計算科学における情報圧縮

Information Compression in Computational Science

2021.10.14

#2:現代物理学と情報圧縮

Information compression in modern physics

理学系研究科　大久保　毅

Graduate School of Science, **Tsuyoshi Okubo**

Outline

- Many body problems
    - Quantum system as an example of huge data
    - Phase transition and statistical mechanics
      (I will skip this part in the class.)
- Review of linear algebra
    - Vector space- Abstract vectors-
        - General vector space (with inner product)
        - Basis and relation to coordinate vector space
        - Vector subspace and spanned vector subspace
    - Matrix and linear map
        - Relation between matrices and linear maps

Many body problem:

Quantum system as an example of huge data

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）

Inner product:

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

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

素粒子

➡ Static problems: Time-independent Schrödinger equation

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

Energy

= Eigenvalue problem

(If you are not familiar with physics, please imagine just an eigenvalue problem with huge matrix.)

Quantum 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.

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

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

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

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

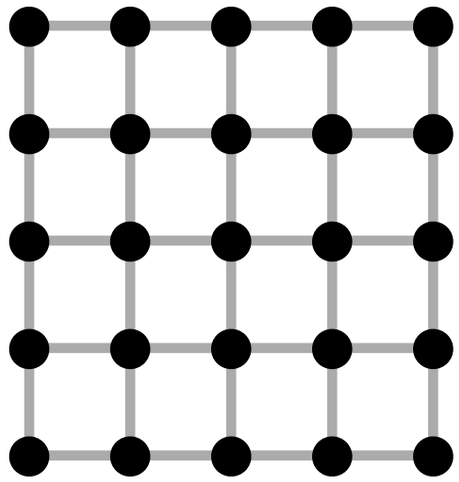
$$\Rightarrow \mathcal{H} \to \begin{pmatrix} H_{0,0;0,0} & H_{0,0;0,1} & H_{0,0;1,0} & H_{0,0;1,1} \\ H_{0,1;0,0} & H_{0,1;0,1} & H_{0,1;1,0} & H_{0,1;1,1} \\ H_{1,0;0,0} & H_{1,0;0,1} & H_{1,0;1,0} & H_{1,0;1,1} \\ H_{1,1;0,0} & H_{1,1;0,1} & H_{1,1;1,0} & H_{1,1;1,1} \end{pmatrix}$$

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

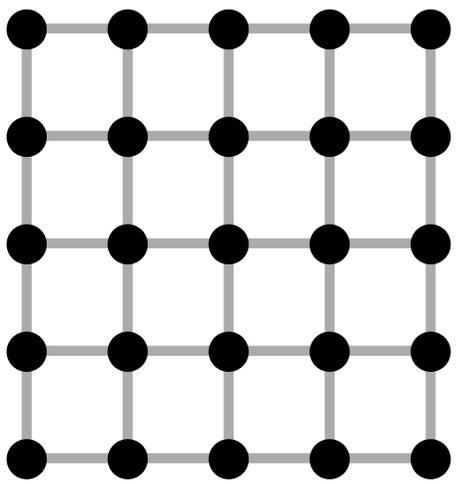
Lattice

1D

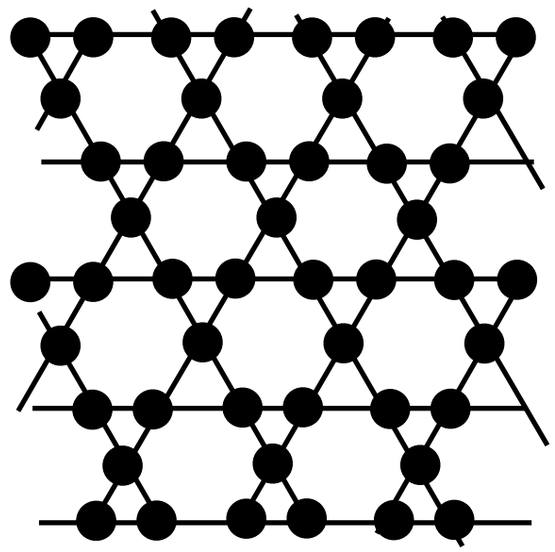
Chain

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 $\hbar = 1$)

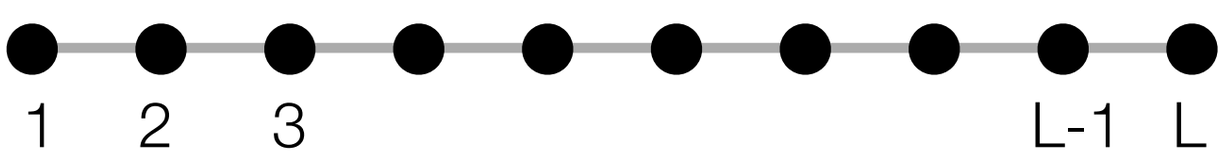
Quantum spin: S=1/2

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:



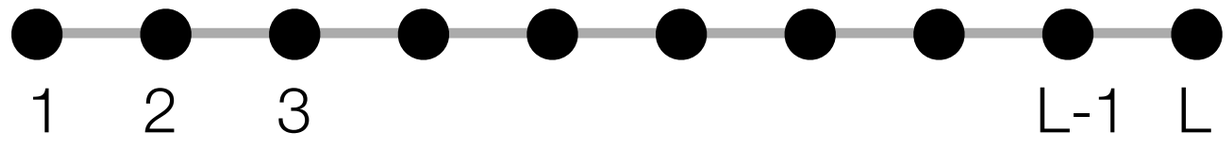
"Transverse field Ising model"　（横磁場イジング模型）

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

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

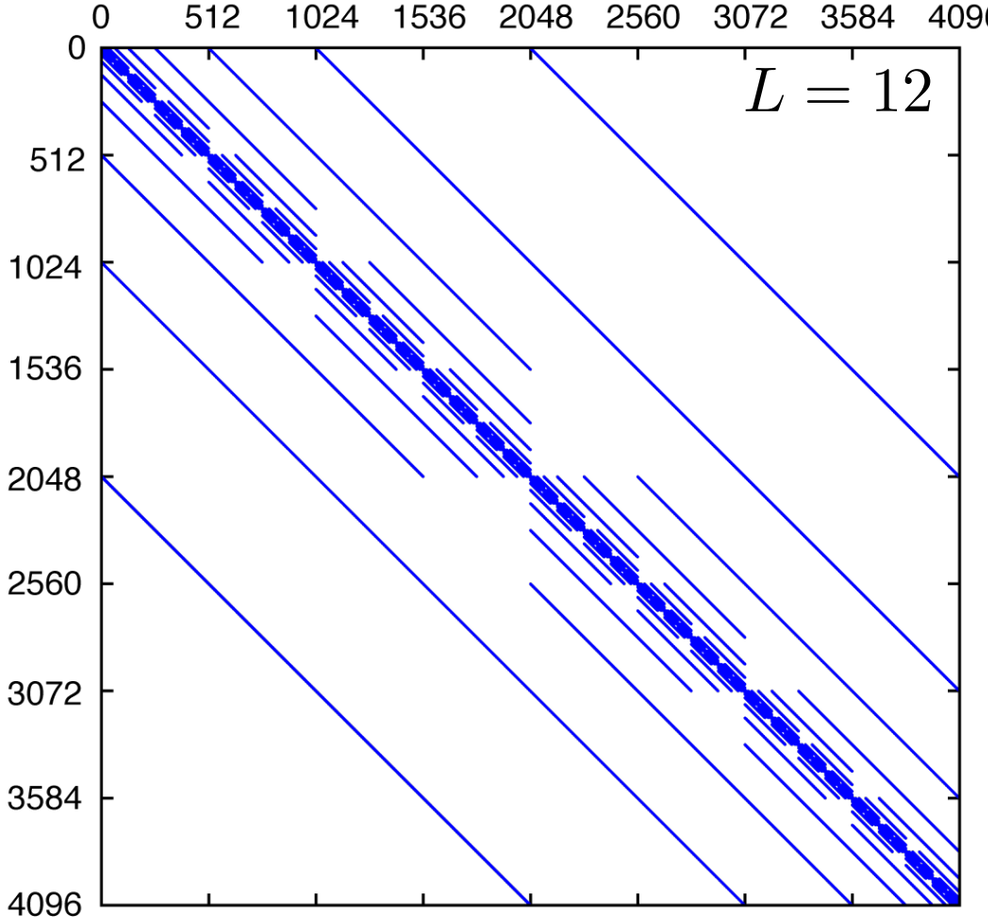


"Transverse field Ising model"

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

Non-zero elements in the Hamiltonian

(Figure from Yamaji-sensei)



Total matrix elements=2^{2L}

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

Sparse!

Classical Ising spins

Classical Ising spin: $S_i = \pm 1 = \uparrow, \downarrow$ (Scaler instead of operator)

It can be considered as

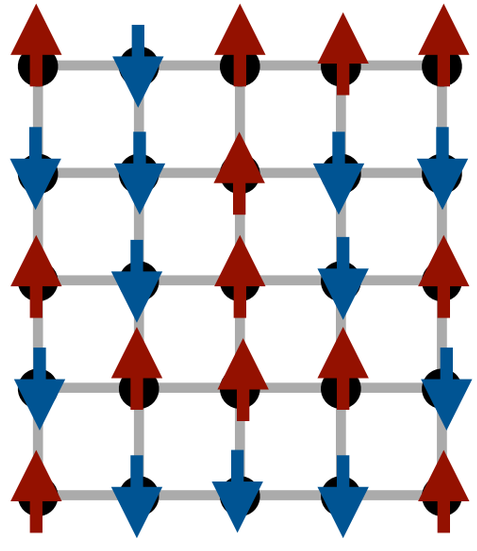
- Approximation of quantum spins under strong easy axis anisotropy
- Object representing underlying Z_2 symmetry for critical phenomena.

A state is characterized by a sequence of ± 1.

$(1, -1, 1, 1, \cdots, -1, 1)$ (N dimensional vector)

*In the case of classical system, there is no superposition.

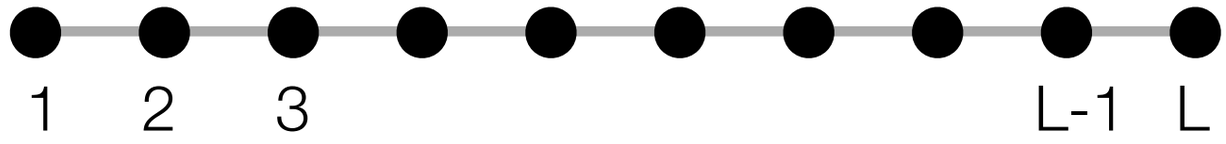
→ In total, there are 2^N states.



Ising spins on the square lattice

Ising spins on a chain

Spins on a chain:



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

"(classical) Ising model"　（（古典）イジング模型）

$$\mathcal{H} = -\sum_{i=1}^{L-1} S_i S_{i+1} - h \sum_{i=1}^{L} S_i$$ (The hamiltonian is not a matrix)

This model can be mapped to a S=1/2 quantum model by $S_i \to S_{i,z}$

(Thermodynamic properties are almost unchanged.)

$$\mathcal{H}' = -\sum_{i=1}^{L-1} S_{i,z} S_{i+1,z} - h \sum_{i=1}^{L} S_{i,z}$$ (The hamiltonian is a matrix)

*The magnetic field is parallel to *z* axis.

Classical Ising spin vs. quantum spin

Ising spin

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

If we consider S_i as $S_{i,z}$ in quantum spins,

"Ising model"

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

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

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 considered as "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** $\sim O(2^L)$

Classification of Information Compression by Memory Costs

Linear algebra for huge data: $\vec{v} \in \mathbb{C}^M$

(1) A matrix can be stored.

Required memory~ $O(M^2)$

(2) Although a matrix cannot be stored, vectors can be stored.

Required memory~ $O(M)$

(3) A vector cannot be stored.

Required memory $\ll O(M)$

Quantum system: $M \sim a^N$ N:problem size (e.g. system size)

Depending on the cases we use different "compression" techniques.

For (1), low rank approximation of M.
For (2), Krylov subspace method.
For (3), tensor network decomposition.

Low rank approximation by singular value decomposition **(特異値分解)**

Singular value decomposition (SVD):

For a K × L matrix M,

$$M = U \Lambda V^\dagger$$

$$M_{i,j} = \sum_m U_{i,m} \lambda_m V^\dagger_{m,j}$$

$U, V^\dagger$: (half) unitary

Λ : Diagonal

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_N \end{pmatrix}$$

Singular values: $\lambda_m \geq 0$

Singular vectors:

$$\sum_i U_{i,m} U^\dagger_{m,j} = \delta_i, j$$

$$\sum_i V_{i,m} V^\dagger_{m,j} = \delta_i, j$$

By taking only several larger singular values,
we can approximate M as a lower rank matrix.

Krylov subspace method

Krylov subspace

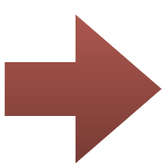
linear subspace generated by a square matrix (M) and a vector (v) as

$$\mathcal{K}_n(M, \vec{v}) = \mathrm{span}\left\{\vec{v}, M\vec{v}, M^2\vec{v}, \ldots, M^{n-1}\vec{v}\right\}$$

For quantum many body problems:

$M = \mathcal{H}$:Hamiltonian

$\vec{v} = |\phi\rangle$:wavevector



Solve the eigenvalue problem within
a restricted space (Krylov subspace)

Lanczos method, Arnoldi method

* In these method, we do not necessarily need explicit matrix.
It is enough to know the result of matrix vector multiplication.

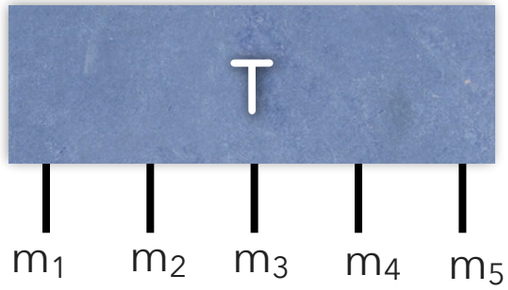
Tensor network decomposition

Wave function: $|\Psi\rangle = \sum_{\substack{\{m_i=\uparrow\downarrow\} \\ \text{or} \\ \{m_i=0,1\}}} T_{m_1,m_2,\cdots,m_N}|m_1,m_2,\cdots,m_N\rangle$

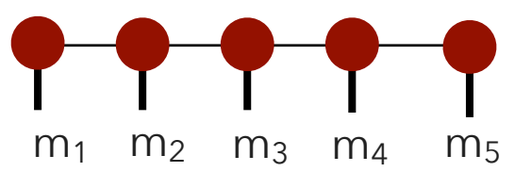
（波動関数）

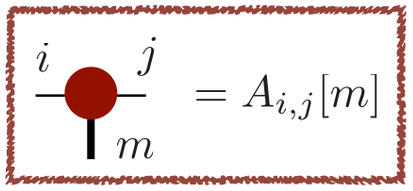
$T_{m_1,m_2,\cdots,m_N}$ N-rank tensor (or Vector)

# of Elements＝2^N



Approximation as
a product of "matrices"





Matrix Product States (行列積状態)

（Tensor train decomposition）

$$T_{m_1,m_2,\cdots,m_N} \simeq A_1[m_1]A_2[m_2]\cdots A_N[m_N]$$

$A[m]$ ：Matrix for state m

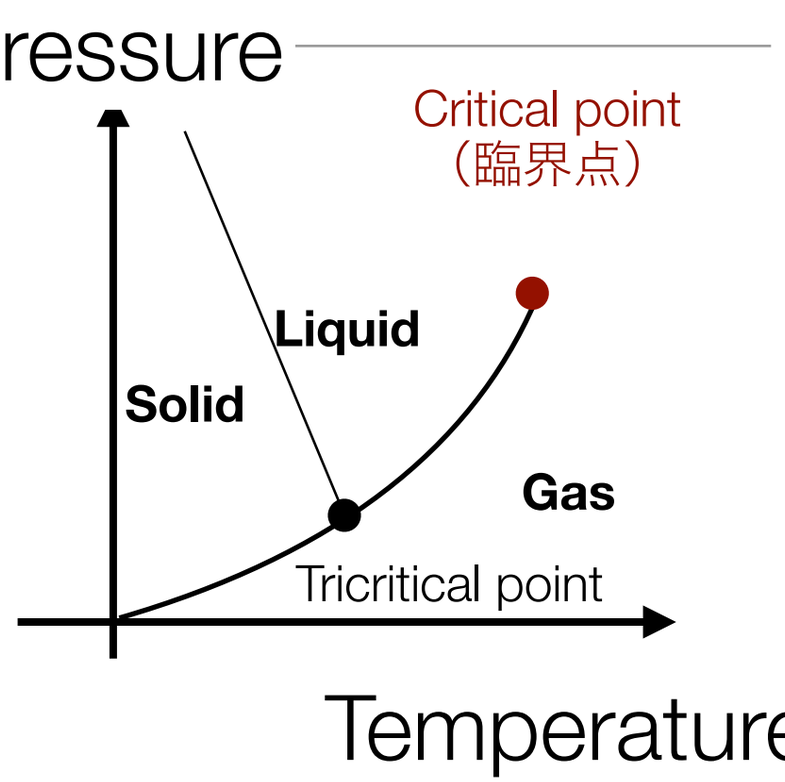
Many body problems:

Statistical mechanics and phase transition

(This section will be skipped in the class.)

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?

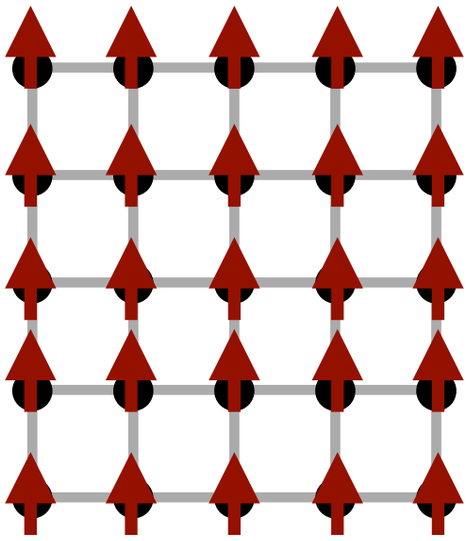
Phases in magnets (spin model)

Typically we have two phases:

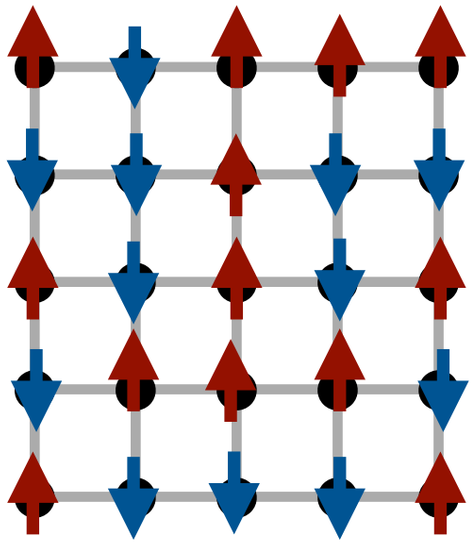
Magnetically ordered phase

Disordered phase

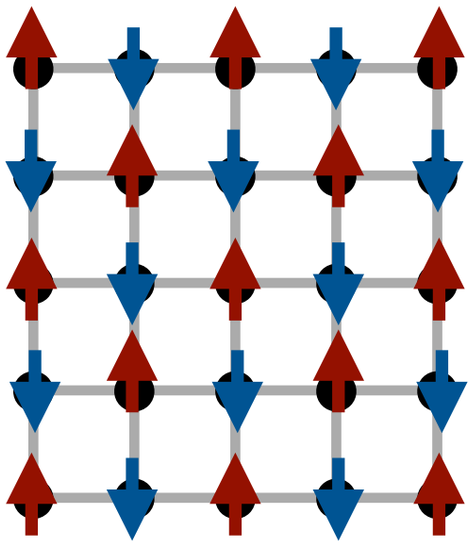
Ferromagnetic
(強磁性)



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 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. {$S_1, S_2, \ldots S_L$})

$P(\Gamma)$: 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**
- **....**

Review of linear algebra

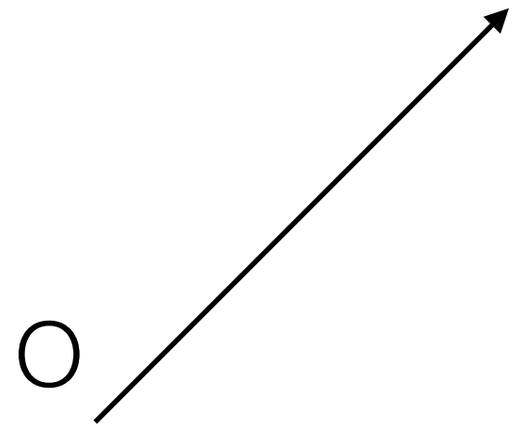
Vector space -Abstract vectors-

Geometric vector

Geometric vector: Arrow on the plane (or the space) ,

which has "Direction" and "Length"

$$\vec{v} \equiv \overrightarrow{OP}$$



We can express a vector by its component:

$$\vec{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} x_p - x_o \\ y_p - y_o \\ z_p - z_o \end{pmatrix}$$

Properties of vector

Properties of addition:

$$\vec{a}+\vec{b}=\vec{b}+\vec{a}$$ Commutative property（交換法則）

$$\left(\vec{a}+\vec{b}\right)+\vec{c}=\vec{a}+\left(\vec{b}+\vec{c}\right)$$ Associative property（結合法則）

$$\vec{a}+\vec{0}=\vec{a}$$ zero vector

$$\vec{a}+(-\vec{a})=\vec{0}$$ inverse vector

Multiplication of scaler $c \in \mathbb{R}$（実数）：

$$c(\vec{a}+\vec{b})=c\vec{b}+c\vec{a}$$
$$(c+d)\vec{a}=c\vec{a}+d\vec{a}$$ Distributive property（分配法則）
$$(cd)\vec{a}=c\,(d\vec{a})$$

Inner product of vector

Inner product:

$$(\vec{a}, \vec{b}) \equiv \vec{a} \cdot \vec{b}$$

$$= a_x b_x + a_y b_y + a_z b_z$$

Example:

$$\vec{a} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}, \vec{b} = \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix}$$

Properties:

$$(\vec{a}, \vec{a}) \geq 0$$

$$(\vec{a}, \vec{b}) = (\vec{b}, \vec{a})$$

$$(\vec{a} + \vec{b}, \vec{c}) = (\vec{a}, \vec{c}) + (\vec{b}, \vec{c})$$

$$(c\vec{a}, \vec{b}) = c(\vec{a}, \vec{b}) \qquad c \in \mathbb{R}$$

Norm (length):

$$\|\vec{a}\| \equiv \sqrt{(\vec{a}, \vec{a})}$$

Vector space (linear space)

Vector space $\mathbb{V}$: generalization of geometric vector

Set of elements (vectors) satisfying following **axioms**（公理）

Properties of addition:

$$\vec{a}+\vec{b}=\vec{b}+\vec{a}$$ Commutative property（交換法則）

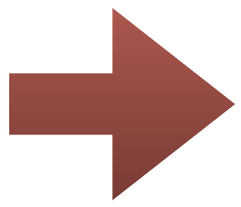
$$\left(\vec{a}+\vec{b}\right)+\vec{c}=\vec{a}+\left(\vec{b}+\vec{c}\right)$$ Associative property（結合法則）

$$\vec{a}+\vec{0}=\vec{a}$$ Existence of unique zero vector

$$\vec{a}+(-\vec{a})=\vec{0}$$ Existence of unique inverse vector

Multiplication of scaler c :

$$c(\vec{a}+\vec{b})=c\vec{b}+c\vec{a}$$
$$(c+d)\vec{a}=c\vec{a}+d\vec{a}$$
$$(cd)\vec{a}=c\,(d\vec{a})$$



$c \in \mathbb{R}$: Real vector space

$c \in \mathbb{C}$: Complex vector space

Inner product space (metric vector space)
(計量空間)

Inner product space:

Vector space + definition of inner product

Inner product: $(\vec{a}, \vec{b})$

Axiom:

$$(\vec{a}, \vec{a}) \geq 0$$

$$(\vec{a}, \vec{b}) = (\vec{b}, \vec{a})^*$$

$$(\vec{a} + \vec{b}, \vec{c}) = (\vec{a}, \vec{c}) + (\vec{b}, \vec{c})$$

$$(c\vec{a}, \vec{b}) = c(\vec{a}, \vec{b})$$

*If a norm defined from the inner product is "complete"（完備）,

that space is called **Hilbert space**.

Examples of vector spaces

(1) Coordinate space（数ベクトル空間） $\mathbb{R}^n, \mathbb{C}^n$

Vector: $\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad v_i \in \mathbb{R} \text{ or } \mathbb{C}$

Inner product: $(\vec{a}, \vec{b}) \equiv \vec{a} \cdot \vec{b}^*$

(2) Wave vectors in quantum physics

Vector: $|\Psi\rangle$

Inner product: $(|a\rangle, |b\rangle) = \langle b|a\rangle$

Linearly independent or dependent
（線形独立）　（線形従属）

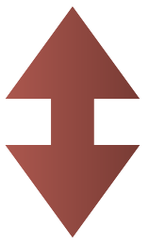
Linear combination:

$$\vec{x} = c_1\vec{v}_1 + c_2\vec{v}_2 + \cdots c_k\vec{v}_k$$

$$\vec{v}_i \in \mathbb{V} \qquad c_i \in \mathbb{R} \text{ or } \mathbb{C}$$

A set $\{\vec{v}_1, \vec{v}_2, \cdots \vec{v}_k\}$ is **linearly independent** when

$\vec{x} = \vec{0}$ is satisfied if and only if $c_1 = c_2 = \cdots = c_k = 0$



A set $\{\vec{v}_1, \vec{v}_2, \cdots \vec{v}_k\}$ is **linearly dependent** when

it is not linearly independent.

Basis of vector space
（基底）

A set $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ $(\vec{e}_i \in \mathbb{V})$ is a basis（基底）of $\mathbb{V}$ when

$\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ is linearly independent.

and

Any vectors in $\mathbb{V}$ are represented by its linear combination.

$\vec{e}_i$: basis vector

# of basis vectors (n) is called **dimension**（次元）of $\mathbb{V}$.

$$n = \dim \mathbb{V}$$

Relation (map) to coordinate vector space

By using a basis $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$, $\vec{v} \in \mathbb{V}$ is uniquely represented as

(* From linear independency)

$$\vec{v} = v_1\vec{e}_1 + v_2\vec{e}_2 + \cdots v_n\vec{e}_n$$

We can represent $\vec{v}$ as a coordinate vector

$$\vec{v} \rightarrow \begin{pmatrix} v_1 \\ v_2 \\ \cdots \\ v_n \end{pmatrix} \in \mathbb{C}^n (\text{ or } \mathbb{R}^n)$$

By selecting a basis, we obtain a "concrete" coordinate vector for an "abstract" vector

Orthonormal basis （正規直交基底）

When a vector space has an inner product,

$\vec{a}, \vec{b}$ is **orthogonal** （直交） if $(\vec{a}, \vec{b}) = 0$.

Orthonormal basis

A basis $\{\vec{e}_1, \vec{e}_2, \cdots \vec{e}_n\}$ is an orthonormal basis when

$$\|\vec{e}_i\| = 1 \qquad (i = 1, 2, \ldots, n)$$
$$(\vec{e}_i, \vec{e}_j) = 0 \qquad (i \neq j; i, j = 1, 2, \ldots, n)$$

*A basis can be transformed into an orthonormal basis.

cf. Gram-Schmidt orthonormalization

Example: wave vector

2 qbits: We can choose following four vectors as the (orthonormal) basis.

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

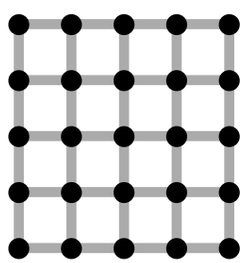
Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

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

$C_{\alpha,\beta} = \langle\alpha\beta|\Psi\rangle$:complex number

$$C \in \mathbb{C}^4$$

Many qbits:



basis: $|m_1, m_2, \cdots, m_N\rangle = |00\cdots0\rangle, |00\cdots1\rangle, |01\cdots0\rangle, \ldots$

$$|\Psi\rangle = \sum_{\{m_i=0,1\}} T_{m_1,m_2,\cdots,m_N}|m_1, m_2, \cdots, m_N\rangle$$

$$T_{m_1,m_2,\cdots,m_N} = \langle m_1, m_2, \cdots, m_N|\Psi\rangle \quad T \in \mathbb{C}^{2^N}$$

Vector subspace (linear subspace)

Vector subspace（ベクトル部分空間）**:**

A subset $\mathbb{W}$ of a vector space $\mathbb{V}$ is a vector subspace of $\mathbb{V}$ when $\mathbb{W}$ satisfies the same axioms of vector space with $\mathbb{V}$.

The following conditions are necessary and sufficient.

$$\vec{a}, \vec{b} \in \mathbb{W} \Rightarrow \vec{a} + \vec{b} \in \mathbb{W}$$

$$\vec{a} \in \mathbb{W}, c \in \mathbb{C} \Rightarrow c\vec{a} \in \mathbb{W}$$

(In the case of complex vector space)

Spanned vector subspace

Spanned subspace:

For a subset $\mathbb{S}$ of a vector space $\mathbb{V}$, a set of linear combinations

$$\{c_1\vec{s}_1 + c_2\vec{s}_2 \cdots + c_k\vec{s}_k | c_i \in \mathbb{C}, \vec{s}_i \in \mathbb{S}\}$$

becomes a vector subspace of $\mathbb{V}$.

We often use

$$\mathrm{Span}\{\vec{s}_1, \vec{s}_2, \cdots, \vec{s}_k\}$$

to represents a vector subspace spanned by a set of vectors

$$\{\vec{s}_1, \vec{s}_2, \cdots, \vec{s}_k\}$$

(This representation will appear in Krylov subspace method.)

Matrix and linear map

Matrix（行列）

Matrix: "Table" of (complex) numbers in a rectangular form

M × N matrix

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & \cdots & A_{2,N} \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{M,N} \end{pmatrix}$$

$A_{ij} \in \mathbb{C}(\text{ or } \mathbb{R})$

Product of matrices: $C = AB$

$$C_{ij} = \sum_{k=1}^{K} A_{ik} B_{kj}$$

$A : M \times K$

$B : K \times N$

$C : M \times N$

In general: $XY \neq YX$

*We also know addition, multiplication of scalar.

Identity matrix（単位行列）

Identity matrix:

N × N matrix
(Square matrix)

$$I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

Product:

$$IA = A \qquad A : N \times M$$

$$BI = B \qquad B : K \times N$$

* Element of the identity matrix: $I_{ij} = \delta_{ij}$ (Kronecker delta)

$$\delta_{ij} = \begin{cases} 1 & (i = j) \\ 0 & (i \neq j) \end{cases}$$

Transpose, complex conjugate and adjoint

Transpose:
(転置)

$$A^t \qquad (A^t)_{ij} = A_{ji}$$

Complex conjugate:
(複素共役)

$$A^* \qquad (A^*)_{ij} = A^*_{ij}$$

Adjoint:
(随伴)

or

Hermitian conjugate:
(エルミート共役)

$$A^\dagger = (A^t)^* = (A^*)^t$$

$$(A^\dagger)_{ij} = A^*_{ji}$$

("Dagger" is convention in physics)

Multiplication to coordinate vector

$$A : M \times N \qquad \vec{v} \in \mathbb{C}^N \qquad \vec{v}' \in \mathbb{C}^M$$

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1,N} \\ A_{21} & A_{22} & \cdots & A_{2,N} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{M,N} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_M \end{pmatrix}$$

M × N matrix transforms a N-dimensional coordinate vector to a M-dimensional coordinate vector.

M × N matrix ⟷ **Linear map:** $\mathbb{C}^N \to \mathbb{C}^M$ （線形写像）

1 to 1

General linear map

Map: $f : \mathbb{V} \to \mathbb{V}'$

$$f(\vec{v}) = \vec{v}' \qquad (\vec{v} \in \mathbb{V}, \vec{v}' \in \mathbb{V}')$$

Linear map:

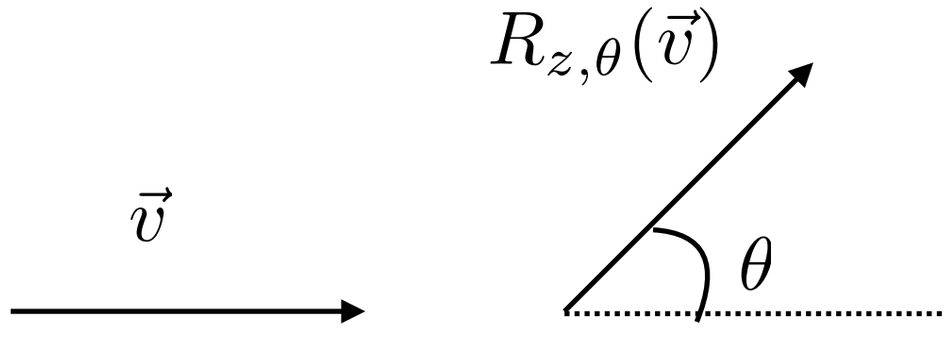
$$f(\vec{x} + \vec{y}) = f(\vec{x}) + f(\vec{y})$$

$$f(c\vec{x}) = cf(\vec{x}) \qquad (\vec{x}, \vec{y} \in \mathbb{V}, c \in \mathbb{C})$$

Examples:

Rotation (e.g. θ rotation around z-axis)

$$R_{z,\theta} : \mathbb{C}^3 \to \mathbb{C}^3$$



Hamiltonian operator

$$\mathcal{H} : \mathbb{V} \to \mathbb{V}$$

$$|\Psi\rangle \qquad \mathcal{H}|\Psi\rangle$$

Next week

1st: Huge data in modern physics (Today)

2nd: Information compression in modern physics

(+review of linear algebra)

3rd: Review of linear algebra (+ singular value decomposition)

4th: Singular value decomposition and low rank approximation

5th: Basics of sparse modeling

6th: Basics of Krylov subspace methods

7th: Information compression in materials science

8th: Accelerating data analysis: Application of sparse modeling

9th: Data compression: Appication of Krylov subspace method

10th: Entanglement of information and matrix product states

11th: Application of MPS to eigenvalue problems

12th: Tensor network representation

13th: Information compression by tensor network renormalization