

計算科学における情報圧縮

Information Compression in Computational Science

**2017.10.5**

**#2:情報圧縮と繰り込み**

**Information compression and renormalization**

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# Outline

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

Many body problems:  
Quantum and Classical systems

# Quantum systems

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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

$$\boxed{\mathcal{H} |\Psi\rangle = \underline{E} |\Psi\rangle} = \text{Eigenvalue problem}$$

Energy

# Quantum systems

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

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

The Hamiltonian can be represented in these bases

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

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

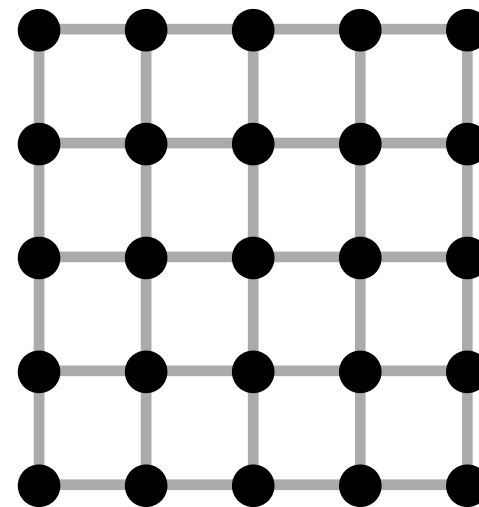
# Quantum systems

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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**)

基底狀態

➡ We can concentrate to a **special state**

- Typical system only has "short range" interactions

➡ Hamiltonian matrix becomes **sparse**

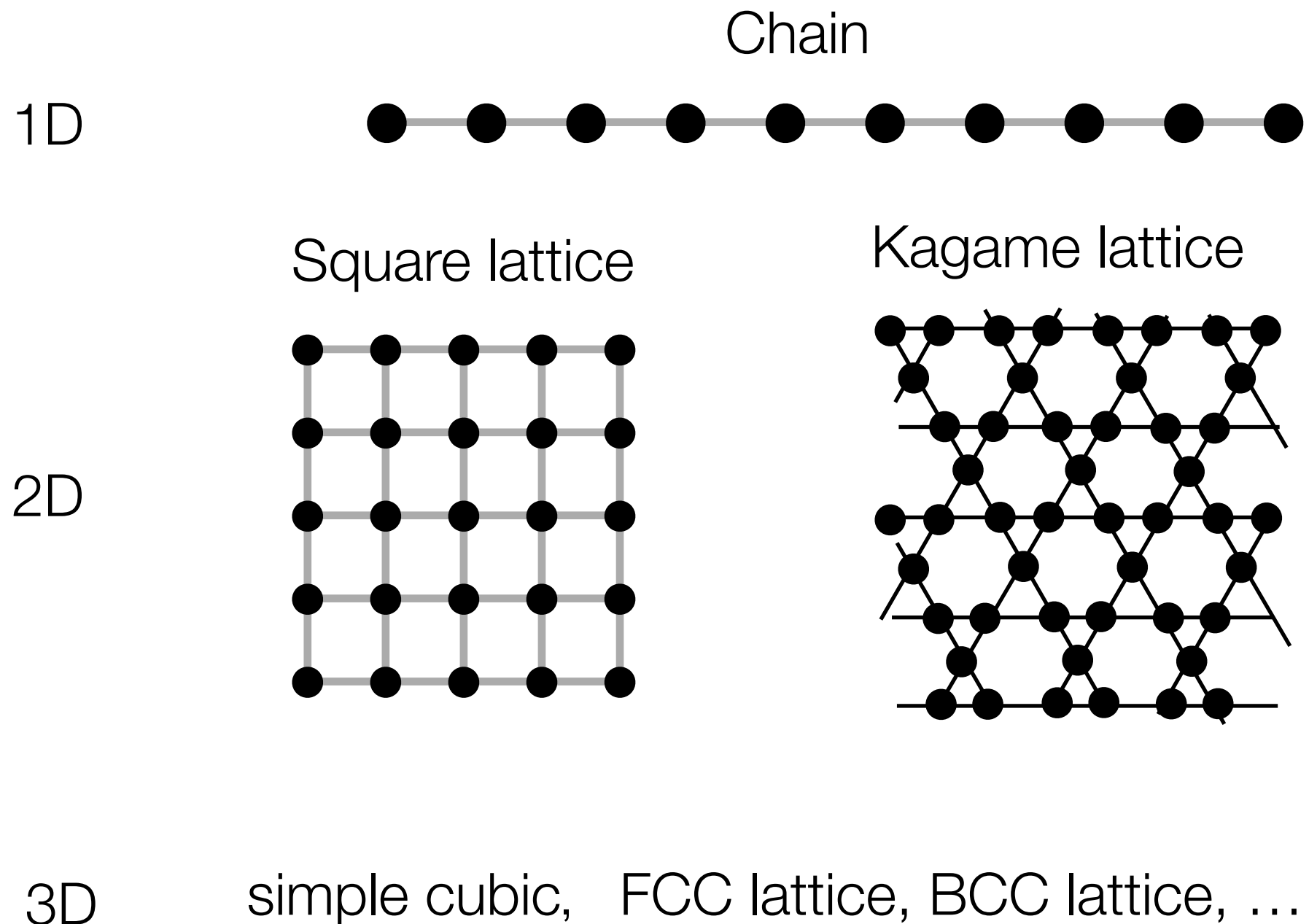
# (Quantum) spin system

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## Spin systems:

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

### **Lattice**



# Quantum spin

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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

$$S = \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$$

$$S_z = -S, -S+1, \dots, S-1, S$$

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



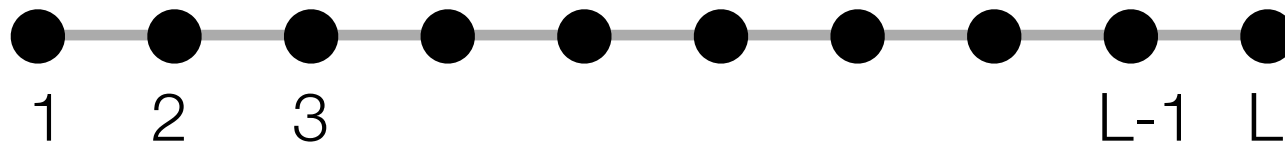
# Quantum spin: $S=1/2$

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:

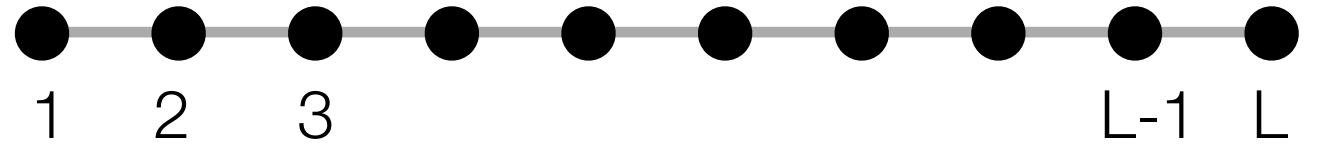


"Transverse field Ising model" (横磁場イジング模型)

$L=2$

$$\mathcal{H} = - \sum_{i=1}^{L-1} S_{i,z} S_{i+1,z} - \Gamma \sum_{i=1}^L S_{i,x} \quad \mathcal{H} = \begin{pmatrix} -1/4 & -\Gamma/2 & -\Gamma/2 & 0 \\ -\Gamma/2 & 1/4 & 0 & -\Gamma/2 \\ -\Gamma/2 & 0 & 1/4 & -\Gamma/2 \\ 0 & -\Gamma/2 & -\Gamma/2 & -1/4 \end{pmatrix}$$

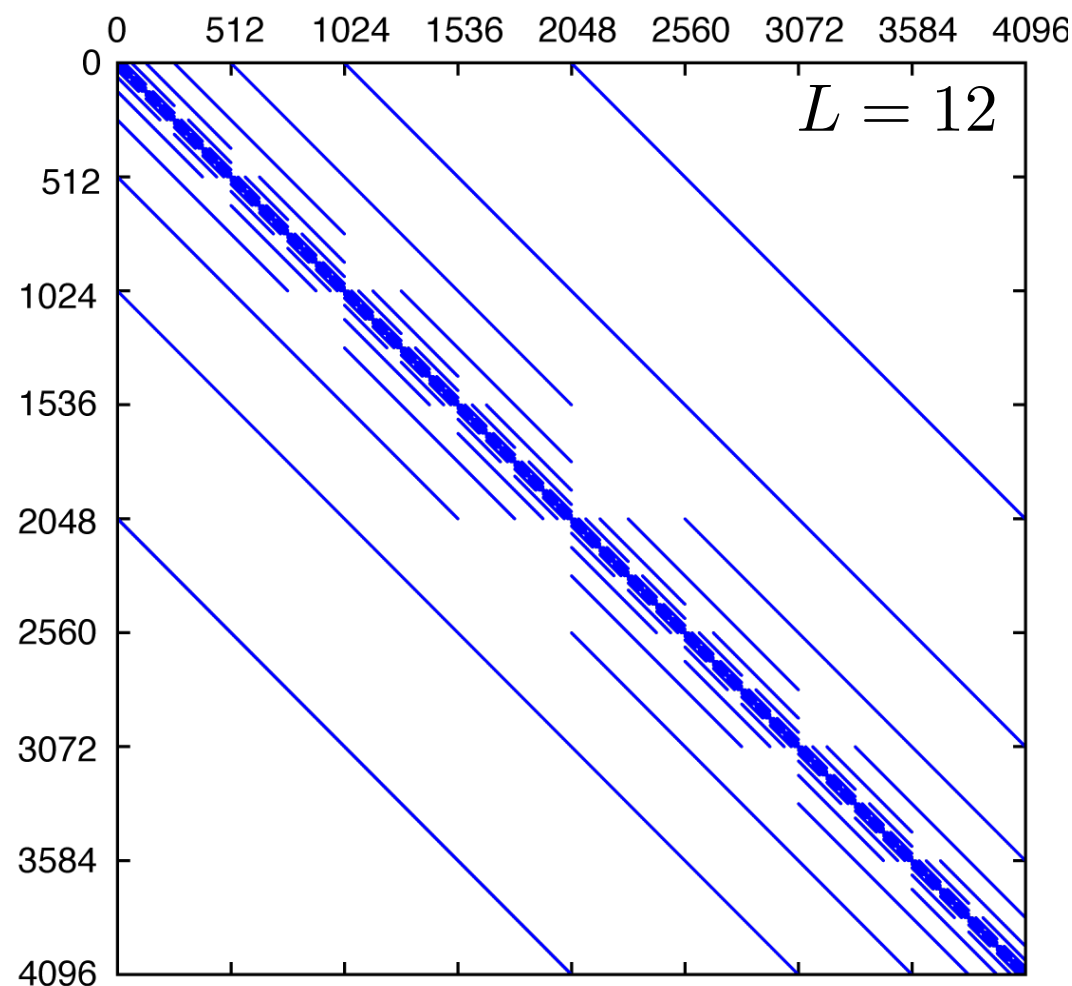
# Quantum spin: $S=1/2$



"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  $\sim O(Le^L)$

Sparse!

# Classical problems

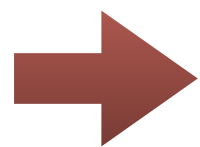
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## Two types of classical many-body problems

### 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**
- ...

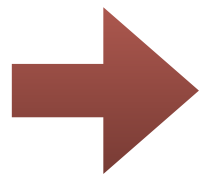
# Classical problems as an approximation: magnetism

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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  $S \rightarrow \infty$ .

“classical” spin model

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

# Classical spin degree of freedom

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Classical spin: 1.  $S \rightarrow \infty$  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 understood 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"

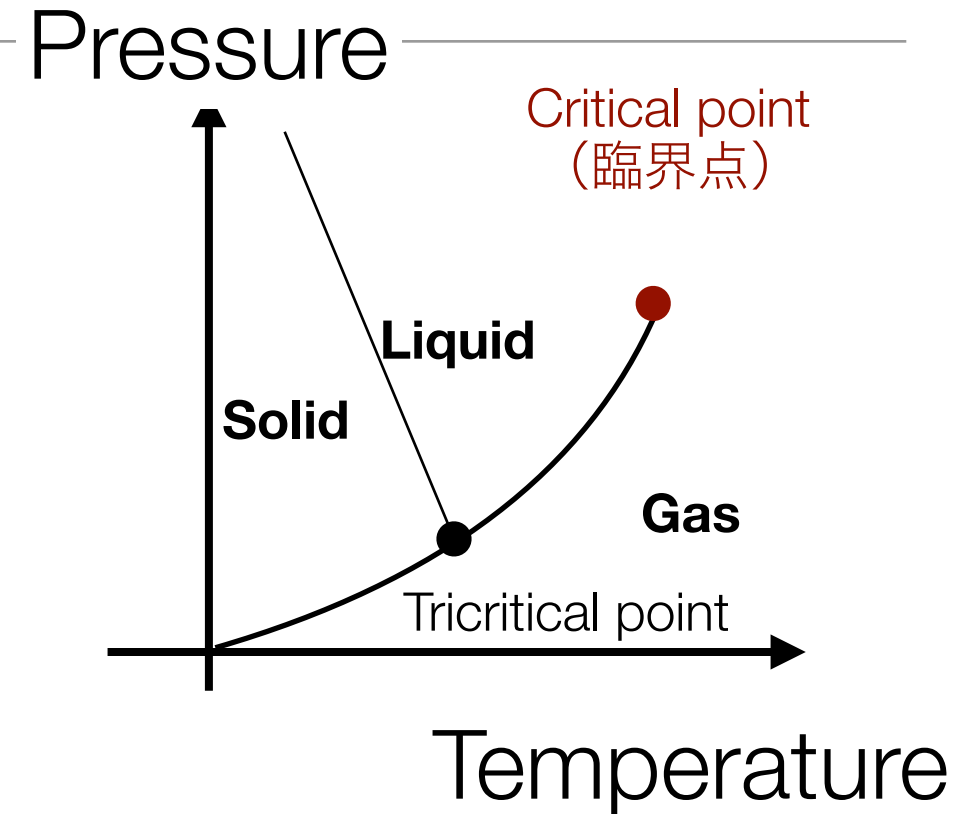


- We do not need explicit diagonalization
- "State" can be represented by a product of local DOF  
 $\sim O(L)$  (Degrees Of Freedom)
- Although, # of states is  $\sim O(2^L)$

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** (相轉移)
- 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)

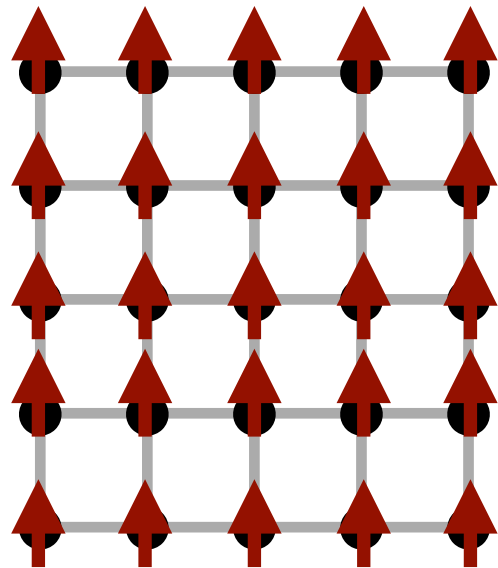
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Typically we have two phases:

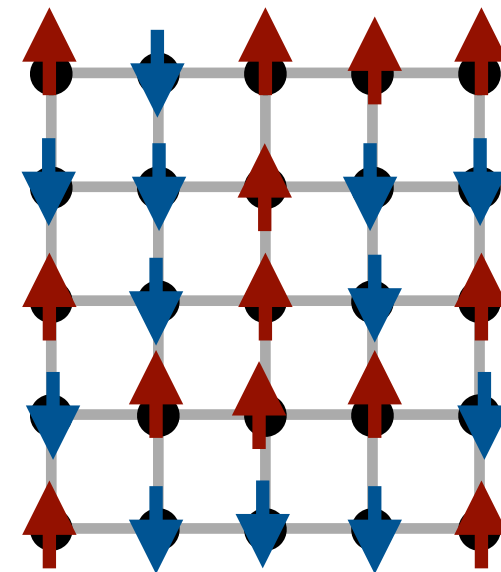
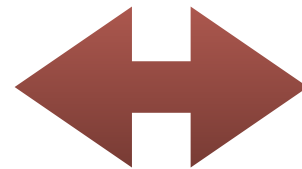
Magnetically ordered phase

Disordered phase

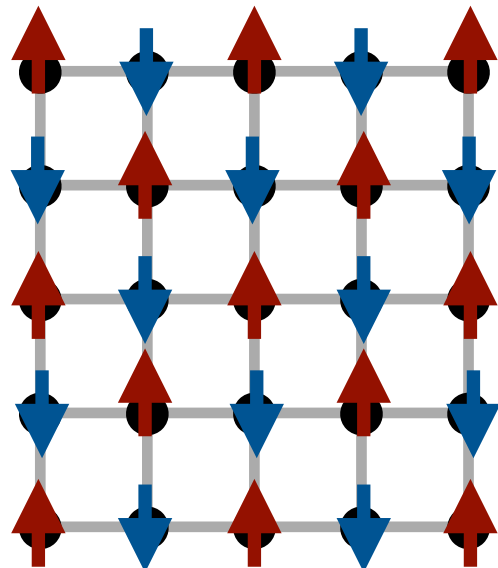
**Ferromagnetic**  
(強磁性)



Phase transition



**Antiferromagnetic**  
(反強磁性)



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

# First order and Second order phase transition

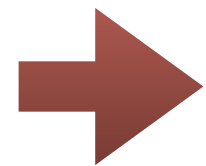
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- There are two types of phase transition: **discontinuous** and **continuous**
  - Discontinuous transition:  
At the phase transition, **the derivative of the free energy changes discontinuously** = First order phase transition
    - Eg. Liquid  $\longleftrightarrow$  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  $\longleftrightarrow$  Liquid critical point, phase transition in Ising model

# Critical phenomena (臨界現象)

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At the critical point, characteristic length diverges



Scale invariance  
(スケール不変性)

Several quantities show **power-law 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)

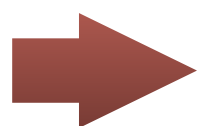
$$\chi \sim |T - T_c|^{-\gamma}$$

exponent = **critical exponent**  
(臨界指数)

exponent > 0: Quantity diverges at  $T_c$

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

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Canonical ensemble:  
(カノニカル分布)

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

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

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

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

Partition function (分配関数)  $\mathcal{H}$  : Hamiltonian

= Normalization factor of the canonical ensemble

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

Relation to the free energy in thermodynamics

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

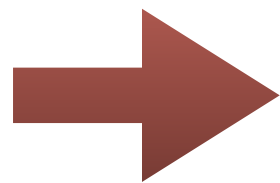
log of the partition function = Free energy

# Expectation value in canonical ensemble

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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  
↔ Macroscopic physical quantities observed in thermodynamics



We can calculate thermodynamic quantities from 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

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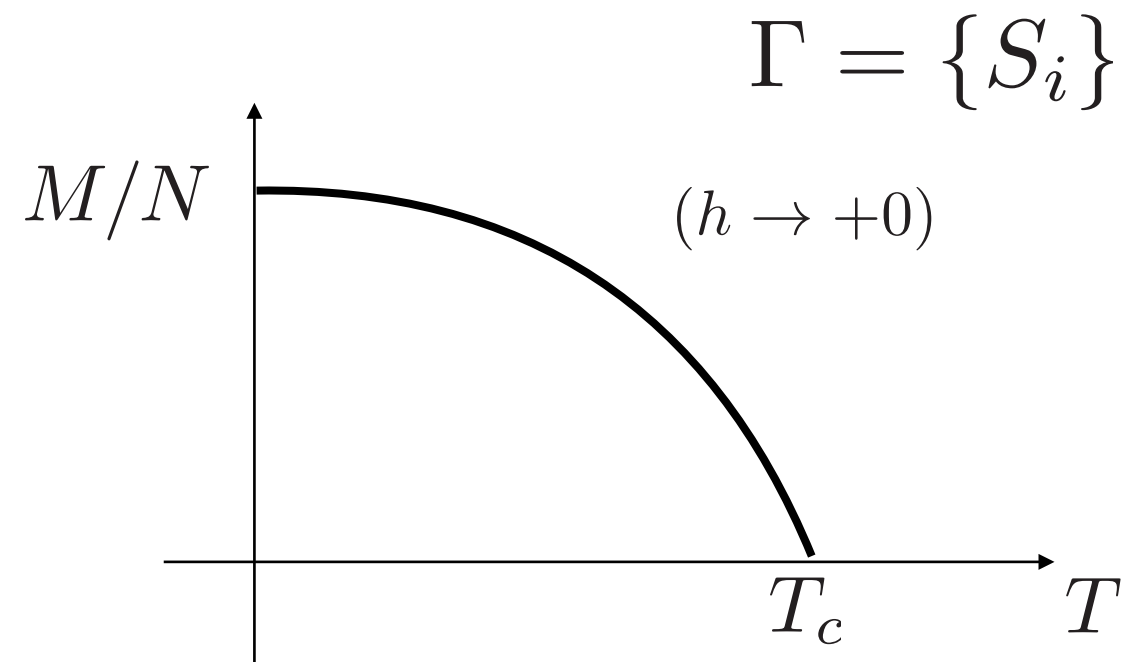
## Ising model

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

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

Magnetization at T:

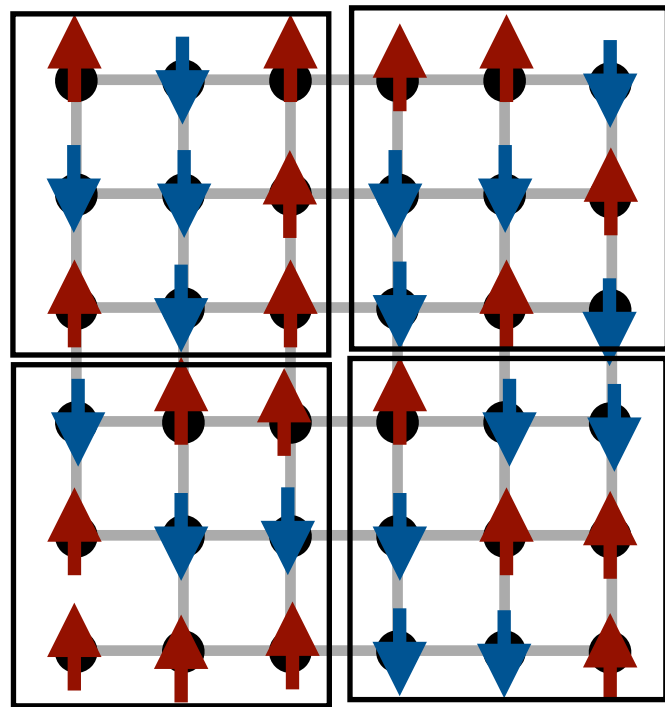
$$\begin{aligned} M(T) &= \left\langle \sum_i S_i \right\rangle_T \\ &= \sum_{\Gamma} \sum_i S_i P(\Gamma; T) \end{aligned}$$



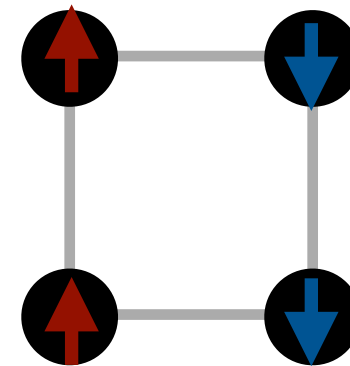
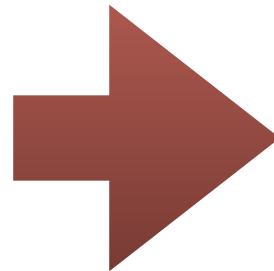
# Coarse graining (粗視化)

Block spin transformation  
(ブロックスピン変換)

↑ : 1    ↓ : -1



6×6 system

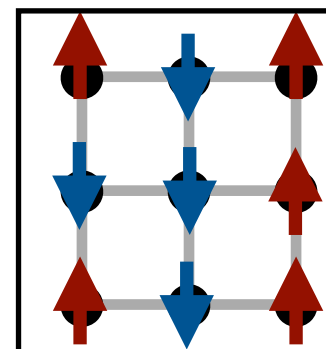


2×2 system

"Length scale"  
changes

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

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



=





# Example of block spin transformation

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

$T=T_c$  (critical point)

$T > T_c$

(befor)

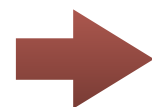
(after)

(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

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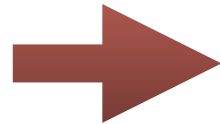
Partition function after a block spin transformation:

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

$$Z = \sum_{\substack{\{S_i = \pm 1\} \\ 2^{L^d}}} e^{K \sum_{\langle i,j \rangle} S_i S_j} = \sum_{\substack{\{S'_i = \pm 1\} \\ 2^{(L/b)^d}}} e^{-\mathcal{H}'(\{S'_i\})}$$

(d-dimensional system with length L)      (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

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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  $\mathcal{H}'$  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 " $K$ "

$$K \rightarrow K' \rightarrow K'' \rightarrow \dots \rightarrow K^\infty$$

"renormalization group"  
(繰り込み群)  $K' = \mathcal{R}_b(K)$

$\mathcal{R}_b$  : transformation with scale  $b$

# Renormalization flow

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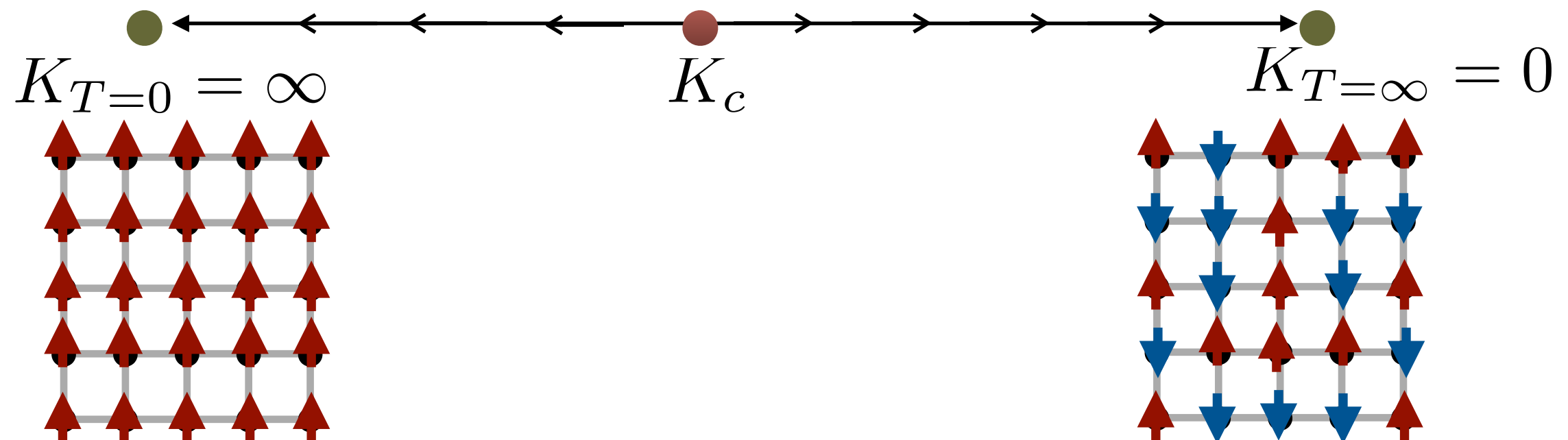
Renormalization group:  $K' = \mathcal{R}_b(K)$

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

Unchanged under renormalization

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

Corresponding  $T=0$ ,  $T=\infty$ , and  $T=T_c$

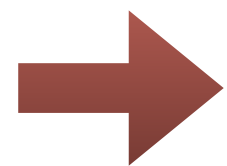


# General case

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

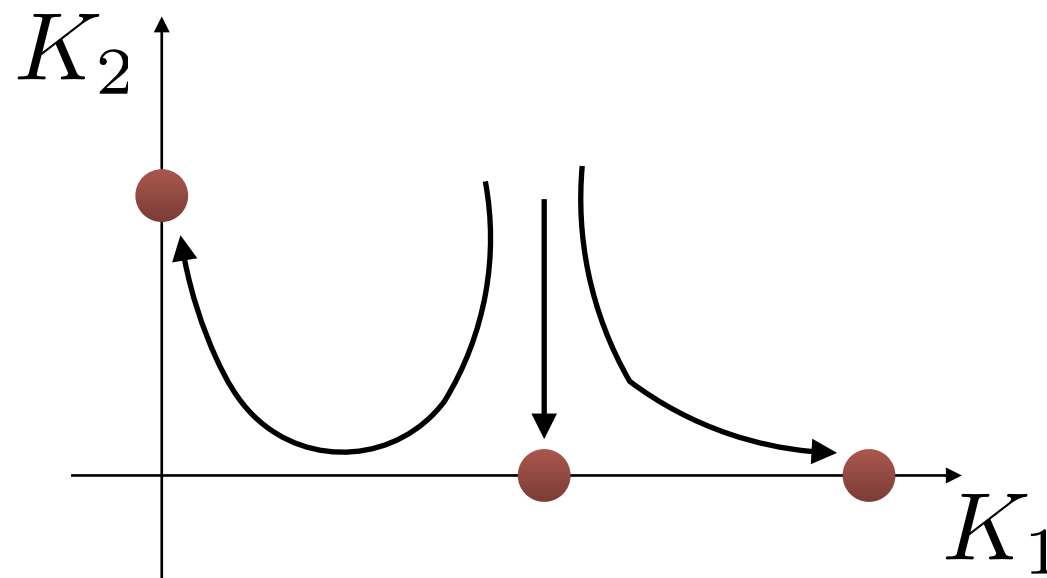
In general,  $\mathcal{H}'$  contains many body interaction such as  $S_i S_j S_k S_l$ .



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

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

RG characterize a flow in parameter space



# Critical exponents and eigenvalues

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

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

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

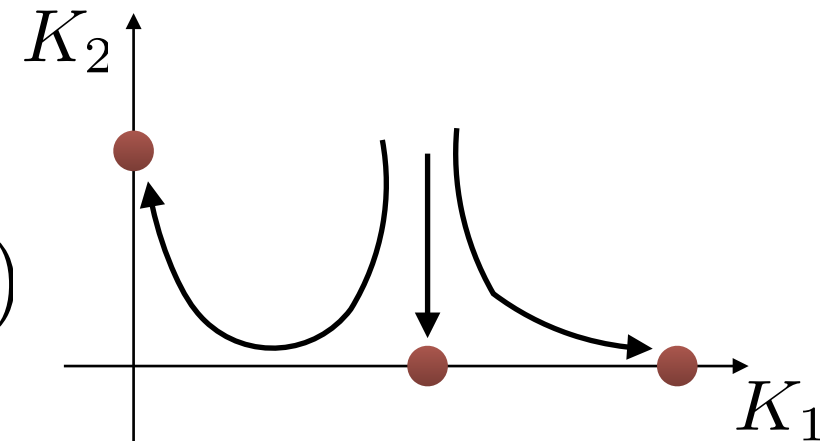
$y_i$  : Eigenvalue of  $\mathcal{M}_b$

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

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

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

Critical exponents relate to relevant eigenvalues!

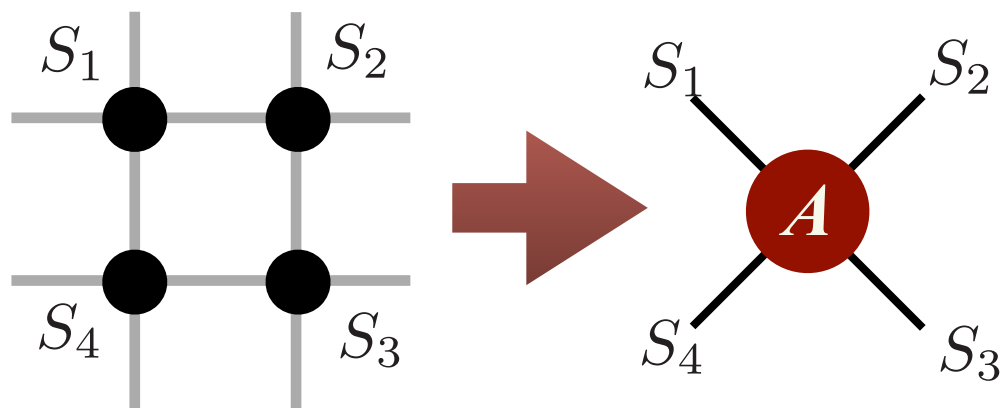


# Tensor network representation of partition function

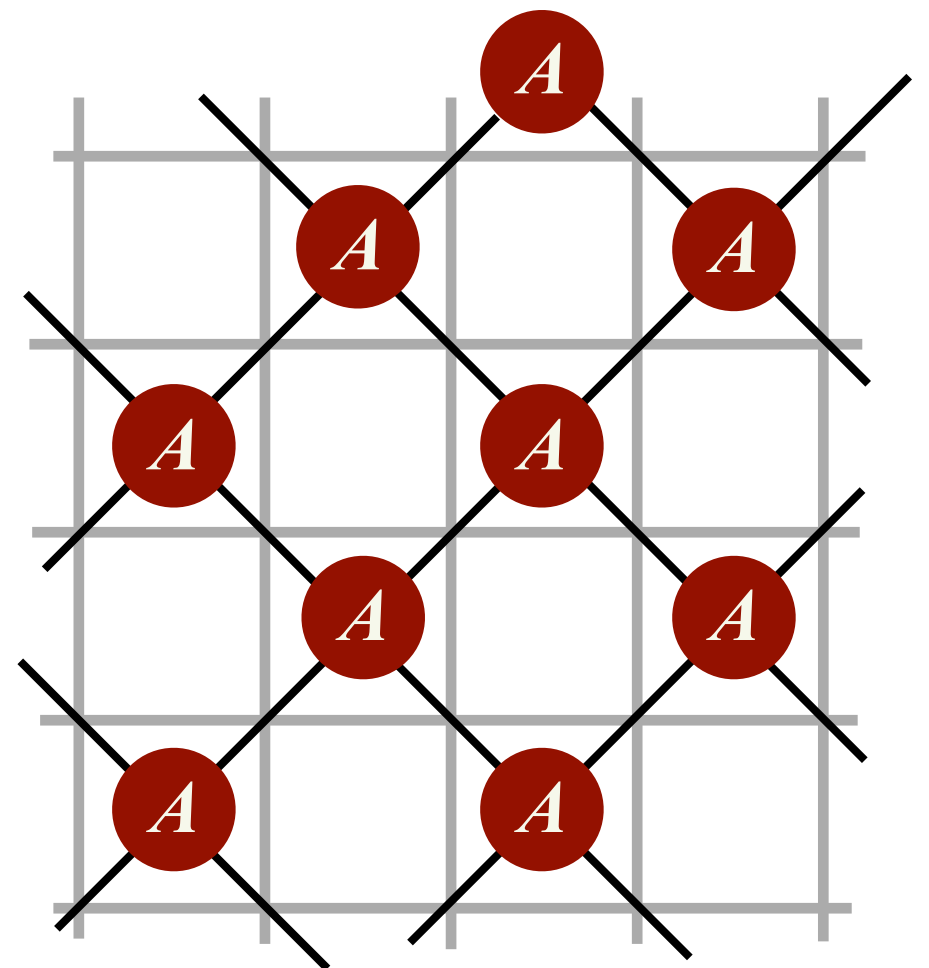
We can represent a partition function in a network of "tensor products"

Example: Ising model on the square lattice

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



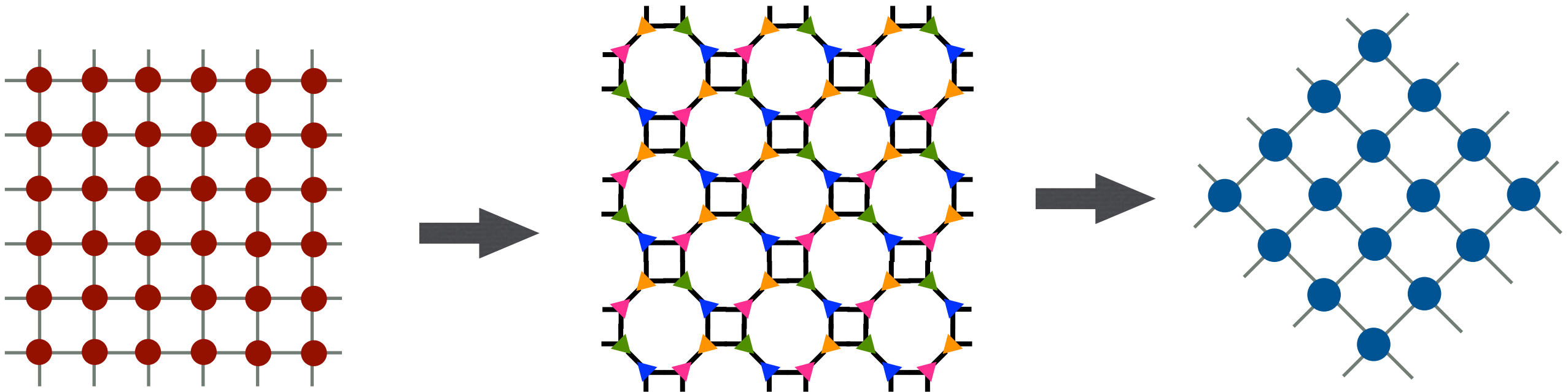
$Z =$



# Real space renormalization of tensor network

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Coarse graining of a tensor network



The coarse graining directly related to  
real space renormalization group

Fixed point Hamiltonian  $\longleftrightarrow$  Fixed point tensor  
Relation?

Important Keyword: **Entanglement of information**



# Next week

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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