

計算科学における情報圧縮

Information Compression in Computational Science

2018.10.4

#2:現代物理学と情報圧縮

Information compression in modern physics

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Lecture schedule

- 第1回： 現代物理学における巨大なデータ
- 第2回： 現代物理学と情報圧縮
- 第3回： 情報圧縮の数理1 (線形代数の復習)
- 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： データ解析の高速化：スパース・モデリングの物質科学への応用
- 第9回： データ空間の圧縮：クリロフ部分空間法の物質科学への応用
- 第10回： 高度なデータ圧縮：情報のエンタングルメントと行列積表現
- 第11回： 行列積表現の固有値問題への応用
- 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による情報圧縮

Outline

- 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

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

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

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

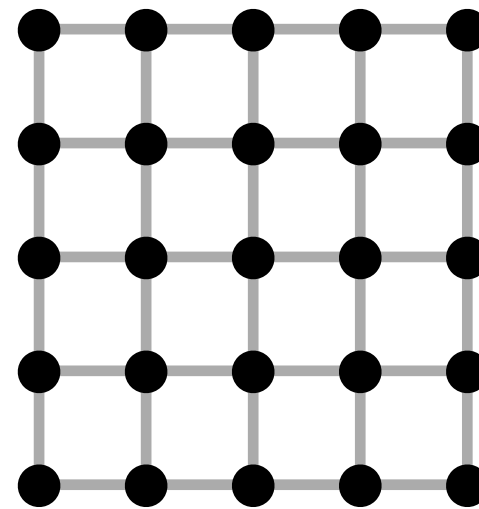
Matrix element: $H_{\alpha, \beta; \alpha', \beta'} \equiv \langle \alpha\beta | \mathcal{H} | \alpha'\beta' \rangle$

Quantum systems

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

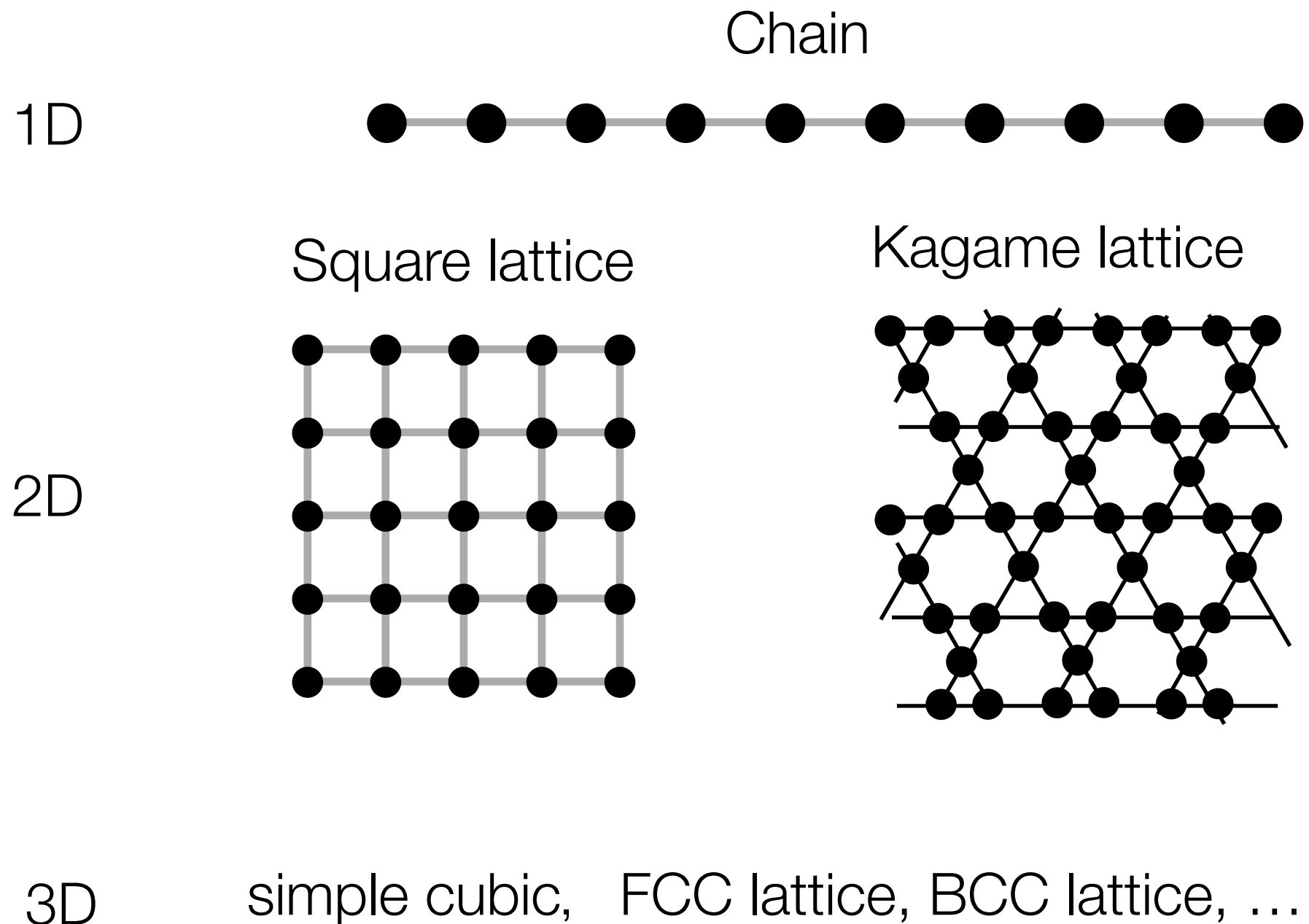
➡ Hamiltonian matrix becomes **sparse**.

(Quantum) spin system

Spin systems:

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

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

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

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

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

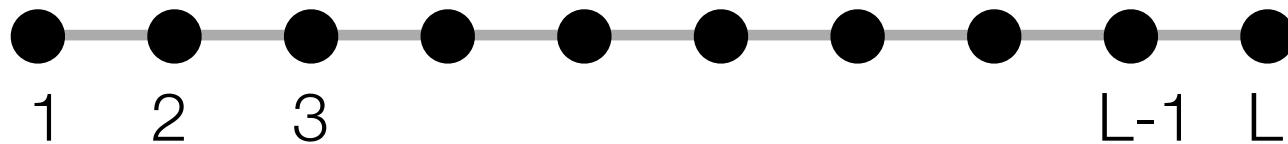
Quantum spin: $S=1/2$

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:

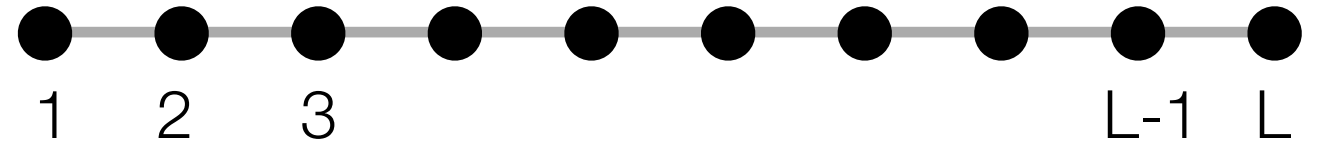


"Transverse field Ising model" (横磁場イジング模型)

$L=2$

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

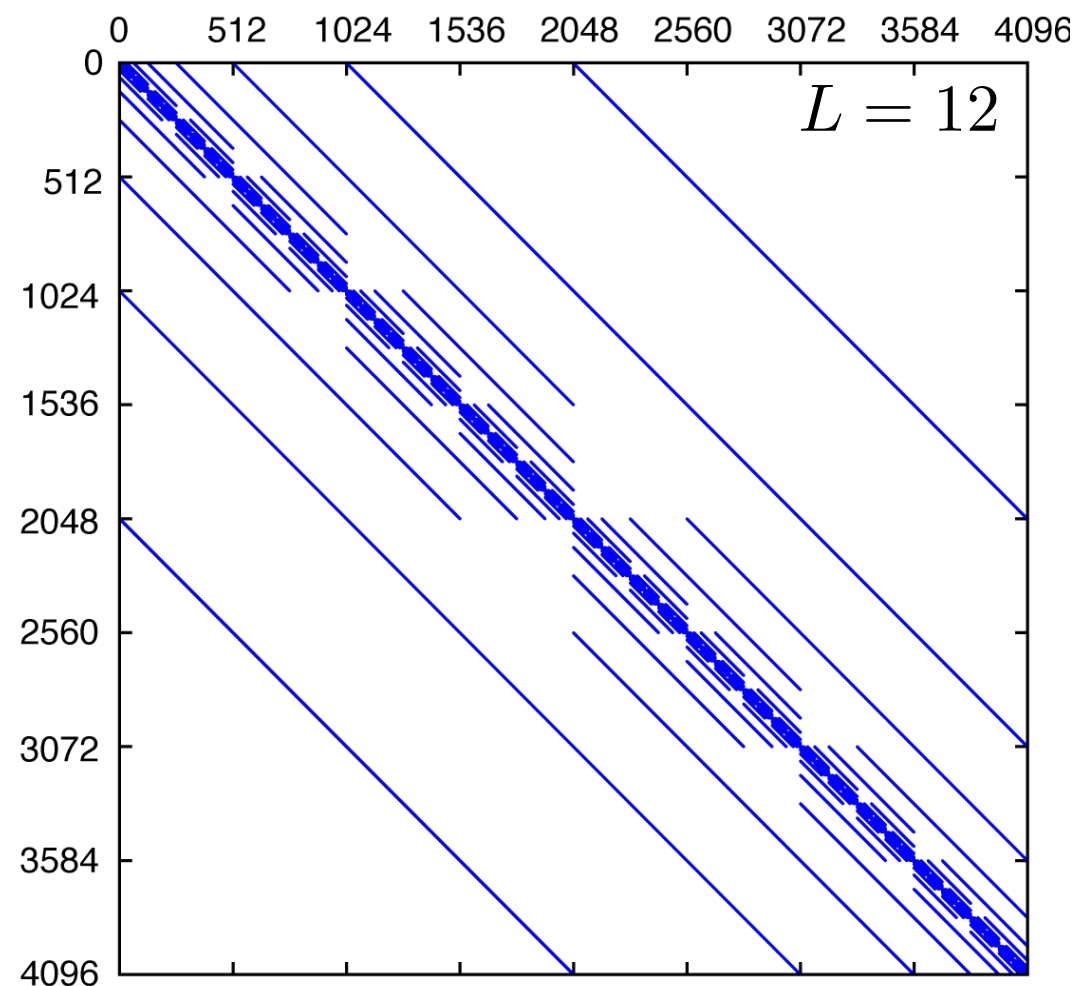
Quantum spin: $S=1/2$



"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!

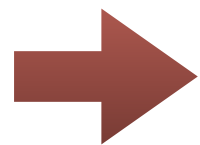
Classical problems

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

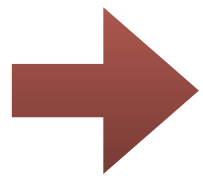
- Percolation, covering, packing, ...
- Stochastic process, “dynamical” system, ..
- **Critical phenomena**
- ...

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 $S \rightarrow \infty$.

“classical” spin model

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

Classical spin degree of freedom

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"

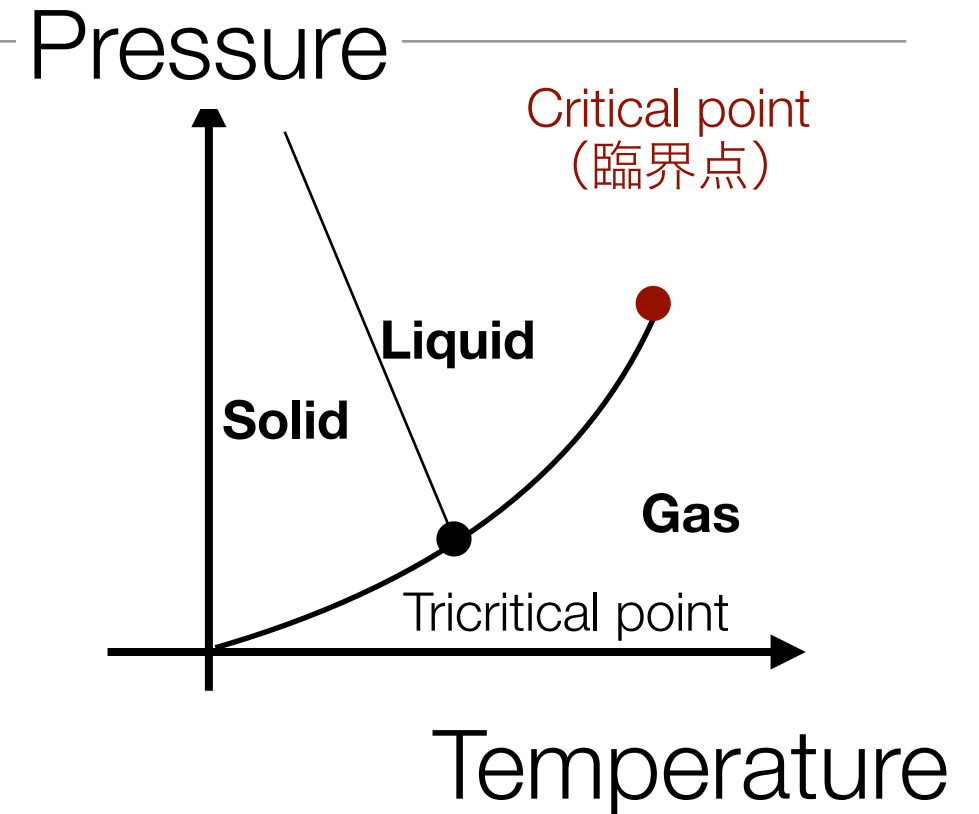


- We do not need explicit diagonalization
- "State" can be represented by a product of local DOF
 $\sim O(L)$ (Degrees Of Freedom)
- Although, # of states is $\sim O(2^L)$

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?

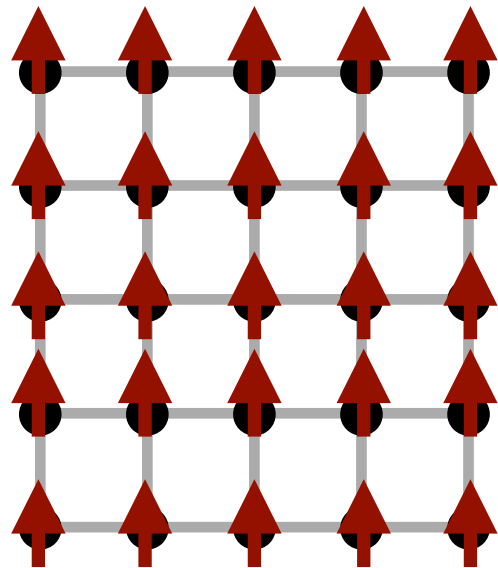
Phases in magnets (spin model)

Typically we have two phases:

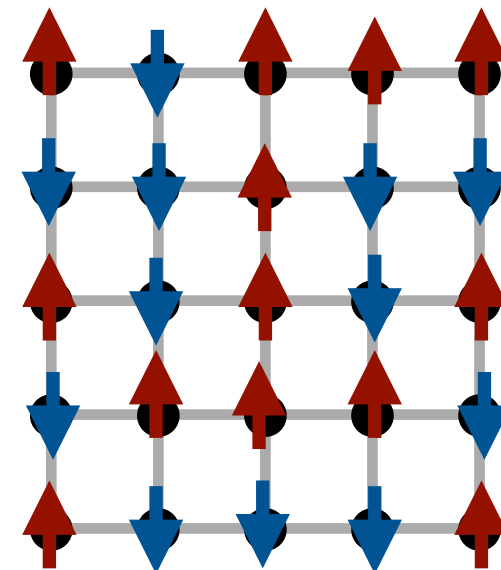
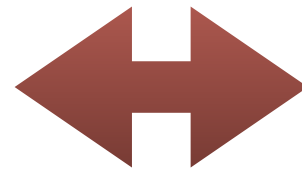
Magnetically ordered phase

Disordered phase

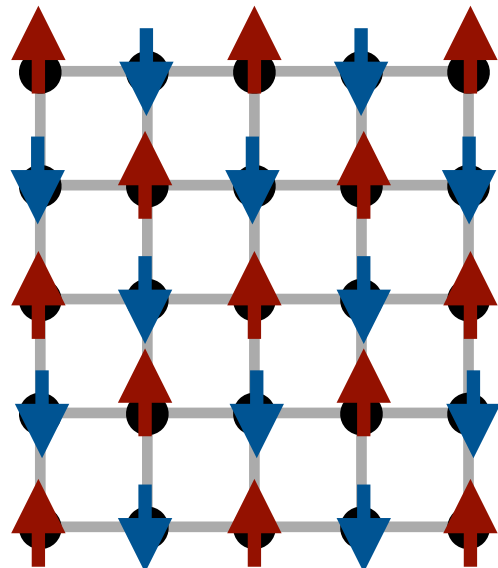
Ferromagnetic
(強磁性)



Phase transition



Antiferromagnetic
(反強磁性)



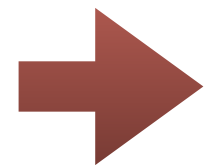
In real matters and complex spin models,
variety of magnetic orders are stabilized

First order and Second order phase transition

- 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)

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)

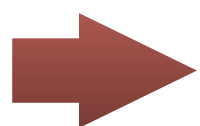
$$\chi \sim |T - T_c|^{-\gamma}$$

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

Canonical ensemble:
(カノニカル分布)

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

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

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

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

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

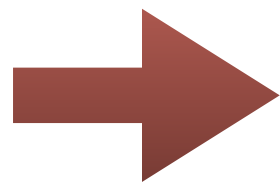
$$F = -k_B T \ln Z$$

log of the partition function = Free energy

Expectation value in canonical ensemble

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_{Γ} 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:

Related to the 13th lecture

Example: Ising model

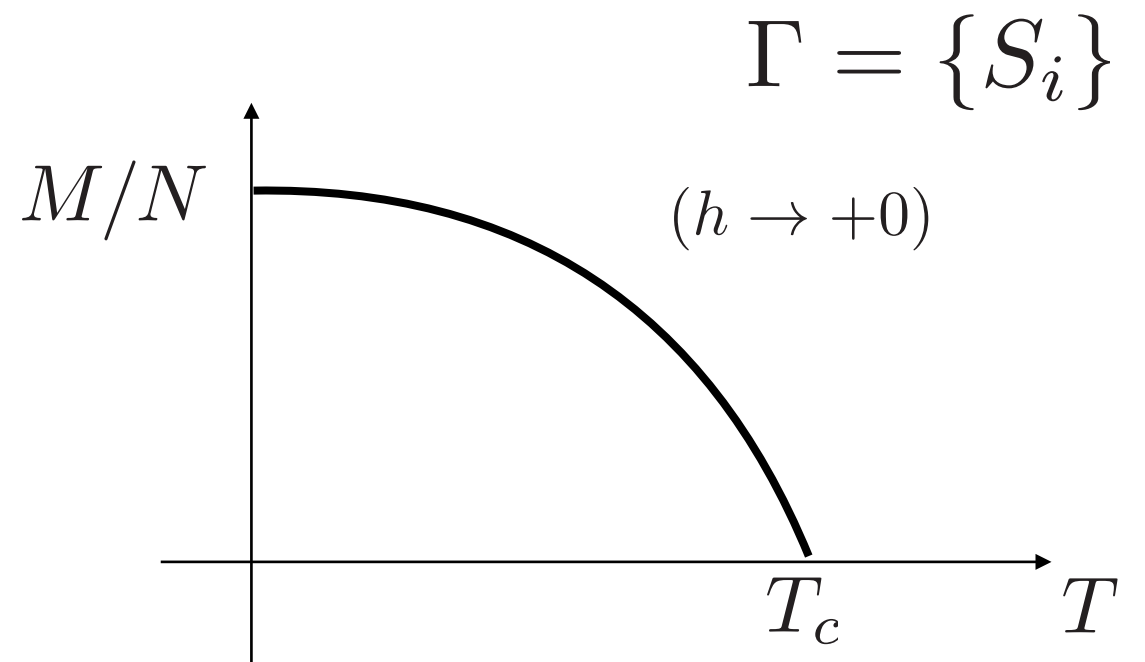
Ising model

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

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

Magnetization at T:

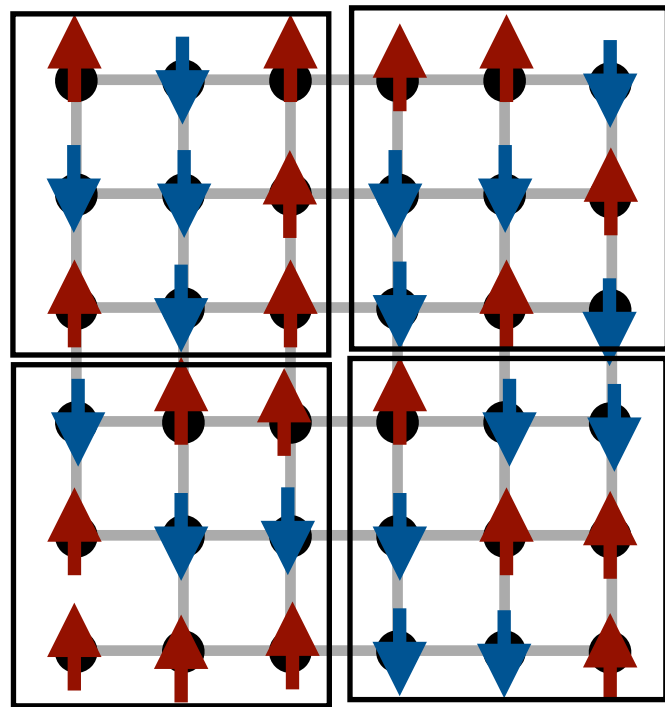
$$\begin{aligned} M(T) &= \left\langle \sum_i S_i \right\rangle_T \\ &= \sum_{\Gamma} \sum_i S_i P(\Gamma; T) \end{aligned}$$



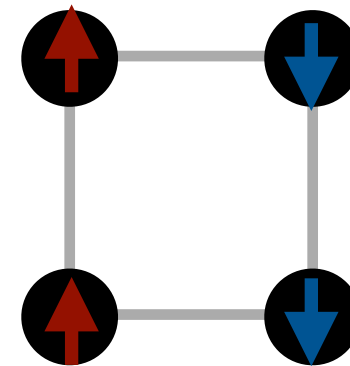
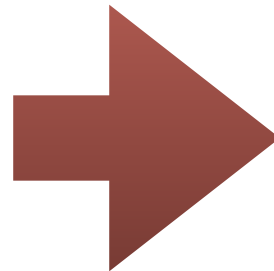
Coarse graining (粗視化)

Block spin transformation (ブロックスピン変換)

↑ : 1 ↓ : -1



6×6 system



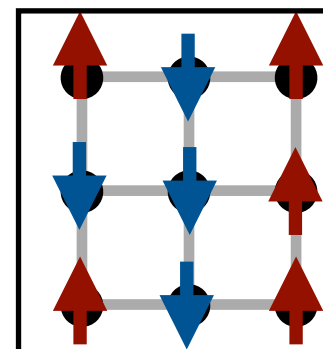
2×2 system

"Length scale" changes

coarse grained spin

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

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



=



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)

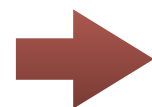
(after)

(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

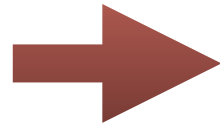
Partition function after a block spin transformation:

(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

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

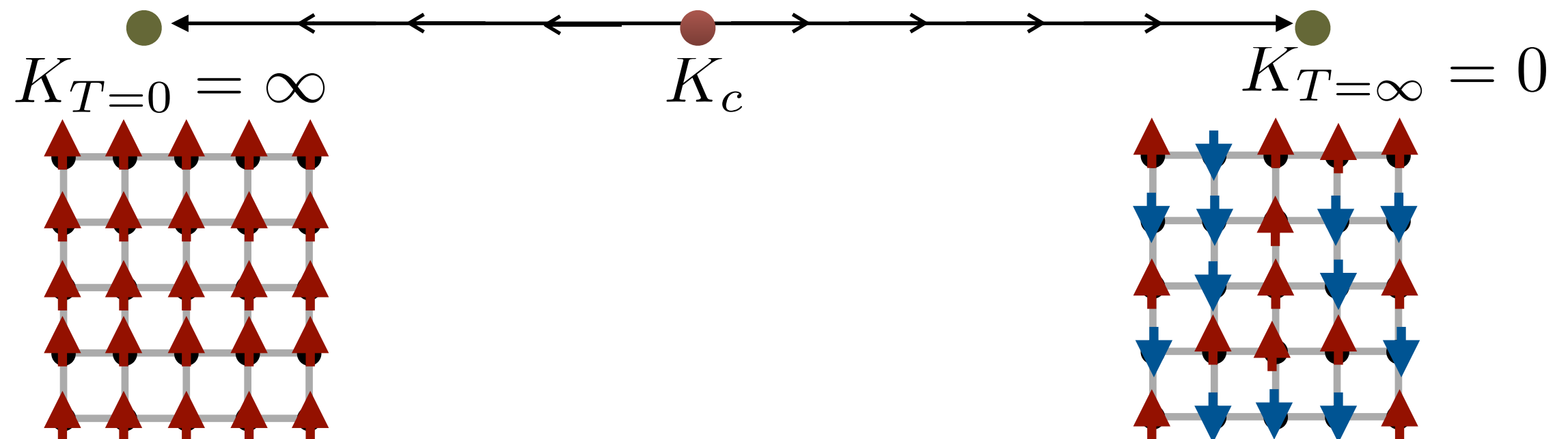
Renormalization group: $K' = \mathcal{R}_b(K)$

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

Unchanged under renormalization

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

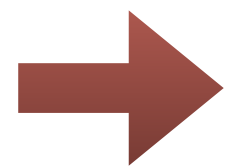
Corresponding $T=0$, $T=\infty$, and $T=T_c$



General case

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

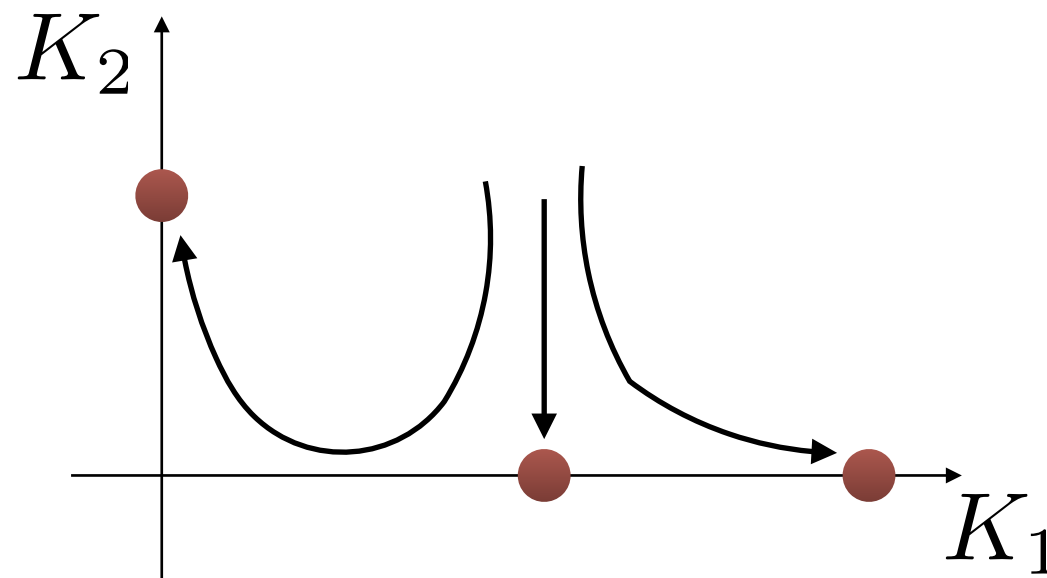
In general, \mathcal{H}' contains many body interaction such as $S_i S_j S_k S_l$.



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

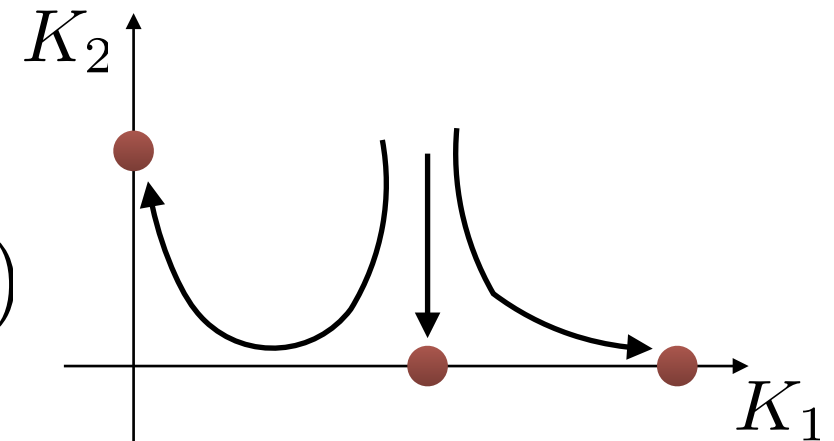


Critical exponents and eigenvalues

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

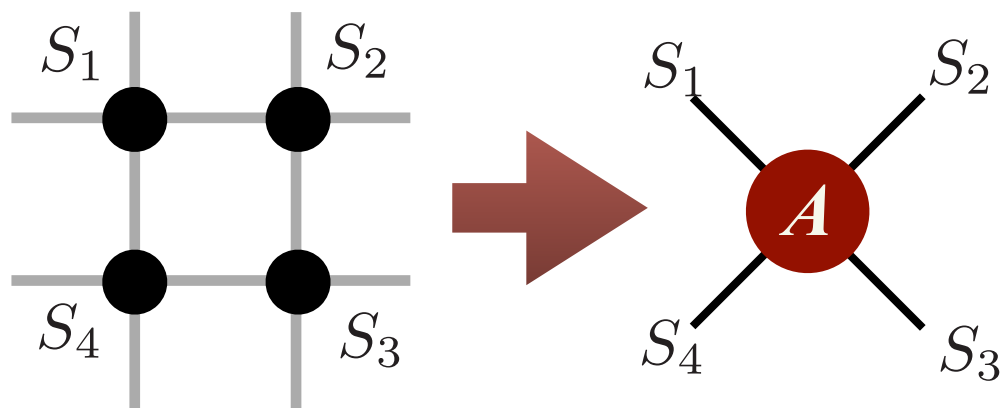
Critical exponents are related to relevant eigenvalues!

Tensor network representation of partition function

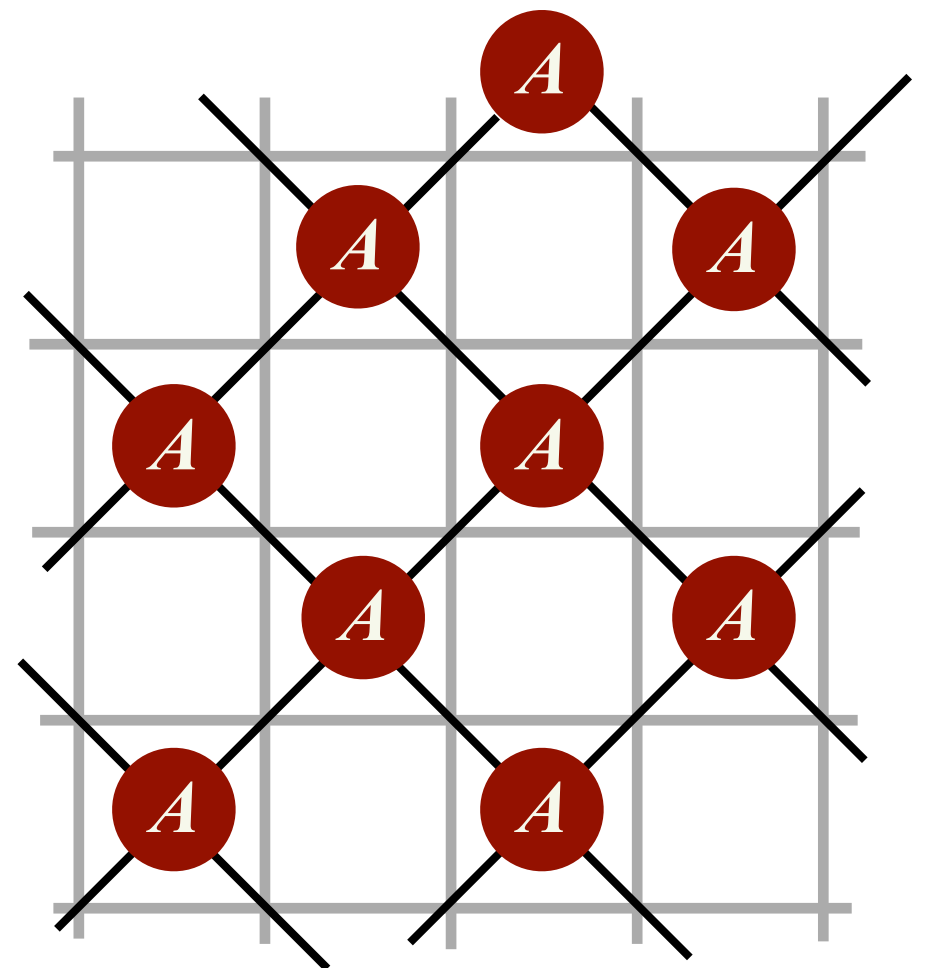
We can represent a partition function in a network of "tensor products"

Example: Ising model on the square lattice

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

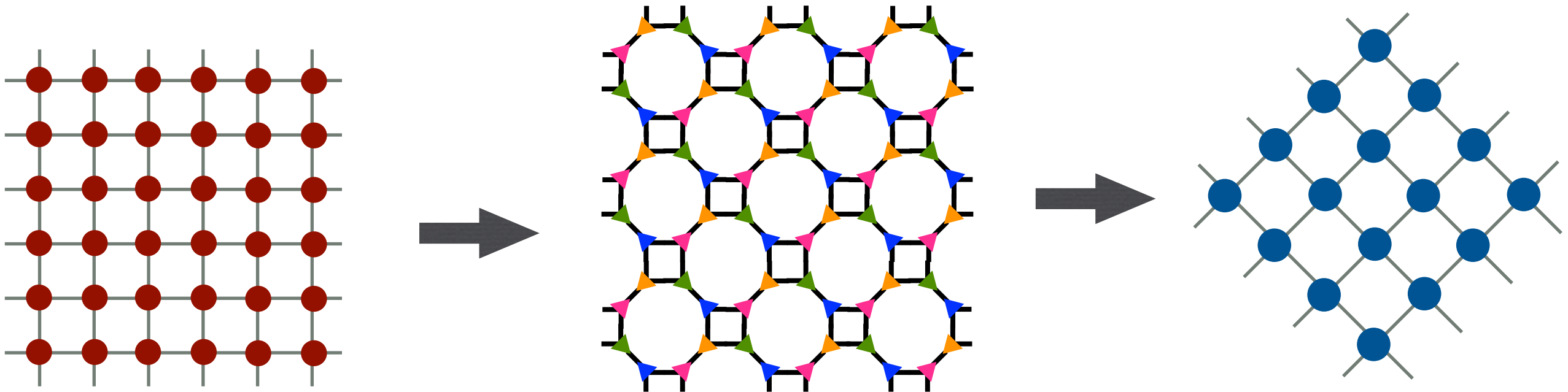


$Z =$



Real space renormalization of tensor network

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2回： 現代物理学と情報圧縮

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)

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第8回： データ解析の高速化：スパース・モデリングの物質科学への応用

第9回： データ空間の圧縮：クリロフ部分空間法の物質科学への応用

第10回： 高度なデータ圧縮：情報のエンタングルメントと行列積表現

第11回： 行列積表現の固有値問題への応用

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による情報圧縮