

多体問題の計算科学

Computational Science for Many-body problems

2023.4.11

#1: 物理学における多体問題とその困難

Many-body problems in physics and why they are hard to solve

理学系研究科 大久保毅

Graduate school of science, **Tsuyoshi Okubo**

email: t-okubo@phys.s.u-tokyo.ac.jp

- This class is from 14:55 to 16:40 (105 min.)

*This lecture will be given by

Tsuyoshi Okubo and Dr. Youhei Yamaji

Outline

- Background
 - Background of the lecture
 - Tentative lecture schedule
 - Evaluation
- Introduction
 - Many-body problems in physics
 - Why are many-body problems hard to solve?
 - Numerical algorithms for many-body problems

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Background of the lecturer

大久保 豪 (OKUBO Tsuyoshi)

Project associate professor,
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Research:

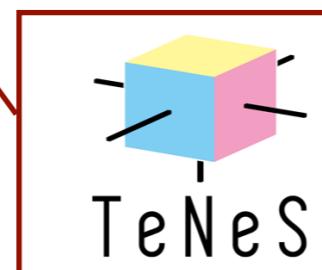
Statistical Physics, Condensed matter physics, Magnetism,
(Computational Physics)

- Random packing of disks
- Mean-filed analysis of hierarchical society
- Ordering of (classical) frustrated spin system
 - Skyrmion, multiple-Q states, Z_2 -vortex, ...
- Deconfined quantum criticality
- Tensor network
-

Monte Carlo

(Spin) dynamics

Quantum Monte Carlo



TeNeS

Massively parallel tensor network solver

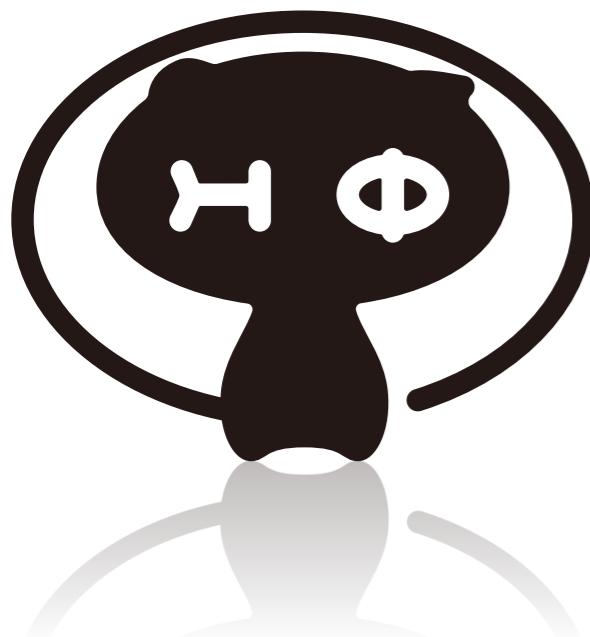
<https://www.pasums.issp.u-tokyo.ac.jp/tenes/en>

山地 洋平 YAMAJI, Youhei
YAMAJI.Youhei@nims.go.jp

Group Leader
Quantum Materials Modeling Group, MANA,
National Institute for Materials Science

Research:
Theoretical condensed matter physics
Computational method of many-body quantum systems

Developer of open source codes for supercomputers



Quantum lattice model solver HΦ
<http://ma.cms-initiative.jp/ja/index/ja/listapps/hphi>

Computational Science Alliance, The University of Tokyo



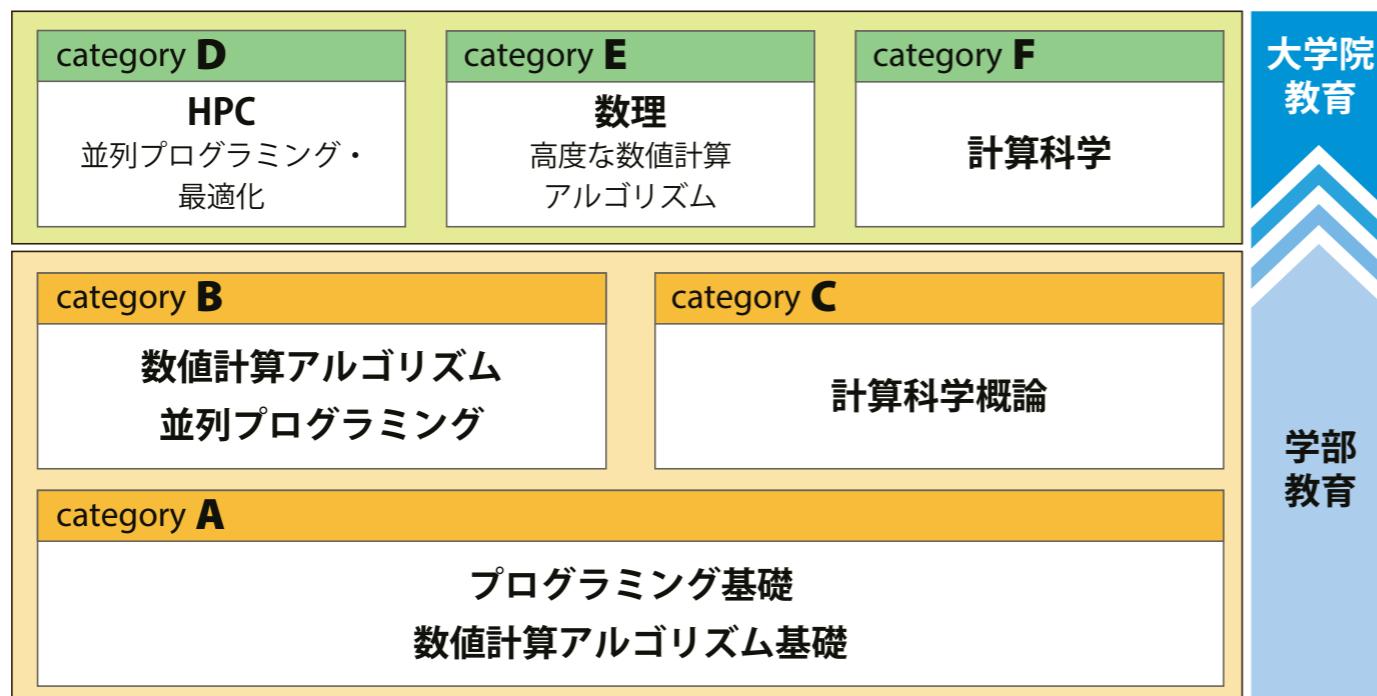
The University of Tokyo

<https://www.compsci-alliance.jp>

Train experts for computational and computer sciences.

計算科学アライアンス認定講義

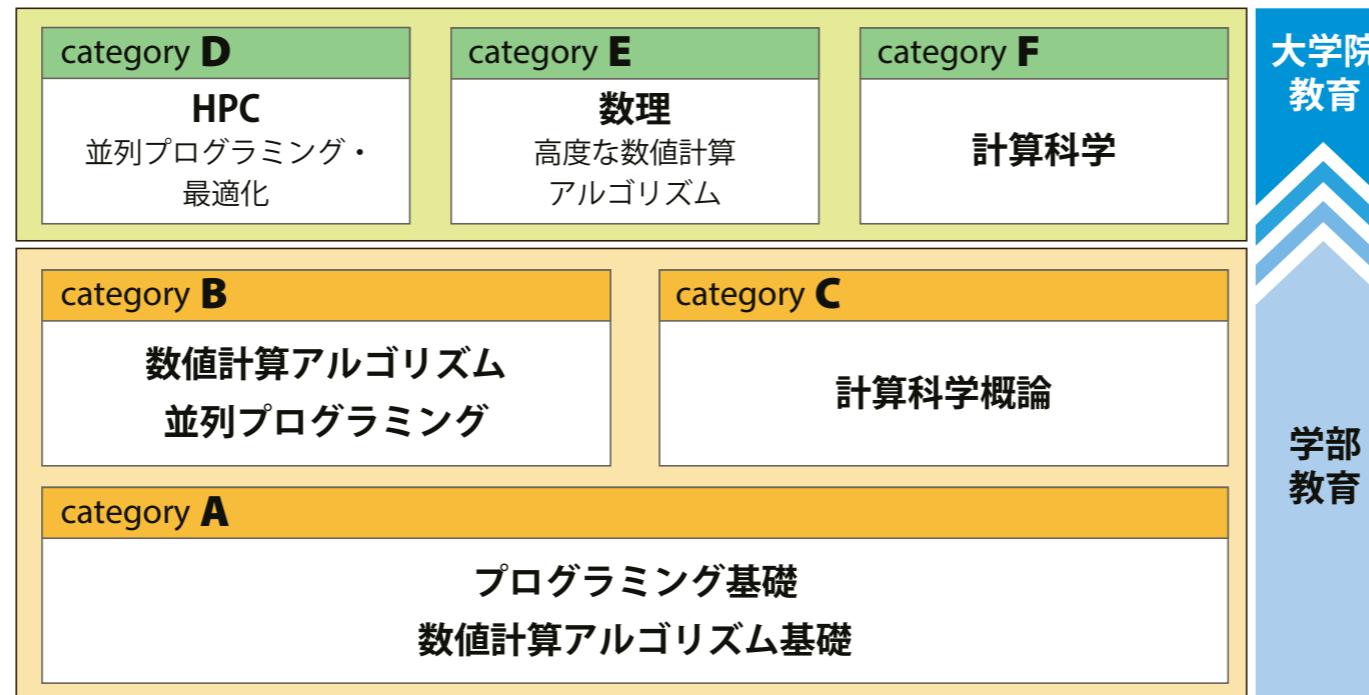
- 平成29年度から実習にも力点をおいた新しい講義を立ち上げ
- 計算科学・計算機科学に関する80以上の学部・大学院講義とあわせ、「計算科学アライアンス認定講義」として体系化
- 認定講義を内容に応じて6つのカテゴリに分類
- 所定の単位を取得した学生には「修了認定証」を発行
- この講義はカテゴリF



- 学部
 - カテゴリA,B,Cからそれぞれ1.5単位以上
- 大学院
 - カテゴリD,E,Fのうち2つのカテゴリを選択しそれぞれから2単位以上

計算科学アライアンス認定講義：大学院

- ・ カテゴリD - 最先端のスーパーコンピュータを駆使するのに必要とされる技術。種々の並列アルゴリズム、MPI並列やOpenMP並列などの並列プログラミング、メモリアクセス最適化などのチューニング
 - ・ 例：**計算科学アライアンス特別講義I、II**
- ・ カテゴリE - 最先端の数値計算アルゴリズムとその数理的基礎付け。差分法・有限要素法・有限体積法、特異値分解、最適化問題などの手法とその応用
 - ・ 例：**計算科学・量子計算における情報圧縮**
- ・ カテゴリF - 各分野におけるシミュレーション手法とその研究成果。電子状態計算、分子動力学、量子多体計算、数値流体力学、構造計算、ゲノム解析など
 - ・ 例：**多体問題の計算科学**



(Tentative)

Lecture schedule

Okubo

1st: Many-body problems in physics and why they are hard to solve

2nd: Classical statistical models and numerical simulation

3rd: Classical Monte Carlo method

4th: Applications of classical Monte Carlo method

5th: Molecular dynamics simulation and its applications

6th: Extended ensemble method for Monte Carlo methods

7th: Tensor Renormalization group

8th: Quantum lattice models and numerical simulation

9th: Quantum Monte Carlo methods

10th: Applications of quantum Monte Carlo methods

11th: Linear algebra of large and sparse matrices for
quantum many-body problems

12th: Large sparse matrices, and quantum statistical mechanics

13th: Advanced algorithms for quantum many-body problems

Classical

Quantum

Yamaji

Important infomations

Style: This course will be

- A hybrid of face-to-face and **online** for #1 - #7.
- Full **online** for #8 - #13.

(Zoom information is on UTAS and ITC-LMS.)

It is from 14:55 to 16:40 (105 min. lecture).

Slides: The lecture slides will be uploaded to

- ITC-LMS (Information Technology Center Learning Management System)
- <https://github.com/compsci-alliance/many-body-problems>

Important infomations

Evaluation: Based on **2 reports**:

Exercises include algorithms and computer simulations.

(I will probably provide **python codes (jupyter notebooks)**.)

Notice!

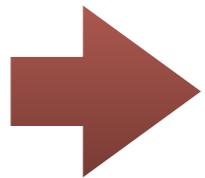
The grade will be evaluated based on
the sum of scores of two reports.

(So, if you will miss one of them, it will be big disadvantage.)

*Past-year report assignments are in the GitHub repository.

Information for future exercises

- **I will provide sample python codes.**



By using these codes, you will experience simulations explained in lectures.

Q. Are you familiar with running python codes?

Unfortunately, there may be **no enough time** to explain "how to use them".

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Many-body problems in physics

Many-body problems in physics

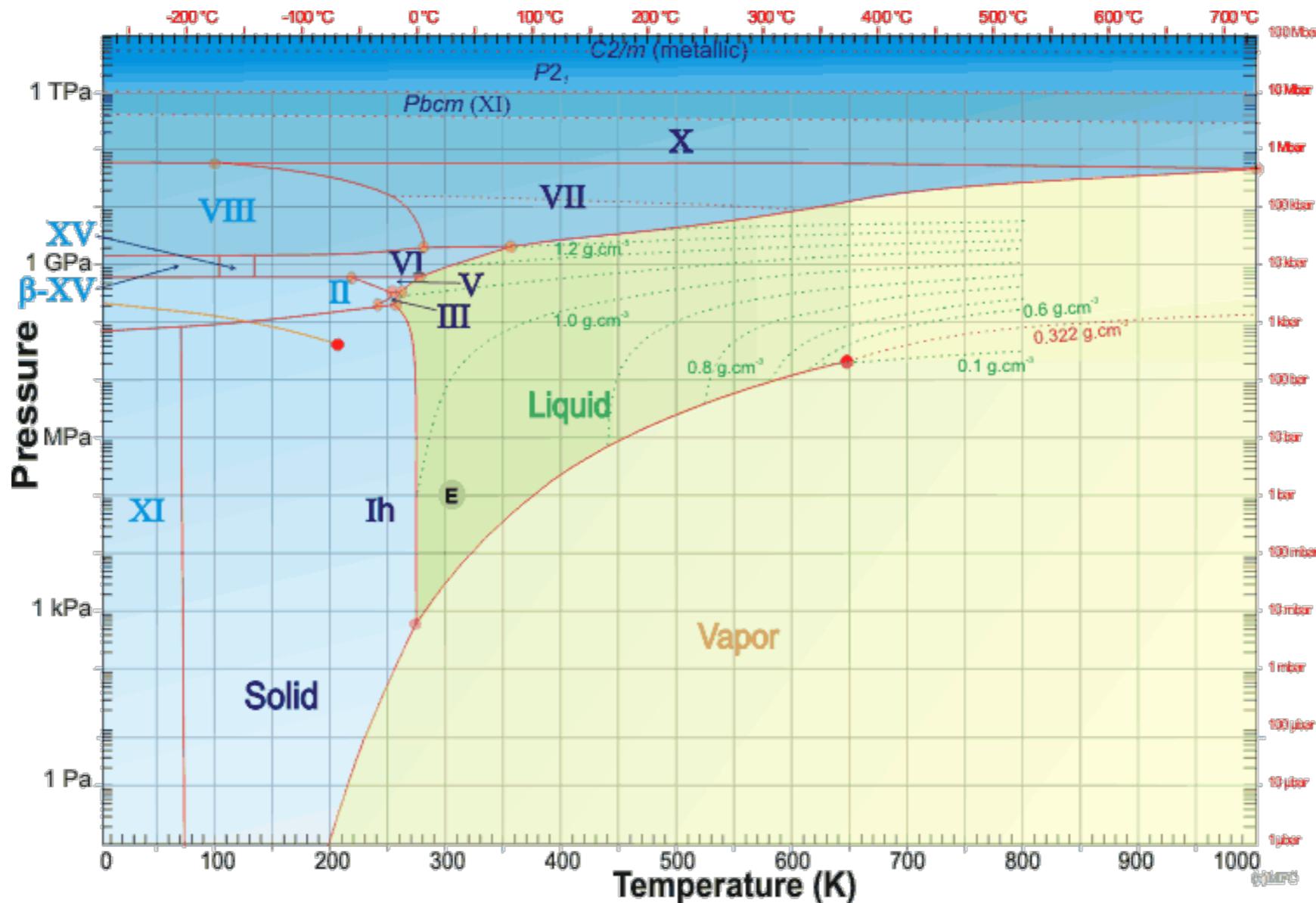
- Celestial movement (天体運動)
- Gases, Liquids
- Molecules, Polymers (eg. Proteins), ...
- Electrons in molecules and solids
- Elemental particles (Quantum Chromo Dynamics)
(量子色力学)

Principles for computations:

- Classical mechanics
 - Newton's equation, Navier-Stokes equation, ...
- Quantum mechanics
 - Schrodinger equation, ...
- Classical/Quantum statistical mechanics

Example: H₂O

Phase diagram of H₂O

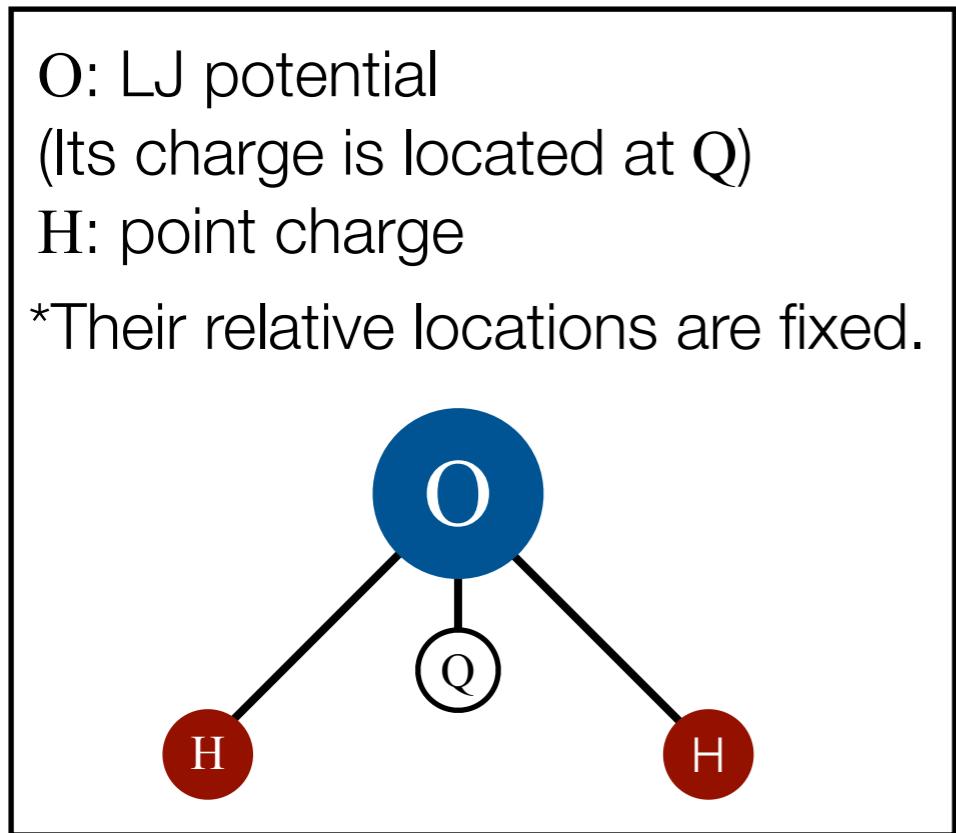


* Taken from “Water Structure and Science” by Martin Chaplin,
https://water.lsbu.ac.uk/water/water_structure_science.html

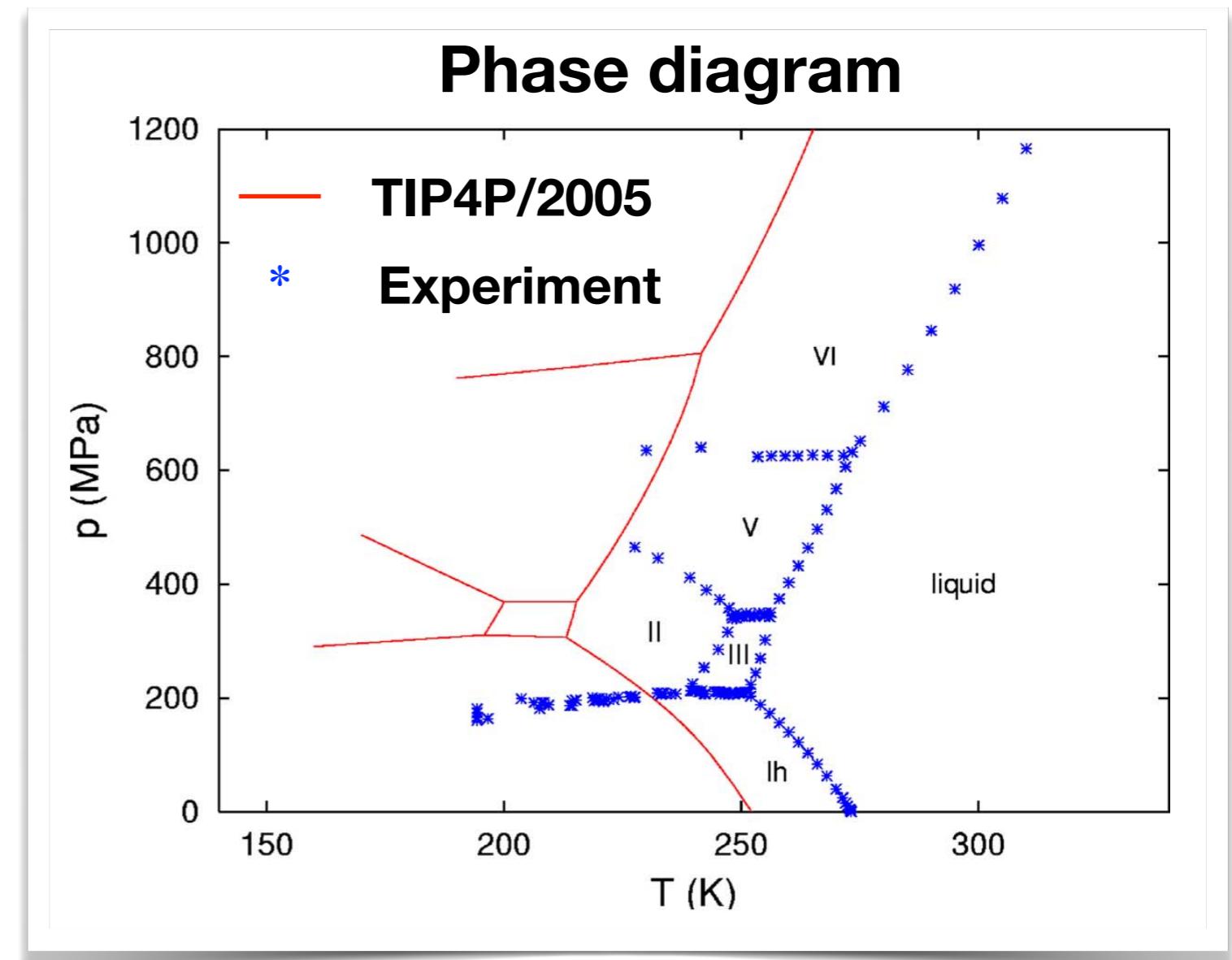
Example: H₂O (numerical simulation)

For H₂O, there are lots of effective potentials

Example: TIP4P/2005 (J. L. F. Abascal and C. Vega, J. Chem. Phys. **123**, 234505(2005))



Phase diagram of water is **qualitatively** reproduced!

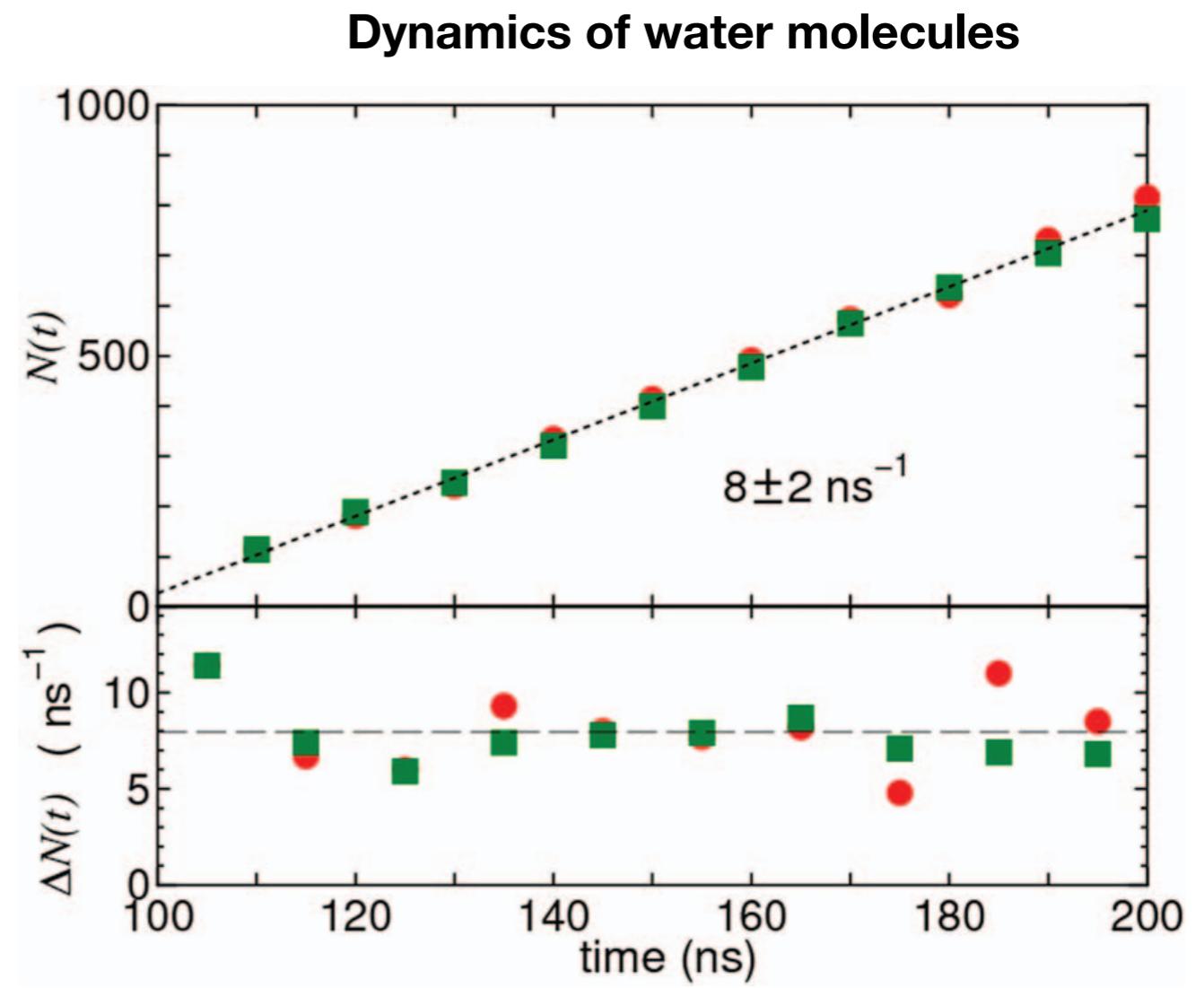
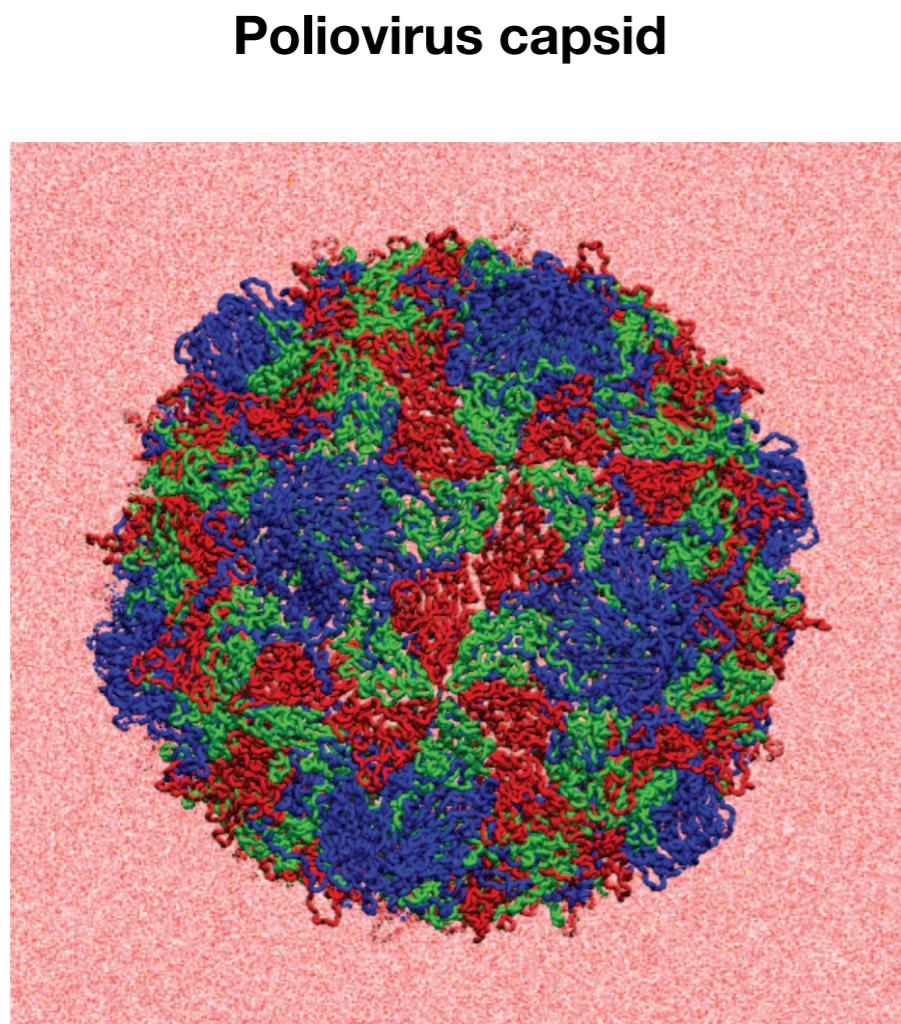


Example: Complex systems

Poliovirus capsid in electrolyte solution (電解質溶液)

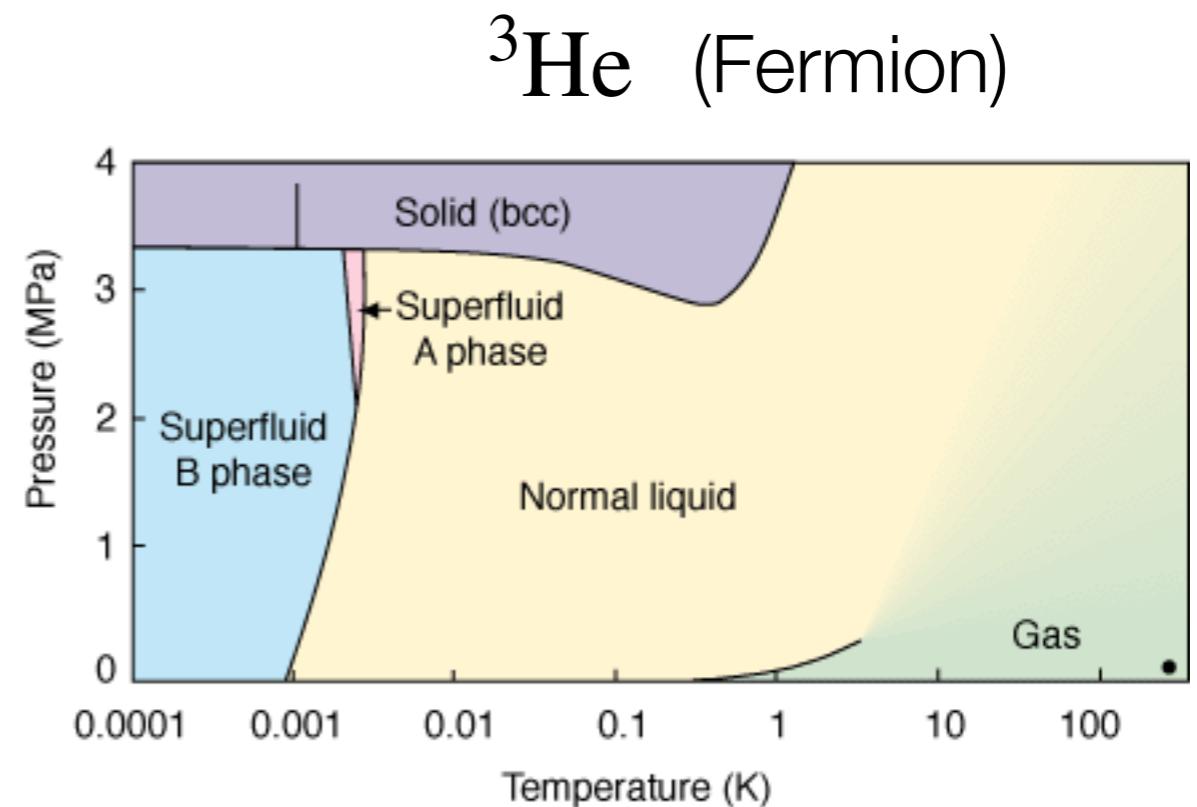
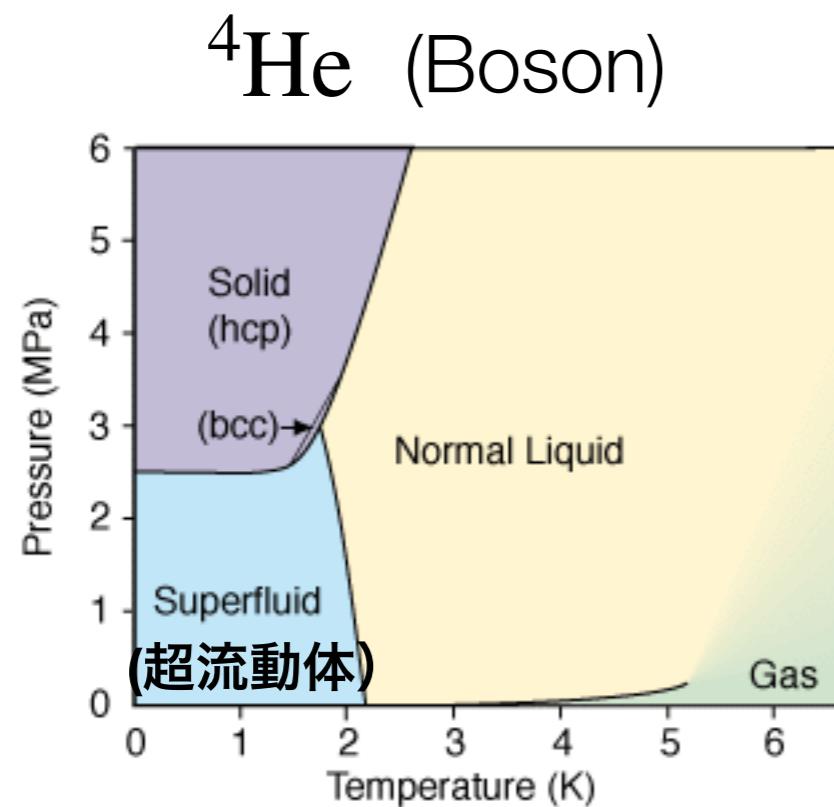
Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

Long-range coulomb interaction



Example: Quantum liquids

Phase diagrams of He.



* Taken from Web page by Erkki Thuneberg,
<http://ltl.tkk.fi/research/theory/helium.html>

Low-temperature behaviors are governed by quantum mechanics.

Example: Localized electrons as spin systems

Antiferromagnetic Mott insulator Na_2IrO_3

(反強磁性)

$$\mathcal{H} = \sum_{i,j} J_{ij} S_i S_j$$

(モット絶縁体)

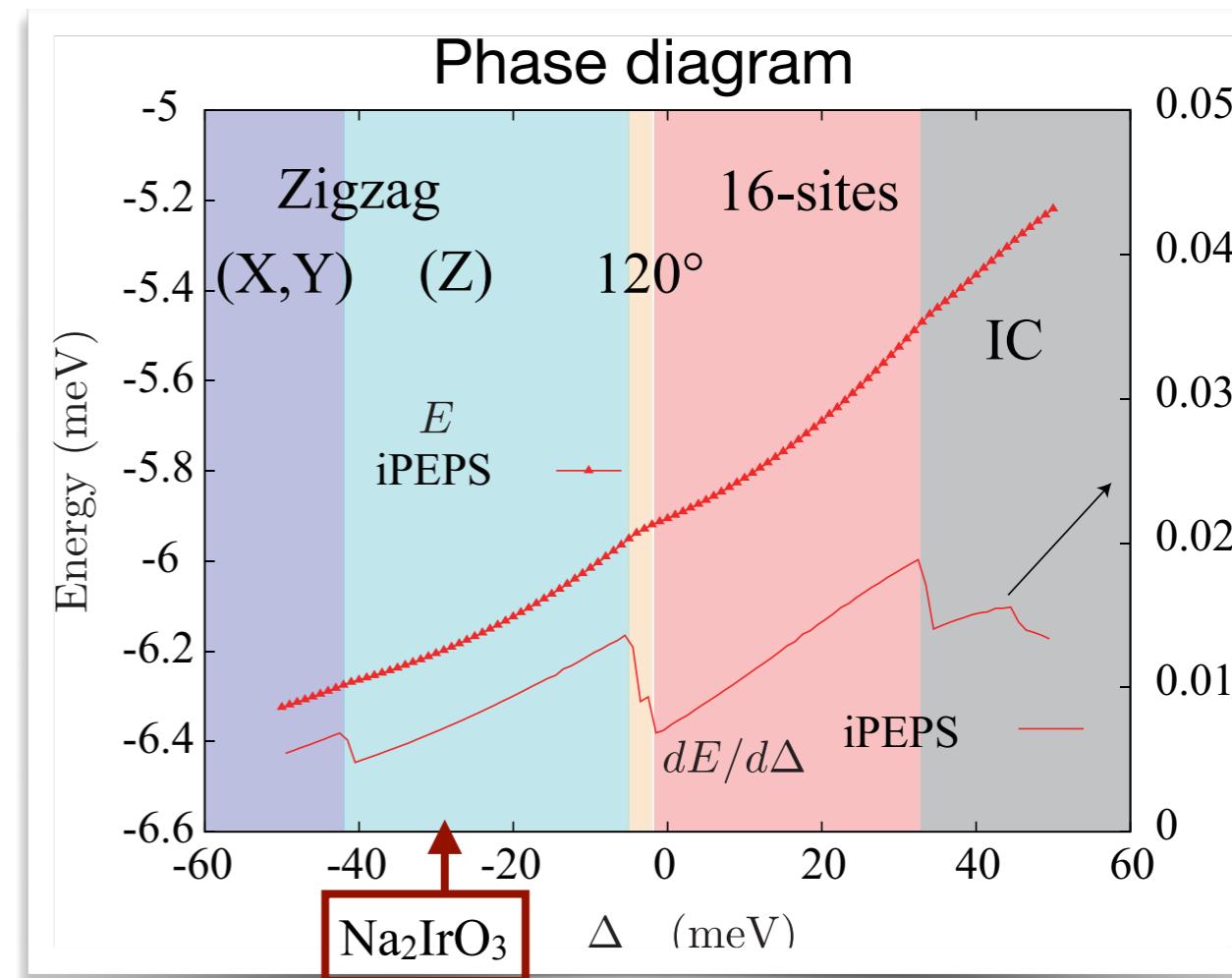
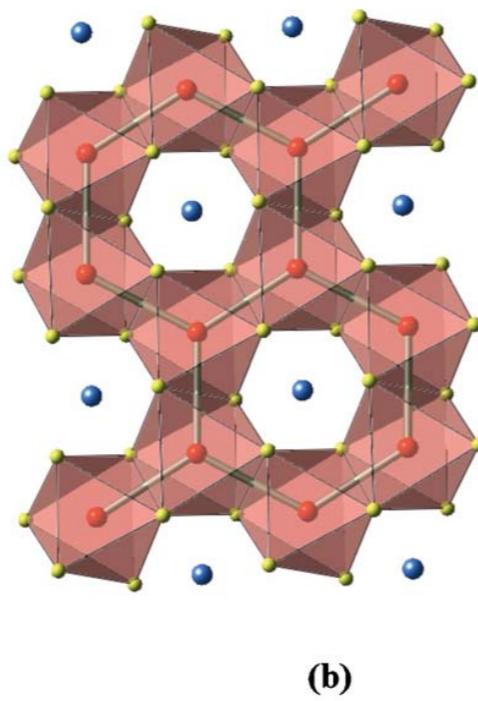
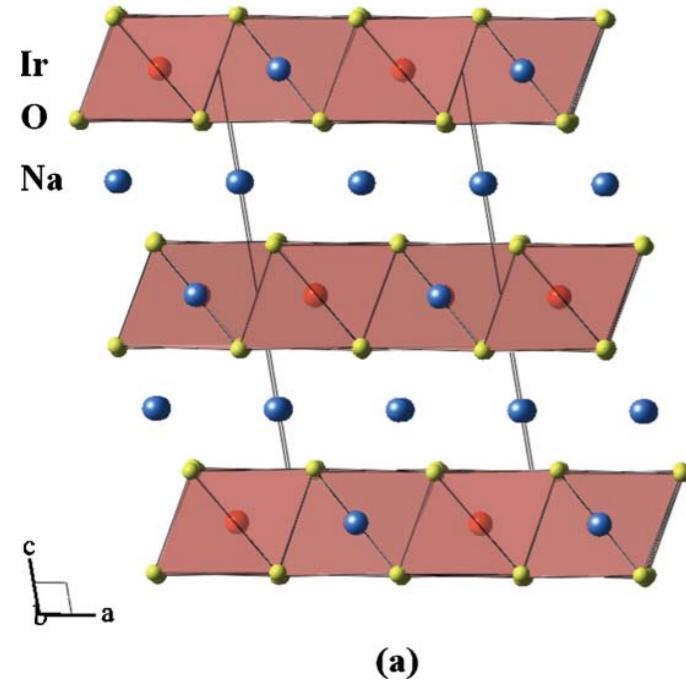
S_i : spin operator

Spins are treated as

- Classical spins
- Quantum spins

Y. Singh and P. Gegenwart, Physical Review B **82**, 064412 (2010)

T. Okubo, et al, Phys. Rev. B **96**, 054434 (2017).



Example: spin models

(Quantum) Spin model:

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

Ex.1: (classical) Ising model

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_{i,z} S_{j,z}$$

$S_{i,z} = \pm 1$

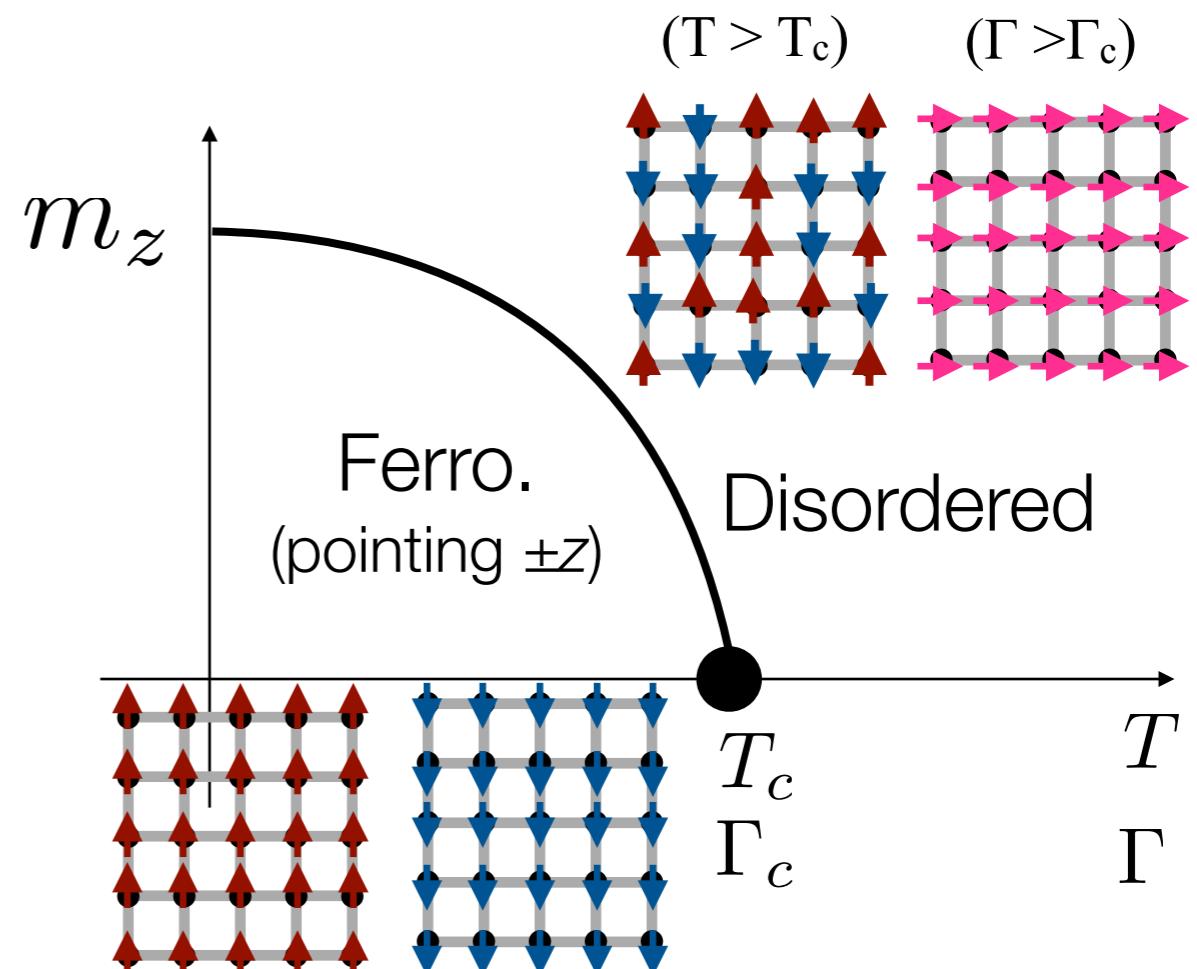
Phase transition **by varying temperature**

Ex.2: Transverse field Ising model

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_{i,z} S_{j,z} - \Gamma \sum_i S_{i,x}$$

$S_{i,z}, S_{i,x}$: spin **operator**

Phase transition by **varying Γ at $T=0$** .



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Target of this lecture

We consider numerical algorithm to deal with

- N -body Newton's equation of motion
 - Ex. Dynamics of classical particles, molecules, ...
- N -body classical statistical mechanics
 - Ex. Thermodynamic properties, ...
- N -body Schrödinger equation
 - Ex. Dynamics of quantum particles, eigenstates, ...
- N -body quantum statistical mechanics
 - Ex. Thermodynamic properties, ...

N -body Newton's equation of motion

N-particle system:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i(\{\mathbf{r}_i\}) \quad i = 1, 2, \dots, N$$

For the three-dimensional space:

The state of the system is determined by $6N$ degrees of freedom.

We need to solve large dimensional differential equations **stably**.

- Depending on the interest, we may need long-time simulations.
 - We need to take care of conserved quantities, such as energy.

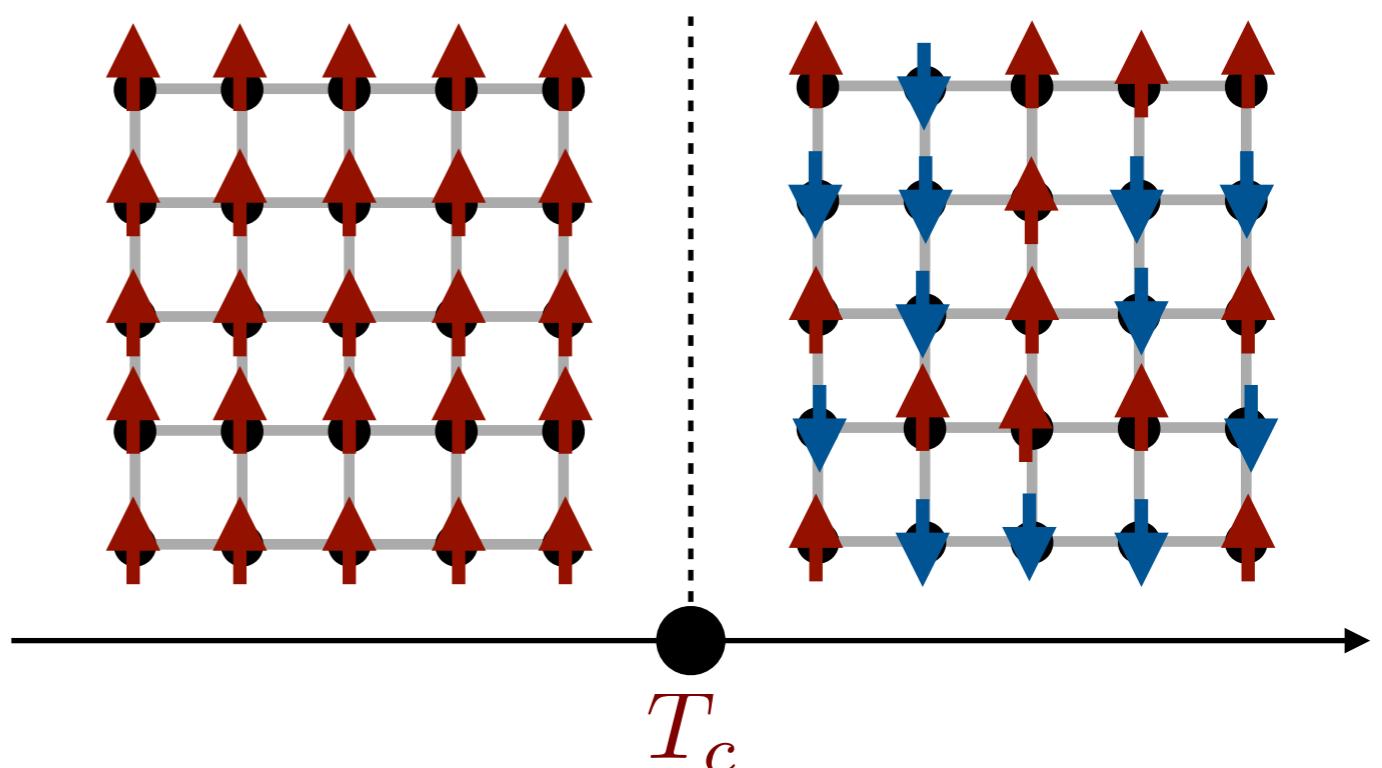
N -body classical statistical mechanics

Classical Ising model (N spins)

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

$S_i = \pm 1$

of possible configurations = 2^N



Statistical mechanics:

Probability distribution function at a temperature T .

$$P(\{S_i\}) = \frac{1}{Z} \exp(-\mathcal{H}/k_B T) = \frac{1}{Z} \exp(-\beta \mathcal{H}) \quad \beta = \frac{1}{k_B T} \quad \text{inverse temperature (逆温度)}$$

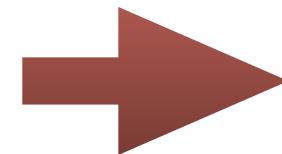
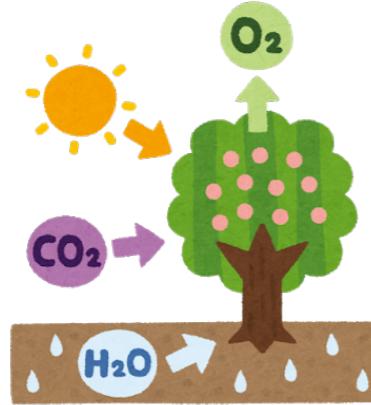
Partition function: $Z = \sum_{\{S_i=\pm 1\}} \exp(-\beta \mathcal{H})$ → Free energy: $F = -k_B T \log Z$
(分配関数) ↓ (自由エネルギー)

For the exact calculation, we need to sum over 2^N configurations.

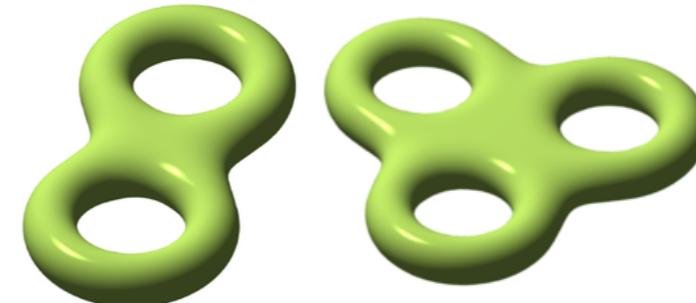
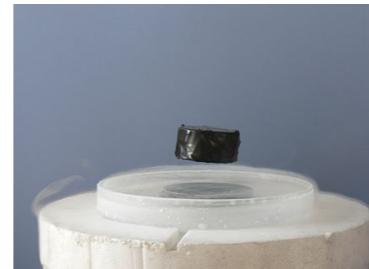
N -body quantum systems

A variety of phenomena in physics

- Chemical reaction
- Superconductivity
- Topological states
- ...



Quantum many-body problems



Cited from wikipedia: "Meisner effect", "Torus"

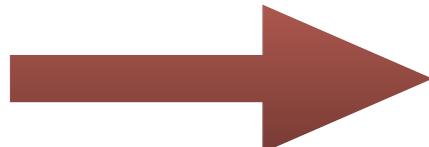
= Eigen value problem

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

$|\Psi\rangle$

:Hamiltonian

:State vector



Time-independent
situation

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

energy

= Eigen value problem

N -body quantum systems

(Time independent) Schrödinger equation = Eigen value problem

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

Ex. Transverse field Ising model:

$$\mathcal{H} = - \sum_{\langle i,j \rangle} S_{i,z} S_{j,z} - \Gamma \sum_i S_{i,x}$$

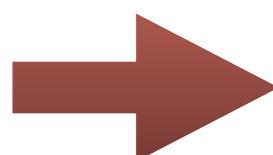
$S_{i,z}, S_{i,x}$: spin operator

$$S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

→ The dimension of the Hamiltonian matrix is $2^N \times 2^N$.

- Dimension of the vector space increases exponentially as # of particles increases
- Quantum many-body problem ~ Eigenvalue problem of huge matrices



To solve the problem numerically by (classical) computer,
we need huge memory and huge computation time.

Summary of difficulties

There are several difficulties in many-body problems:

- For large N , it is usually difficult (impossible) to solve them by hand.
 - We solve the problem by computer simulation!
- Even if we can calculate Newton's equation, we may need to continue long-time simulations to observe physics.
 - We need algorithms suitable for long-time simulations.
- In (classical) statistical mechanics, we need to sample 2^N configurations.
 - Calculation of the partition function is almost impossible.
- For quantum systems, we deal with a huge vector space.
 - For $S=1/2$ spins, the dimension is 2^N
 - Again, it is almost impossible to solve the Schrödinger equation for large N .

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(Tentative)

Lecture schedule

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Classical

Quantum

Yamaji

Markov Chain Monte Carlo (#3)

Probability distribution function at a temperature T .

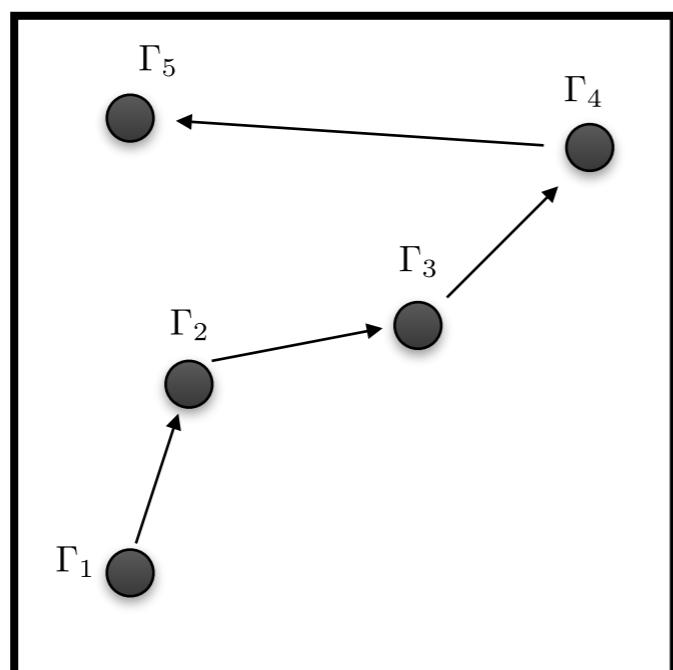
$$P(\{S_i\}) = \frac{1}{Z} \exp(-\mathcal{H}/k_B T) = \frac{1}{Z} \exp(-\beta \mathcal{H})$$

The calculation of the partition function, Z , is difficult.

→ Can we sample the configurations without knowing Z ?

Markov Chain Monte Carlo (MCMC)!

We might generate a $P(\{S_i\})$ as the steady state of a stochastic process.



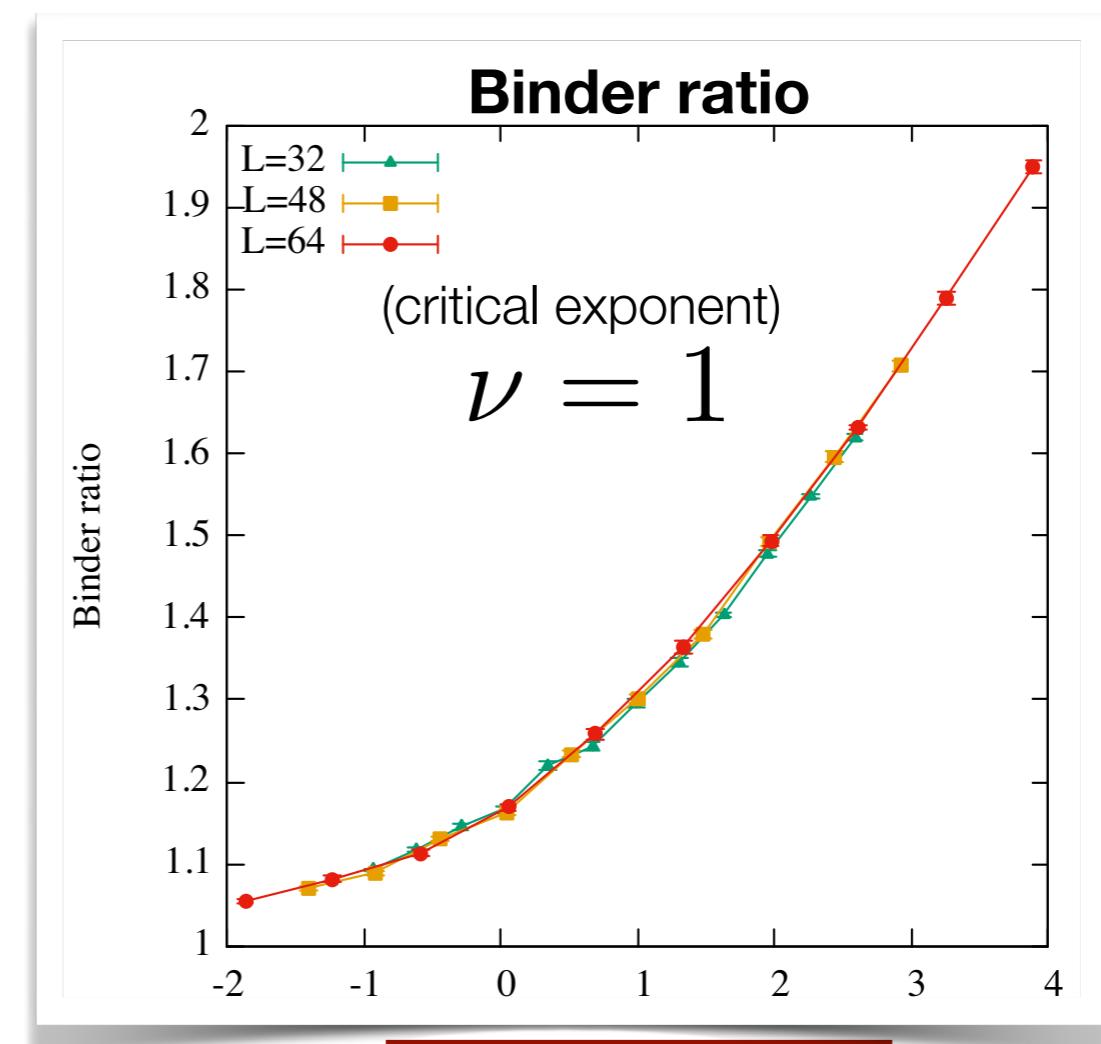
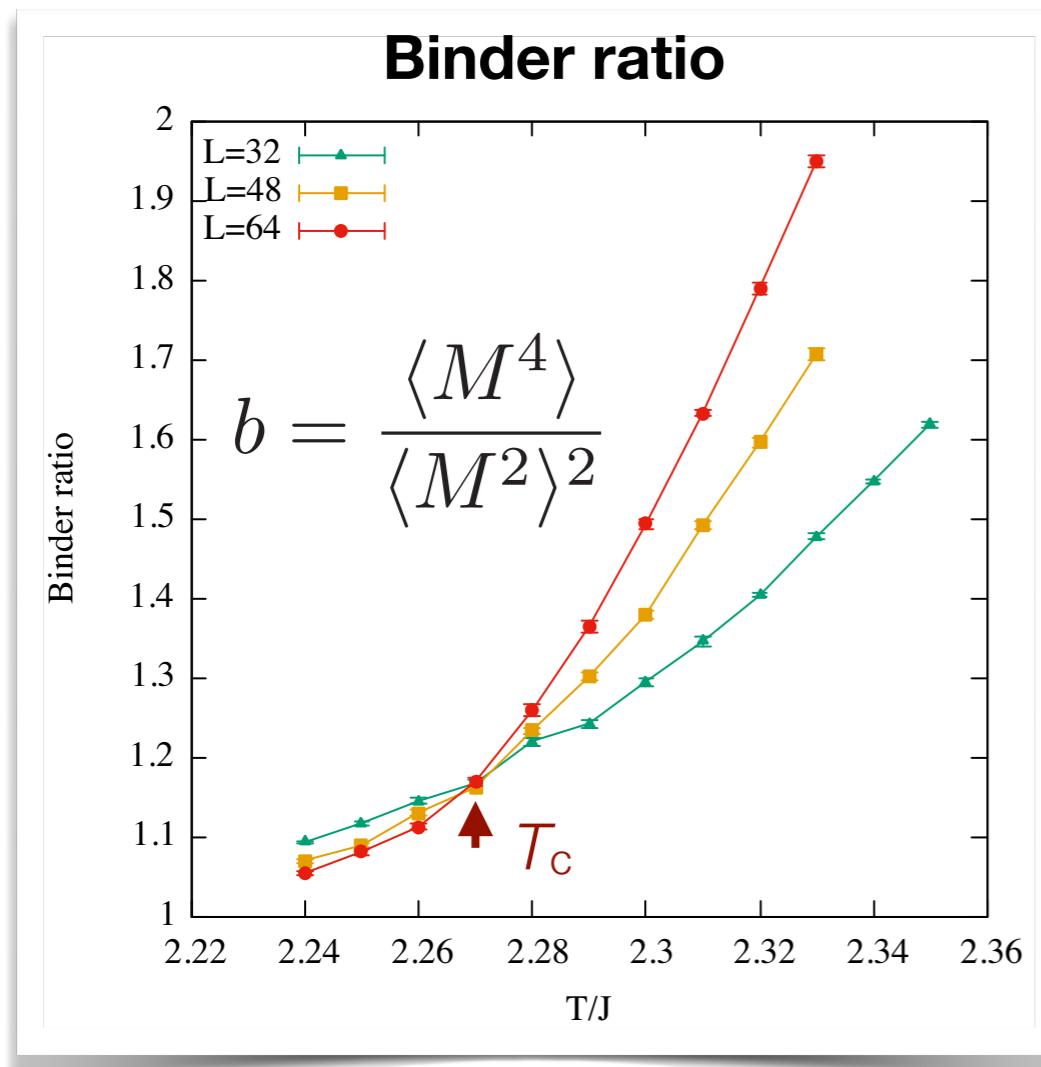
A sampling point moves “randomly”.

Finite-size scaling of the data (#4)

From the data obtained by MCMC, we can extract much information.

→ Ex. **Finite-size scaling** $b = f((T - T_c)L^{1/\nu})$

By this scaling, we extract information about the infinite-size system from data of finite-size simulations.



$$(T - T_c)L^{1/\nu}$$

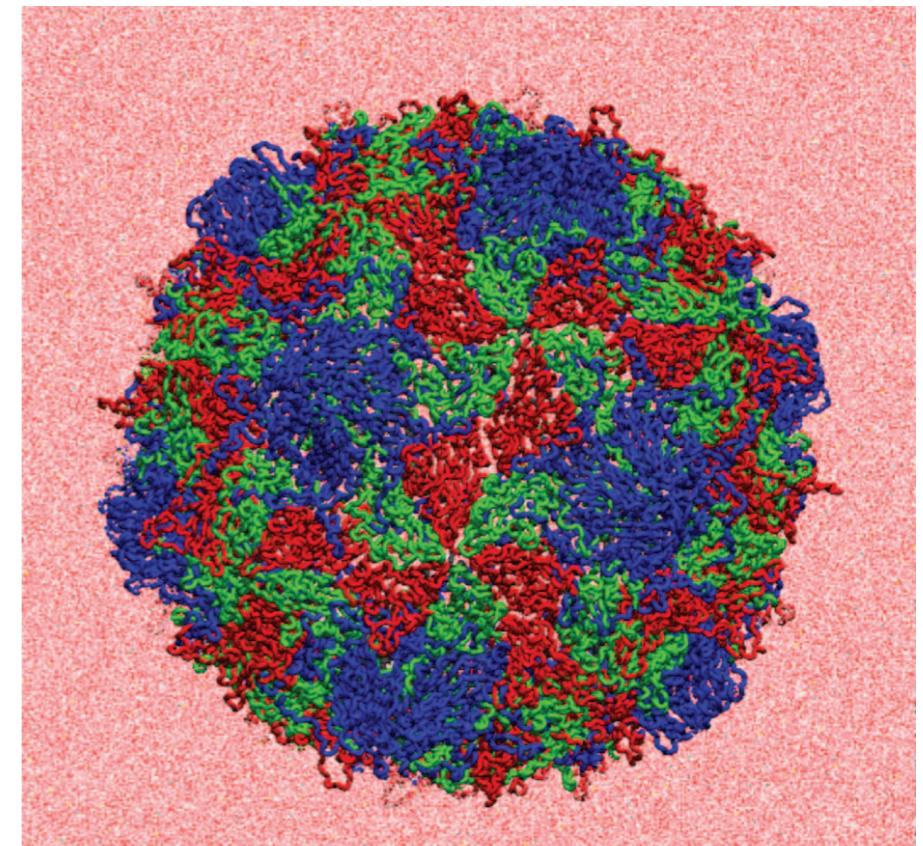
Molecular dynamics simulation (#5)

Molecular Dynamics (MD) simulation:

Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

Solving Newton's equation **numerically**.

Poliovirus capsid



By MD, we can calculate equilibrium properties:

Usual Newton's equation gives us the NVE ensemble
(Micro canonical ensemble).

$$\langle \hat{O} \rangle_{NVE} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \hat{O}(\Gamma(t))$$

By temperature or pressure controls,
we can also obtain other ensemble averages.

$$\langle \hat{O} \rangle_{NVT} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \hat{O}(\underline{\Gamma_{NVT}(t)})$$

$$\langle \hat{O} \rangle_{NPT} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \hat{O}(\underline{\Gamma_{NPT}(t)})$$

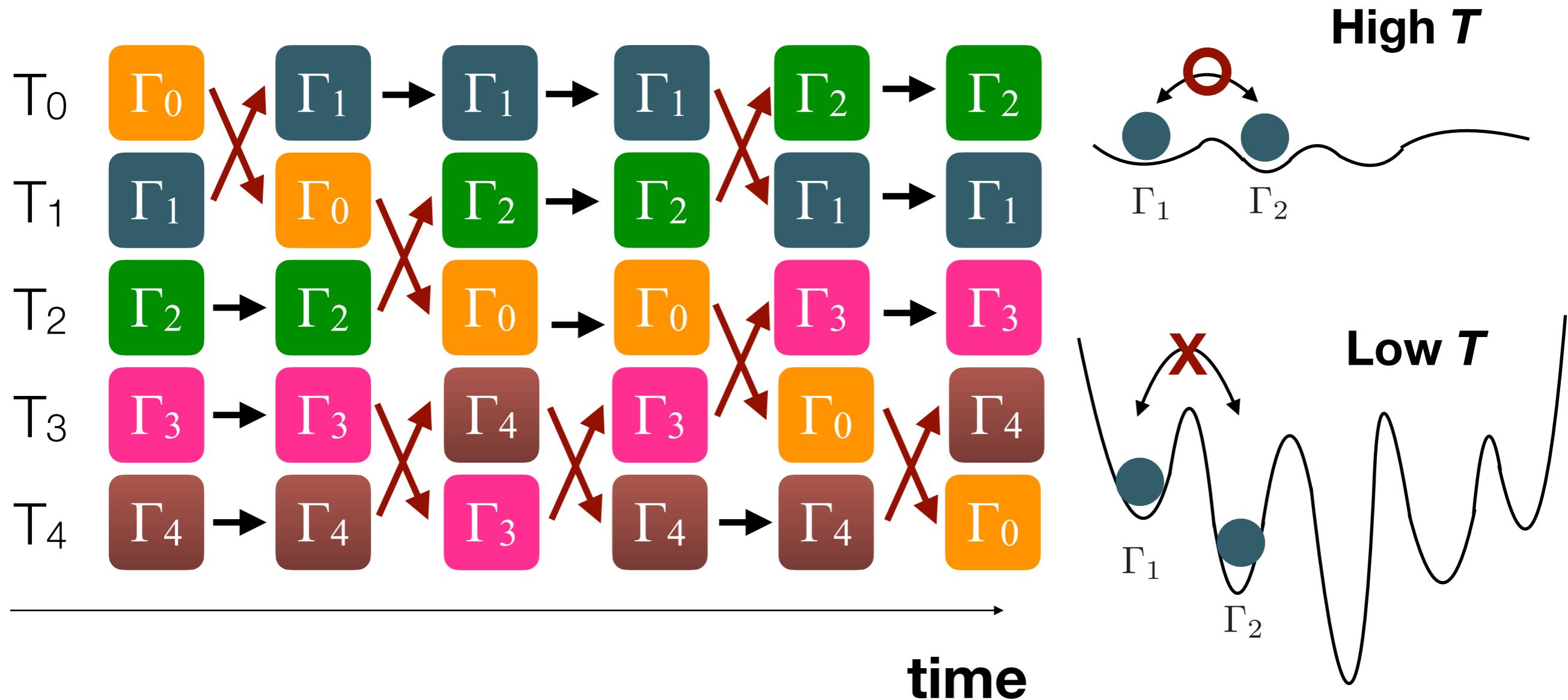
Modified dynamics!

Extended ensembles (#6)

To improve sampling efficiency in MCMC and MD simulations,
we can use many “extended” ensembles:

Ex. Replica exchange simulation

Along simulation, we “exchange” the relationship between parameter and realization

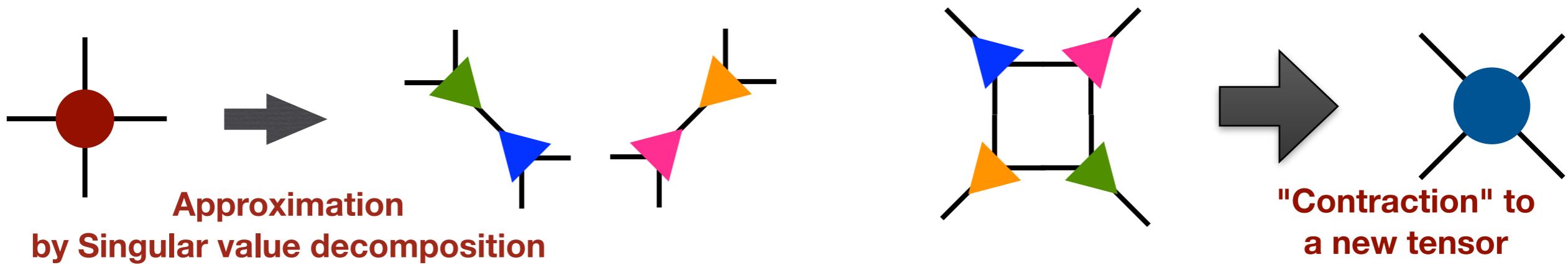
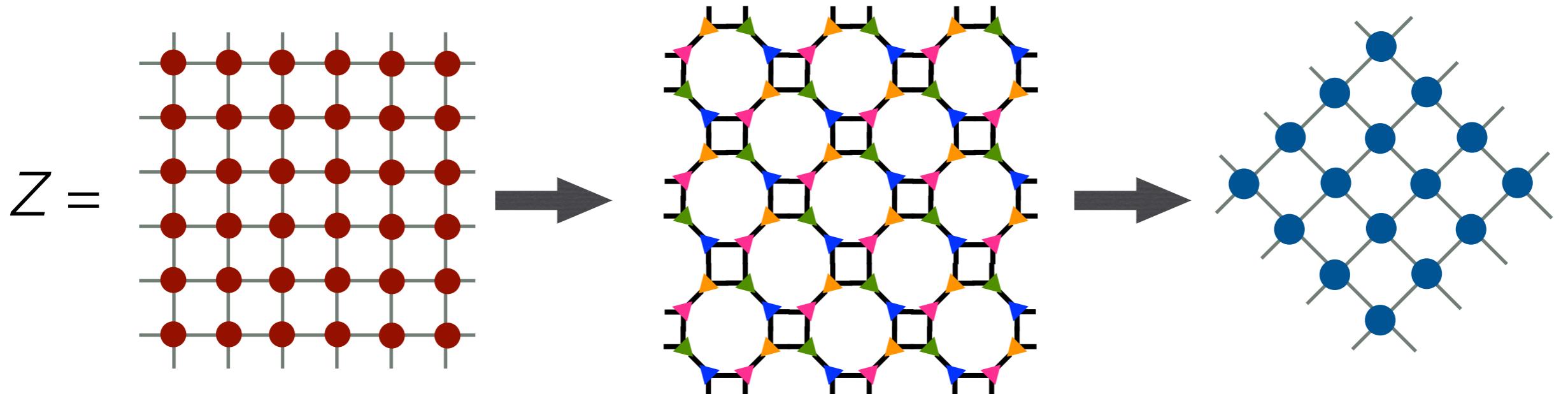


Tensor renormalization group (#7)

Tensor renormalization group (テンソル繰り込み群)

We can efficiently calculate the partition function numerically!

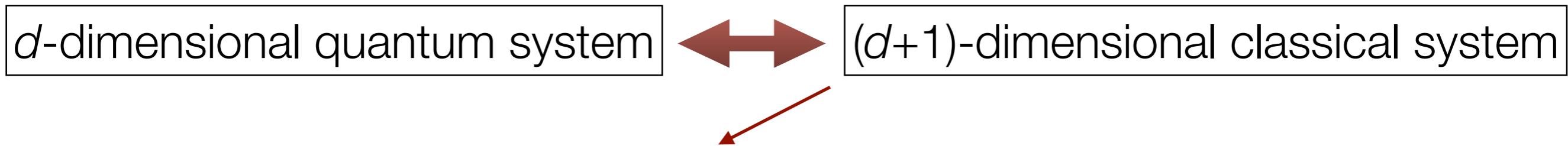
- We can represent the partition function as **a tensor network**
- We can calculate the contraction (縮約) of the network through coarse-graining.



Quantum Monte Carlo (#9 and #10) by Yamaji-san

We can apply MCMC algorithms even for a quantum system.

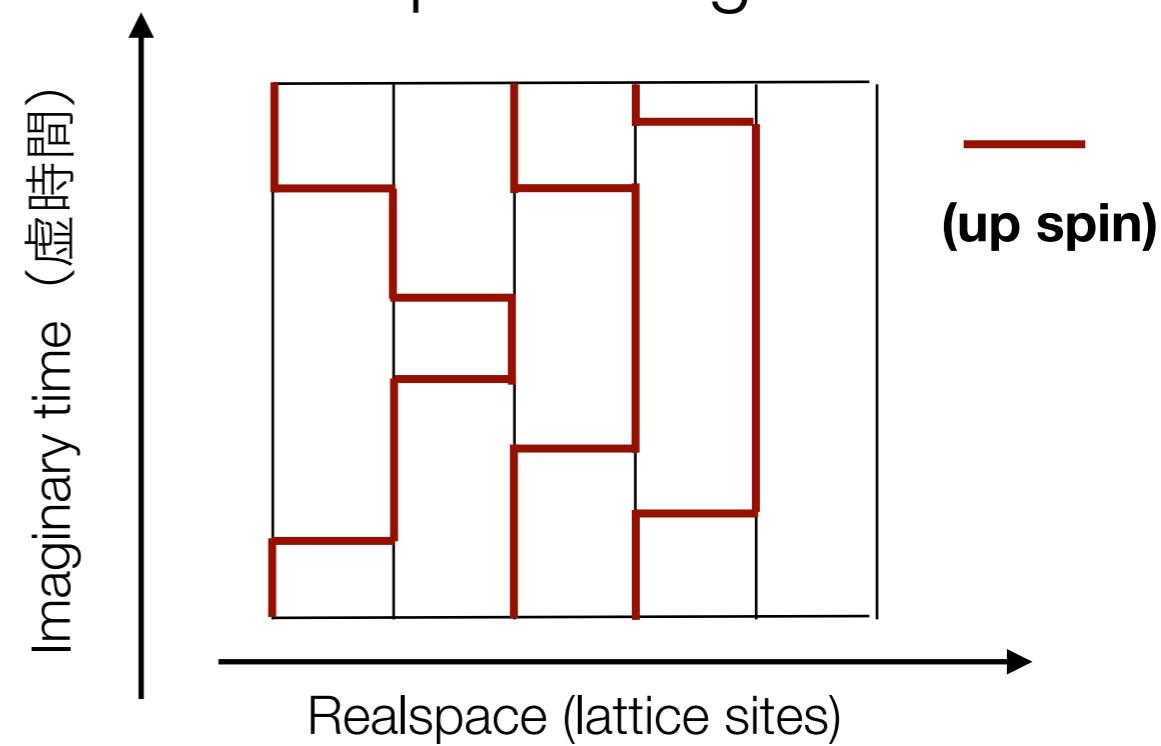
Through Feynman's path integral (経路積分) :



For such a $(d+1)$ -dimensional system, we perform **classical MCMC simulation**.

1d quantum spin chain

$$\mathcal{H} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z)$$



Krylov subspace method (#11- #12) by Yamaji-san

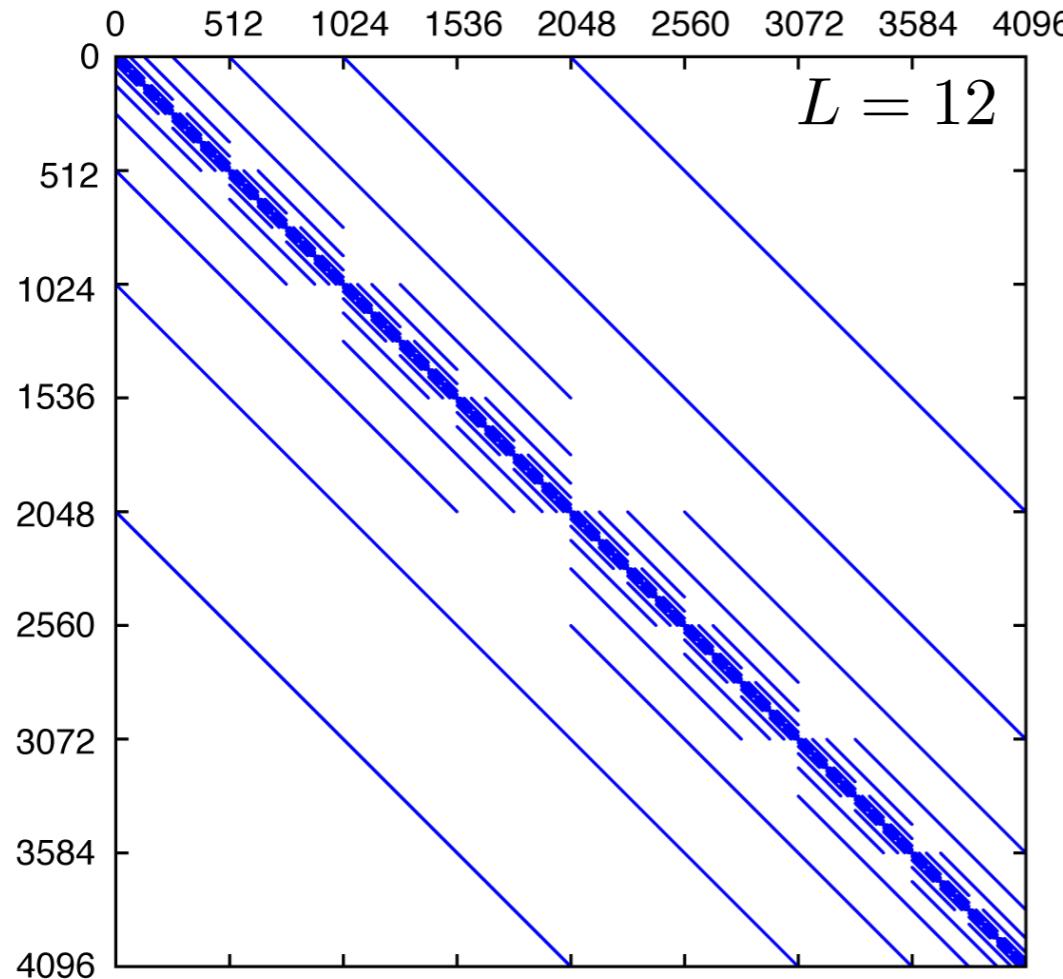
Typical Hamiltonian in quantum many-body problem is **sparse**.

"Transverse field Ising model"

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

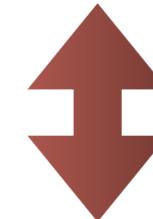
Non-zero elements in the Hamiltonian

(Figure from Yamaji-sensei)



Total matrix elements = 2^{2L}

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



Sparse!

Krylov subspace method (#11- #12) by Yamaji-san

Krylov subspace

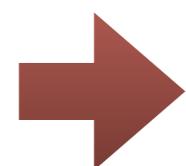
linear subspace generated by a square matrix (M) and a vector (v) as

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

For quantum many body problems:

$M = \mathcal{H}$:Hamiltonian

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



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

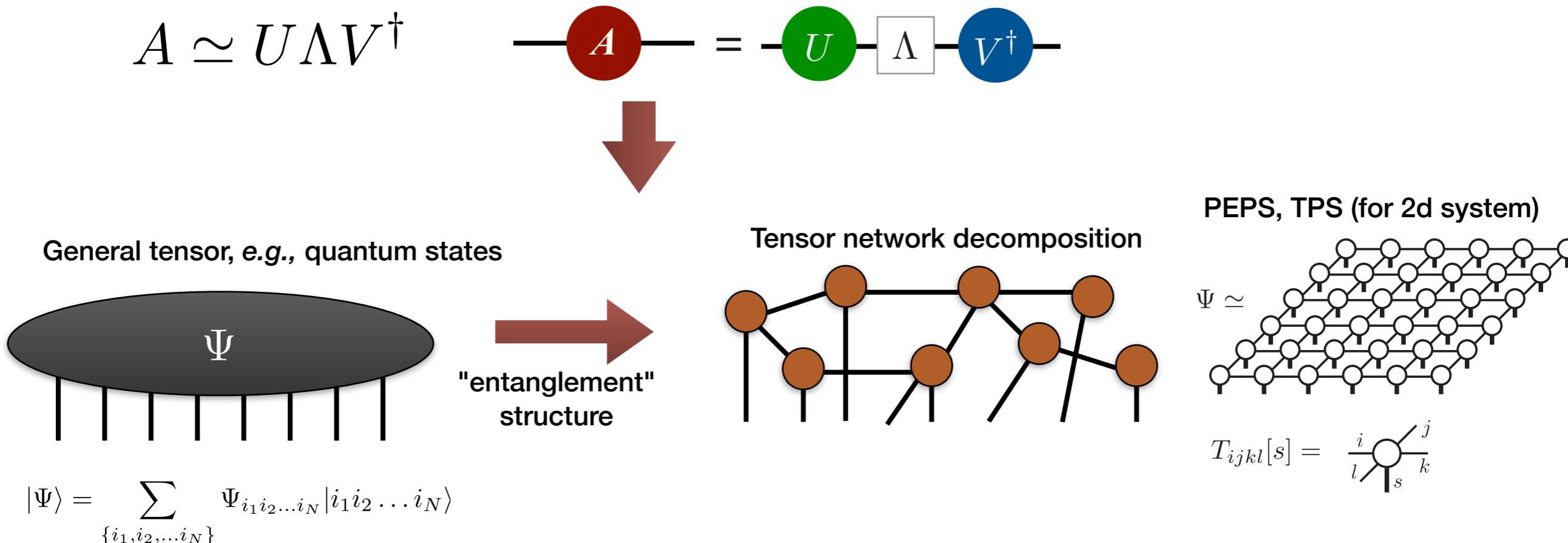
Lanczos method, Arnoldi method

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

Advanced algorithms for quantum many-body problems

Ex. Tensor network method (This will be discussed in another lecture in A semester)

Generalization of the low-rank approximation of matrices to tensors



By choosing a “good” network, we can express G.S. wave function efficiently.

ex. TPS: # of elements $\sim ND^4$

D : dimension of the tensor T

Exponential \rightarrow Linear

Next week (4/18)

Classical

Quantum

1st: Many-body problems in physics and why they are hard to solve

2nd: Classical statistical models and numerical simulation

3rd: Classical Monte Carlo method

4th: Applications of classical Monte Carlo method

5th: Molecular dynamics simulation and its applications

6th: Extended ensemble method for Monte Carlo methods

7th: Tensor Renormalization group

8th: Quantum lattice models and numerical simulation

9th: Quantum Monte Carlo methods

10th: Applications of quantum Monte Carlo methods

11th: Linear algebra of large and sparse matrices for
quantum many-body problems

12th: Large sparse matrices, and quantum statistical mechanics

13th: Advanced algorithms for quantum many-body problems