How to study a tensor-network wavefunction?

Example: Heisenberg model

Heisenberg

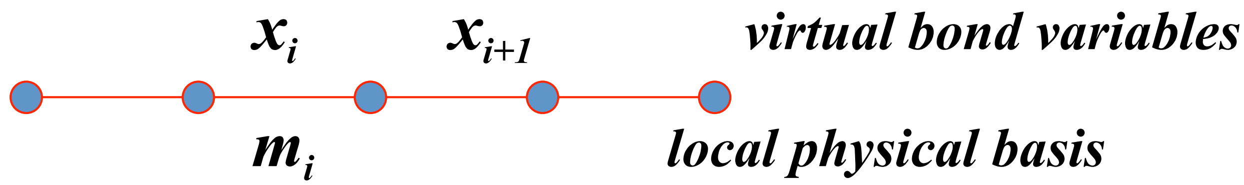
$$H = J\sum_{i=1}^{N}\vec{S}_i\cdot\vec{S}_{i+1}$$

quantum spin operators

1D Wavefunction: Matrix Product State

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

$A_{x_1x_2}[m_1]$ ***D×D matrix***



$$\boxed{S \sim L^0 < \ln D}$$

- **MPS: is the wavefunction determined by the DMRG**
- **Bond dimension *D* measures the upper bound of the entanglement entropy**

MPS is not a good representation in 2D

$$\boxed{\begin{aligned} &S \sim L^{d-1} \sim \ln D \\ &D \sim \exp\left(L^{d-1}\right) \end{aligned}}$$

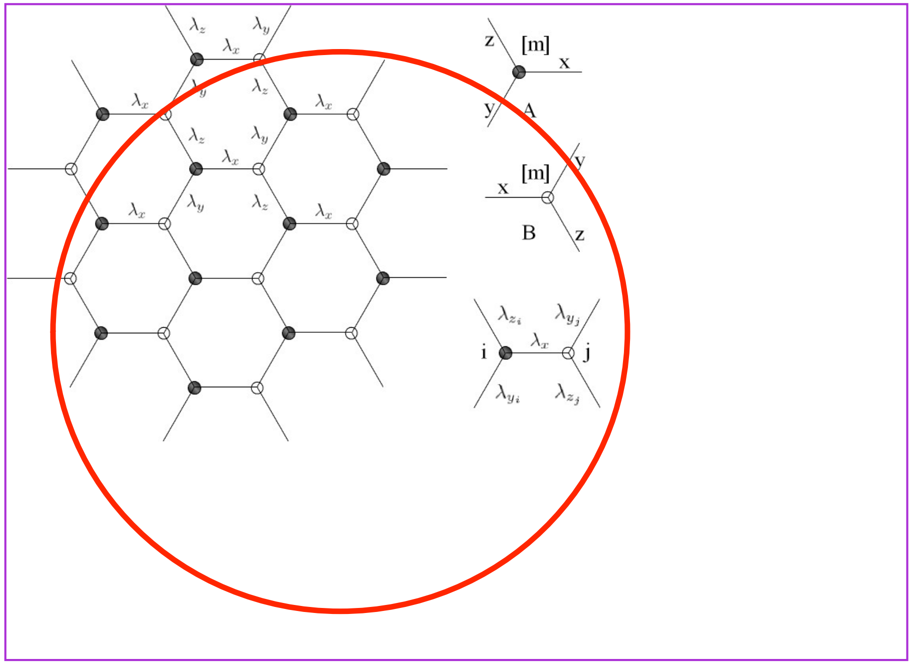
$$d = 2$$

- **Number of basis states needed for describing a 2D system grows exponentially with the system size**
- **Breaks the locality of local interactions**

2D: Tensor-Network Wavefunction

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

bond vector



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

The number of dangling bonds is proportional to the cross section

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?

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

1. Variational approach

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

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

$D \le 5$

Verstraete, Cirac, arXiv:0407066
Gu, Levin, Wen, PRB 78, 205116 (2008)
……

How to determine the local tensor?

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

"Entanglement" measure

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

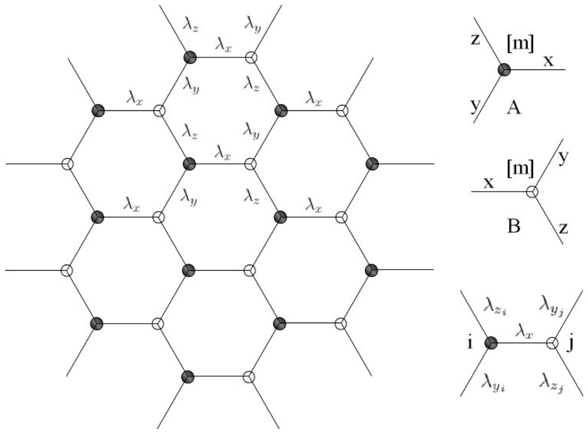
Projection Operator

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

$D \sim 70$ (honeycomb lattice) $D \sim 20$ (square or Kagome lattice)

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

Entanglement Weighted Projection



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

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

Heisenberg model

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

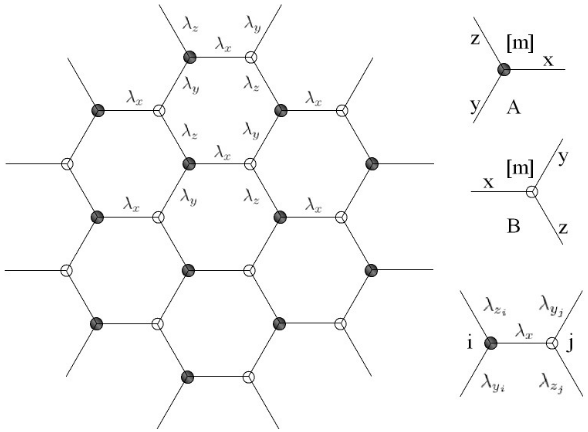
$$H_{ij} = J S_i \cdot S_j$$

Projection

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

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

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: Poor Man's Approach

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

Step I

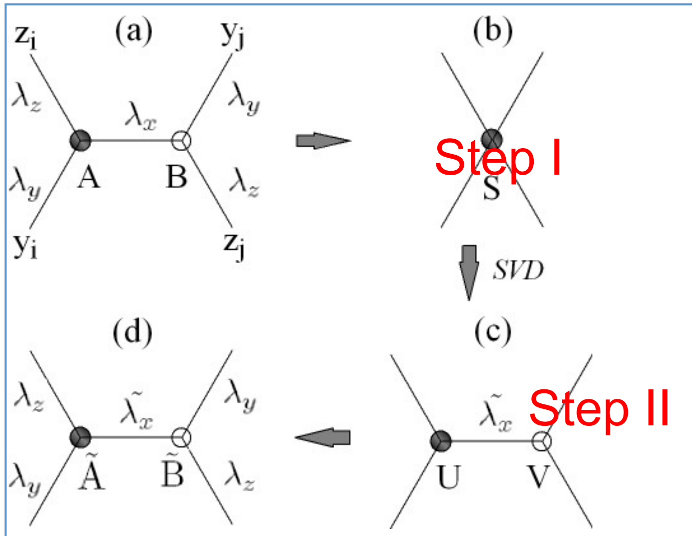
$$S_{y_i z_i m_i', y_j z_j m_j'} = \sum_{m_i m_j} \sum_{x} \langle m_i' m_j' | e^{-H_{ij}\tau} | m_i m_j \rangle \lambda_{y_i} \lambda_{z_i} A_{x y_i z_i}[m_i] \lambda_x B_{x y_j z_j}[m_j] \lambda_{y_j} \lambda_{z_j}$$

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

$$\begin{aligned} A_{x y_i z_i}[m_i] &= \lambda_{y_i}^{-1} \lambda_{z_i}^{-1} U_{y_i z_i m_i, x}, \\ B_{x y_j z_j}[m_j] &= \lambda_{y_j}^{-1} \lambda_{z_j}^{-1} V_{y_j z_j m_j', x}. \end{aligned}$$

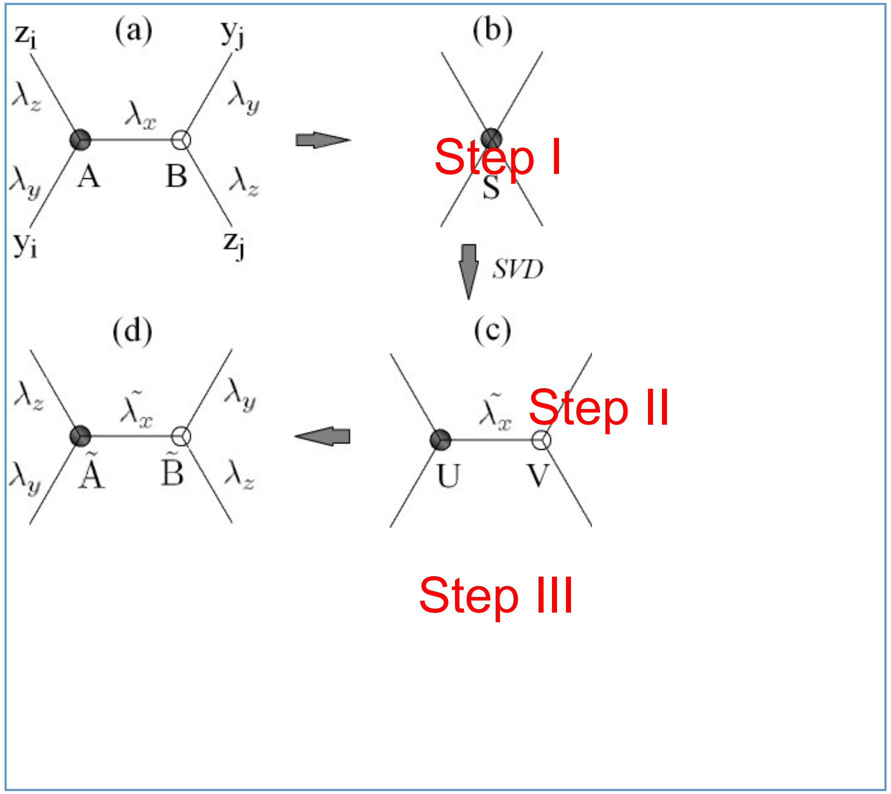


Step III

SVD: singular value decomposition

Projection:Poor Man's Approach

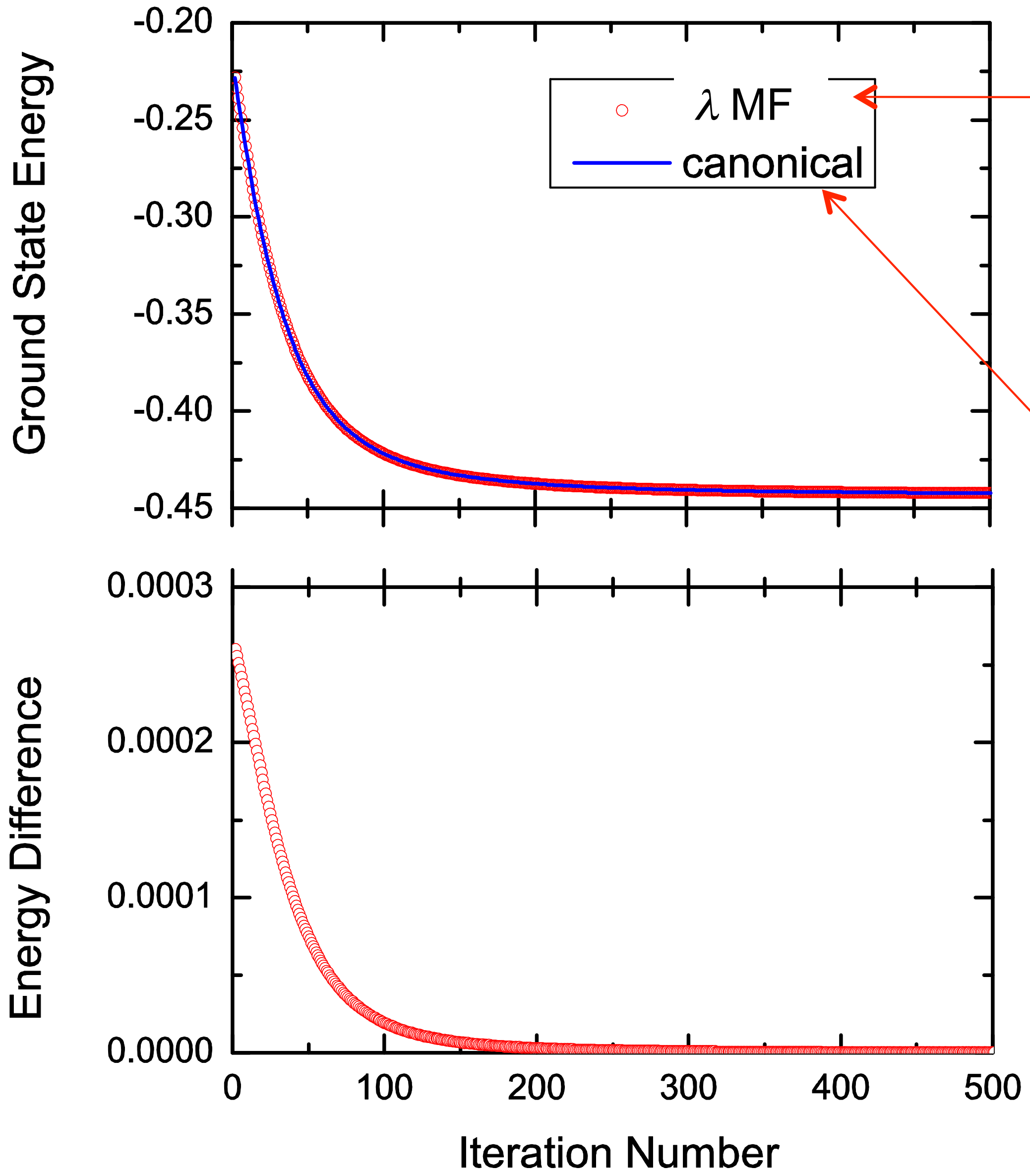
$$e^{-\tau H_x}\left|\Psi\right\rangle = Tr\prod_{\substack{i\in black\\ j=i+\hat{x}}}\left\langle m_i' m_j'\right|e^{-\tau H_{i,j}}\left|m_i m_j\right\rangle \lambda_{x_i}\lambda_{y_i}\lambda_{z_i}A_{x_i y_i y_i}[m_i]B_{x_j y_j y_j}[m_j]\left|m_i' m_j'\right\rangle$$



SVD: singular value decomposition

- To use bond vector λ as effective fields to take into account the environment contribution
- The projection is done locally. This keeps the locality of wavefunction, making the calculation very efficient
- Truncation error is not accumulated

How accurate is this approach



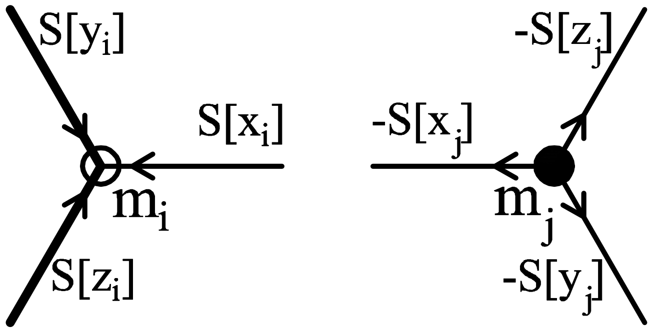
Without performing the canonical transformation for the matrix product state

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

1D Heisenberg model

Symmetry Implementation

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



$$S\left[x_i\right] + S\left[y_i\right] + S\left[z_i\right] = m_i$$

$$-S\left[x_j\right] - S\left[y_j\right] - S\left[z_j\right] = m_j$$

$$\sum_i m_i = 0$$

Expectation Value

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

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

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

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

Bond dimension D^2

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

Can be evaluated using

- TRG

  Gu et al, PRB 78, 205116 (2008)

  Jiang et al, PRL **101**, 090603 (2008)

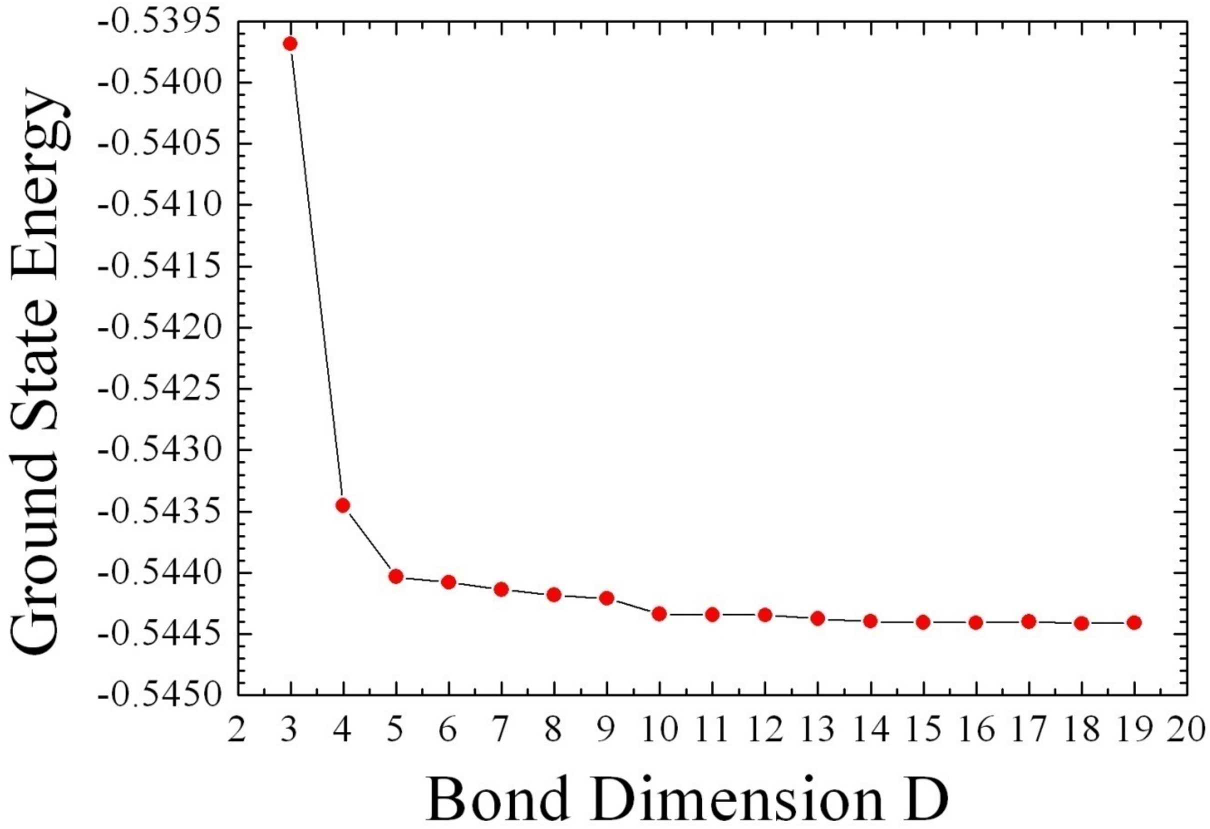
- SRG

  Xie et al, PRL 103, 160601 (2009)

  Zhao, et al, PRB 81, 174411 (2010)

- TMRG
- Monte Carlo

Quantum Heisenberg Model on Honeycomb Lattice



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

SRG D = 19
E = -0.544410

SRG D = 30 (right D=2)
E = -0.54442

Monte Carlo:
E = -0.54454 (± 20)

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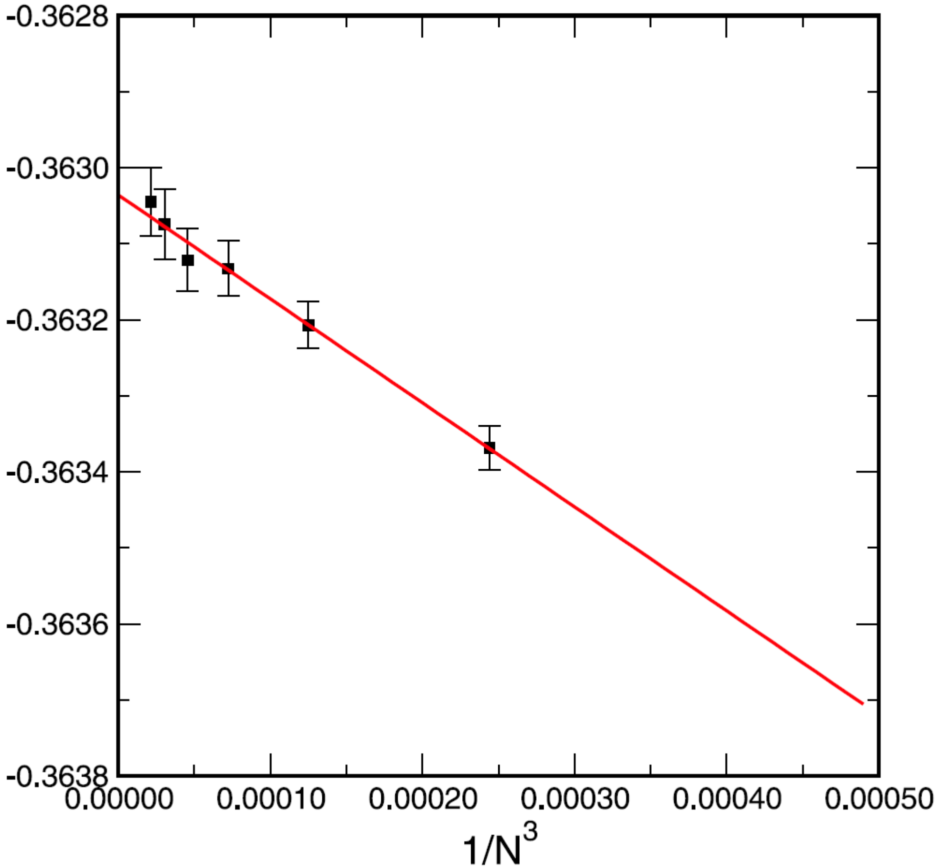
Lattice size $N = 2 \times 3^{30}$

Heisenberg Model on Honeycomb Lattice

Quantum Monte Carlo Result



E = -0.36303 (± 13) per bond

= -0.54454 (± 20) per site

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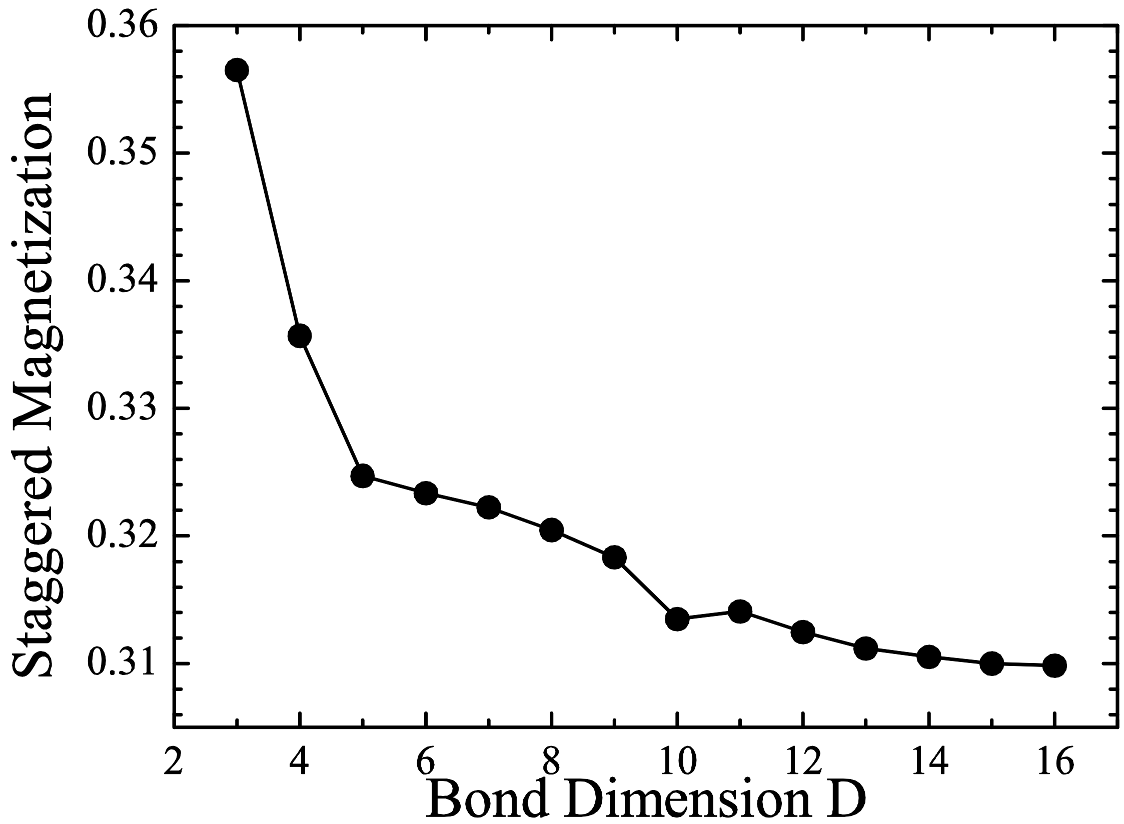
Staggered Magnetization



SRG D = 16

M = 0.3098

Monte Carlo:

M = 0.2681

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M = 0.22

Reger, Riera, Young, JPC 1989

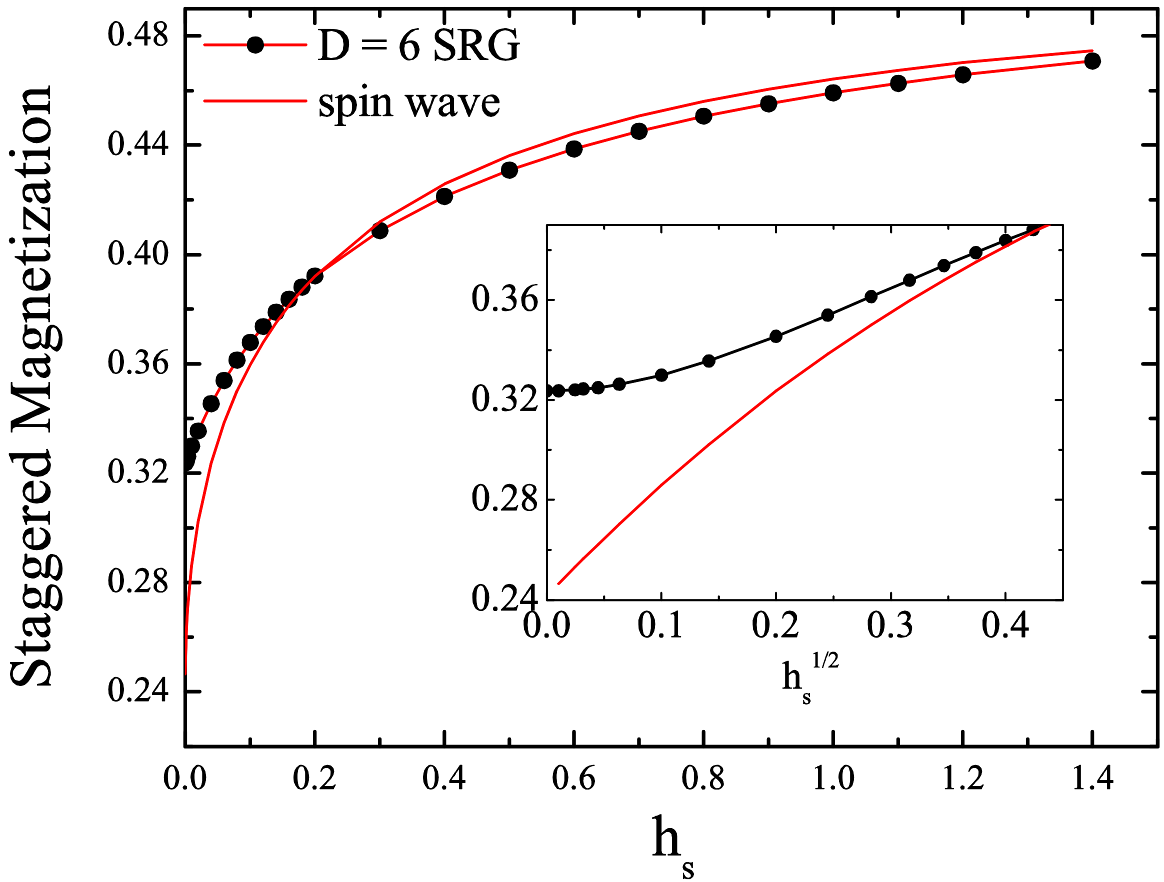
Spin Wave:

M = 0.24

Series expansion

M = 0.27

Staggered Magnetization

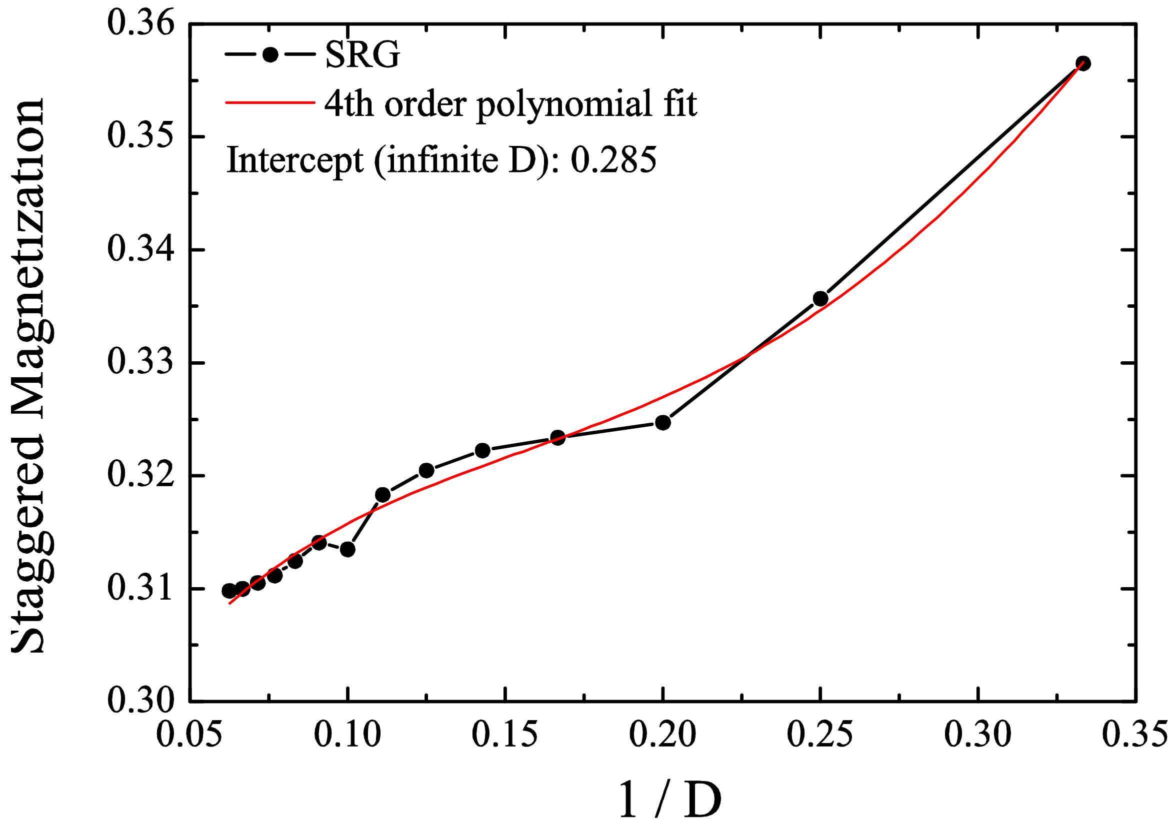


The tensor-network state cuts the long-range correlation

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



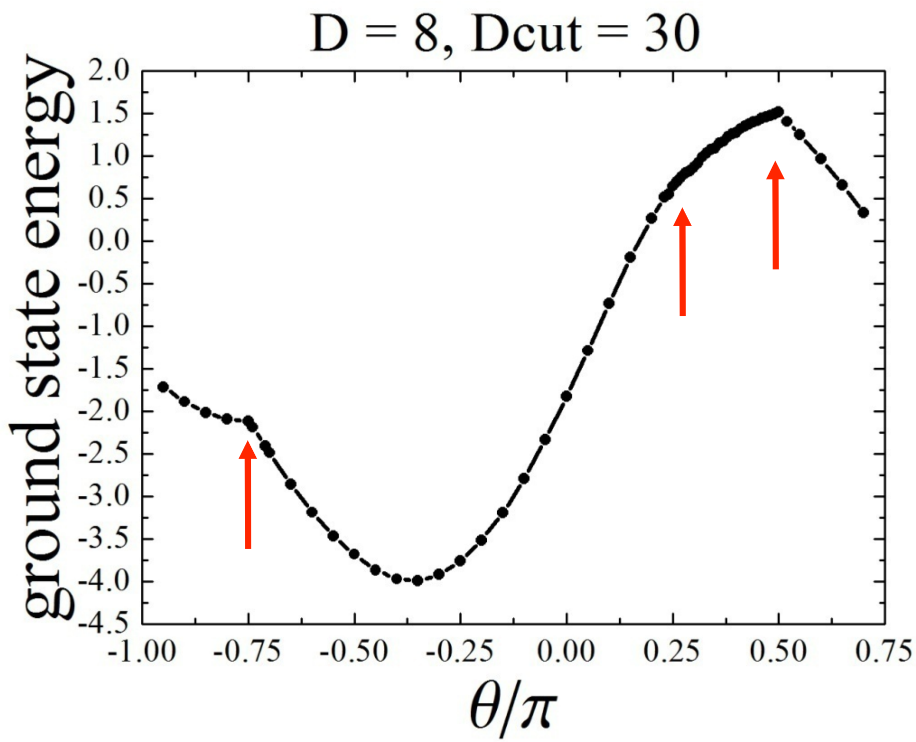
4^{th} order polynomial fit
M = 0.285

Monte Carlo:
M = 0.2681

Spin-1 Heisenberg Model with Biquadratic Interaction

$$\boxed{H = \sum_{\langle ij \rangle} \left[\cos\theta S_i \cdot S_j + \sin\theta \left(S_i \cdot S_j \right)^2 \right]}$$

✓ What is the phase diagram?



There are 3 phase transition points, 4 phases

Possible Order Parameters

✓ Ferromagnetic or antiferromagnetic order

✓ uniform or staggered quadrupole order $\boxed{\langle Q_i \cdot Q_j \rangle}$

$$\boxed{\langle Q \rangle = \begin{pmatrix} \langle Q_{z^2} \rangle \\ \langle Q_{x^2-y^2} \rangle \\ \langle Q_{xy} \rangle \\ \langle Q_{xz} \rangle \\ \langle Q_{yz} \rangle \end{pmatrix} = \begin{pmatrix} \langle S_z^2 \rangle \\ \langle S_x^2 - S_y^2 \rangle \\ \langle S_x S_y \rangle \\ \langle S_x S_z \rangle \\ \langle S_y S_z \rangle \end{pmatrix}}$$

$$\boxed{Q_i \cdot Q_j = 2\left(S_i \cdot S_j\right)^2 + S_i \cdot S_j - \frac{8}{3}}$$

Quadrupole Hamiltonian

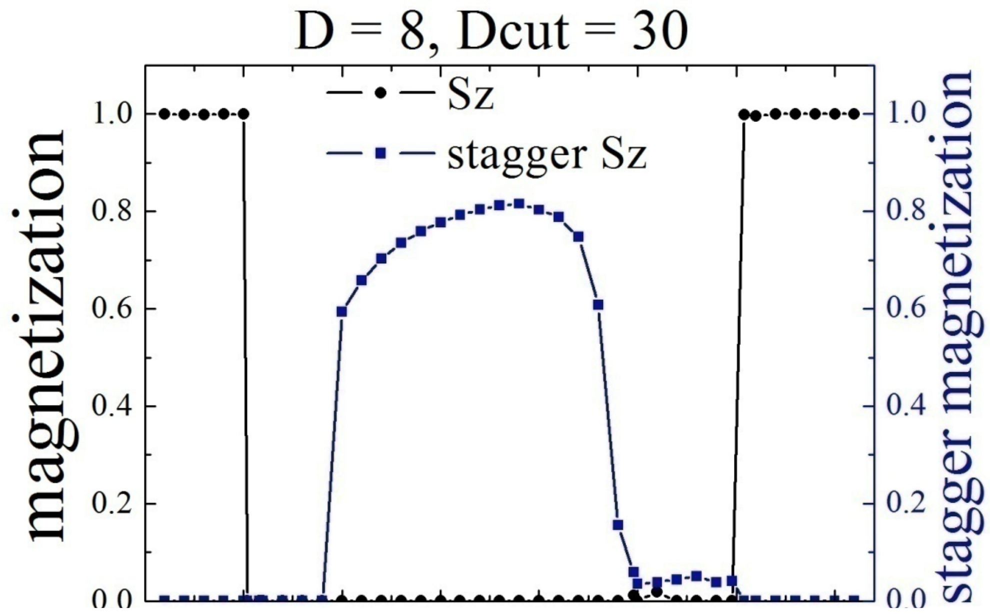
$$H = \sum_{\langle ij \rangle} \left[\left(J_1 - \frac{J_2}{2} \right) \left(S_i \cdot S_j \right) + \frac{J_2}{2} \left(Q_i \cdot Q_j \right) \right]$$

$$J_1 = \cos\theta$$

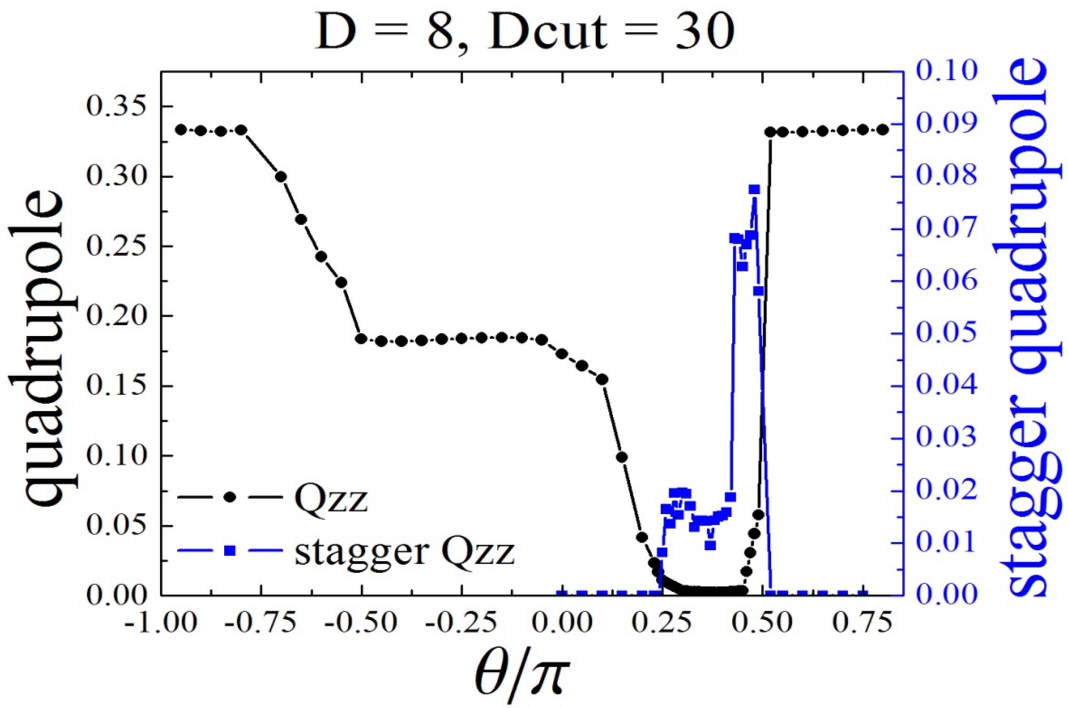
$$J_2 = \sin\theta$$

Pure quadrupole Hamiltonian for $J_1 = J_2 / 2$ ($\theta \sim 0.35\pi$)

- uniform quadrupole, if $J_2 < 0$
- staggered quadrupole, if $J_2 > 0$



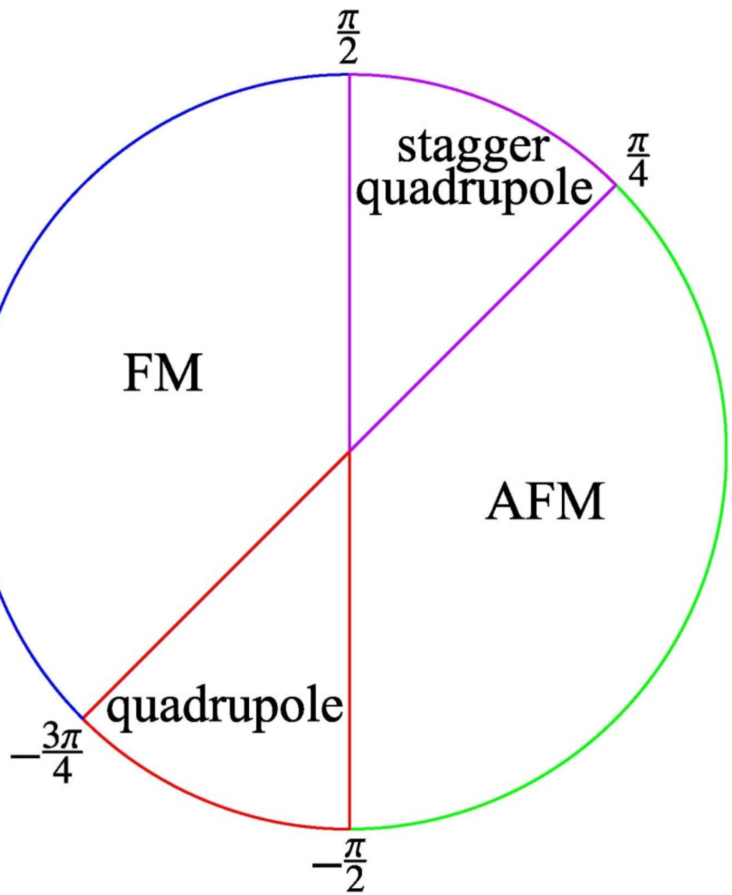
Uniform and staggered magnetization



Uniform and staggered quadrupole order

Phase Diagram

$$H = \sum_{\langle ij \rangle} \left[\cos\theta S_i \cdot S_j + \sin\theta \left(S_i \cdot S_j \right)^2 \right]$$



Summary

An accurate and efficient numerical method for evaluating tensor network states in 2D (either finite or infinite) is introduced. It contains two parts

1. SRG: the second normalization of tensor network state

   for determining the partition function of classical statistical models or the expectation values of quantum tensor network states

2. The entanglement projection method

   for determining quantum tensor network wavefunctions

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