計算科学における情報圧縮

Information Compression in Computational Science

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#2:情報圧縮と繰り込み

Information compression and renormalization

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Outline

- Many body problems
    - Quantum and classical systems
    - Phase transition and statistical mechanics
- (Real space) Renormalization group
  - Example: 1D-Ising spin
  - General case
  - Relation to tensor network
  - Comments

Many body problems:
Quantum and Classical systems

Quantum systems

Quantum system: governed by Schrödinger equation

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

$\mathcal{H}$:Hamiltonian

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

(波動関数 or 状態ベクトル)

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

素粒子

Static problems: Time-independent Schrödinger equation

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

Quantum systems

Example of quantum system: Array of quantum bits

1 bit

A quantum bit has two eigenstates $|0\rangle, |1\rangle$

$$\mathcal{H}^{(1)}|i\rangle = E_i|i\rangle \quad i = 0, 1$$

2 bits

The Hilbert space is spanned by four basis vectors
ヒルベルト空間

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

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

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

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

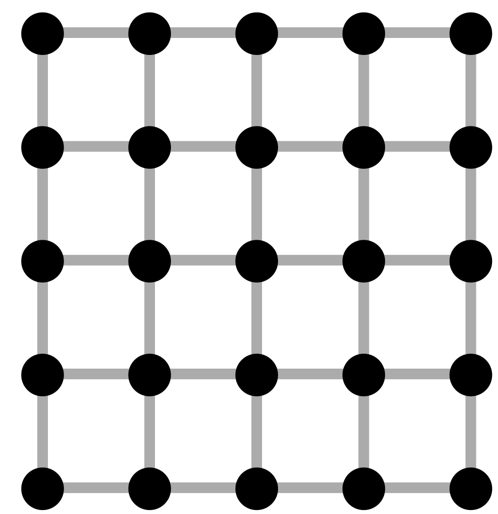
The Hamiltonian can be represented in these bases

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

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

Quantum 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

(Quantum) spin system

Spin systems:

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

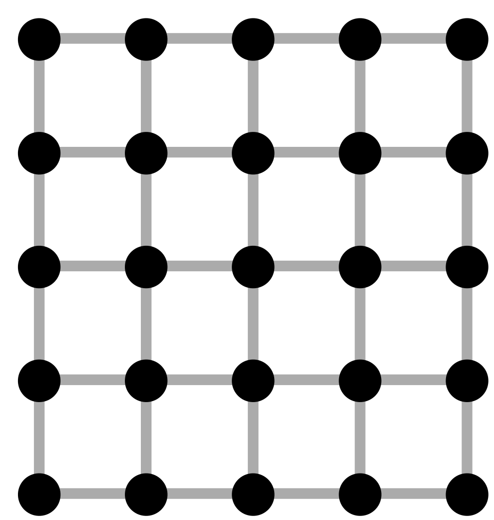
Lattice

1D

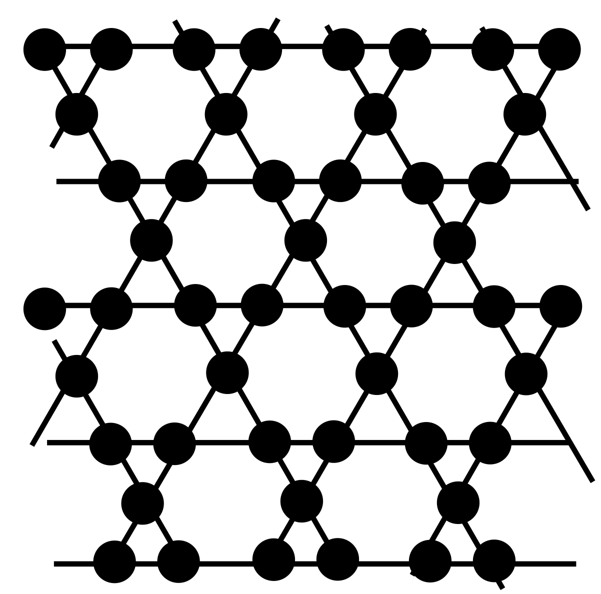
Chain

2D

Square lattice



Kagame lattice



3D simple cubic, FCC lattice, BCC lattice, …

Quantum spin

Spin operator: (S_x, S_y, S_z)

Commutation relation
（交換関係）

$$[S_x, S_y] = i\hbar S_z, [S_y, S_z] = i\hbar S_x, [S_z, S_x] = i\hbar S_y$$

$$[A, B] \equiv AB - BA$$

Spin quantum number operator:
（スピン量子数）

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

Simultaneous eigenstate of S^z and S^2: $|S_z, S\rangle$

$$S^2|S_z, S\rangle = \hbar^2 S(S+1)|S_z, S\rangle$$
$$S_z|S_z, S\rangle = \hbar S_z|S_z, S\rangle$$

Quantized spin number

$$S = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$$
$$S_z = -S, -S+1, \ldots, S-1, S$$

(Hereafter, we set $\hbar = 1$)

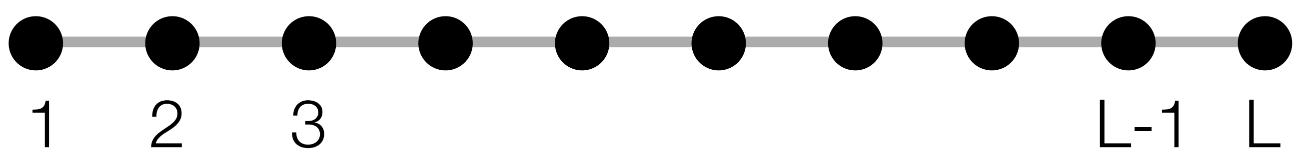
Quantum spin: S=1/2

Matrix representation of the spin operators: $S = \frac{1}{2}$

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can consider S=1/2 spin as a quantum bit : $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Spins on a chain:



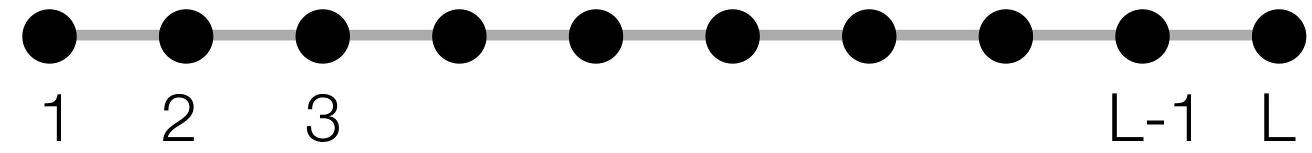
"Transverse field Ising model"　（横磁場イジング模型）

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

L=2

$$\mathcal{H} = \begin{pmatrix} -1/4 & -\Gamma/2 & -\Gamma/2 & 0 \\ -\Gamma/2 & 1/4 & 0 & -\Gamma/2 \\ -\Gamma/2 & 0 & 1/4 & -\Gamma/2 \\ 0 & -\Gamma/2 & -\Gamma/2 & -1/4 \end{pmatrix}$$

Quantum spin: S=1/2

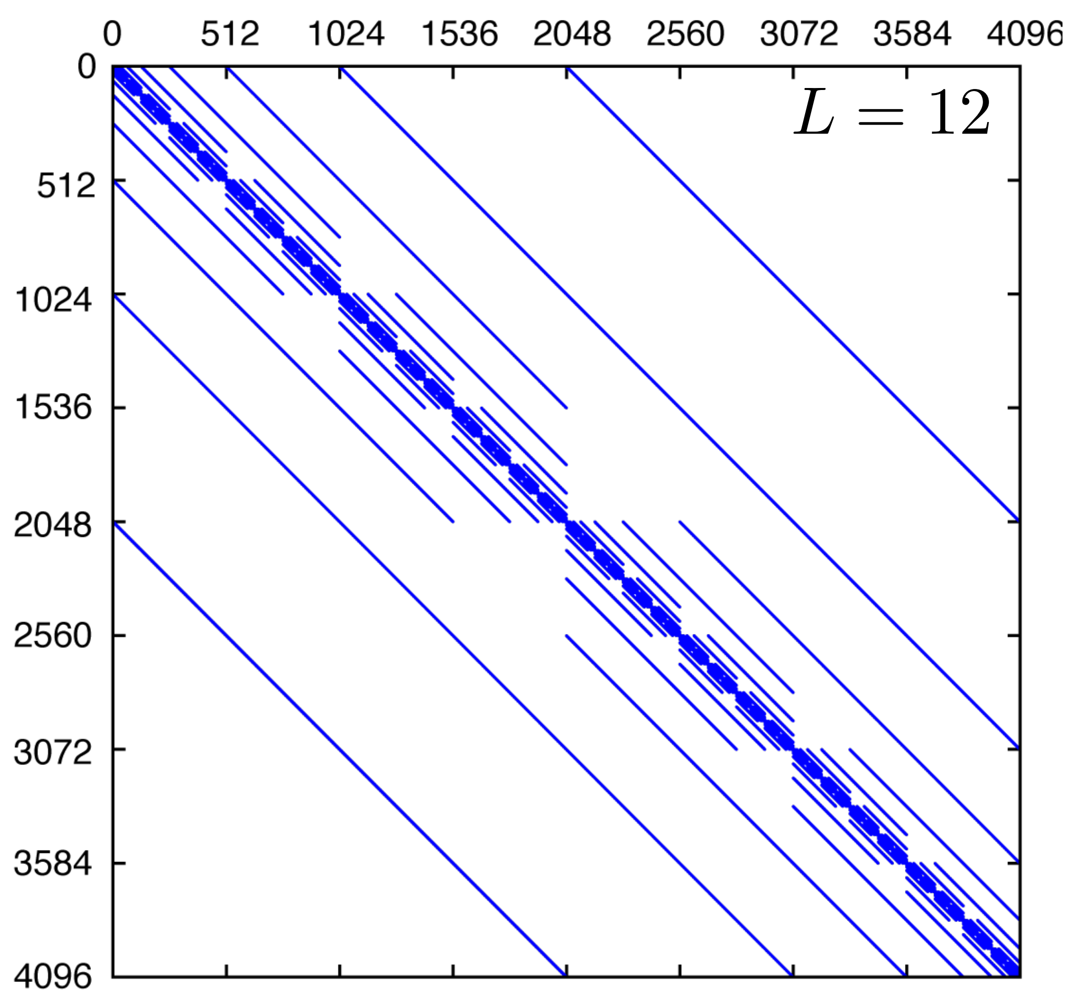


"Transverse field Ising model"

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

Non-zero elements in the Hamiltonian

(Figure from Yamaji-sensei)



Total matrix elements=2^{2L}

# of non-zero elements $\sim O(L)$

Sparse!

Classical problems

Two types of classical many-body problems

1. Approximation of quantum problems

Nature: Elementary particles obey quantum mechanics.

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

⇒ Classical mechanics is an approximation

2. Pure classical problems

Classical problems not necessary based on quantum mechanics

- Percolation, covering, packing, …
- Stochastic process, “dynamical” system, ..
- Critical phenomena
- …

Classical problems as an approximation: magnetism

Electron Spin: “Quantum” degree of freedom

For accurate treatment, the spin quantum number S is important

$S=1/2, 1, 3/2, \dots$

However, we can approximate the system by taking the limit of $S \to \infty$.
“classical” spin model

- Classical Heisenberg model
- Anisotropy: Ising model, XY model
- ….

Classical spin degree of freedom

Classical spin:
1. $S \to \infty$ limit of quantum spin
2. simple degree of freedom reflecting symmetry

1. Heisenberg spin $S_i = (S_i^x, S_i^y, S_i^z)$

Three component unit vector: $(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1$

A lot of magnetism can be understand through classical Heisenberg spin

2. Ising spin $S_i = \pm 1 = \uparrow, \downarrow$

- Strong easy axis anisotropy
- Representing underlying Z_2 symmetry

3. XY spin $S_i = (S_i^x, S_i^y)$ Two component unit vector: $(S_i^x)^2 + (S_i^y)^2 = 1$

- Strong easy plane anisotropy
- Representing underlying U(1) symmetry

Classical Ising spin vs. quantum spin

Ising spin

$$S_i = \pm 1 = \uparrow, \downarrow$$

"Ising model"

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

$$\mathcal{H} = \begin{pmatrix} -1-2h & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1+2h \end{pmatrix}$$

S=1/2 quantum spin

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

"Transverse field Ising model"

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

$$\mathcal{H} = \begin{pmatrix} -1/4 & -\Gamma/2 & -\Gamma/2 & 0 \\ -\Gamma/2 & 1/4 & 0 & -\Gamma/2 \\ -\Gamma/2 & 0 & 1/4 & -\Gamma/2 \\ 0 & -\Gamma/2 & -\Gamma/2 & -1/4 \end{pmatrix}$$

In the case of classical system, the Hamiltonian is "diagonal"

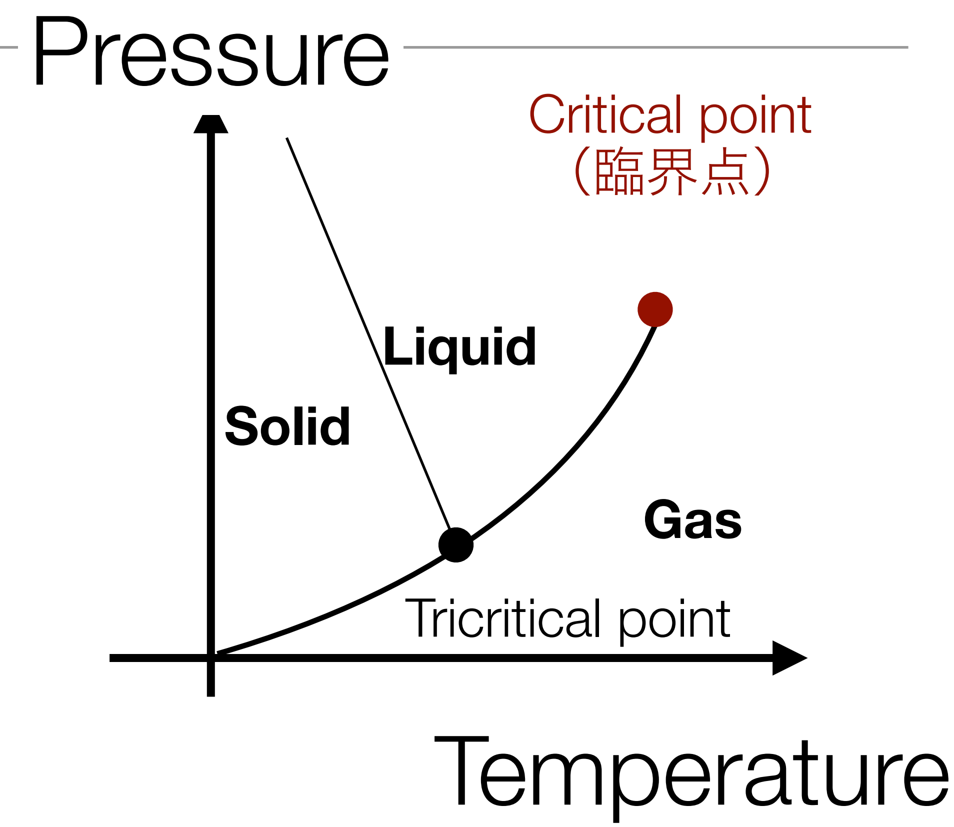
- We do not need explicit diagonalization
- "State" can be represented by a product of local DOF $\sim O(L)$ (Degrees Of Freedom)
- Although, # of states is $\sim O(2^L)$

Many body problems:

Statistical mechanics and phase transition

Phase transition

- By changing parameter, such as temperature or pressure, a singularity appears in thermodynamic free energy →Phase transition （相転移）
    - States separated by a phase transition ＝ Phase
    - Water
        - At the atmospheric pressure (大気圧）, as temperature is decreased three phases appear: gas → liquid → solid



Target of (condensed matter) physics

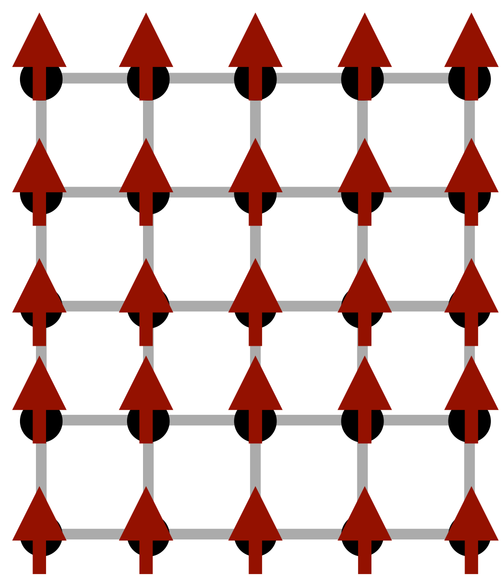
- What kinds of phases are stabilized？
    - Long range order（長距離秩序）、Topological order, ...
- Nature of phase transitions in between them?

Phases in magnets (spin model)

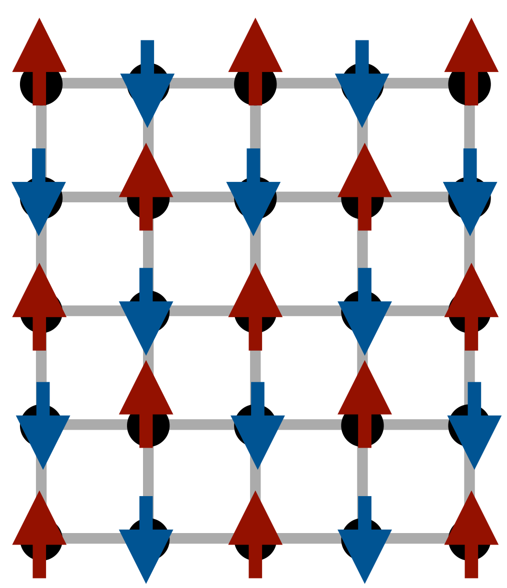
Typically we have two phases:

Magnetically ordered phase

Ferromagnetic
(強磁性)

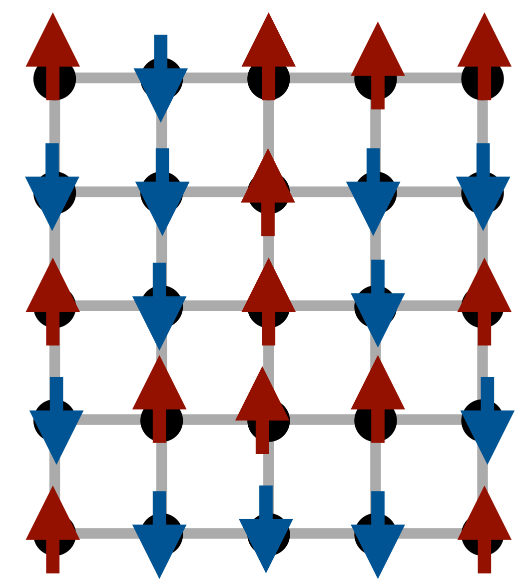


Antiferromagnetic
(反強磁性)



Phase transition

Disordered phase



In real matters and complex spin models,
variety of magnetic orders are stabilized

First order and Second order phase transition

- There are two types of phase transition: discontinuous and continuous
  - Discontinuous transition:
    At the phase transition, the derivative of the free energy changes discontinuously = First oder phase transition
    - Eg. Liquid ⟷Solid phase transition of water
  - Continuous transition：

    The derivative of the free energy is continuous
    - In many case, the second derivative changes discontinuously
      ＝Second order phase transition
    - Eg. Gas⟷Liquid critical point, phase transition in Ising model

Critical phenomena（臨界現象）

At the critical point, characteristic length diverges

→ Scale invariance（スケール不変性）

Several quantities show power-low behaviors

Correlation length :（相関長） $\xi \sim |T - T_c|^{-\nu}$

Specific heat :（比熱） $C \sim |T - T_c|^{-\alpha}$

Susceptibility :（感受率） $\chi \sim |T - T_c|^{-\gamma}$

exponent＝critical exponent（臨界指数）

exponent > 0: Quantity diverges at Tc

Universality（普遍性）

Critical exponents depends only on “symmetry” and “spacial dimensions”

→ A lot of critical phenomena are exactly understood from classical models

Statistical mechanics and canonical ensemble

Canonical ensemble:
（カノニカル分布）

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

Γ ：State (e.g. {S_1, S_2, ... S_L})

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

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

$\mathcal{H}$ ：Hamiltonian

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

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

log of the partition function＝Free energy

Expectation value in canonical ensemble

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

Expectation value of physical quantity
$\longleftrightarrow$ Macroscopic physical quantities observed in thermodynamics

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

(Even if we use super computer)

Calculate partition function and expectation values approximately

- Monte Carlo method
- Molecular dynamics method
- Tensor network method
- ....

(Real space) Renormalization group

Example: Ising model

Ising model

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

$$(S_i = \pm 1 = \uparrow, \downarrow)$$

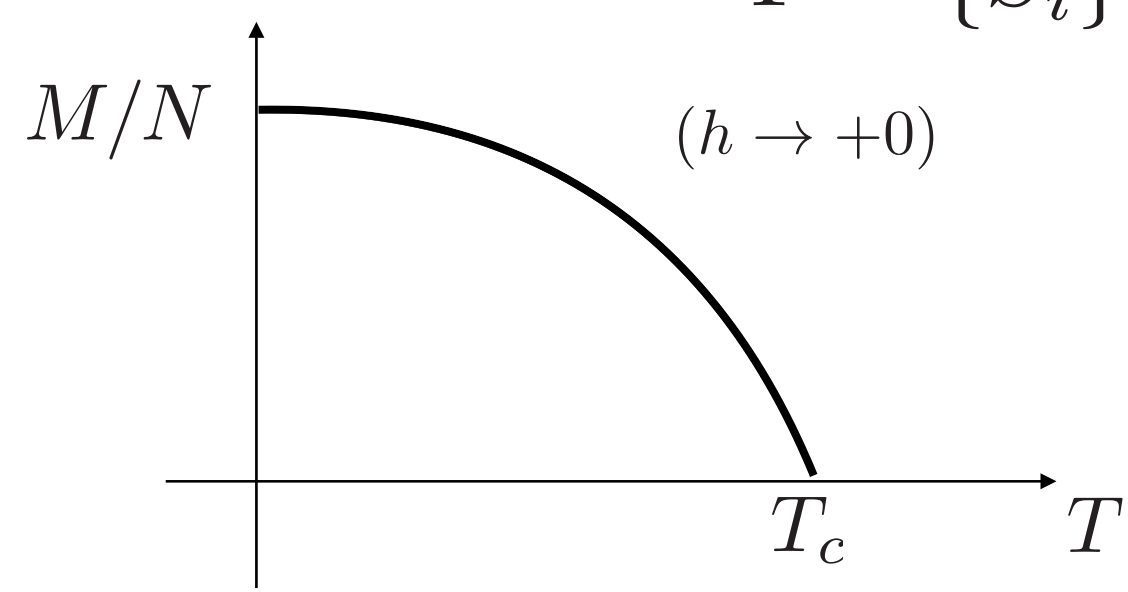
Canonical ensemble: $P(\Gamma; T) = \dfrac{1}{Z} \exp\left(-\dfrac{1}{k_B T} \mathcal{H}(\Gamma) \right)$

Magnetization at T:

$$\Gamma = \{S_i\}$$

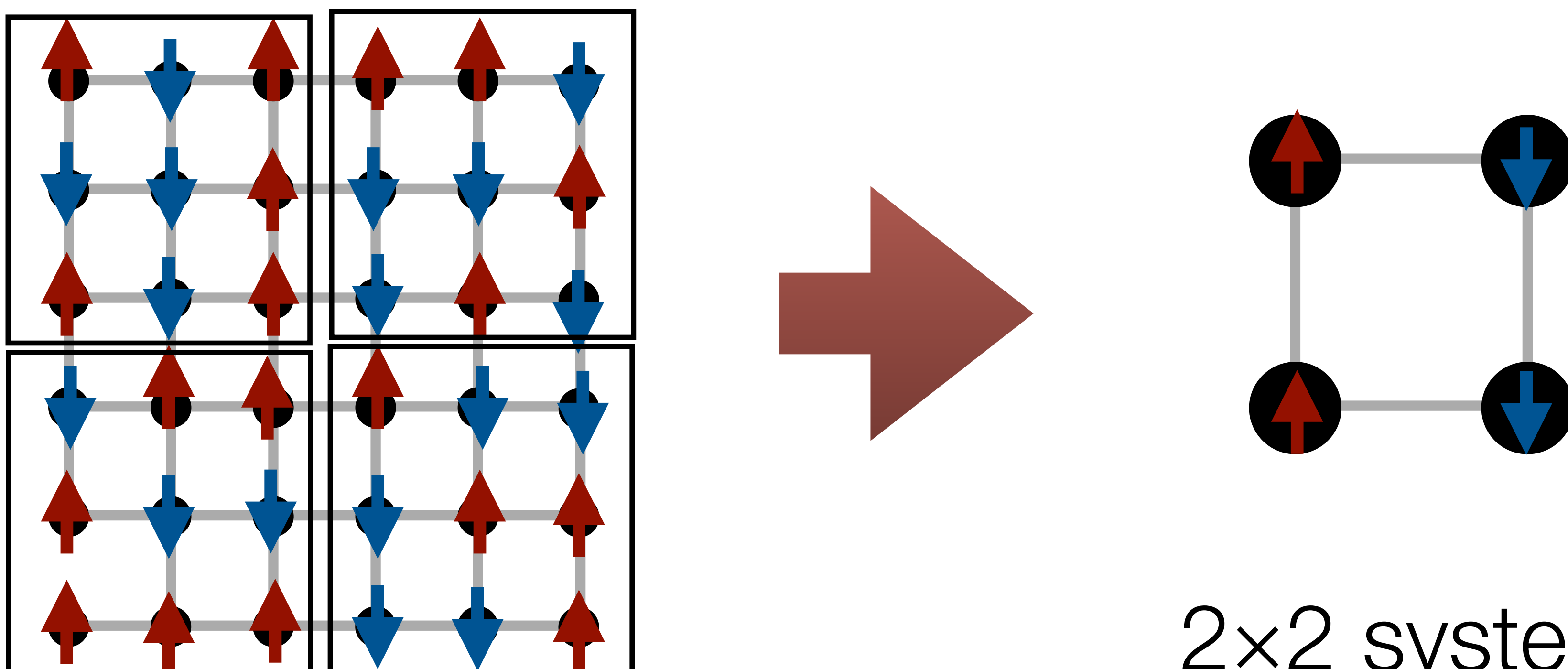
$$M(T) = \left\langle \sum_i S_i \right\rangle_T$$

$$= \sum_\Gamma \sum_i S_i P(\Gamma; T)$$



Coarse graining （粗視化）

Block spin transformation ↑ :1 ↓ :-1
（ブロックスピン変換）



"Length scale" changes

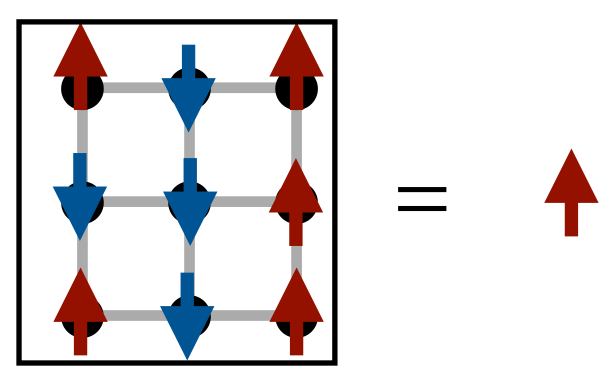
6×6 system

2×2 system

coarse grained spin

$$\sum_{i\in\mathrm{block}} S_i > 0 \quad : \quad \uparrow$$

$$\sum_{i\in\mathrm{block}} S_i < 0 \quad : \quad \downarrow$$



Example of block spin transformation

Figure taken from a book "Scaling and Renormalization in Statistical Physics", John Cardy

$T = T_c$ (critical point)

(befor) (after)

$T > T_c$

(befor) (after)

- At the critical point, the block spin transformation does not change"image" qualitatively.

  → "Scale invariance"

- At $T > T_c$, the block spin transformation changes typical "cluster size"

Partition function after coarse graining

Partition function after a block spin transformation:

(for simplicity, we set $J/k_BT = K$)

$$Z = \sum_{\{S_i=\pm 1\}} e^{K\sum_{\langle i,j\rangle} S_i S_j} = \sum_{\{S'_i=\pm 1\}} e^{-\mathcal{H}'(\{S'_i\})}$$

2^{L^d} (d-dimensional system with length L)

$2^{(L/b)^d}$ (d-dimensional system with length L/b)

By block spin transformation, the partition function is represented by smaller # of spins with a modified Hamiltonian

→ Information compression by "tracing out" short range fluctuations

Coarse grained Hamiltonian

Partition function after a block spin transformation:

$$e^{-\mathcal{H}'(\{S_i'\})} = \sum_{\{S_i\}\in\{S_i'\}} e^{K\sum_{\langle i,j\rangle} S_i S_j}$$

Sum over spin configurations corresponds to {S'}

Suppose H' has the same form with the original Hamiltonian, which characterized only one parameter K:

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

By repeating the procedure, we can draw a flow of "K"

$$K \to K' \to K'' \to \cdots \to K^{\infty}$$

"renormalization group"
(繰り込み群)

$$K' = \mathcal{R}_b(K)$$

R_b : transformation with scale *b*

Renormalization flow

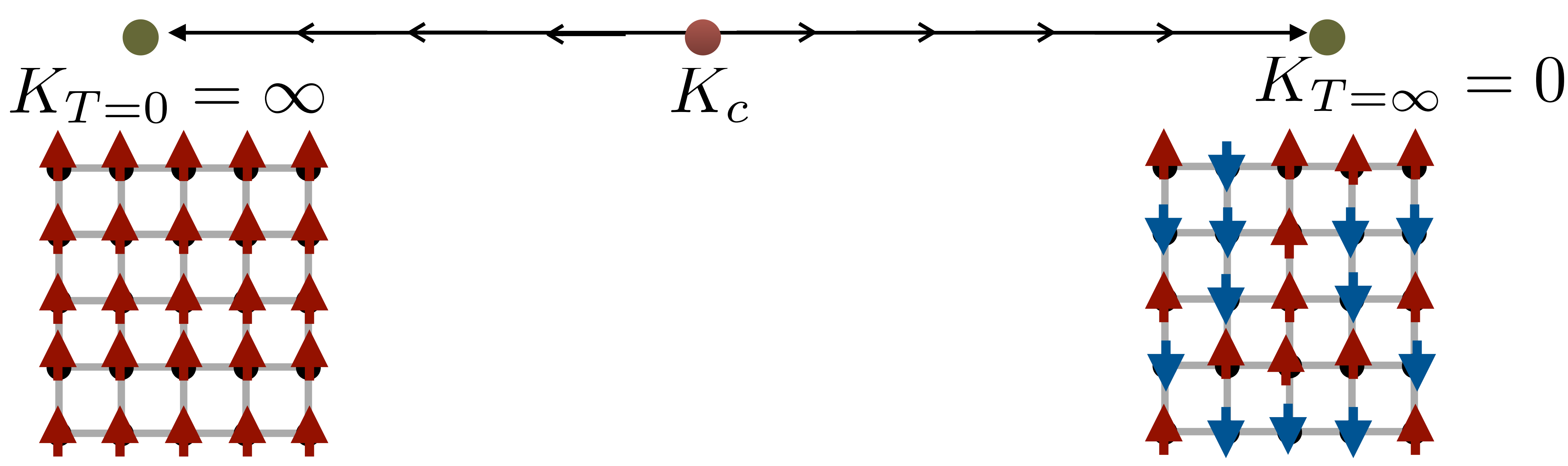
Renormalization group: $K' = \mathcal{R}_b(K)$

Fixed point（固定点）: $K^* = \mathcal{R}_b(K^*)$

Unchanged under renormalization

Typically, we have three fixed points for a phase transition:

Corresponding T=0, T=∞, and T=Tc



General case

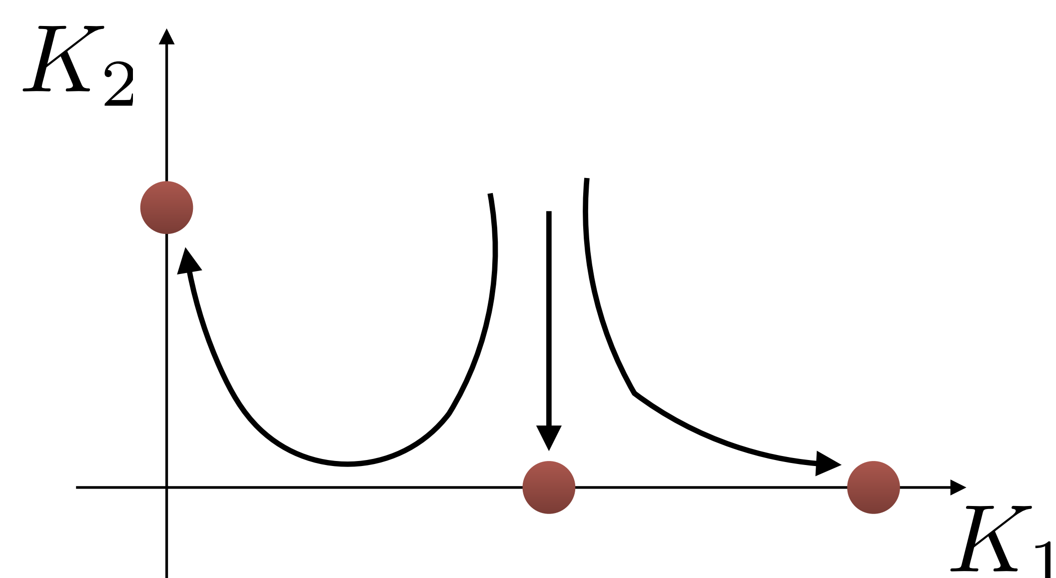
$$e^{-\mathcal{H}'(\{S_i'\})} = \sum_{\{S_i\}\in\{S_i'\}} e^{K\sum_{\langle i,j\rangle} S_i S_j}$$

In general, H' contains many body interaction such as $S_iS_jS_kS_l$.

We need more than one parameter: $\{K_1, K_2, \ldots\}$

Renormalization group: $\vec{K}' = \mathcal{R}_b(\vec{K})$

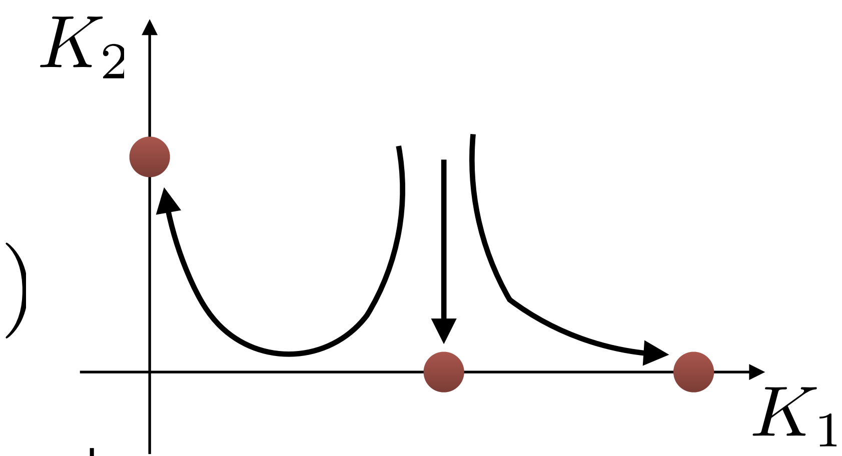
RG characterize a flow in parameter space



Critical exponents and eigenvalus

Linearization around Kc: $\vec{K}' = \mathcal{R}_b(\vec{K})$

$$\vec{K}' - \vec{K}_c \simeq \mathcal{M}_b(\vec{K} - \vec{K}_c)$$



$\mathcal{M}_b$:Matrix applied in parameter space

y_i :Eigenvalue of $\mathcal{M}_b$

$\delta\vec{K}_i$:Eigenvector

"Relevant" $|y_i| > 1$ ➡ $\delta\vec{K}_i$ increases along renormalization

"Irrelevant" $|y_i| < 1$ ➡ $\delta\vec{K}_i$ decreases along renormalization

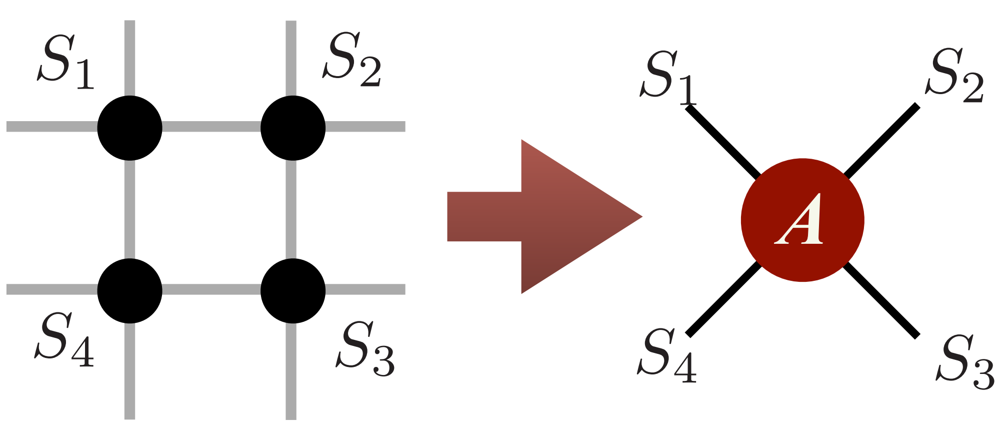
Critical exponents relate to relevant eigenvalues!

Tensor network representation of partition function

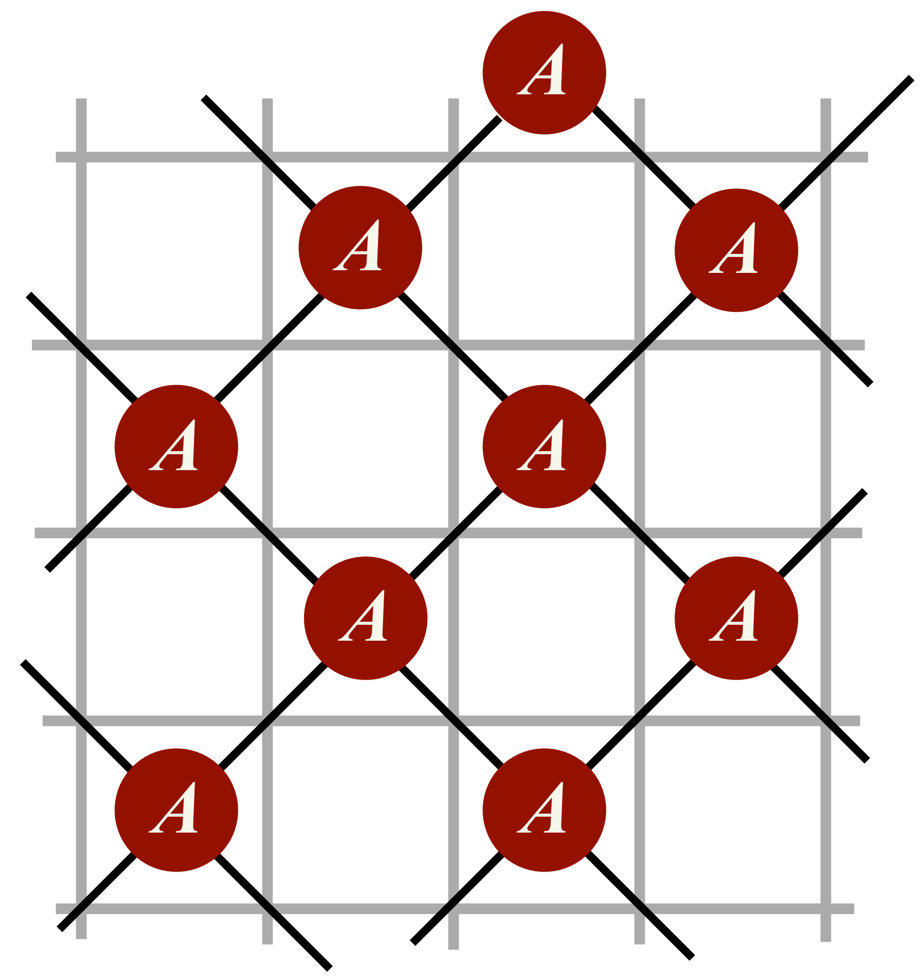
We can represent a partition function in a network of "tensor products"

Example: Ising model on the square lattice

$$A_{S_1,S_2,S_3,S_4} = e^{\beta J(S_1 S_2 + S_2 S_3 + S_3 S_4 + S_4 S_1)}$$

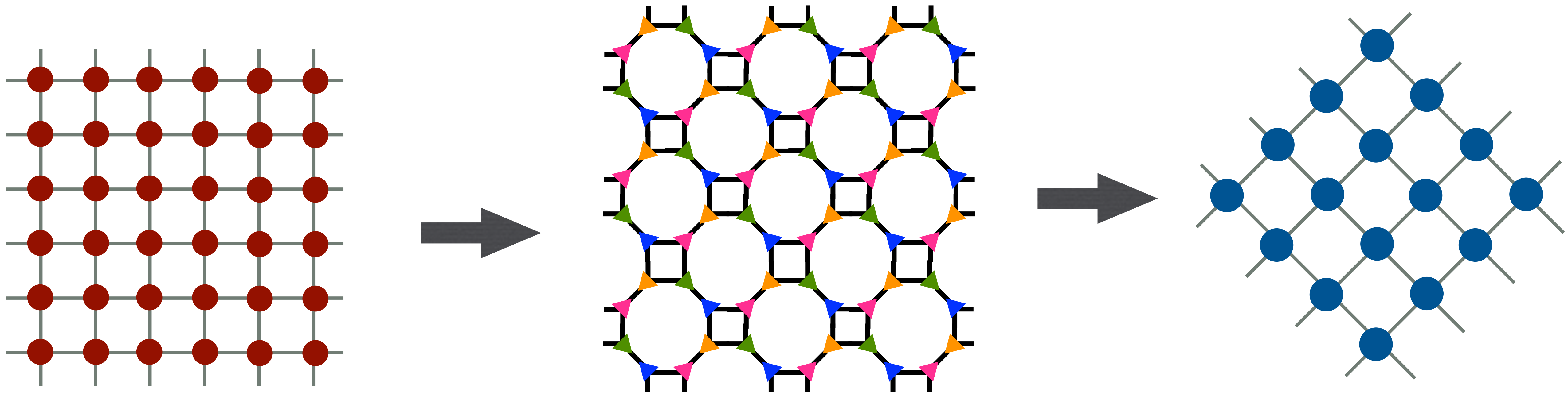


$Z =$



Real space renormalization of tensor network

Corse graining of a tensor network



The coarse graining directly related to
real space renormalization group

Fixed point Hamiltonian ⟷ Fixed point tensor

Relation?

Important Keyword: Entanglement of information

Next week

第１回：　現代物理学における巨大なデータ
第２回：　情報圧縮と繰り込み
第３回：　情報圧縮の数理１　(線形代数の復習)
(Review of linear algebra)
第４回：　情報圧縮の数理２　(特異値分解と低ランク近似)
第５回：　情報圧縮の数理３　(スパース・モデリングの基礎)
第６回：　情報圧縮の数理４　(クリロフ部分空間法の基礎)
第７回：　物質科学における情報圧縮
第８回：　スパース・モデリングの物質科学への応用
第９回：　クリロフ部分空間法の物質科学への応用
第１０回：　行列積表現の基礎
第１１回：　行列積表現の応用
第１２回：　テンソルネットワーク表現への発展
第１３回：　テンソルネットワーク繰り込みと低ランク近似の応用