テンソルネットワークによる情報圧縮と物性物理への応用

東大理, JST さきがけ　大久保毅

Contents

- Huge data in physics
- Information compression
  - Basics: singular value decomposition
  - Tensor network renormalization
  - Tensor network quantum states
- Applications
- Summary and outlook

Contents

Huge data in physics

Many-body problems in physics

- Celestial movement
- Gases, Liquids
- Molecules, Polymers (eg. Proteins), ...
- Electrons in molecules and solids
- Elemental particles (Quantum Chromo Dynamics)

In these problems, "systems" contain huge degrees of freedoms:

$6N$-dimensional phase space for classical mechanics

$O(e^N)$-dimensional Hilbert space for quantum systems

(Classical) statistical mechanics

Canonical ensemble:

Γ : State (e.g. $\{S_1, S_2, \dots S_L\}$)

$P(\Gamma)$: Probability to appear state Γ

$$P(\Gamma) \propto e^{-\beta \mathcal{H}(\Gamma)}$$

$\beta = \dfrac{1}{k_B T}$: Inverse temperature

$\mathcal{H}$: Hamiltonian (Energy)

Partition function（分配関数）

＝Normalization factor of the canonical ensemble

$$Z = \sum_{\Gamma} e^{-\beta \mathcal{H}(\Gamma)}$$

Relation to the free energy in thermodynamics

$$F = -k_B T \ln Z$$

If we can calculate Z, we can easily estimate thermodynamic properties.

Expectation value in canonical ensemble

Expectation value of O: $\langle O \rangle \equiv \frac{1}{Z} \sum_{\Gamma} O(\Gamma) e^{-\beta \mathcal{H}(\Gamma)}$

$$\boxed{\begin{array}{c}\text{Expectation value of physical quantity} \\ \longleftrightarrow \text{Macroscopic physical quantities observed in thermodynamics}\end{array}}$$

We can calculate thermodynamic quantities form microscopic model,
if we can calculate the sum of all states

Real problems : $\sum_{\Gamma}$ is too huge to calculate exactly $\|\Gamma\| \sim e^N$

(Even if we use super computer)

Standard procedures: MD or MC samplings

Quantum systems

Quantum system: governed by Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$$

$\mathcal{H}$:Hamiltonian (Energy)

$|\Psi\rangle$:Wave function (state vector)

Inner product:

$$(|a\rangle, |b\rangle) = \langle b|a\rangle$$

Nature: Elementary particles, e.g. electrons, obey quantum mechanics.

Static problems: Time-independent Schrödinger equation

$$\boxed{\mathcal{H}|\Psi\rangle = \underbrace{E}_{\text{Energy}}|\Psi\rangle}$$

= Eigenvalue problem

Quantum many-body systems

Example of quantum system: Array of quantum bits

1 bit — A quantum bit is represented by two basis vectors.

$$|0\rangle, |1\rangle \quad \text{or} \quad (|\uparrow\rangle, |\downarrow\rangle)$$

2 bits — The Hilbert space is spanned by four basis vectors.

$$|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle$$

Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$$|\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta}|\alpha\beta\rangle$$

$C_{\alpha,\beta}$:complex number

The Hamiltonian for 2 bits system can be represented in these bases.

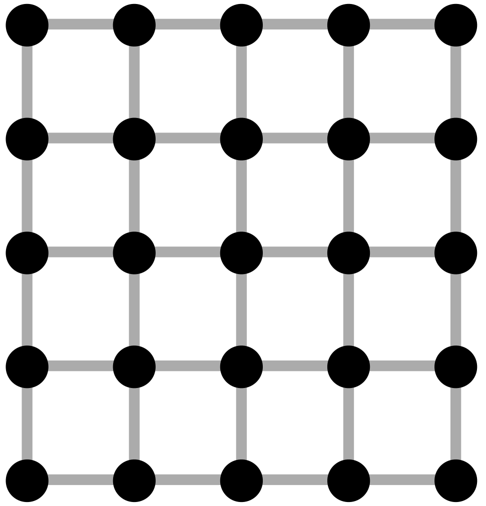
$$\mathcal{H} \to \begin{pmatrix} H_{0,0;0,0} & H_{0,0;0,1} & H_{0,0;1,0} & H_{0,0;1,1} \\ H_{0,1;0,0} & H_{0,1;0,1} & H_{0,1;1,0} & H_{0,1;1,1} \\ H_{1,0;0,0} & H_{1,0;0,1} & H_{1,0;1,0} & H_{1,0;1,1} \\ H_{1,1;0,0} & H_{1,1;0,1} & H_{1,1;1,0} & H_{1,1;1,1} \end{pmatrix}$$

Matrix element: $H_{\alpha,\beta;\alpha',\beta'} \equiv \langle\alpha\beta|\mathcal{H}|\alpha'\beta'\rangle$

Quantum many-body systems

Example of quantum system: Array of quantum bits

N bits: Dimension of the Hilbert space $= 2^N$



➡ Hamiltonian is $2^N \times 2^N$ matrix

Need to solve eigenvalue problem of huge matrix!

In physics,

- We often interested in the "ground state" (smallest eigenvalue)

基底状態

➡ We can concentrate to a special state.

- Typical system only has "short range" interactions

➡ Hamiltonian matrix becomes sparse.

Information compression by tensor network

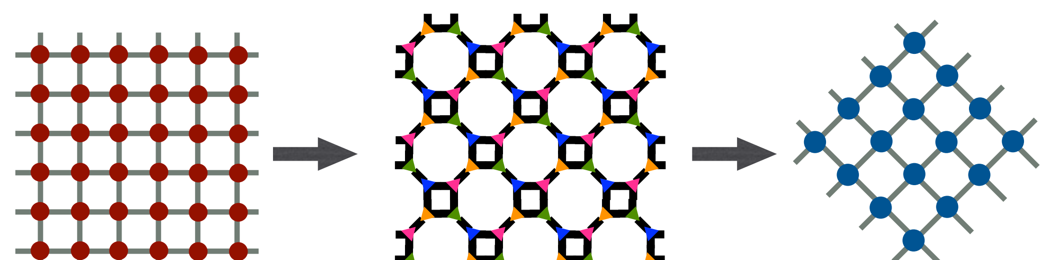
How can we treat and calculate such e^N data in numerics?

One of the methods is an approximate information compression by **tensor network representations**

Calculation of the partition function:

$$Z = \sum_{\Gamma} e^{-\beta \mathcal{H}(\Gamma)}$$

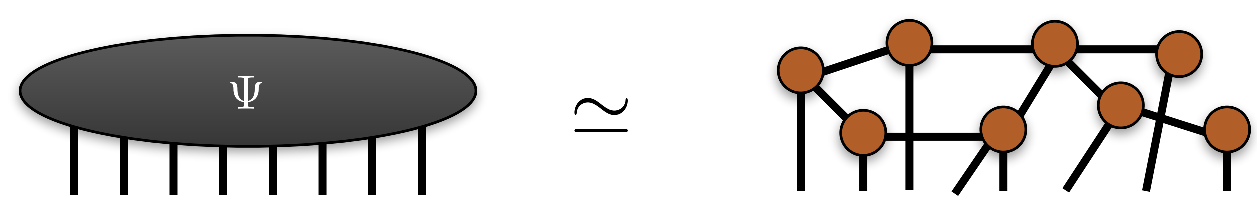
- Tensor network representation of Z
- Approximated contraction of it trough a coarse graining

$Z =$ 

Eigen value problem:

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

- Tensor network representation of an eigenvector
- Variational optimization of it



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Singular value decomposition (SVD)

Singular value decomposition (SVD):

Any matrices are uniquely decomposed as $A = \underbrace{U}_{U : M \times M}\Sigma\underbrace{V}_{V : N \times N}^\dagger$

$$A : M \times N$$

$$A_{ij} \in \mathbb{C}$$

$U : M \times M$ **Unitary**

$V : N \times N$ **Unitary**

$$\Sigma = \begin{pmatrix} \Sigma_{r\times r} & 0_{r\times(N-r)} \\ 0_{(M-r)\times r} & 0_{(M-r)\times N-r} \end{pmatrix}$$

$\boxed{\textbf{\textit{r}=rank(\textit{A})}}$

$$\Sigma_{r\times r} = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{pmatrix}$$

Diagonal matrix with
non-negative real elements

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

Singular values

Amount of data in SVD representation

$$A : M \times N$$

$$A = U\Sigma V^\dagger = U \begin{pmatrix} \Sigma_{r\times r} & 0_{r\times(N-r)} \\ 0_{(M-r)\times r} & 0_{(M-r)\times N-r} \end{pmatrix} V^\dagger$$

$$\boxed{\begin{aligned} U &= (\vec{u}_1, \vec{u}_2, \cdots, \vec{u}_M) \\ V &= (\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_N) \end{aligned}}$$

neglect zero singular values

$$= \bar{U}\Sigma_{r\times r}\bar{V}^\dagger$$

$$\bar{U} : M \times r, \bar{V}^\dagger : r \times N$$

$$\boxed{\begin{aligned} \bar{U} &= (\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r) \\ \bar{V} &= (\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_r) \end{aligned}}$$

If rank(A) is much smaller than M and N,

$$r \ll M, N$$

we can reduce the data to represent A.

(At this stage, no data loss)

Low rank approximation by SVD

Consider a matrix obtained by neglecting smaller singular values

$$A = \bar{U}\Sigma_{r\times r}\bar{V}^{\dagger} \quad \Rightarrow \quad \tilde{A} = \tilde{U}\Sigma_{k\times k}\tilde{V}^{\dagger} \qquad (k < r)$$

$$\boxed{\begin{aligned}\Sigma_{r\times r} &= \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)\\ \bar{U} &= (\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_r)\\ \bar{V} &= (\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_r)\end{aligned}}$$

$$\boxed{\begin{aligned}\Sigma_{k\times k} &= \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)\\ \tilde{U} &= (\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_k)\\ \tilde{V} &= (\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_k)\end{aligned}}$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

$$\mathrm{rank}(A) = r$$

Keep the largest k singular values
(and corresponding singular vectors).

$$\mathrm{rank}(\tilde{A}) = k < r$$

This approximation is one of the best low rank approximation.

$$\min\{\|A - B\|_F : \mathrm{rank}(B) = k\} = \sqrt{\sum_{i=k+1}^{\min(N,M)} \sigma_i^2} = \|A - \tilde{A}\|_F$$

Image compression: grayscale image

Image: 1024 × 768 pixels

768 x1024 matrix A

$$\mathrm{rank}(A) = 768$$

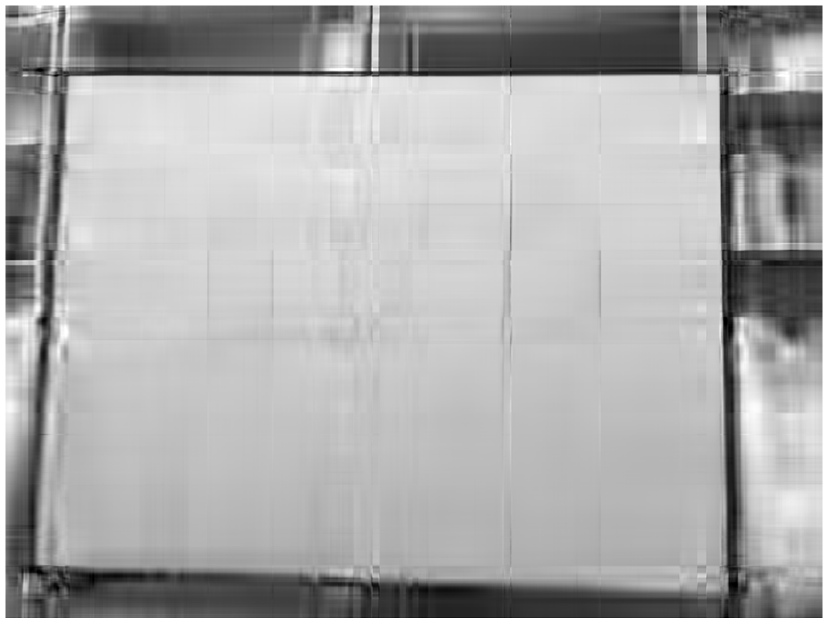
Amount of data=786,432

Perform SVD of A: $A = U\Sigma V^\dagger$

$\mathrm{rank}(\chi)$ approximation

Amount of data=(768 +1024 + 1)×χ

Image compression: grayscale image



Rank: $\chi = 768$ $\chi = 100$ $\chi = 10$

Data: **786,432** **179,300** **179,30**

(Original)

Scalar, Vector, Matrix, Tensor,...

i

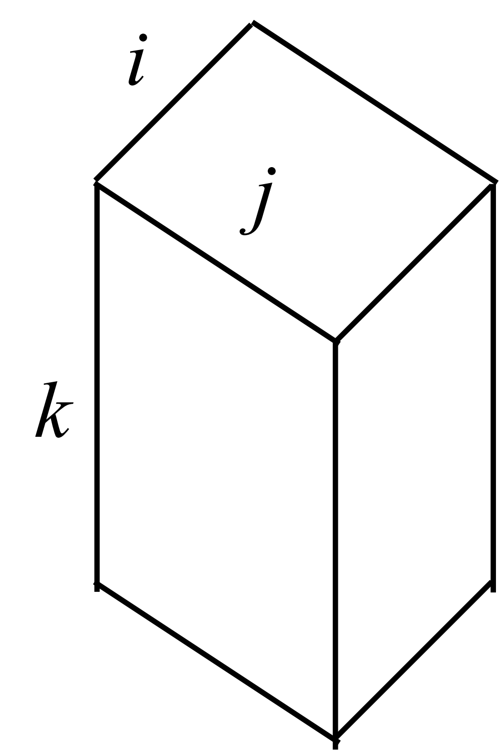
Scalar: c — Number

Vector: v_i — One dimensional array of numbers

Matrix: M_{ij} — Two dimensional array of numbers

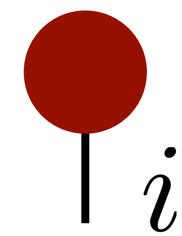
Tensor: $T_{ijk\ldots}$ — Higher dimensional array of numbers

Scalar: 0-dim. tensor
Vector: 1-dim. tensor
Matrix: 2-dim. tensor

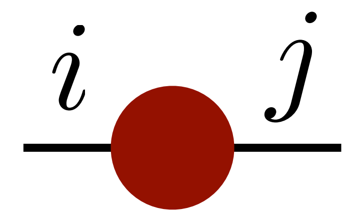


Graphical representations for tensor network

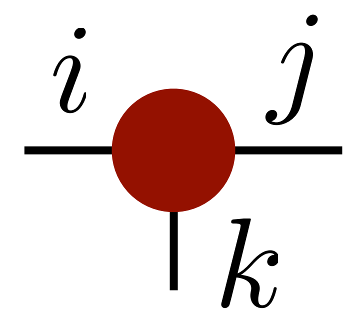
- Vector $\vec{v}$: v_i



- Matrix M : $M_{i,j}$

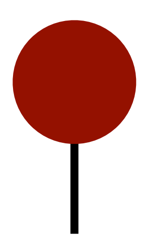
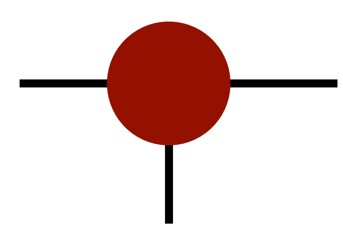


- Tensor T : $T_{i,j,k}$



*** n-rank tensor = n-leg object**

When indices are not presented in a graph, it represent a tensor itself.

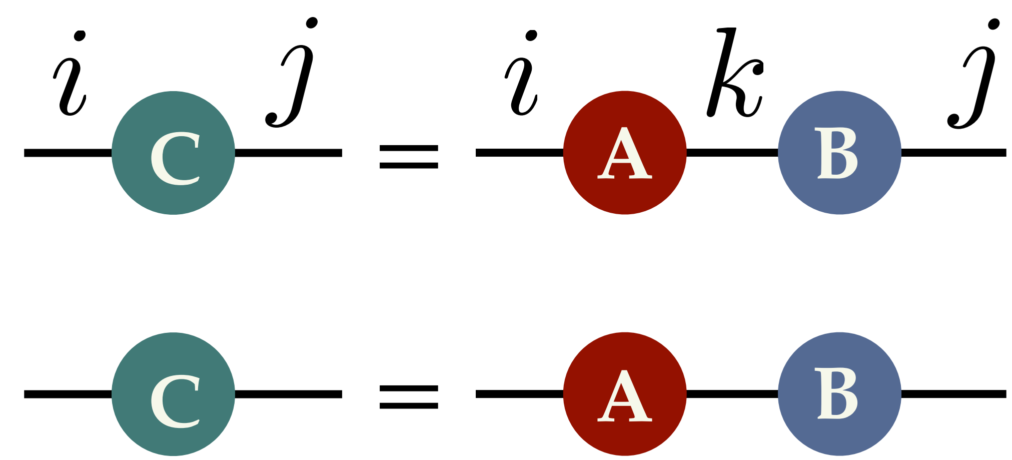
$\vec{v} =$  $T =$ 

Graphical representations for tensor network

Matrix product

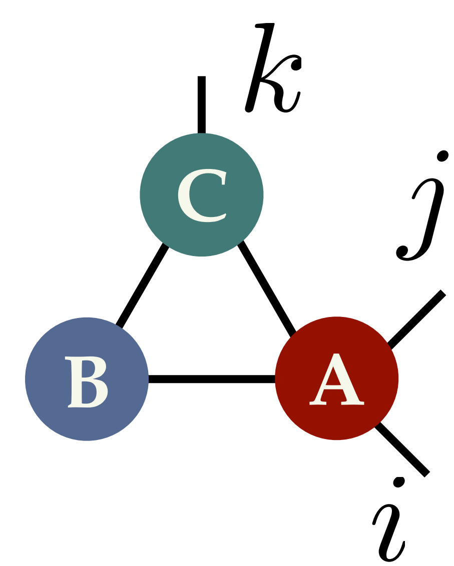
$$C_{i,j} = (AB)_{i,j} = \sum_k A_{i,k} B_{k,j}$$

$$C = AB$$



Generalization to tensors

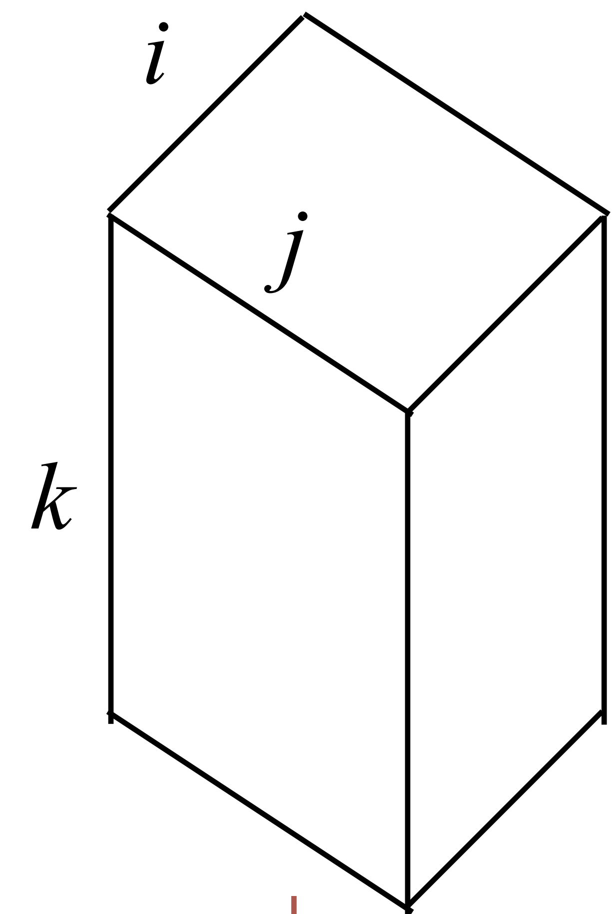
$$\sum_{\alpha,\beta,\gamma} A_{i,j,\alpha,\beta} B_{\beta,\gamma} C_{\gamma,k,\alpha}$$



Contraction of a network = **Calculation of a lot of multiplications**

Low rank approximation: generalization to tensor

Tensor: $T_{ijk\ldots}$

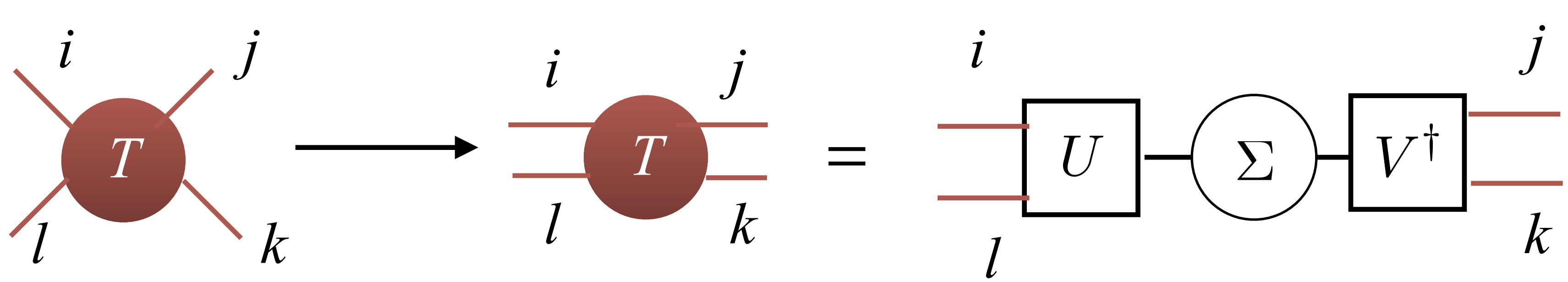


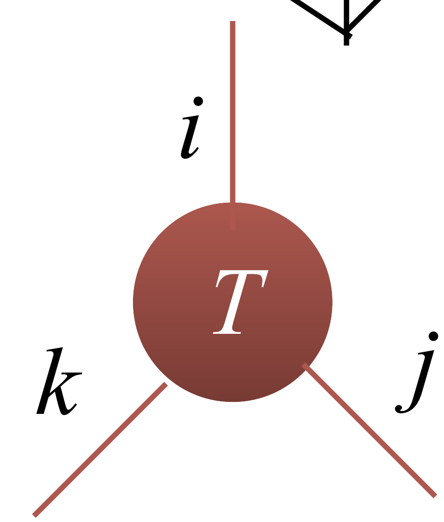
Naive application of SVD:

Make a matrix by dividing indices into two parts.

$$T_{ijkl} \to T_{(il),(jk)}$$

Then apply SVD (and low rank approximation).





Note: The result depends on the initial mapping to a matrix.

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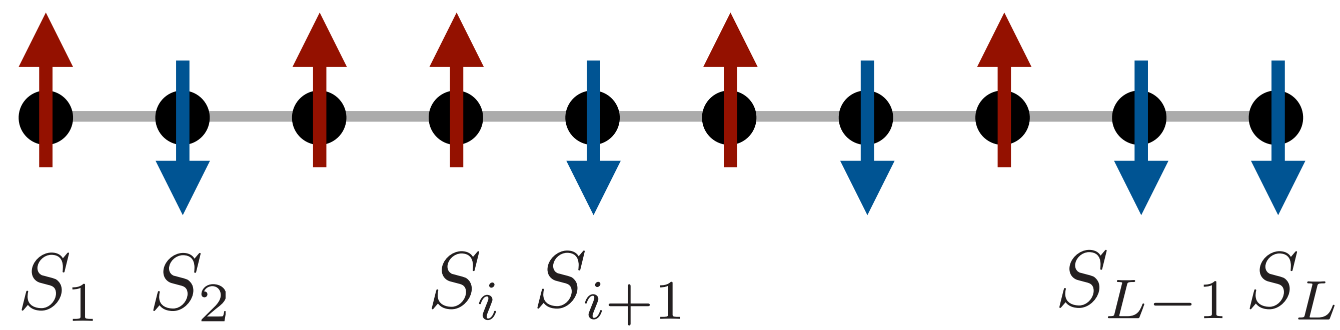
Tensor network representation of partition function

Classical Ising model on a chain



$$\mathcal{H} = -J \sum_{i=1}^{L-1} S_i S_{i+1}$$

$$S_i = 1, -1$$

$$1 = \uparrow \qquad -1 = \downarrow$$

Partition function:

$$Z = \sum_{\{S_i = \pm 1\}} e^{\beta J \sum_i S_i S_{i+1}}$$

$$= \sum_{\{S_i = \pm 1\}} \prod_{i=1}^{L-1} e^{\beta J S_i S_{i+1}}$$

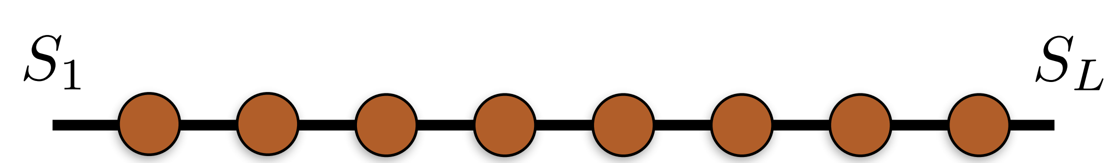
$$= \sum_{S_1 = \pm 1, S_L = \pm 1} \left(T^{L-1}\right)_{S_1, S_L}$$

Transfer matrix
(転送行列)

$$T_{S_i, S_{i+1}} = e^{\beta J S_i S_{i+1}}$$

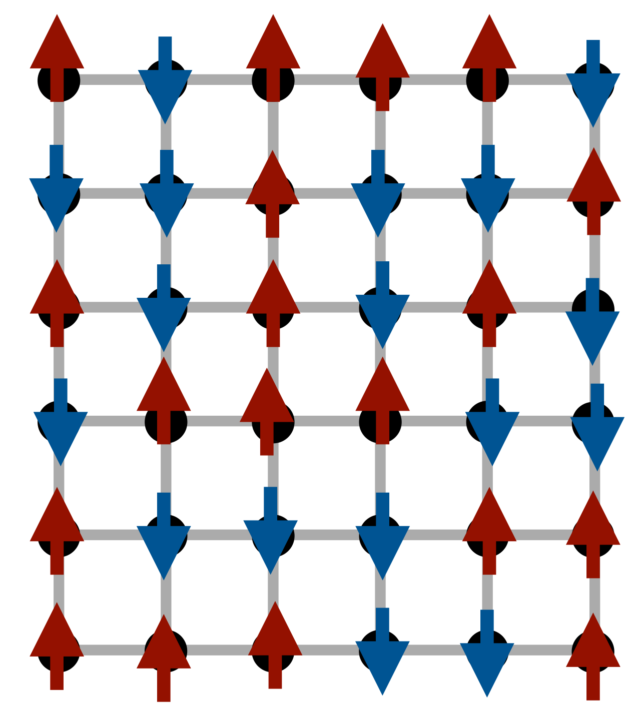
$$T = \begin{array}{cc} +1 & -1 \\ \end{array}$$
$$T = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \begin{array}{c} +1 \\ -1 \end{array}$$

$$\sum_{S_1 = \pm 1, S_L = \pm 1}$$



Tensor network representation in two dimension

Classical Ising model on the square lattice



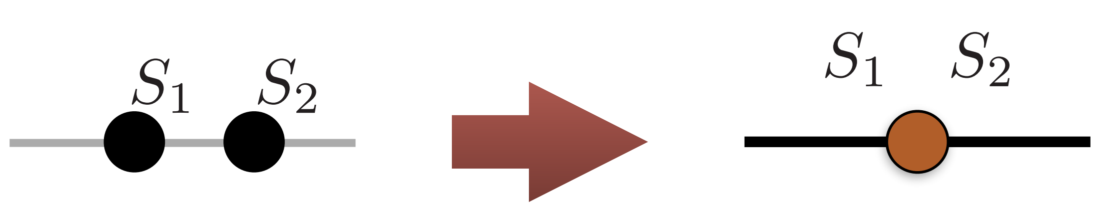
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j \quad (S_i = \pm 1 = \uparrow, \downarrow)$$

$$Z = \sum_{\{S_i = \pm 1\}} e^{\beta J \sum_{\langle i,j \rangle} S_i S_j}$$

We can use a tensor instead of the transfer matrix.

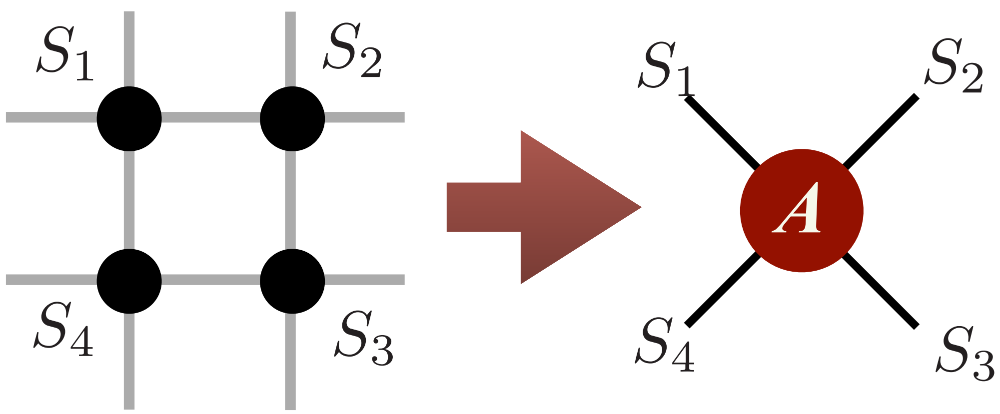
$$e^{\beta J S_1 S_2} = T_{S_1 S_2}$$

Tensor?

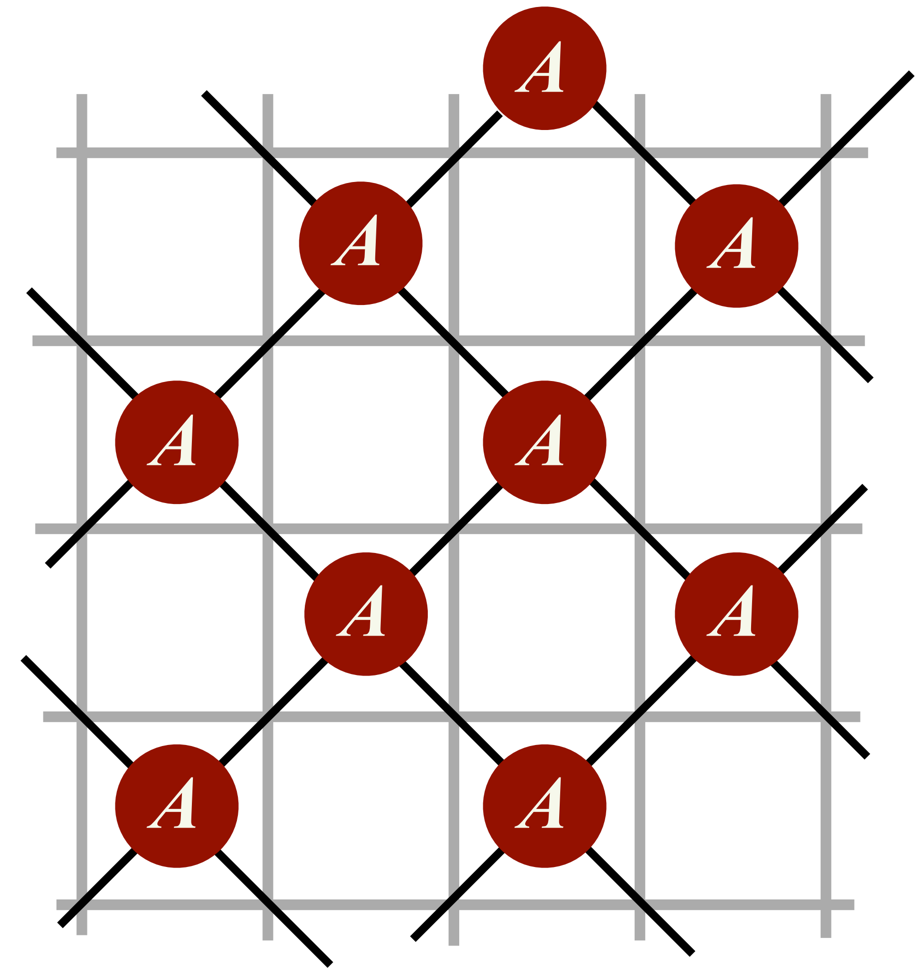


Tensor network representation in two dimension

$$e^{\beta J(S_1S_2+S_2S_3+S_3S_4+S_4S_1)} = A_{S_1S_2S_3S_4}$$



$Z =$



Partition function = Tensor network of tensor A

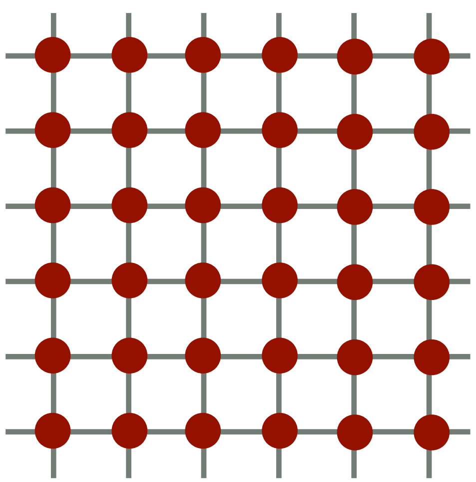
Square lattice Ising model→Square lattice tensor network rotating 45 degrees.

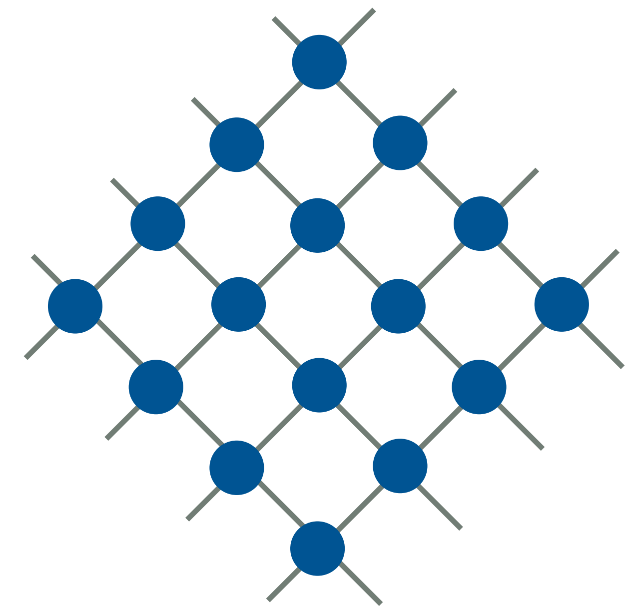
*We can construct a tensor network where tensors are on the nodes of original lattice.

Outline of tensor network renormalization

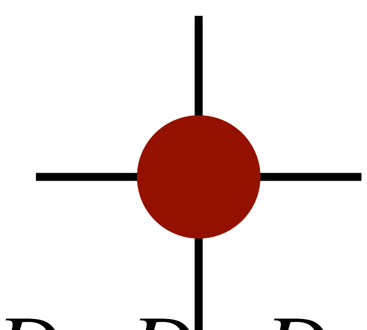
Scaler represented by $L \times L$ tensors

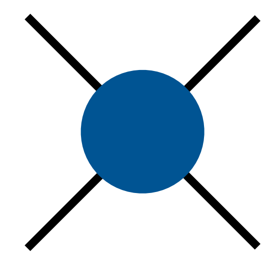
$(L \times L)/2$ tensors





Corse graining (Renormalization) into $\sqrt{2}$ times longer scale.





A: $D \times D \times D \times D$

Approximation

$\tilde{A} : D \times D \times D \times D$

Reduce the number of tensors keeping their size constant

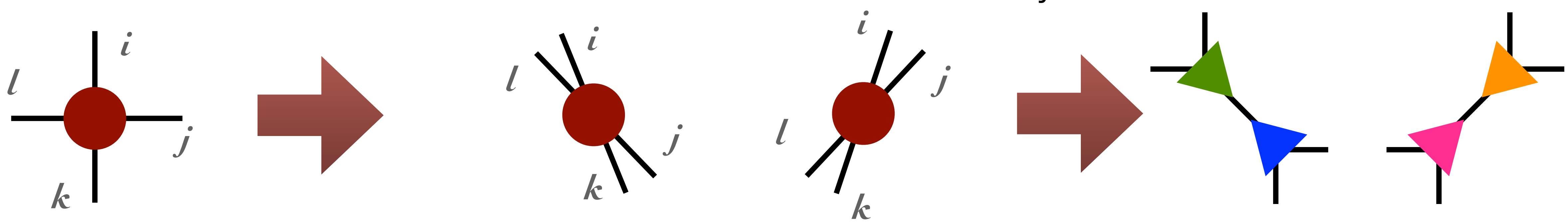
Recipe of Tensor Renormalization Group (TRG)

M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007)
Z.-C. Gu, M. Levin and X.-G. Wen, Phys. Rev. B **78**, 205116 (2008)

1. Decomposition

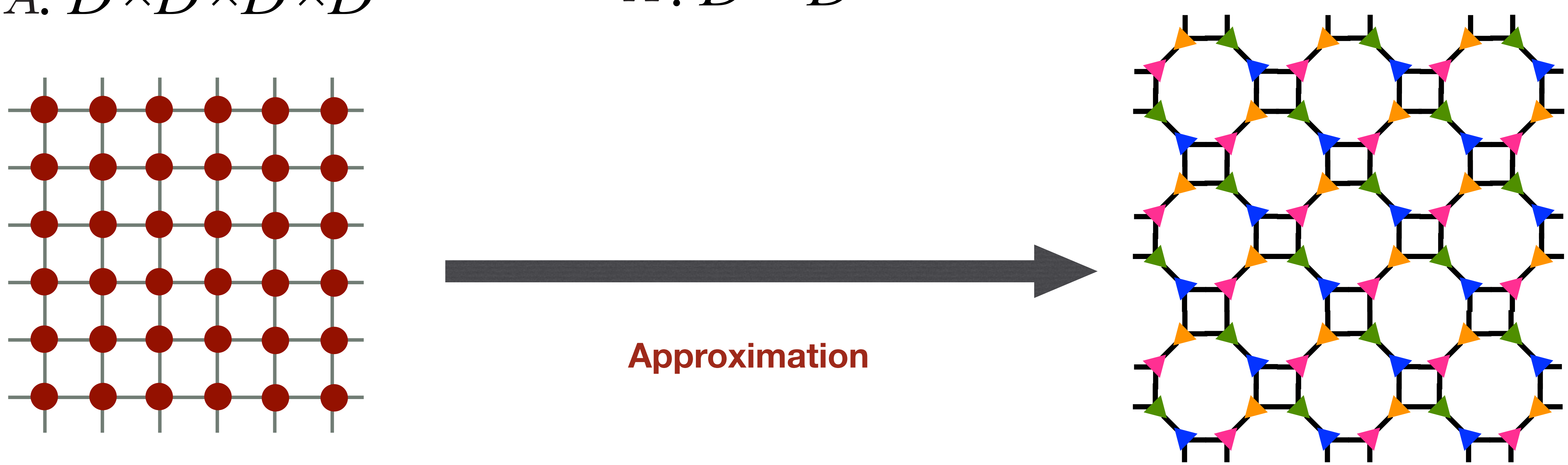
Regard a tensor as a matrix

D-rank approximation by SVD



$A_{i,j,k,l}$ $\quad$ $A_{(i,l),(j,k)}$ $\quad$ $A_{(i,j),(k,l)}$

A: $D \times D \times D \times D$ $\quad$ $A: D^2 \times D^2$



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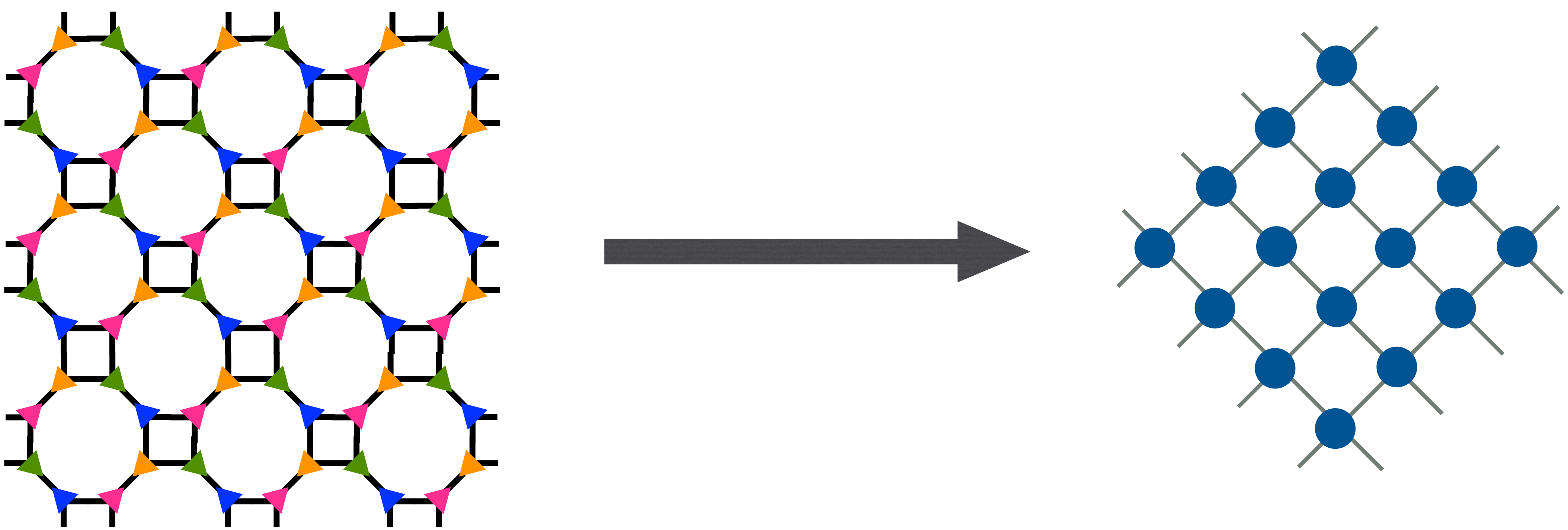
2. Coarse graining

$$\tilde{A} : D \times D \times D \times D$$

In total, two original tensors are coarse grained into a new tensor.



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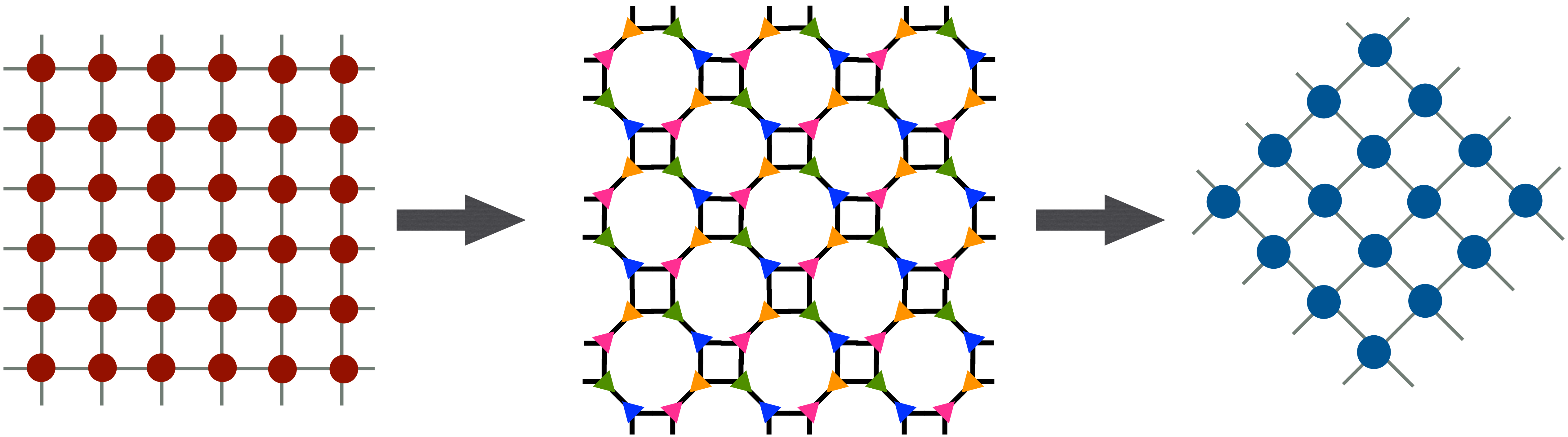


Calculation cost: SVD= $O(D^6)$

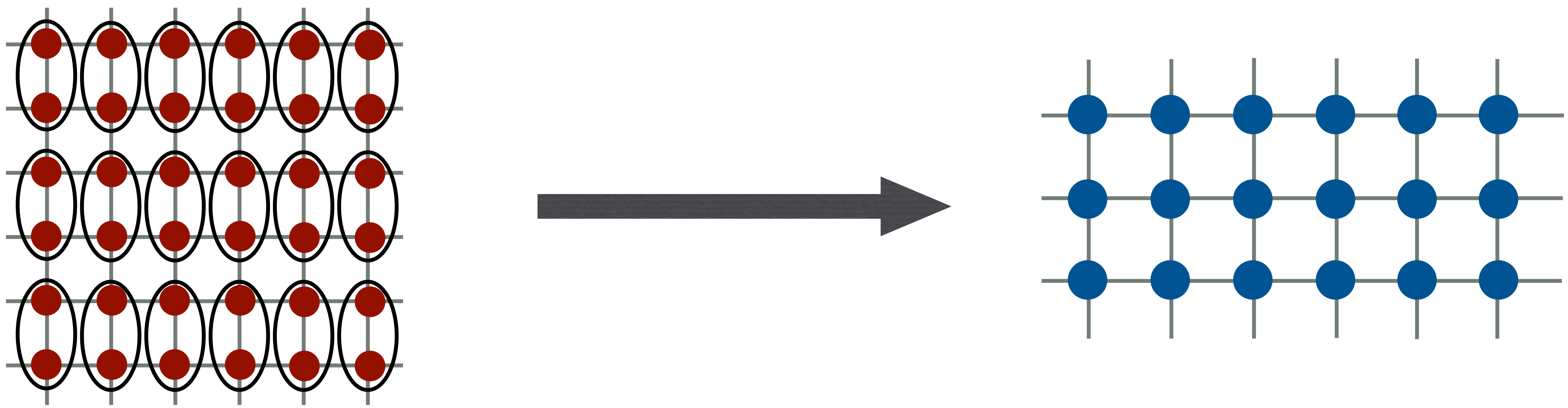
Contraction= $O(D^6)$ (per tensor)

*By one TRG step, # of tensors is reduced by 1/2.

We can calculate the contraction in polynomial cost!

HOTRG and Anisotropic TRG

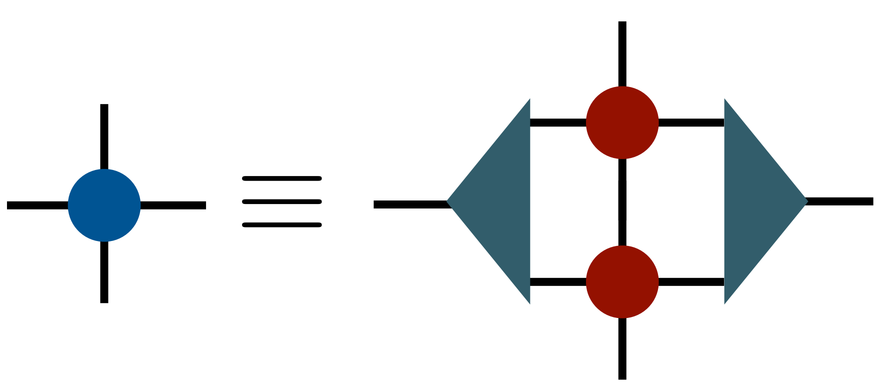
Coarse-graining tensors anisotropically:



This approach can be easily generalized to high dimensions.

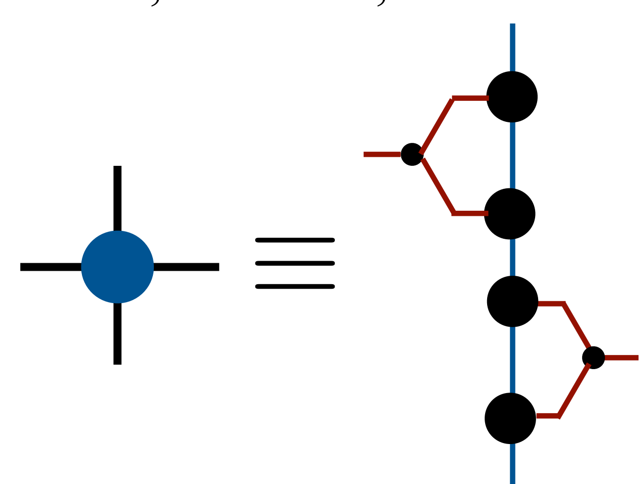
HOTRG $O(D^{4d-1})$

Z. Y. Xie *et a*l, Phys. Rev. B **86**, 045139 (2012)



ATRG $O(D^{2d+1})$

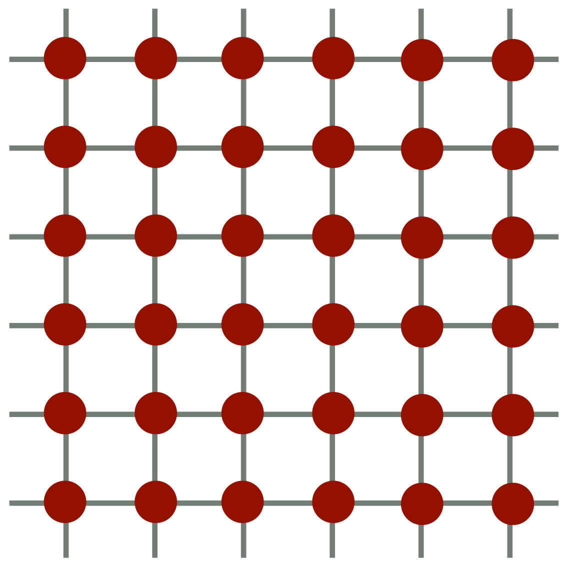
D. Adachi, T. Okubo, and S. Todo, arXiv:1906.02007



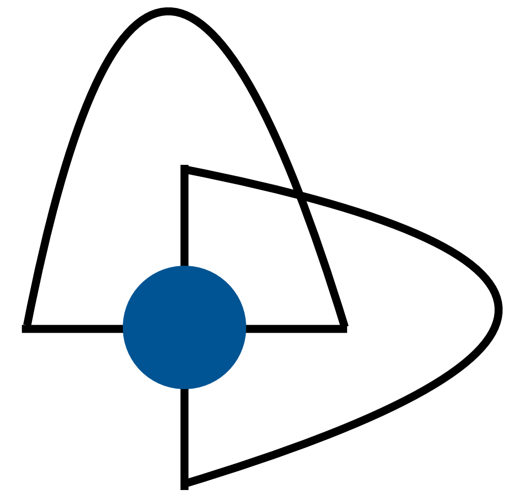
Application to a classical partition function

Partition function

(Periodic boundary condition)

$Z =$ 

Repeat TRG step until only a few tensors remain.



We can easily calculate physical quantities from Z.

Free energy: $F = -k_B T \ln Z$

Energy: $$E = -\frac{\partial \ln Z}{\partial \beta}$$

Specific heat: $$C = \frac{1}{k_B T^2}\frac{\partial^2 \ln Z}{\partial \beta^2}$$

(Use difference approximation or auto differentiation)

H.-J. Liao *et a*l, Phys. Rev. X **9**, 031041(2019)

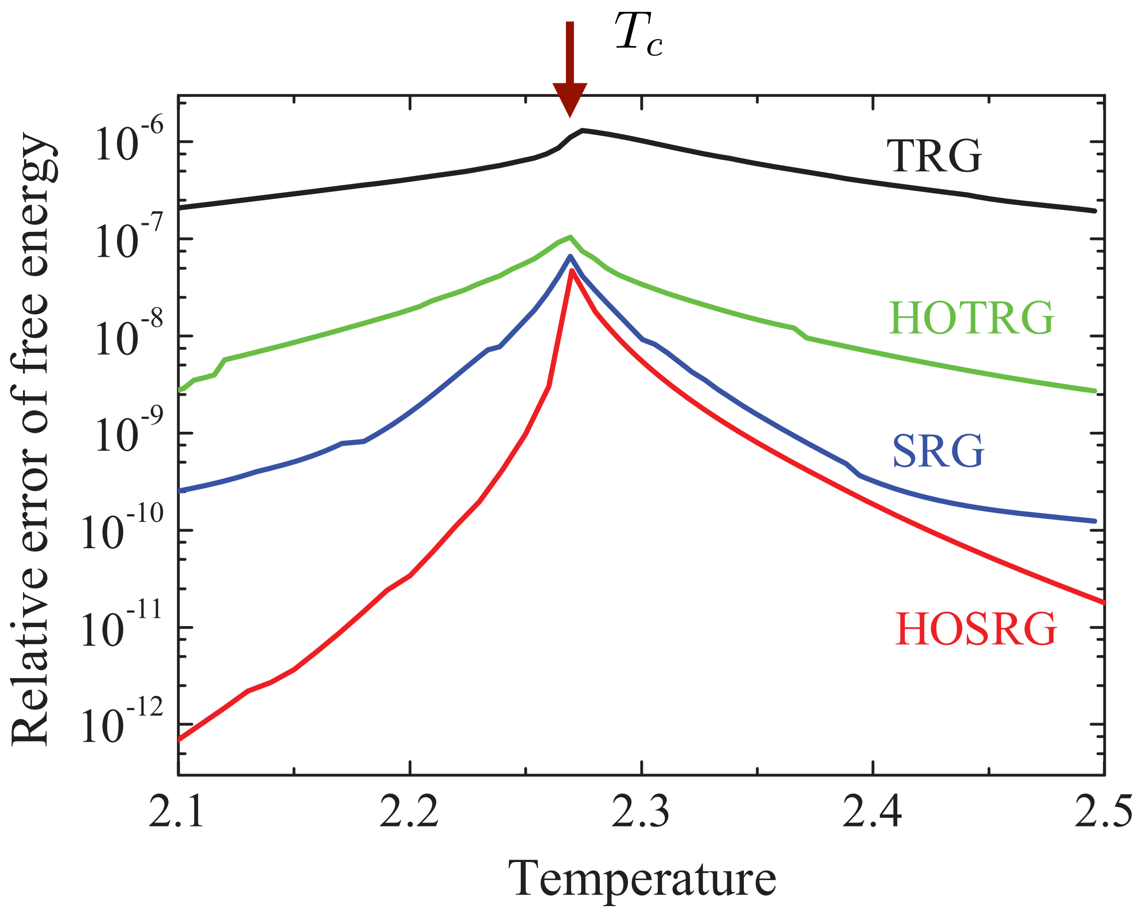
Example of calculation

Ising model in infinite size

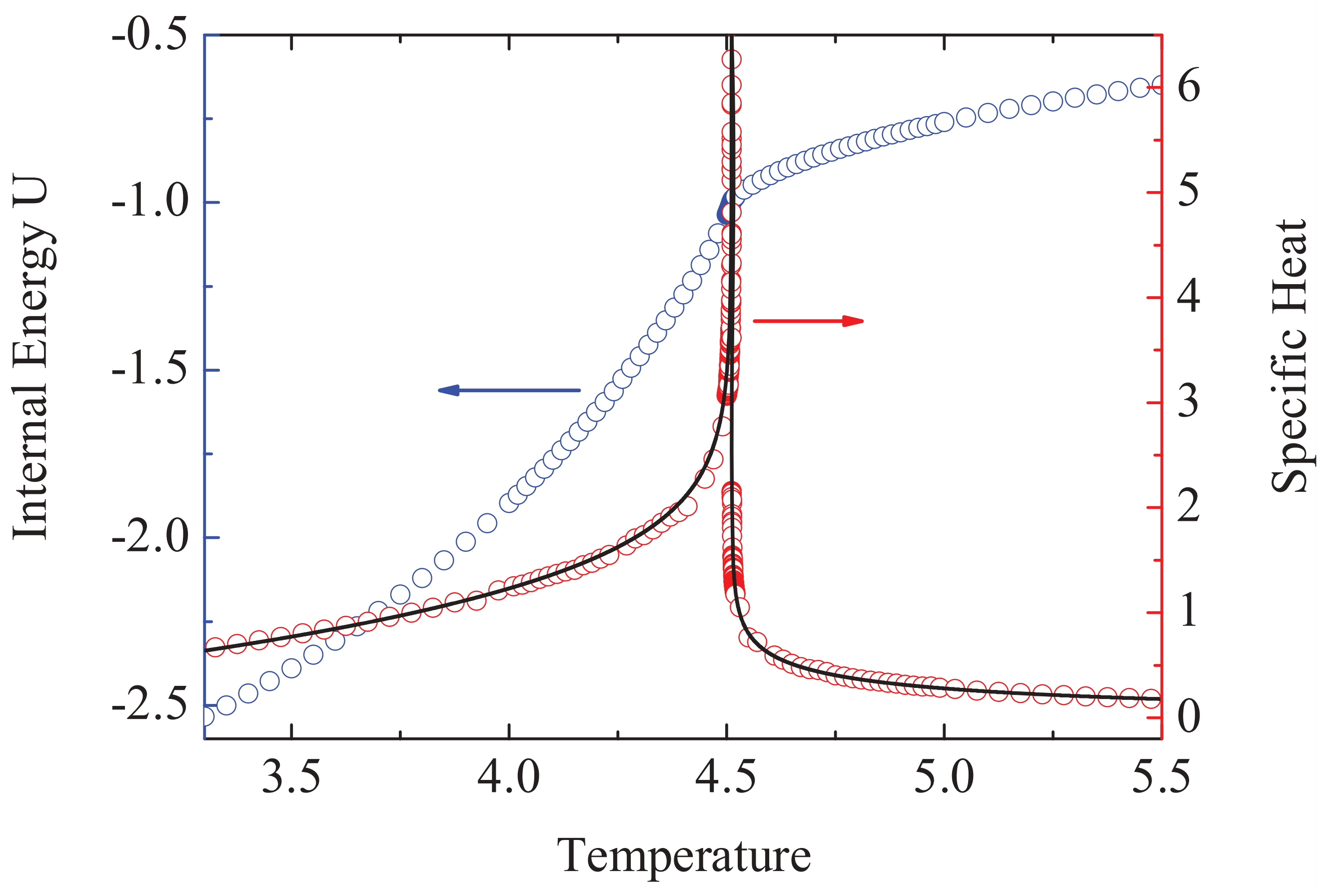
$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j$$

Z. Y. Xie *et al*, Phys. Rev. B **86**, 045139 (2012)

Error of free energy for 2D Ising model



Energy and specific heat of 3D Ising model



$$T_c/J = \frac{2}{\ln(1+\sqrt{2})} \simeq 2.269$$

Interesting topics in tensor network renormalization

- Try to find efficient algorithm to remove "short range" entanglement
  - TNR, Loop-TNR, GILT, Gauge fixing

TNR: G. Evenbly and G. Vidal, Phys. Rev. Lett. **115**, 180405 (2015)

Loop-TNR: S. Yang, Z.-C. Gu and , X.-G. Wen, Phys. Rev. Lett. **118**, 110504 (2017)

GILT: M. Hauru, C. Delcamp. S. Mizera Phys. Rev. B **97**, 045111 (2018)

Gauge fixing: G. Evenbly, Phys. Rev. B **98**, 085155 (2018)

- Application to lattice QCD
  - TRG with Grassmann algebra

Z.-C. Gu, F. Verstraete, and X.-G. Wen, arXiv:1004.2563

S. Takeda, and Y. Yoshimura PTEP **2015**, 043B1 (2015).

- Property at the criticality
  - Relation to Conformal invariance

G. Evenbly and G. Vidal,Phys. Rev. Lett. **115**, 200401 (2015)

G. Evenbly, Phys. Rev. B **95**, 045117 (2017)

Contents

- Huge data in physics
- Information compression
  - Basics: singular value decomposition
  - Tensor network renormalization
  - Tensor network quantum states
- Applications
- Summary and outlook

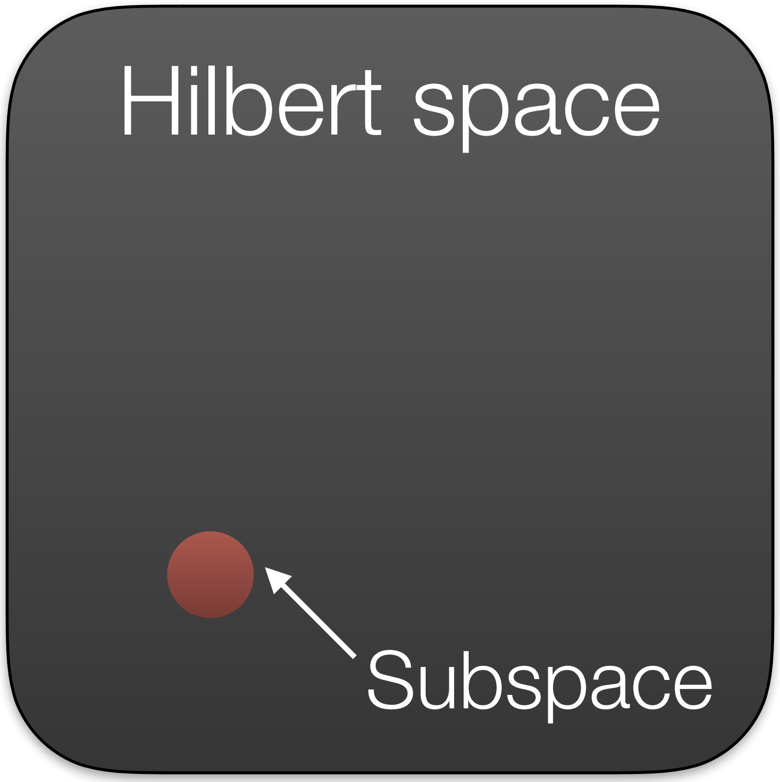
Information compression by tensor networks

We can not treat entire data in the present computers.

Try to reduce the "effective" dimension of (Hilbert) space

By considering proper subspace of the Hilbert space, we can represent a quantum state efficiently.

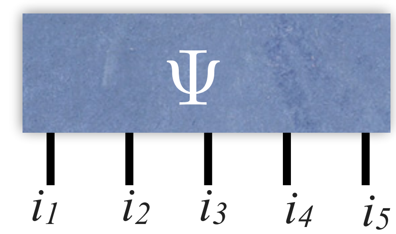
Tensor network quantum states!



Tensor network state

G.S. wave function: $|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$

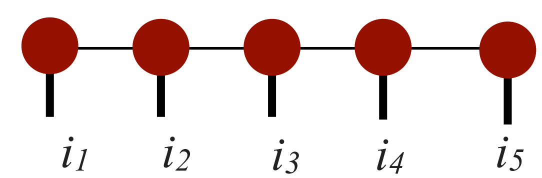
Vector (or N-rank tensor): $\Psi_{i_1 i_2 \ldots i_N}$ =



# of Elements = a^N

\`\`Tensor network" decomposition

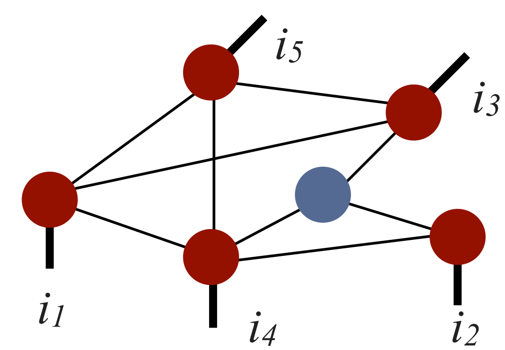
- Matrix Product State (MPS) $A_1[i_1]A_2[i_2]\cdots A_N[i_N]$ =



$A[m]$: Matrix for state m

- General network

$\mathrm{Tr}X_1[i_1]X_2[i_2]X_3[i_3]X_4[i_4]X_5[i_5]Y$



X,Y : Tensors

Tr : Tensor network contraction

By choosing a \`\`good" network, we can express G.S. wave function efficiently.

ex. MPS: # of elements $= 2ND^2$ D: dimension of the matrix A

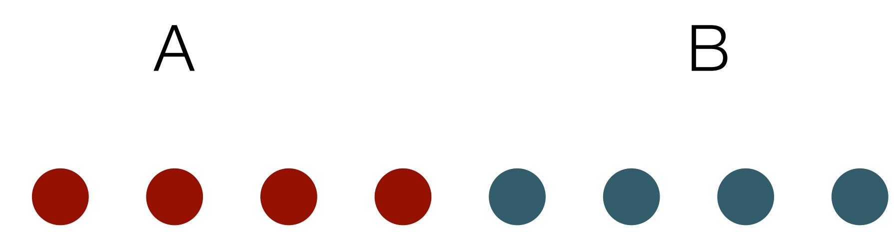
Exponential → Linear *If D does not depend on N…

Area law of the entanglement entropy

Entanglement entropy:

Reduced density matrix of a sub system (sub space):

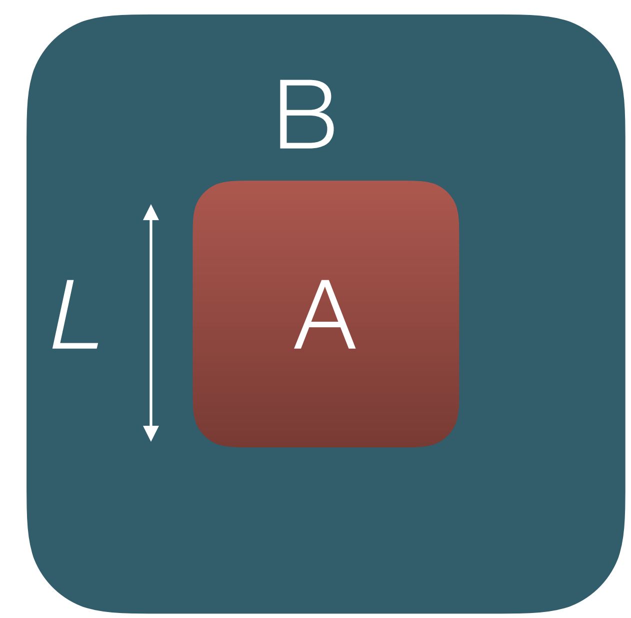
$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$$



Entanglement entropy = von Neumann entropy of ρ_A

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right)$$

General wave functions:



EE is proportional to its **volume (# of spins)**.

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right) \propto L^d$$

(c.f. random vector)

Ground state wave functions:

For a lot of ground states, EE is proportional to its area.

J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys, 277, **82** (2010)

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right) \propto L^{d-1}$$

Ground state are in a small part of the huge Hilbert space!

Matrix product state (MPS)

Good reviews:

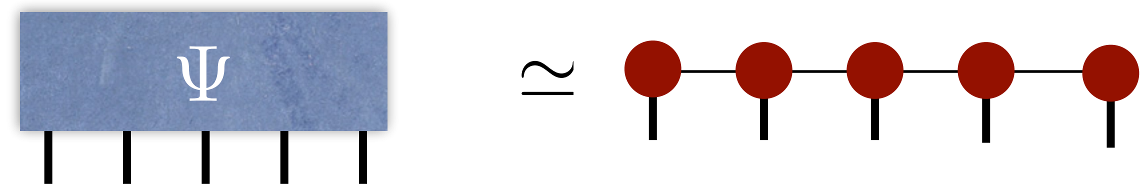
(U. Schollwöck, Annals. of Physics **326**, 96 (2011))
(R. Orús, Annals. of Physics **349**, 117 (2014))

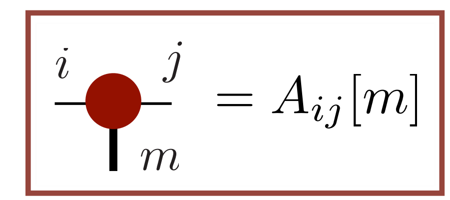
$$|\Psi\rangle = \sum_{\{i_1, i_2, \dots i_N\}} \Psi_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

$$\Psi_{i_1 i_2 \dots i_N} \simeq A_1[i_1] A_2[i_2] \cdots A_N[i_N]$$

$A[i]$: Matrix for state i

MPS





Note:

- MPS is called as "tensor train decomposition" in applied mathematics

(I. V. Oseledets, SIAM J. Sci. Comput. **33**, 2295 (2011))

- A product state is represented by MPS with 1×1 "Matrix" (scalar)

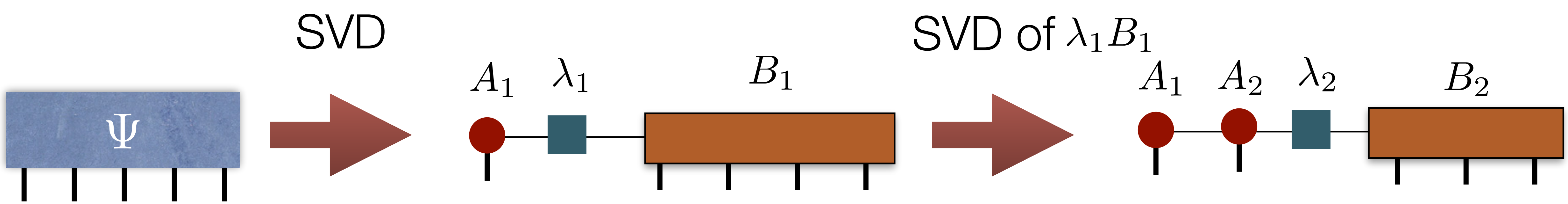
$$|\Psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots$$

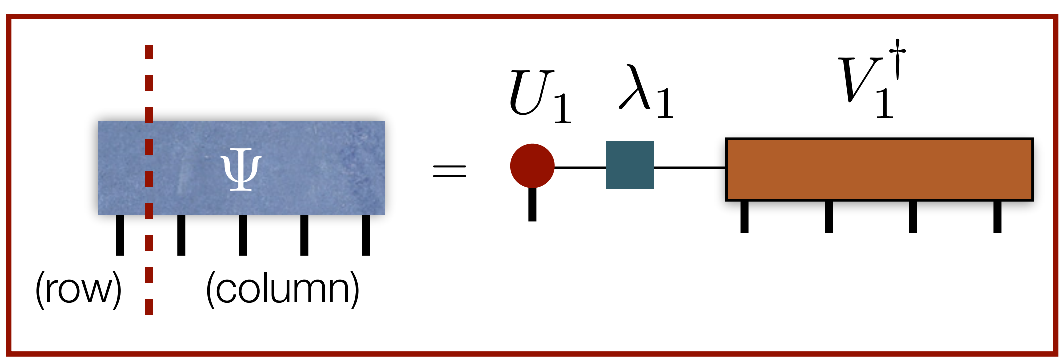
$$\Psi_{i_1 i_2 \dots i_N} = \phi_1[i_1] \phi_2[i_2] \cdots \phi_N[i_N]$$

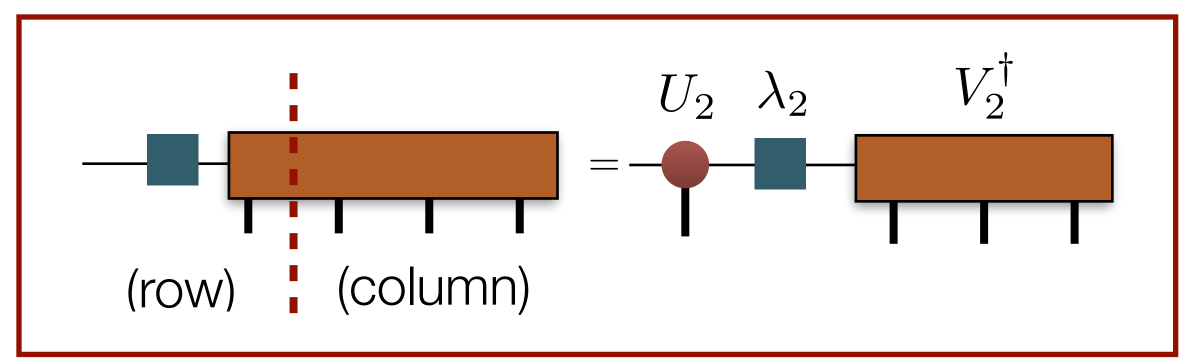
$$\phi_n[i] \equiv \langle i | \phi_i \rangle$$

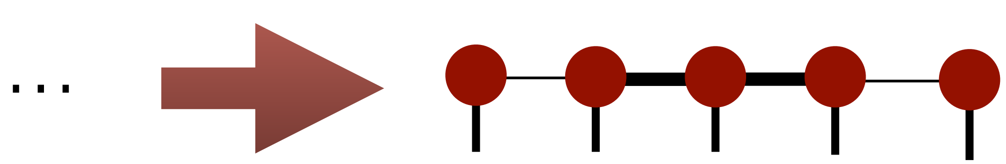
Matrix product state without approximation

General wave function (or vector) can be represented by MPS exactly through successive Schmidt decompositions







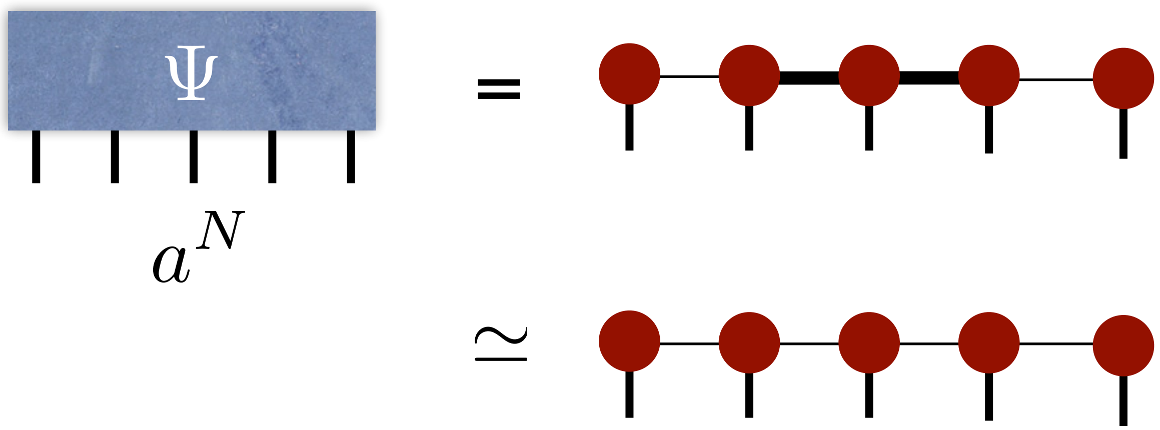


In this construction, the sizes of matrices depend on the position.

$\boxed{\text{Maximum bond dimension} = a^{N/2}}$

At this stage, **no data compression.**

Matrix product state: Low rank approximation



Maximum bond dimension = $a^{N/2}$

a^N

Constant bond dimension = χ

$\propto N a \chi^2$

If the entanglement entropy of the system is **O(1)** (independent of *N*), matrix size "χ" can be small for accurate approximation.

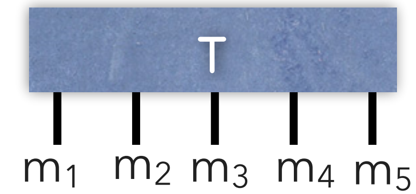
➡ MPS is good for gapped 1d systems.

On the other hand, if the EE increases as increase *N*, "χ" must be increased to keep the same accuracy.

Tensor Product State

$$|\Psi\rangle = \sum_{\{m_i=\uparrow\downarrow\}} T_{m_1,m_2,\cdots,m_N}|m_1,m_2,\cdots,m_N\rangle$$

N-rank tensor: $T_{m_1,m_2,\cdots,m_N}$ =



TPS (Tensor Product State) (AKLT, T. Nishino, K. Okunishi, …)

PEPS (Projected Entangled-Pair State)

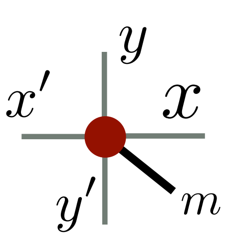
(F. Verstraete and J. Cirac, arXiv:cond-mat/0407066)

d-dimensional tensor network representation
for the wave function of a d-dimensional quantum system

$$|\Psi\rangle = \sum_{\{m_i=1,2,\cdots,m\}} \mathrm{Tr}\ A_1[m_1]A_2[m_2]\cdots A_N[m_N]|m_1m_2\cdots m_N\rangle$$

Tr: tensor network "contraction"

$A_{x_i x'_i y_i y'_i}[m_i]$: Rank 4+1 tensor

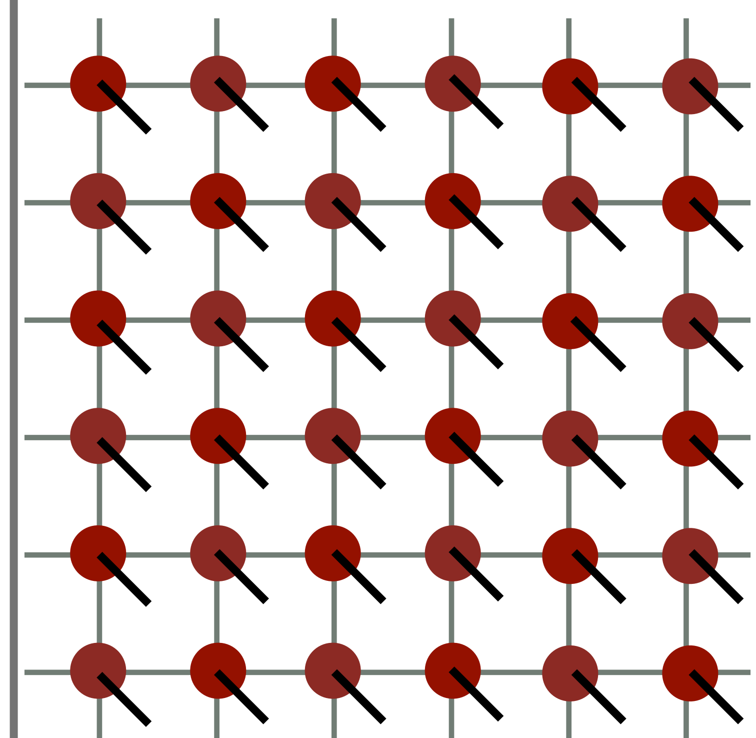


$x,y,x',y' = 1,2,\ldots D$ D = "bond dimension"

$m_i = 1,2,\ldots m$ m = dimension of the local Hilbert space

*D can be larger than m. "Virtual state "

TPS on square lattice



It satisfies the area low!

Enough large, but finite, D, a lot of G.S. can be represented by TPS

＊Finite D even for infinite system!

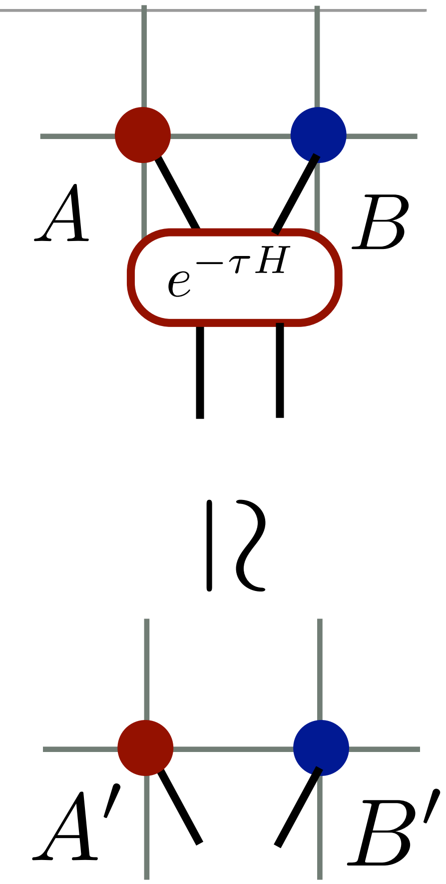
Variational calculation using TPS

(Typical) Optimization: **Imaginary time evolution**

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

Approximatin	Cost	information	Accuracy
Simple update	**O(D^5)**	local	bad
Full update	**O(D^{10})**	global	better

We repeat updates about 10^3~ 10^5 steps



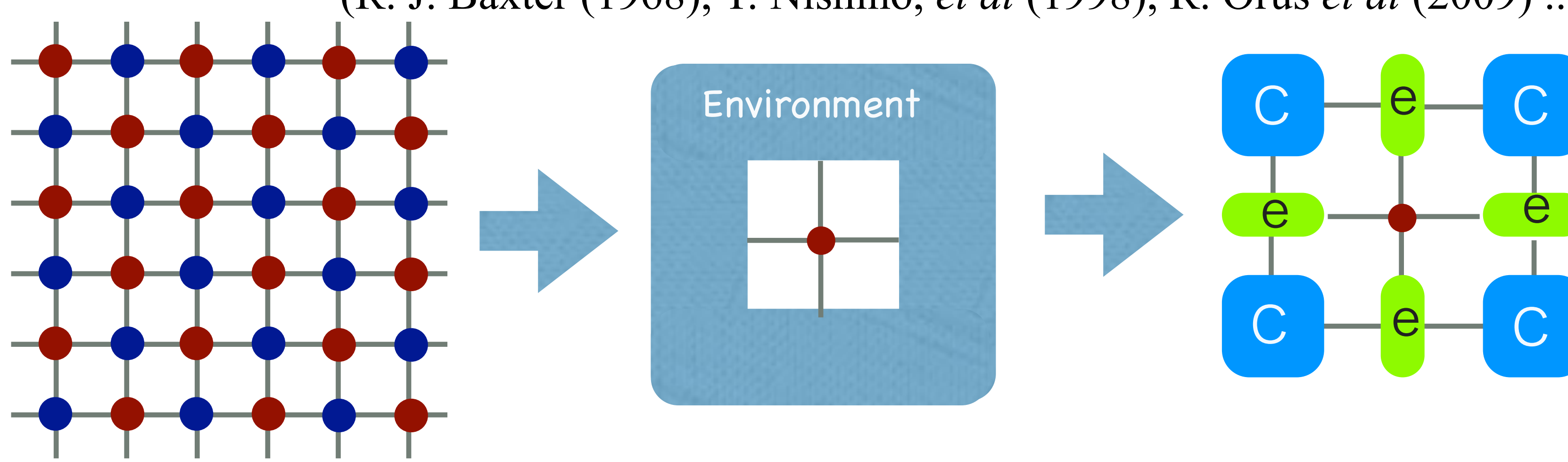
Evaluation: **Contraction of the whole network**

We use the **corner transfer matrix** method.

(R. J. Baxter (1968), T. Nishino, *et al* (1998), R. Orus *et al* (2009) ...)

Cost ~ O(D^{10})

Only a few calculations



TeNeS: Tensor Network Solver

We are developing a open source software for massively parallel tensor network solver for 2D quantum lattice system.

(C++)

https://github.com/issp-center-dev/TeNeS

So far, it is version 0.1.

Update to version 1.0 is scheduled on March.

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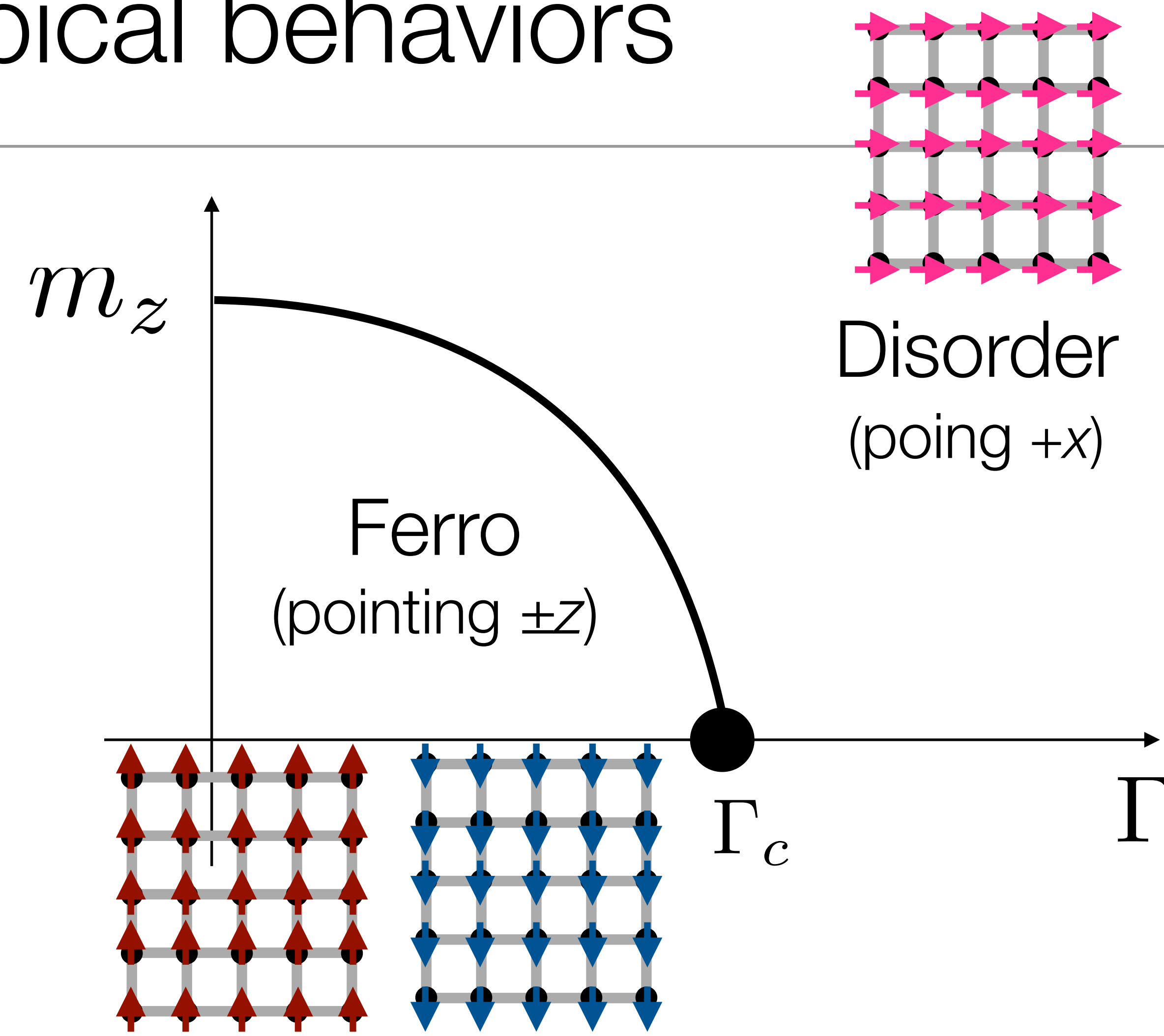
Quantum spin system: typical behaviors

(Quantum) spin system:

Spin degree of freedoms defined on a lattice and interact each other

Example: "Transverse field Ising model"

$$\mathcal{H} = -\sum_{i=1}^{L-1} S_{i,z} S_{i+1,z} - \Gamma \sum_{i=1}^{L} S_{i,x}$$



Usually, the ground states have (magnetic) long range orders:
They may appear as a result of spontaneous symmetry breaking.
or
They may be induced by external fields.

Frustration in spin system

Frustration：Competition among several optimization conditions

Optimization：minimization of the total energy

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j$$

$J > 0$

Antiferromagnetic

local energy minimization ： anti-parallel spin pair

Frustration in spin system

Frustration : Competition among several optimization conditions

Optimization : minimization of the total energy

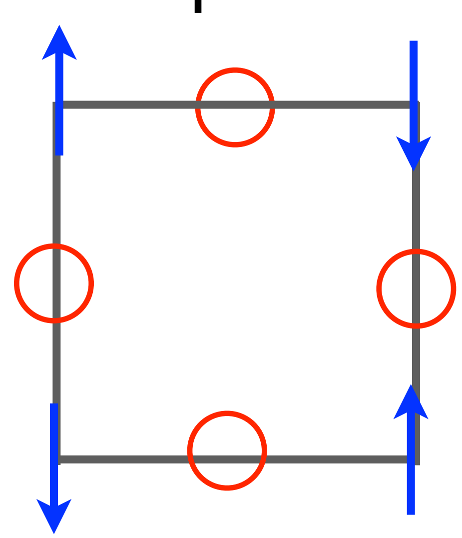
$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \qquad J > 0$$

Antiferromagnetic

local energy minimization : anti-parallel spin pair

Ising spins

Square



All pairs can be anti-parallel

No frustration

Frustration in spin system

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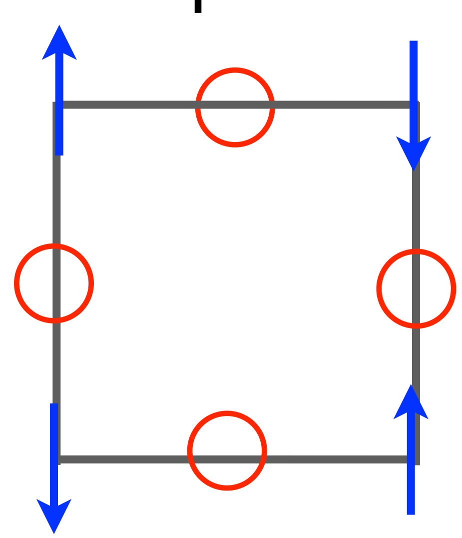
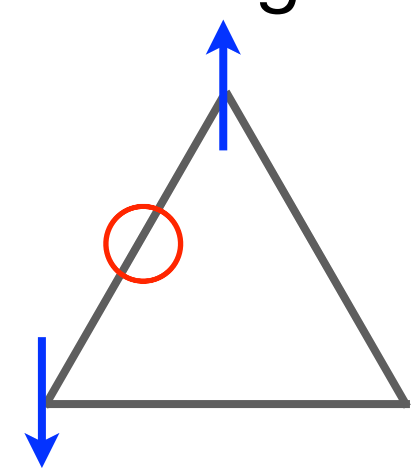


All pairs can be anti-parallel

No frustration

Triangle



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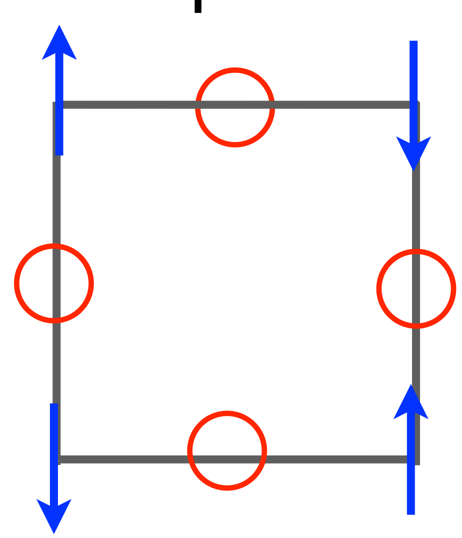

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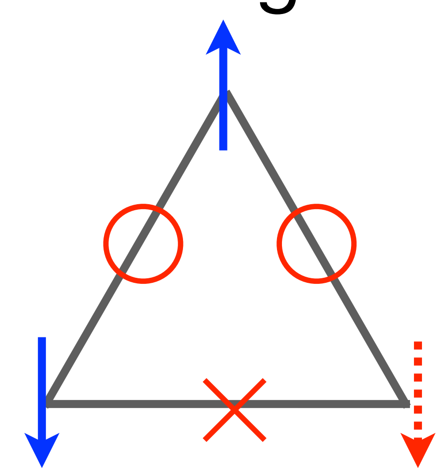

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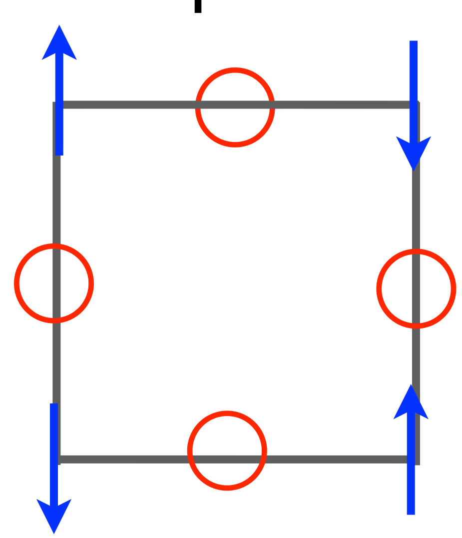

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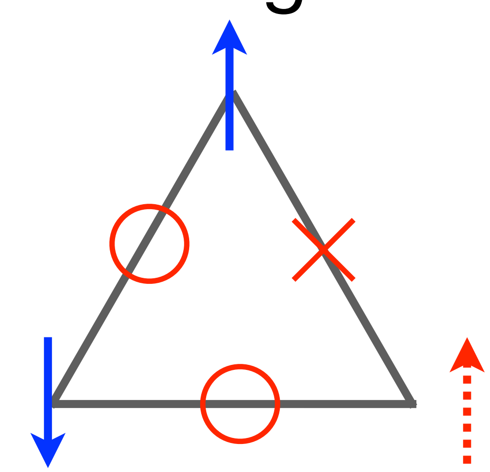

Frustration in spin system

Frustration：Competition among several optimization conditions

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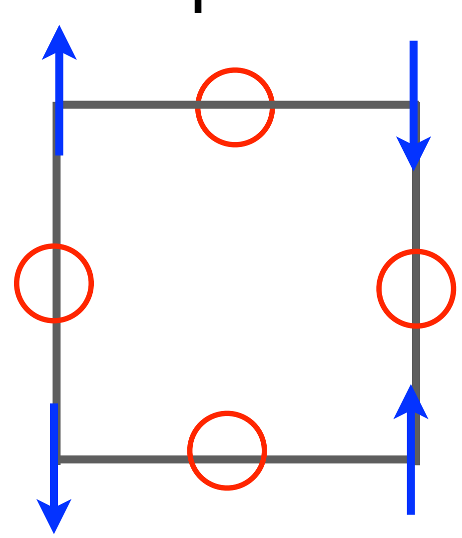
Antiferromagnetic

local energy minimization ： anti-parallel spin pair

Ising spins

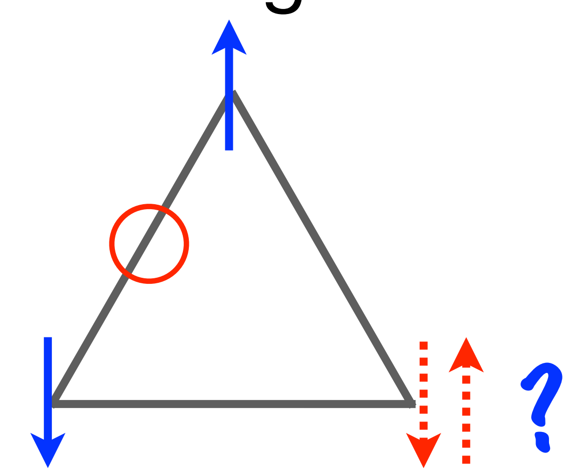
Square



All pairs can be anti-parallel

No frustration

Triangle



One of three pairs is necessarily parallel

Frustration!

Frustration in spin system

Frustration：Competition among several optimization conditions

Optimization：minimization of the total energy

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j \qquad J > 0$$

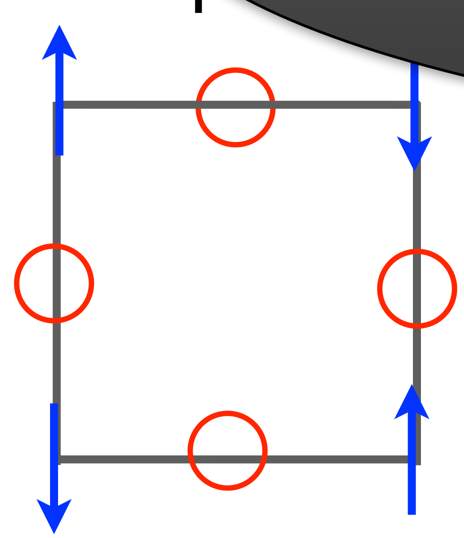
Antiferromagnetic

local

Ising spins

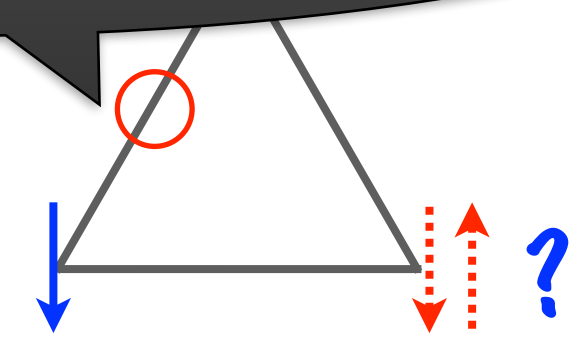
Sq

Huge degeneracy in the ground state.
Large fluctuations!



All pairs can be anti-parallel

No frustration



One of three pairs is necessarily parallel

Frustration!

Quantum spin liquid

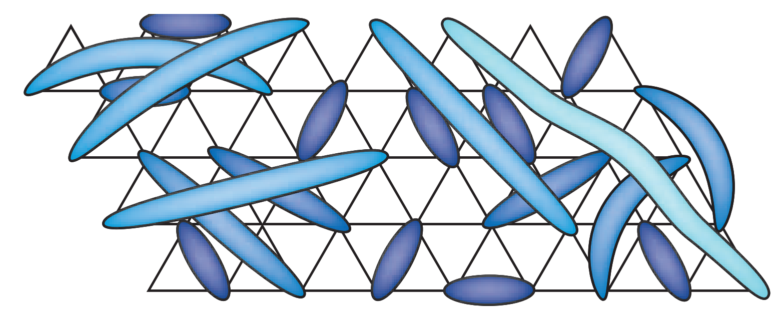
If interactions of the (quantum) spin systems contain frustrations:

⇒ Their ground states might not have any long range order.

Quantum spin liquid

There are a lot of spin liquids based on the mean field theory.

- Z2 spin liquid
- Chiral spin liquid
- U(1) spin liquids
- ...



Spin liquid (RVB)
(L. Balents, Nature (2010))

- We want to find novel states of the matter
  - Quantum spin liquid
  - Topological phase
- We want to investigate phase transitions between them
  - (Quantum) critical phenomena
  - Topological phase transition

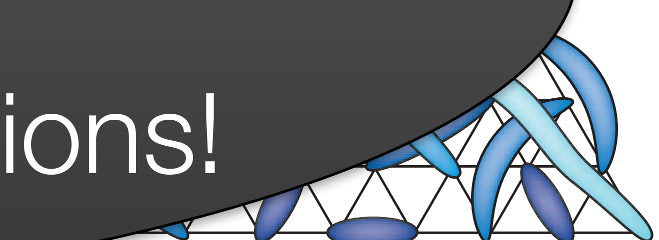
Quantum spin liquid

If interactions of the (quantum) spin systems contain frustrations:

➡ Their ground states might not have any long range order.

Th

A lot of
interesting things occur
in the Avogadro scale ~ 10^{23}
→We need large scale calculations!



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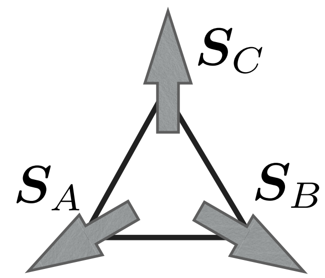
- We want to find novel states of the matter
  - Quantum spin liquid
  - Topological phase
- We want to investigate phase transitions between them
  - (Quantum) critical phenomena
  - Topological phase transition

Kagome lattice Heisenberg model

Hamiltonian

$$\mathcal{H} = J\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j - h\sum_i S_{i,z}$$



- Ground state at zero field

Classical GS: All states satisfying "120 degree structure"

→ Macroscopic degeneracy

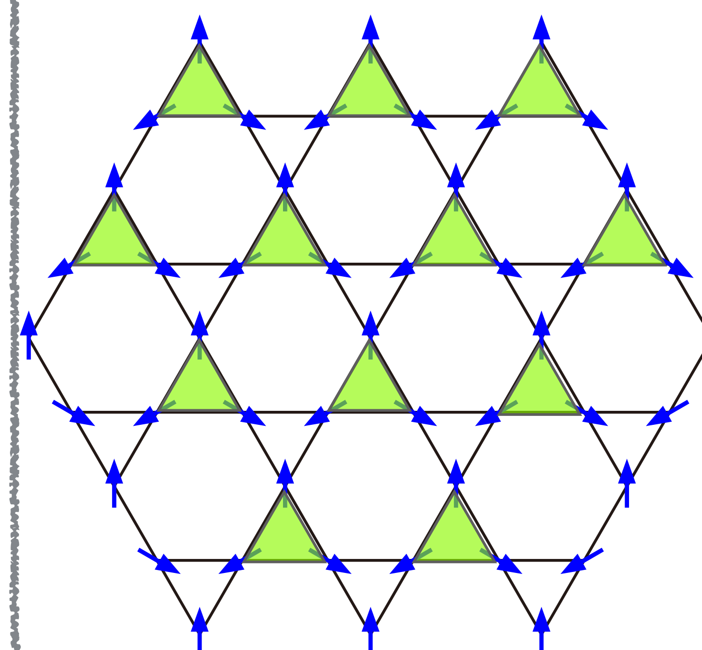
Quantum fluctuation:

S=1/2 quantum spin：

Spin liquid?

- Z_2 spin liquid
- U(1) spin liquid
- …

Kagome lattice



Kagome

Taken from http://koharu2009.blogspot.jp/

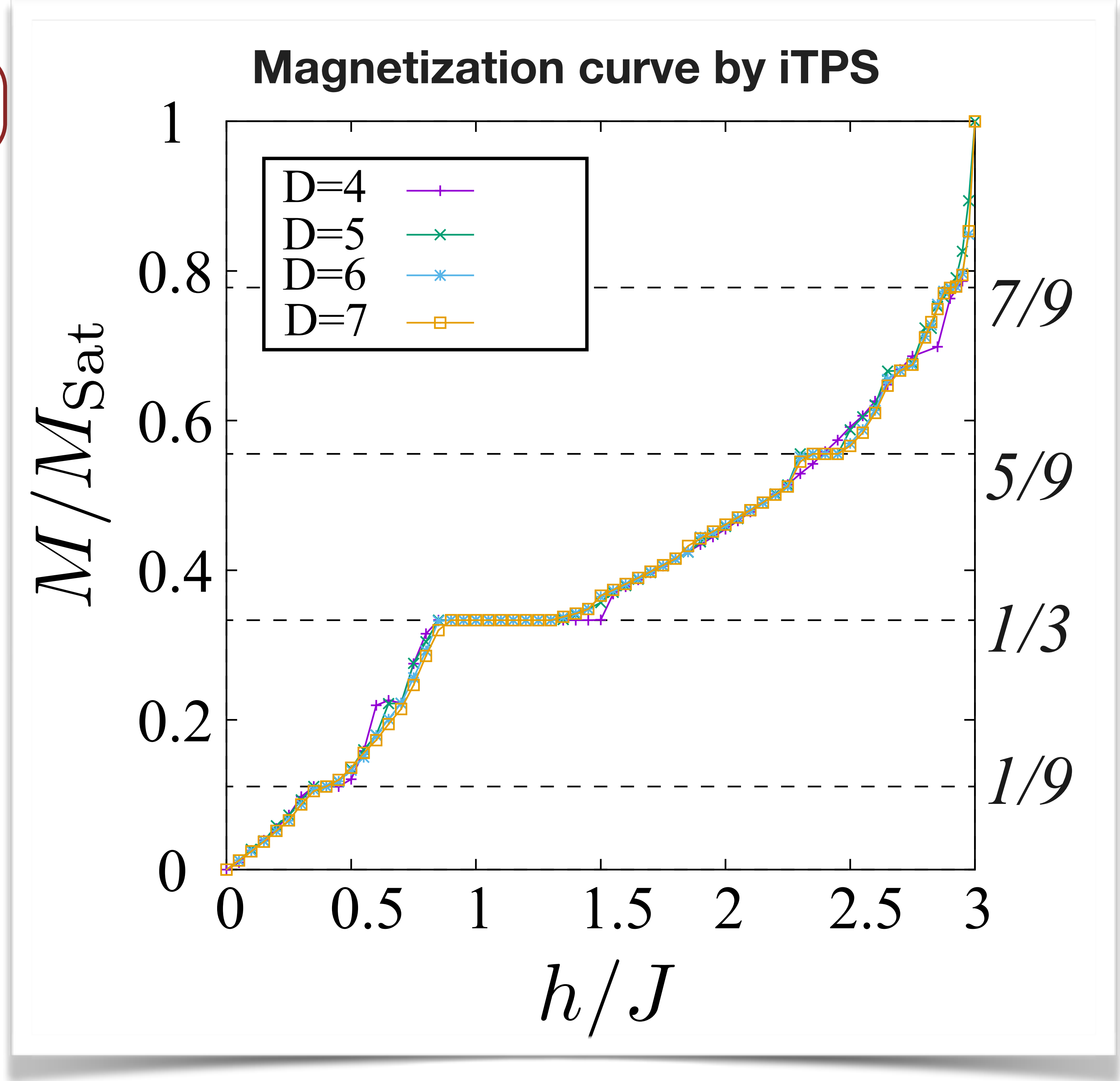
Results : Magnetization curve

(R. Okuma, D. Nakamura, T. Okubo, et al, Nat. Commun. **10,** 1229 (2019))

Several magnetization plateaus are stabilized

- Almost converged data up to D=7

1/9, 1/3, 5/9 :clear plateaus
7/9: weak anomaly



Results：Magnetization curve

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Several magnetization plateaus are stabilized

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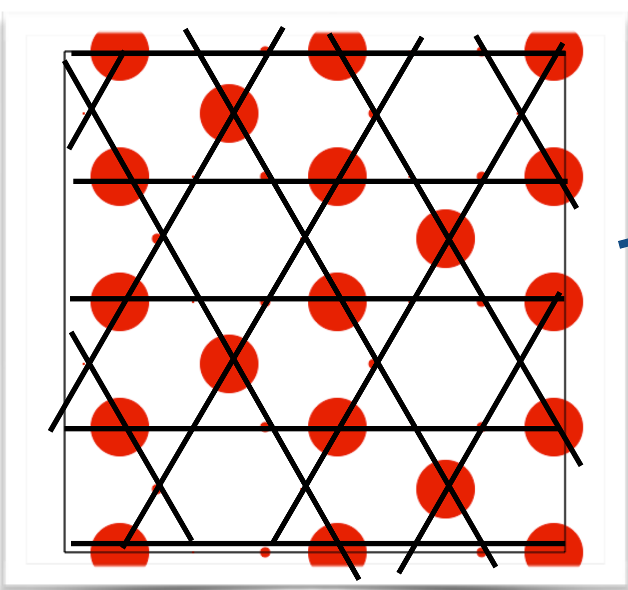
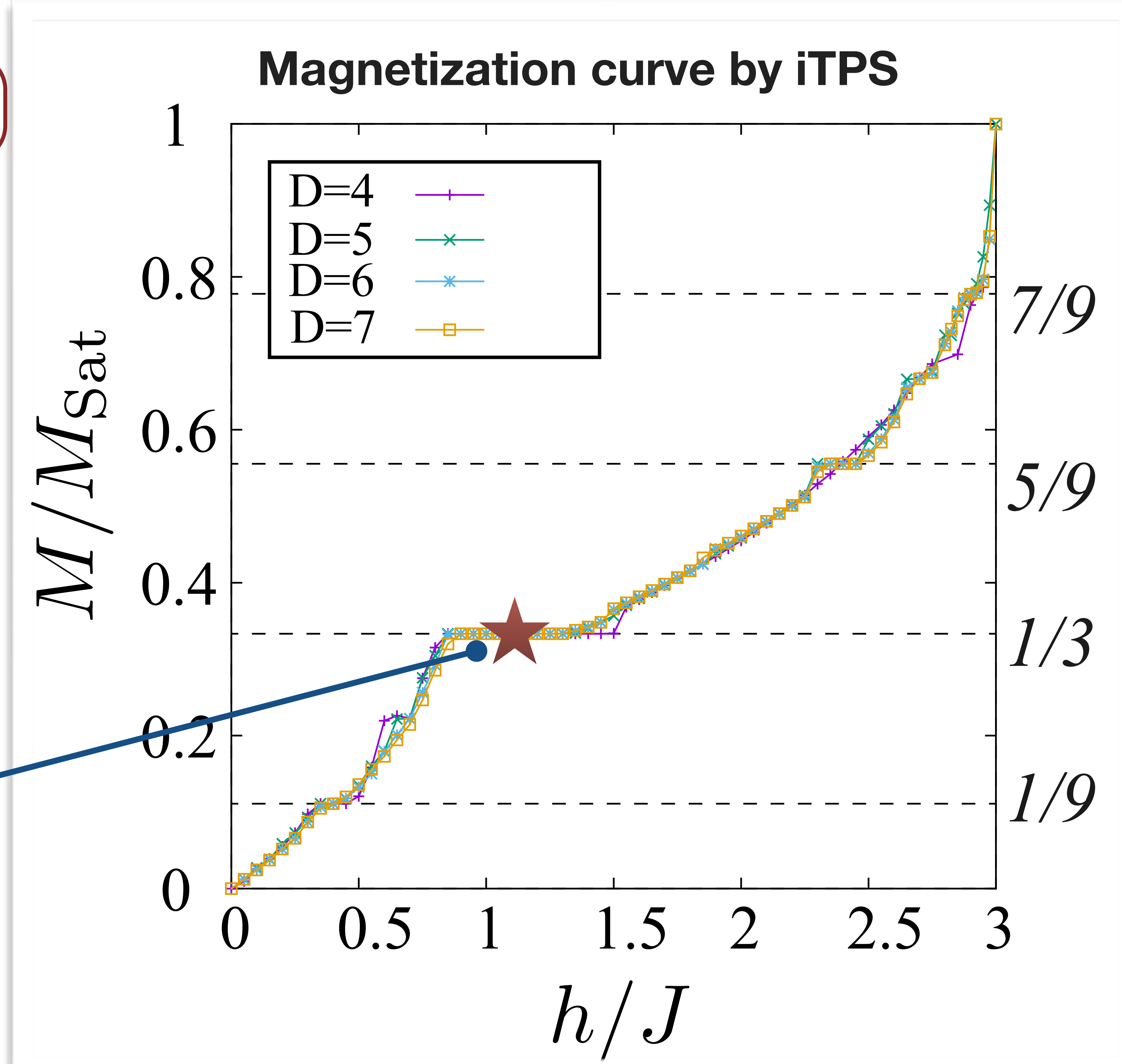
1/9, 1/3, 5/9 :clear plateaus
7/9: weak anomaly

1/3 plateau state is a resonated state.





A_2IrO_3

Iridium Oxides

Strong spin-orbit coupling → Effective "spin" moment: $J_{\mathrm{eff}} = \frac{1}{2}$

Na_2IrO_3

G.Jackeli, et al., PRL 102, 017205 (2009)
J. Chaloupka, et al., PRL 105, 027204 (2010)

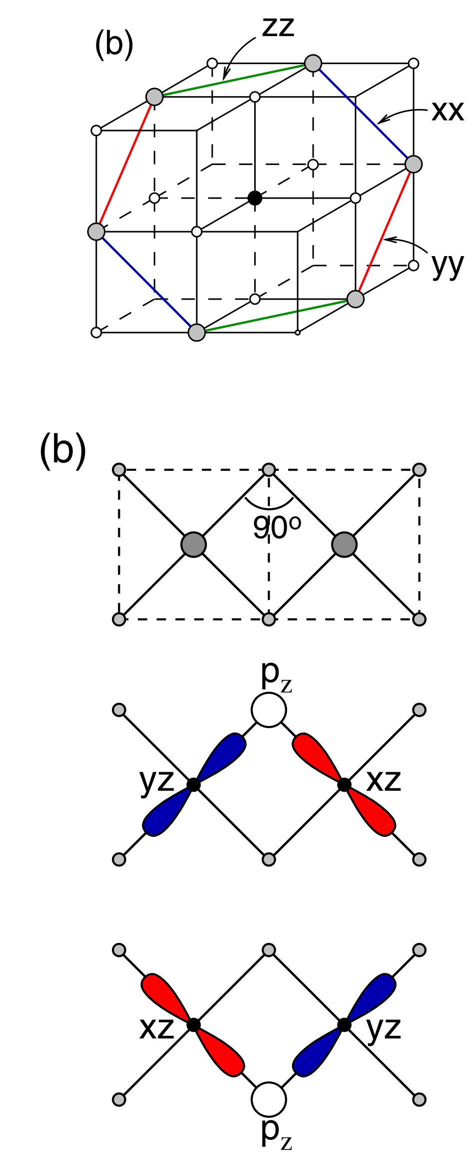
Ir ions form an honeycomb lattice.

Ir - Ir direct exchange: Heisenberg interaction

Ir - O - Ir exchange: Anisotropic Kitaev interaction

Depending on the bond direction, only specific spin component interact.

$$H_K^{(\gamma)} = -J S_i^\gamma S_j^\gamma$$



Ground state of the pure Kitaev model: Spin liquid

A_2IrO_3

Iridium Oxides

Strong spin-orbit coupling → Effective ``spin” moment: $J_{\mathrm{eff}} = \frac{1}{2}$

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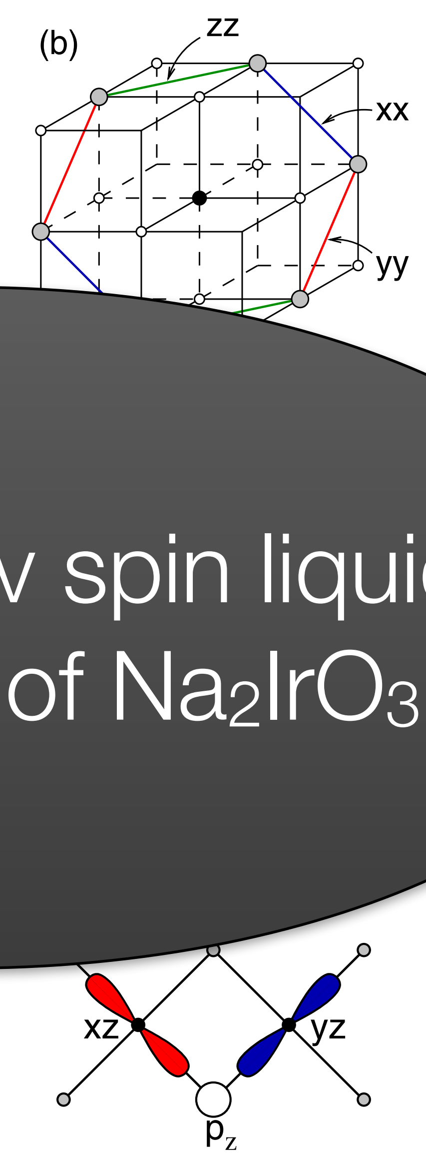
G.Jackeli, et al., PRL 102, 017205 (2009)
J. Chaloupka, et al., PRL 105, 027204 (2010)



Ir ions form an honeycomb lattice.

Ir - Ir direct exchange: Heisenberg interacti

Ir - O - Ir exchange: Anisotropic K

Depending on the bond
specific spin component

$$H_K^{(\gamma)} = -JS_i^\gamma S_j^\gamma$$

Is there Kitaev spin liquid in the vicinity of Na_2IrO_3?

Ground state of the pure Kitaev model: Spin liquid

ab initio Hamiltonian of Na_2IrO_3

(Y. Yamaji et al. Phys. Rev. Lett. **113**, 107201(2014))

ab initio Hamiltonian

$$\hat{H} = \sum_{\Gamma=X,Y,Z} \sum_{\langle \ell,m \rangle \in \Gamma} \vec{\hat{S}}_{\ell}^{T} \mathcal{J}_{\Gamma} \vec{\hat{S}}_{m},$$

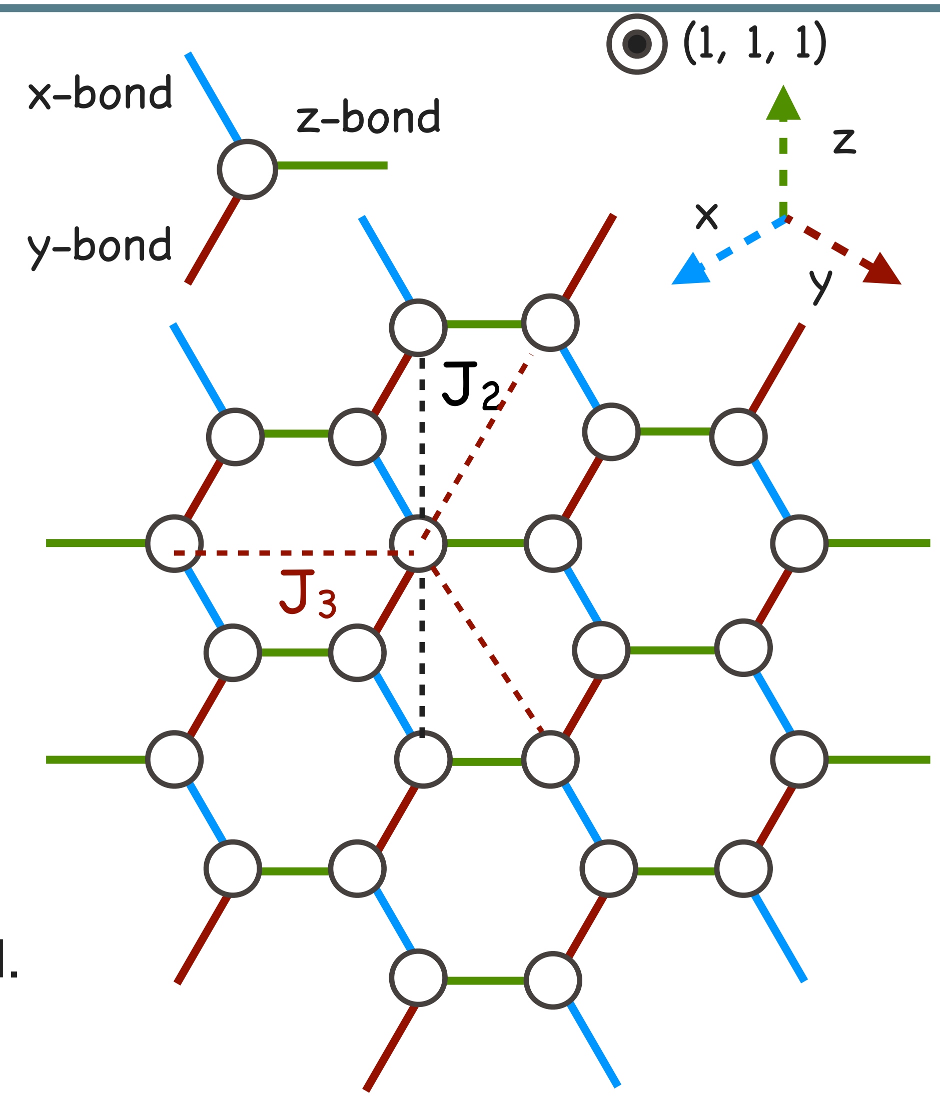
$$\mathcal{J}_Z = \begin{bmatrix} J & I_1 & I_2 \\ I_1 & J & I_2 \\ I_2 & I_2 & K \end{bmatrix}, \mathcal{J}_X = \begin{bmatrix} K' & I_2'' & I_2' \\ I_2'' & J'' & I_1' \\ I_2' & I_1' & J' \end{bmatrix}, \mathcal{J}_Y = \begin{bmatrix} J'' & I_2'' & I_1' \\ I_2'' & K' & I_2' \\ I_1' & I_2' & J' \end{bmatrix},$$

Kitaev coupling K and Heisenberg like coupling J
+
Off-diagonal couplings I_1 and I_2

It also contains J_2 and J_3 interaction term.

J_2 : only "z-bond" which is perpendicular to NN z-bond.

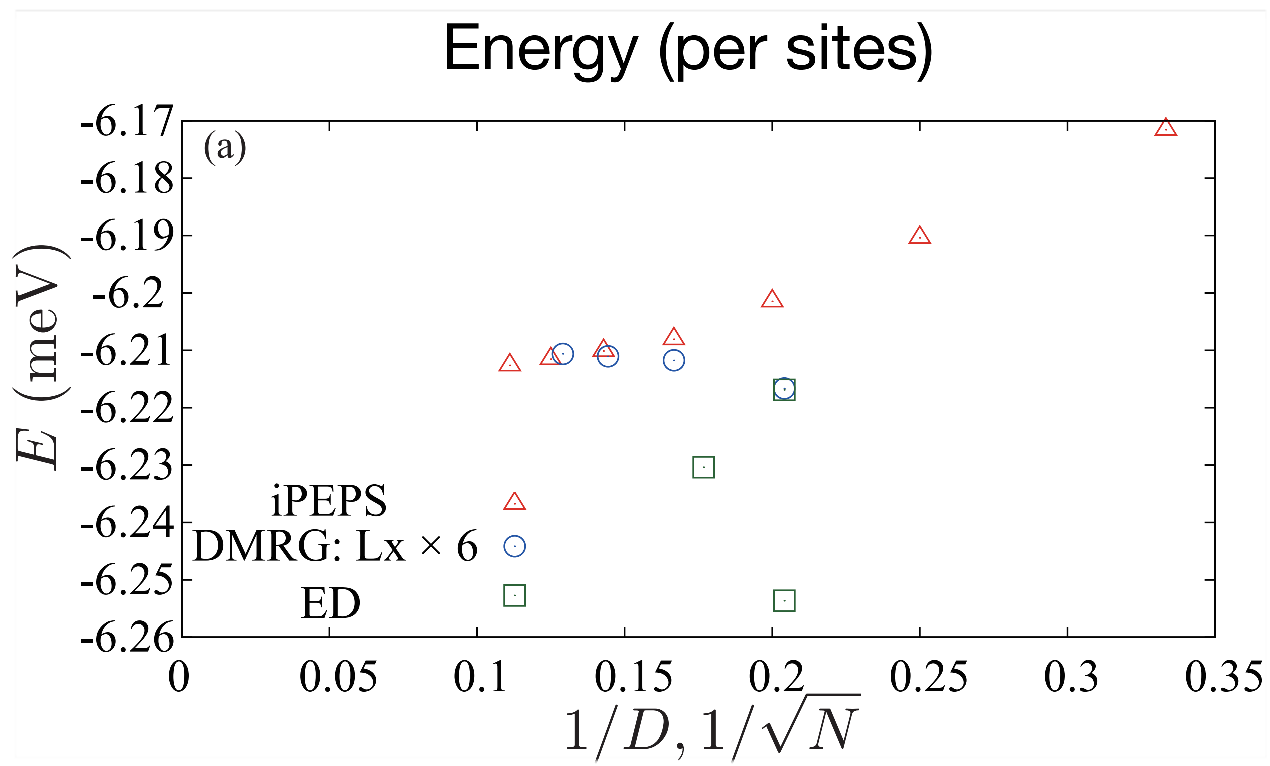
J_3 : all of the three third neighbors

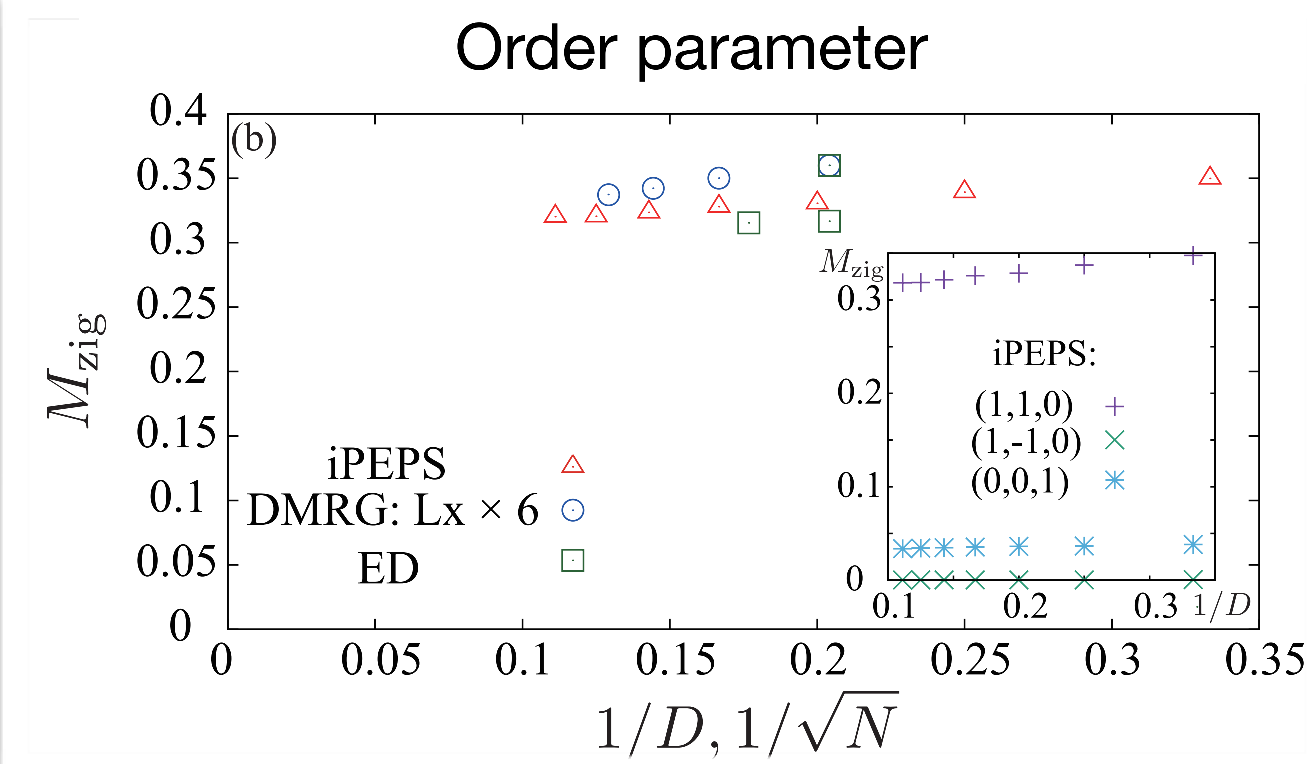


Due to the trigonal distortion, the *ab initio* Hamiltonian contains strong off-diagonal couplings, together with J_2 and J_3 interaction

Results: comparison with other methods

T. Okubo *et al*, PRB **96**, 054434 (2017).





Energies of iTPS, DMRG and ED are consistent.

- For 4 × 6 lattice, DMRG and ED give almost same energy.
- Finite D of iTPS and finite Lx of DMRG are overlapped.

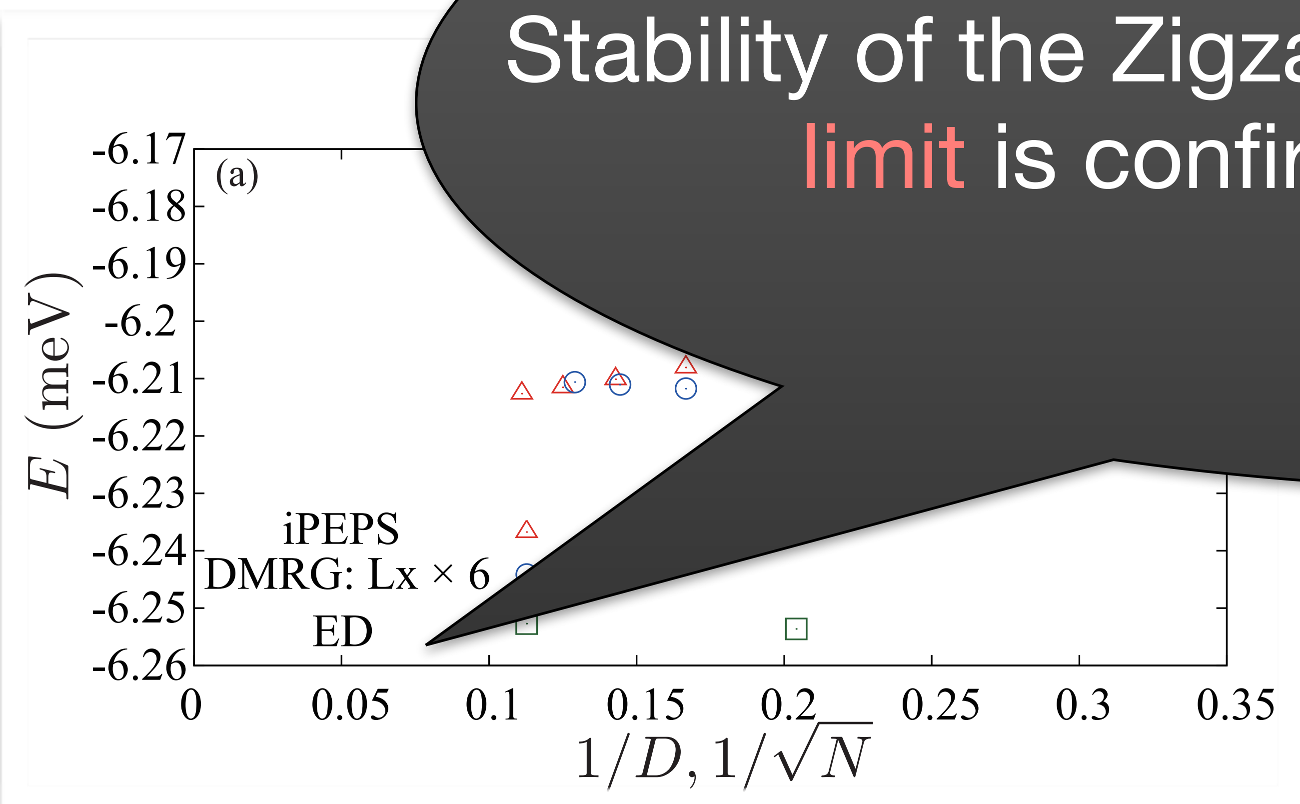
Zigzag(Z) order parameters are consistent.

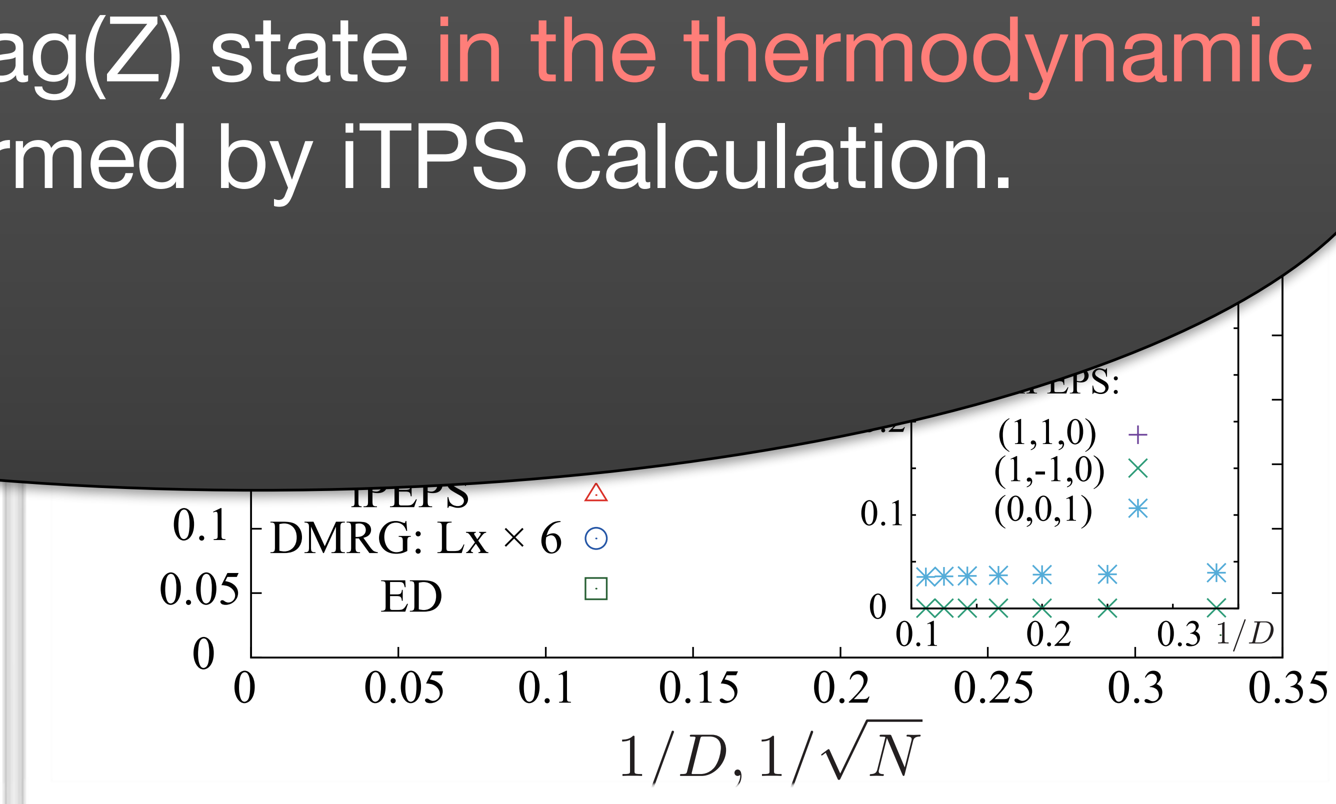
- Extrapolations of them are <M> ~ 0.3
- Spins are almost along (1,1,0) direction, which is consistent with the experimental observations.

Results: comp

(2017).

Stability of the Zigzag(Z) state in the thermodynamic limit is confirmed by iTPS calculation.





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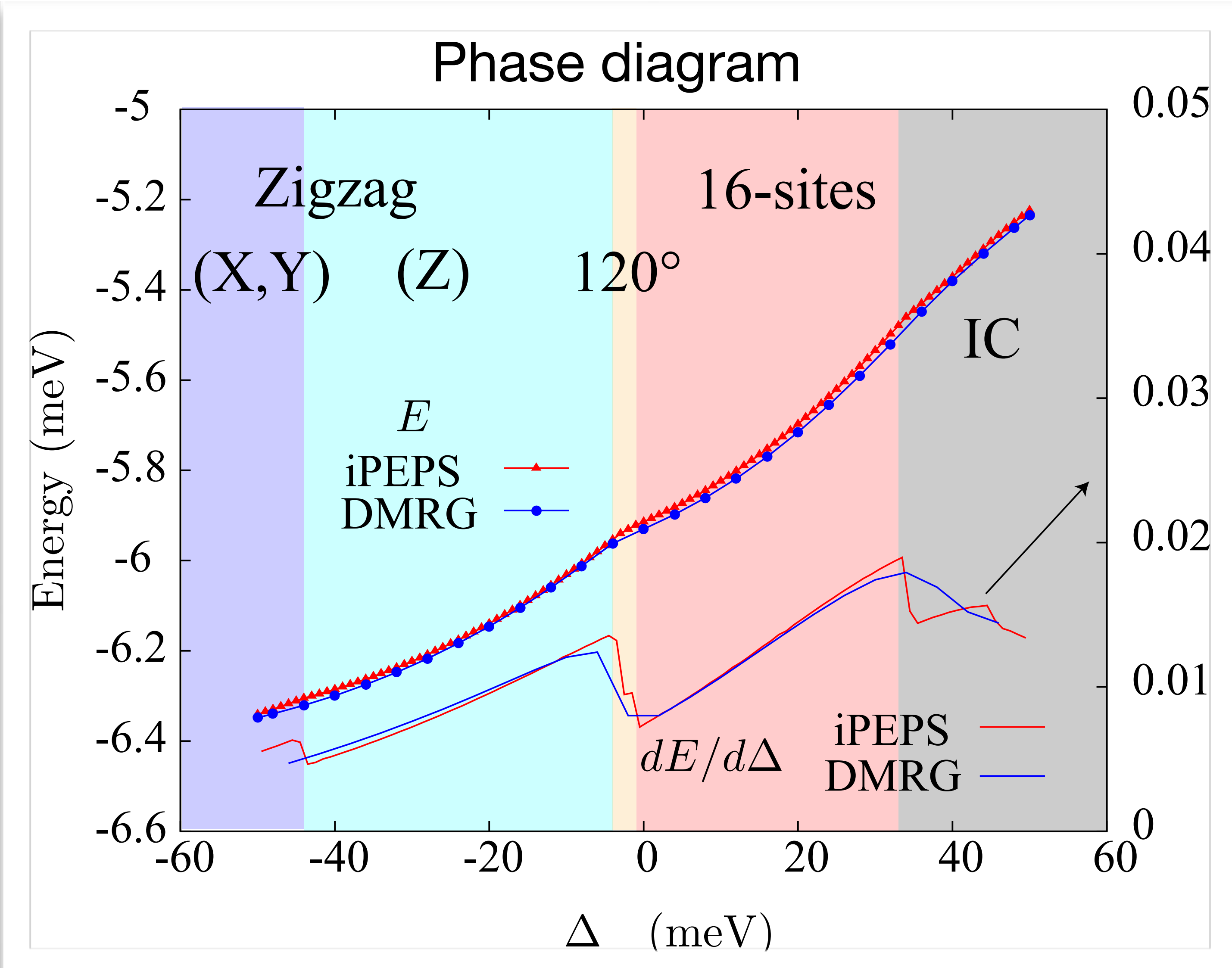
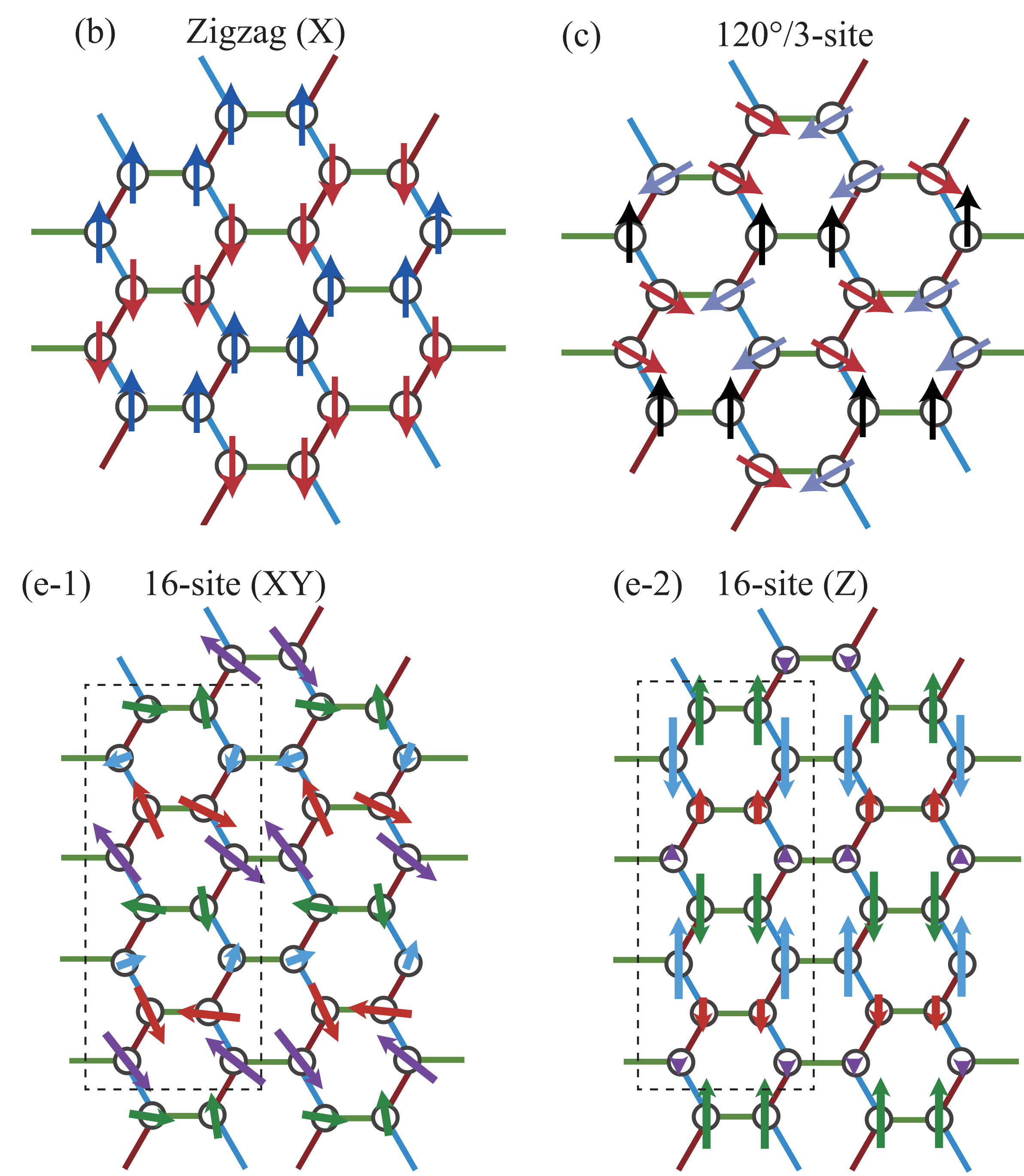
Phase diagram varying the trigonal distortion

T. Okubo *et al,* PRB **96**, 054434 (2017).

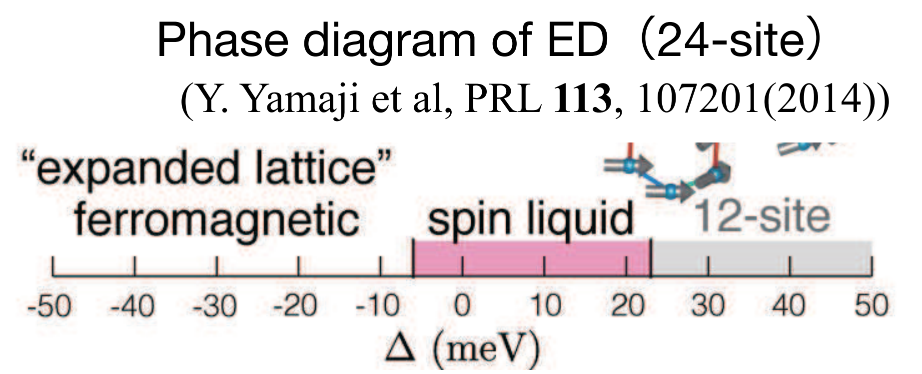




DMRG: 6x8 cluster
iTPS: 4x4, 2x6, 6x8, 8x12, 6x10 unit cells

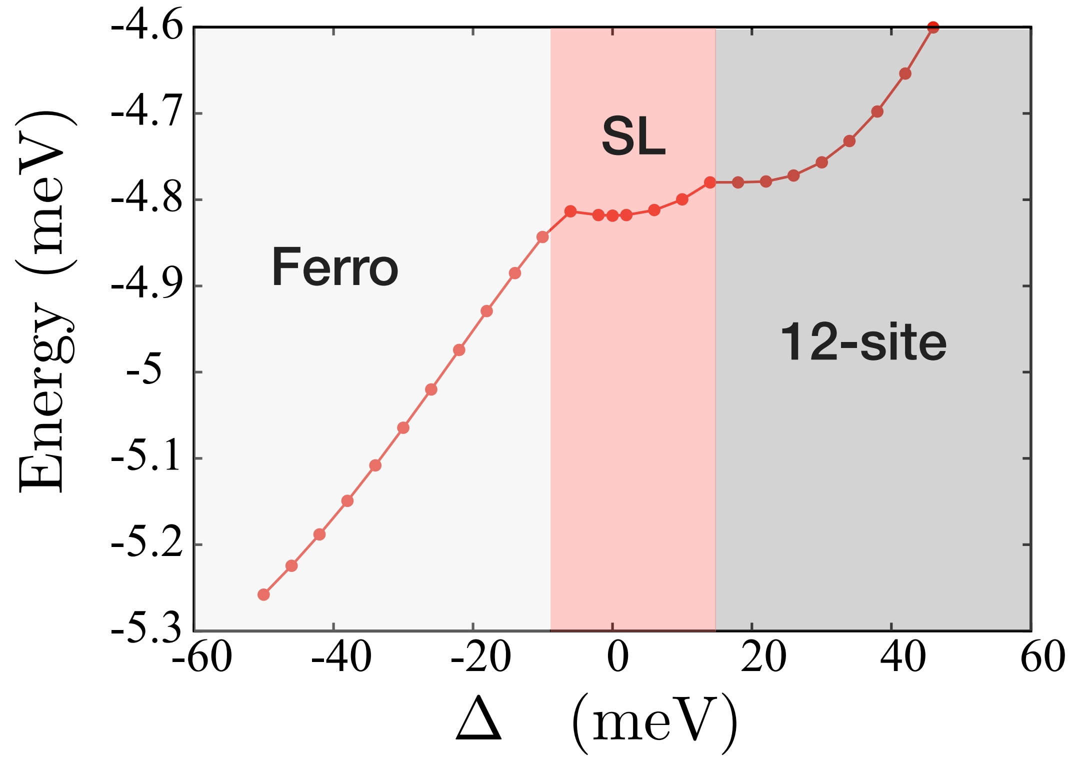
- Energies obtained by iTPS and DMRG are consistent
- New phases are stabilized compared with the previous ED reports

Lattice expansion

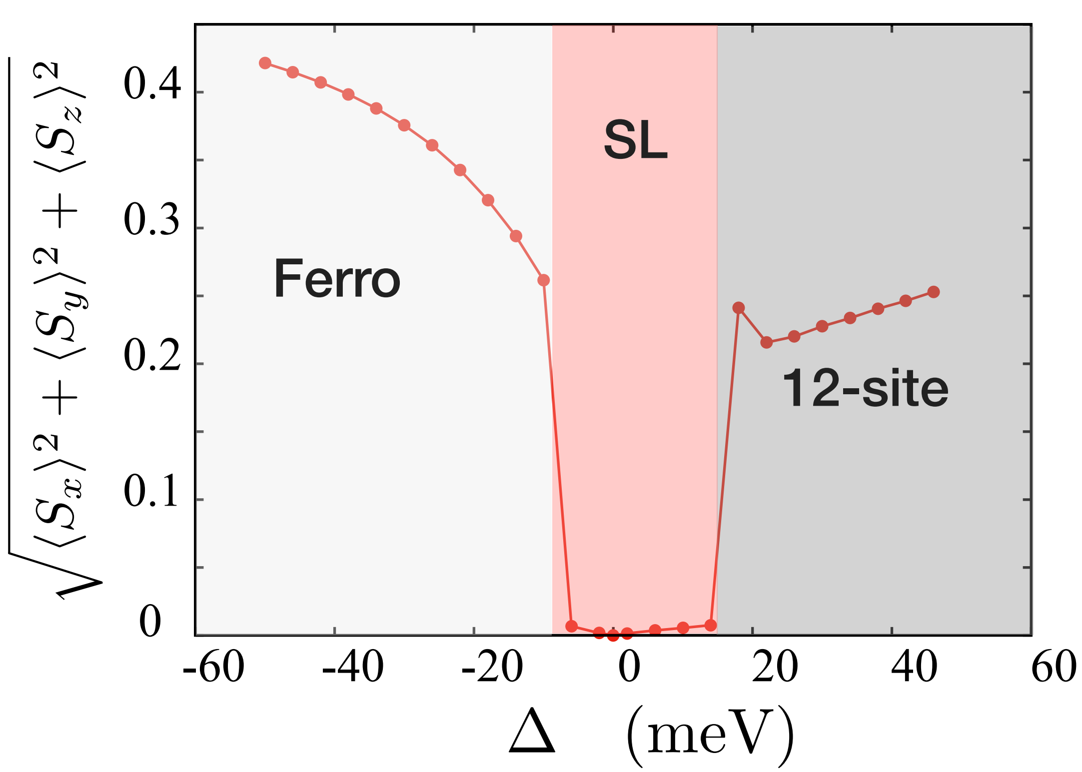


ab-initio Hamiltonian for Na_2IrO_3 (with lattice expansion)

Energy and Phase diagram

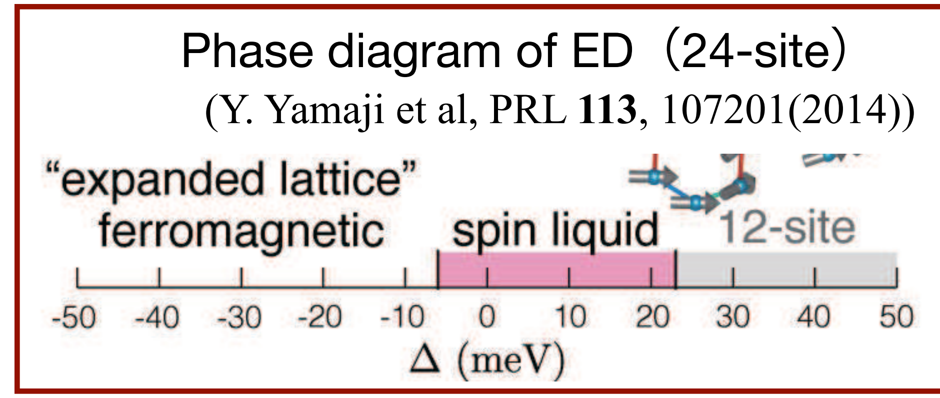


Local magnetization



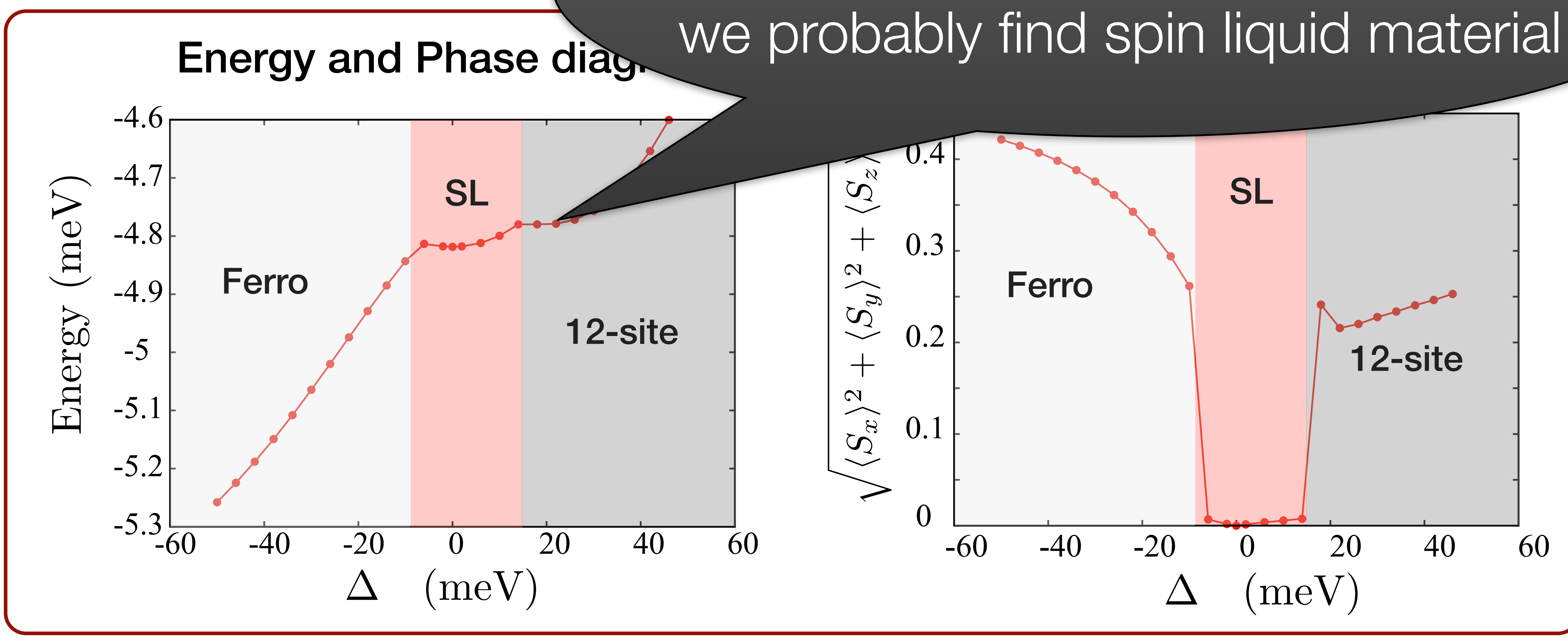
- iTPS phase diagram is qualitatively consistent with the ED.
  - Around Δ=0, a Kitaev spin liquid phase is clearly stabilized.

Lattice expansion



ab-initio Hamiltonian for Na_2IrO_3 (with lattice expansion)

If we can expand
the lattice constant,
we probably find spin liquid material !



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Contents

- Huge data in physics
- Information compression
  - Basics: singular value decomposition
  - Tensor network renormalization
  - Tensor network quantum states
- Applications
- Summary and outlook

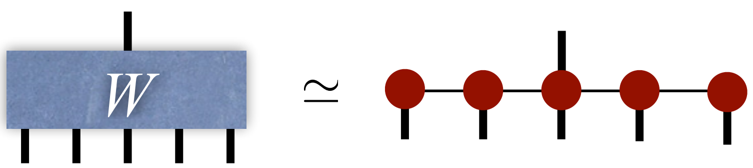
Summary

- By using tensor network representation, we can largely compress the information into compact forms.
  - A partition function in the statistical physics can be represented by a tensor network
    - Its contraction can be done efficiently by tensor network renormalization technique.
    - By using MPI parallelization, 4d (3+1 d) calculation becomes realistic.
  - We can approximate low energy wave function by using tensor network states.
    - Efficiency is guaranteed by the area law of the entanglement entropy
    - We can represent infinite systems with finite bond dimensions D.
    - MPI parallel code TeNeS is available.
    - For 2d frustrated spin systems, iTPS is one of the most powerful methods.

Outlook

- Application to difficult problems
  - Excitation spectrums
  - Finite temperature properties
  - (Lattice QCD)
- Nowadays, tensor network representations expand their application to other fields.
  - Machine learning for classification problem with MPS
    - E. Miles Stoudenmire and D. J. Schwab, NIPS 2016
  - Unsupervised Generative Modeling
    - Born machine instead of Boltzmann machine
      - S. Cheng et al, Phys. Rev. B **99**, 155131 (2019)
      - Z.-Y. Han et al, Phys. Rev. X **8**, 031012 (2018).
  - Quantum circuit simulation
    - A. McCaskey et al, PLoS One **13** e0206704 (2018). (MPS)
    - C. Guo et al, Phys. Rev. Lett. **123**, 190501 (2019). (TPS)

$$f^l = W^l \vec{\psi}(\boldsymbol{x})$$



$$P(\vec{v}) = \frac{|\Psi(\vec{v})|^2}{Z} \qquad \left(Z = \sum_{\vec{v}} |\Psi(\vec{v}_i)|^2\right)$$