古典統計力学模型と数値計算

Classical Statistical Models and Numerical Simulation

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Background of the lecturer

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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

Outline

- Many-body problems: Quantum or Classical ?
  - When we can use classical “models” ?
- Targets of this lecture
  - Targets of computational sciences
  - Examples of classical models
- Computational science for classical statistical models
  - Statistical ensembles
  - Long time average and relaxation time

Many body problems: Quantum or Classical?

Many-body problems: Quantum or Classical?

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

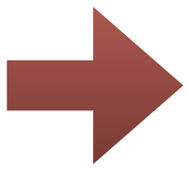
- Percolation, covering, packing, …
- Stochastic process, dynamical system (力学系）, ..
- Critical phenomena (臨界現象）
- …

Classical problems as an approximation: molecules

Interaction of molecules:

- Coulomb interactions of charges
- Van der Waals force
- …

For accurate treatments, we need to consider quantum mechanics.



However, we can approximate the system as a set of **“classical” point particles.**

Approximated two-body interactions between classical particles:

- Lennard-Jones potential for noble gas
- Effective potential for water
- ….

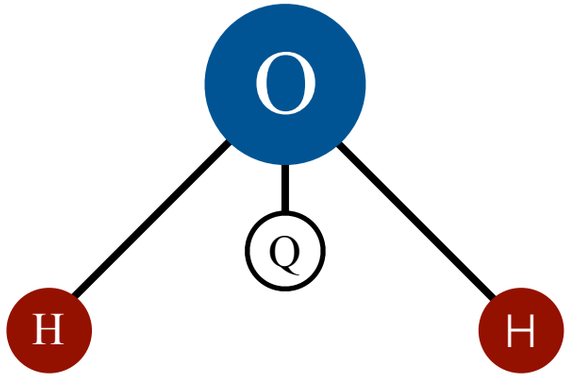
Example: water (H_2O)

For H_2O, there are lots of effective potentials

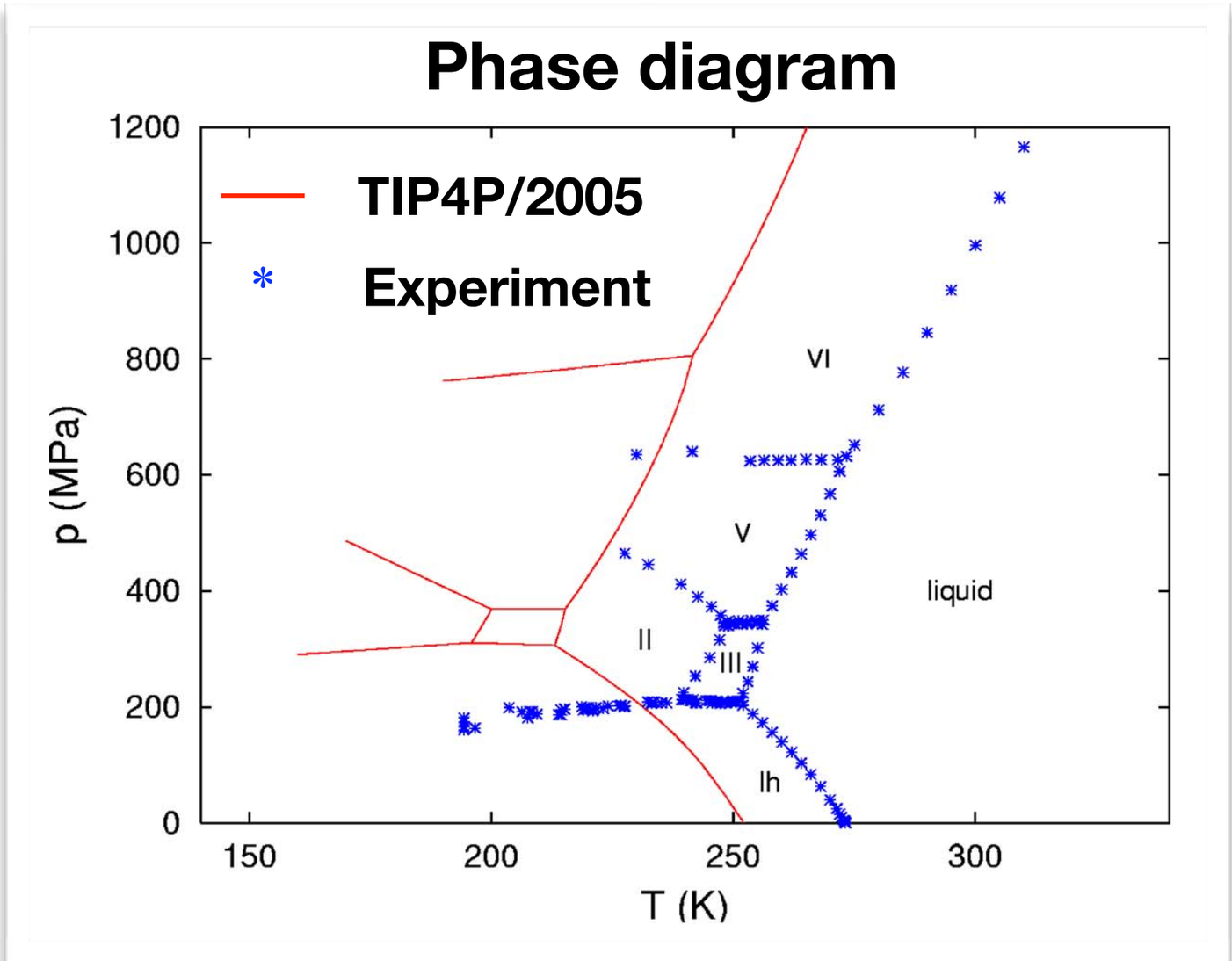
Example: TIP4P/2005 (J. L. F. Abascala and C. Vega, J. Chem. Phys. **123**, 234505(2005))

O: LJ potential
(Its charge is located at Q)
H: point charge

*Their relative locations are fixed.



Phase diagram of water is qualitatively reproduced!

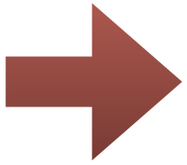


Classical problems as an approximation: magnetism

(Electron) spins:"Quantum" degree of freedom

For accurate treatment, the spin quantum number S is important:

S=1/2, 1, 3/2, …



However, we can approximate the system by taking the limit of $S \to \infty$.

"classical" spin model

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

Example: ferromagnetism

Iron (Fe): Ferromagnet （強磁性体）

Below the Curie temperature $T_c \simeq 1043\ \mathrm{K}$,
it exhibit spontaneous magnetization （自発磁化）.

→ The most simple approximation for the ferromagnet:

Classical Heisenberg model

$$\mathcal{H} = -\sum_{(i,j)} J_{ij} S_i \cdot S_j$$

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

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

→ The Heisenberg model on the bcc lattice shows
a phase transition at $T_c \simeq 2.054\, J$.

(K. Chen, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **48**, 3249 (1993))

Classical problems as an approximation

When a classical approximation becomes accurate?

- High temperature
  - We safely neglect quantum nature compared with thermal fluctuations.
- Low density
  - The interaction between particles is small (rare).
- Classical order (magnetism)
  - If the ground state is classical magnetic long range order, typically, classical approximation is not so bad.

Pure classical problems: Critical phenomena

Critical phenomena:

At the critical point, characteristic length scale diverges

→ Scale invariance

Several quantities show power-low behaviors

Correlation length : $\xi \sim |T - T_c|^{-\nu}$

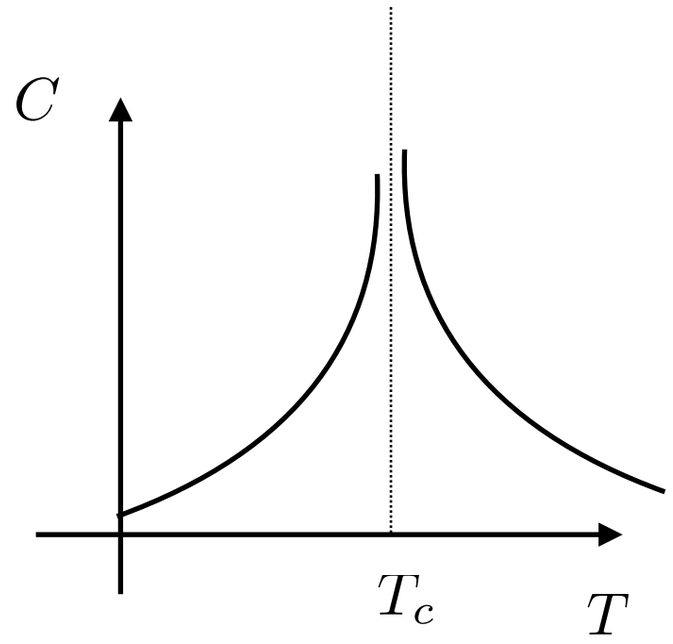
Specific heat : $C \sim |T - T_c|^{-\alpha}$

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

Order parameter: $M \sim (T_c - T)^{\beta}$

Exponent: $\alpha, \nu, \gamma, \beta, \ldots$

= Critical exponent



Pure classical problems: Critical phenomena

Universality

Critical exponents depends only on
symmetry and **spacial dimensions**.

Ising model: the order parameter has Z_2 symmetry

Ising systems	α	β	γ	ν	η
2D-Ising(exact)	0	1/8=0.125	7/4=1.75	1/2=0.5	0
Fe film[a]	N/A	0.13±0.02	1.74±0.05	N/A	N/A
3D-Ising[b]	*0.10994	*0.3264	*1.23719	0.63002(10)	0.03627(10)
$Dy_3Al_5O_{12}$[c,d]	0.12±0.03	0.26±0.02	1.16±0.04	0.61±0.02	N/A
LJ(model liquid)[e]	*0.11	0.3285(7)	*1.2	0.63(4)	*0.1
Xe[f]	0.110±0.003	0.325±0.002	1.241±0.002	0.630±0.002	N/A

a:C.H. Back et al Nature (1995), b:M. Hasenbusch,PRB (2010), c:A Guttmann, J.Phys.C(1975), d:J.C.Norvell et al, Phys.Rev. (1969). e:H. Watanabe et al, JCP(2012), f: taken from table in K. Gills et al, PRE(2004).*: calculated assuming scaling relations.

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

Pure classical problems: other examples

- Percolation problem
  - Physics of Bingo game
- Sphere packing
  - What is the most dense packing in a box?
  - Packing structure of poly-disperse systems?
- Stochastic process
  - Dynamics of financial trades
  - Dynamics of population, society, …

Target of this lecture

Target of studies: Static or Dynamic

Static properties:

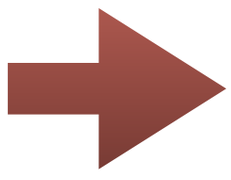
Physical properties independent on time.

(free) energy, specific heat, (static) susceptibilities, …

Dynamical properties:

Related to a response to external forces.

Time-dependent susceptibilities, Time-Correlations,



By computational science, both types of quantities can be calculated, although the method could depend on the type.

(Typically, dynamical properties are more difficult to obtain.)

Target of studies: Equilibrium or Non-Equilibrium

Equilibrium system:

Systems are described by thermodynamics

Non-Equilibrium system:

Systems are not described by thermodynamics

Steady state:

Its physical quantities are independent of time.

Non-steady state:

Its physical quantities depend on time.

Typically, treatment of non-steady state is very difficult.

Target of my lecture

Steady state of classical system (not necessarily in equilibrium)

→ Physical quantities are calculated through steady state distribution $P(\Gamma)$

$$O = \langle \hat{O} \rangle = \mathop{\mathrm{Tr}}_{\Gamma} \left(\hat{O}(\Gamma) P(\Gamma) \right)$$

$$C(\tau) = \langle \hat{A}(t=0) \hat{B}(t=\tau) \rangle = \mathop{\mathrm{Tr}}_{\Gamma} \left(\hat{A}(\Gamma) \hat{B}(\Gamma(\tau)) P(\Gamma) \right)$$

$\Gamma = \{S_i\}, \{q_i, p_i\}, \ldots$:state in the phase space

Q. Are you familiar with statistical physics?

Examples of classical statistical models

Statistical mechanical models:

Models considered in this lecture:

- Classical Spin systems
  - **Ising**, XY, Heisenberg, …
  - Frustration, DM interactions, Anisotropy, …
- Particle systems
  - **Point particles**, Molecules, hard spheres,…

Models related to the methods presented in this lecture:

- Agent models of socio-physics
- Lattice models representing (non-equilibrium) steady state
  - ASEP (ASymmetric Exclusion Process), lattice gas, …
- Langevin dynamics (Stochastic differential equation)
  - Brownian motion, econophysics, …

Classical spin system: spin model on lattice

Spin systems:

Spin degree of freedoms defined on a **lattice** (they **interact** each other).

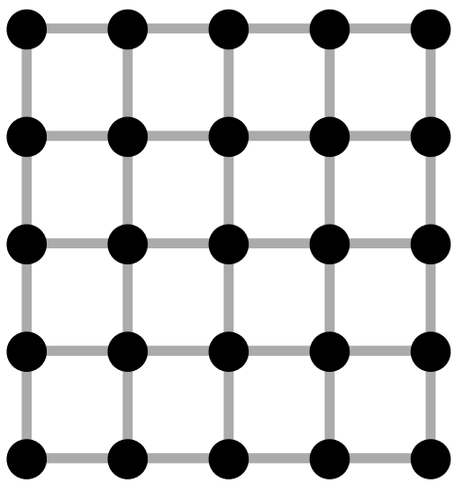
Lattice

1D

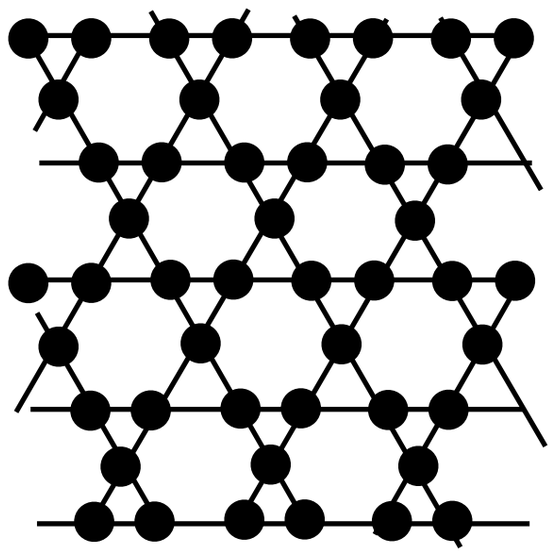
Chain

2D

Square lattice



Kagame lattice



3D

Simple cubic, FCC lattice, BCC lattice, …

Classical spin degree of freedom

Spin: 1. $S \to \infty$ limit of quantum spin

2. simple degree of freedom reflecting symmetry

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

- Strong easy axis anisotropy
- Representing underlying Z_2 symmetry

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

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

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

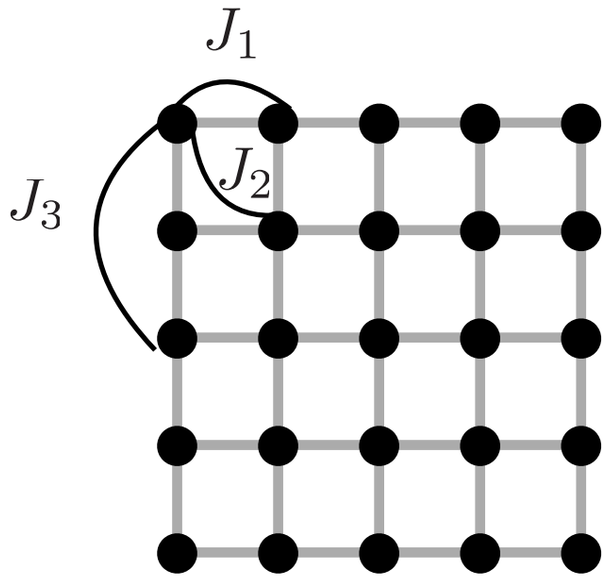
- Strong easy plane anisotropy
- Representing underlying U(1) symmetry

Classical spin model: interactions

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

Heisenberg interaction:

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$



Single ion anisotropy

$$D \sum_i (S_i^z)^2 + E \sum_i \left[(S_i^x)^2 - (S_i^y)^2 \right]$$

$D \rightarrow +\infty$: XY spins

$D \rightarrow$ -∞ : Ising spins

Dzyaloshinskii-Moriya interaction

$$\sum_{\langle i,j \rangle} \vec{D} \cdot (S_i \times S_j)$$

A lot of “novel” magnetism appears even in classical spin system

Example: Magnetic skyrmion

T. Okubo et al Phys. Rev. Lett. **108**, 017206 (2012).

Classical antiferromagnetic Heisenberg model on triangular lattice under magnetic fields

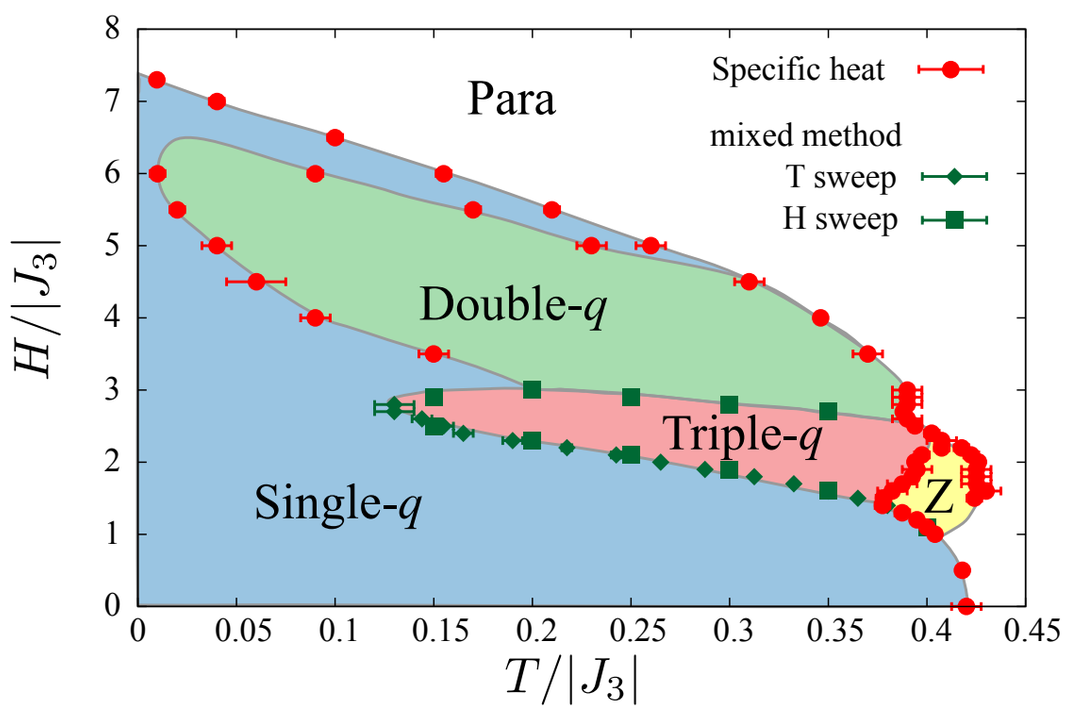
By considering J_1 and J_2 (or J_3) interaction

(effective model for $NiGa_2S_4$)

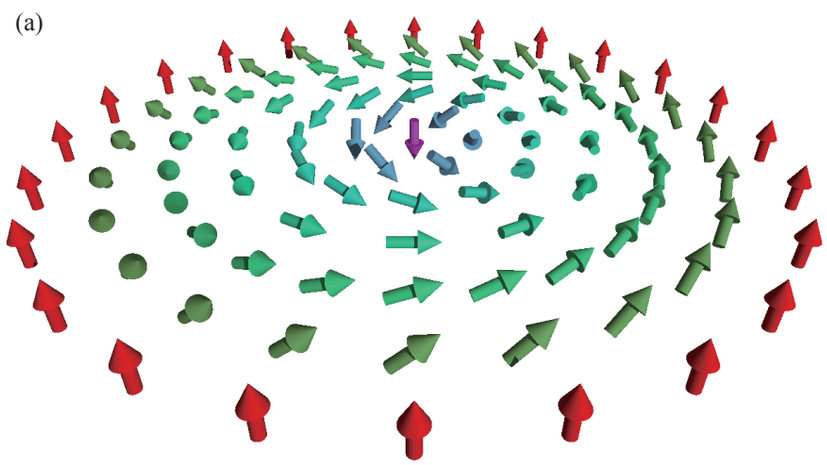
→ Novel multiple-q states are stabilized

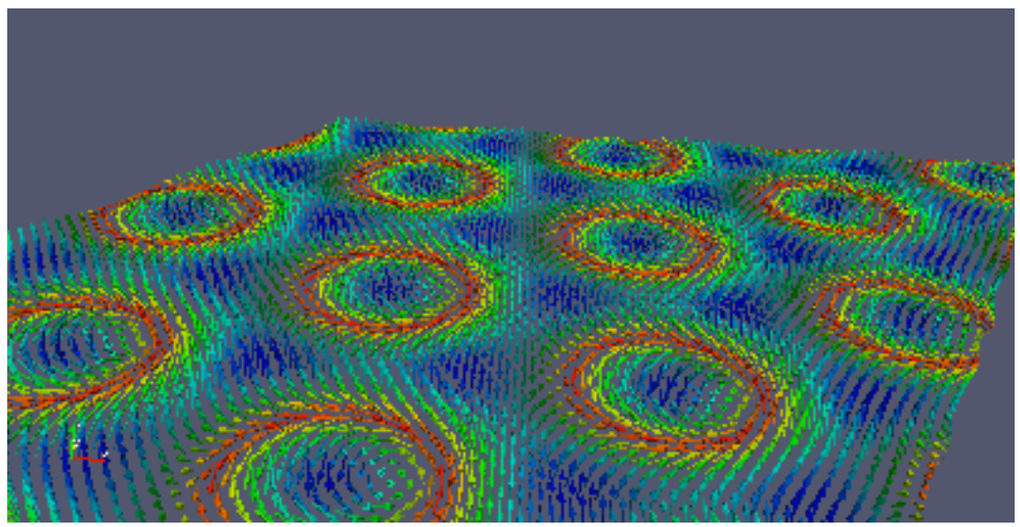
One of them is identical with
"magnetic skyrmion lattice"

Phase diagram



This has been also investigated by **Monte Carlo simulation**.





Particle system:

Particle systems:

Particles moving in continuous space by interacting each other

Typically, their degree of freedoms are “positions” and “momentum”

Two components in Hamiltonian

Interacting potential: $V(\boldsymbol{r}_i - \boldsymbol{r}_j)$

Kinetic Energy: $\dfrac{p_i^2}{2m_i}$

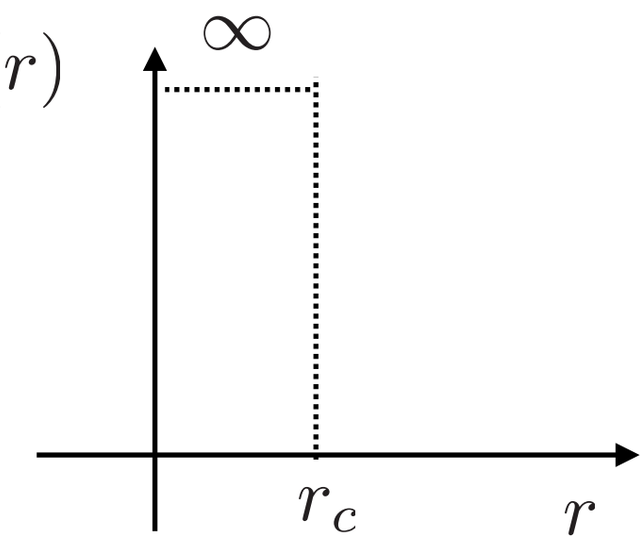
Phase space: $\Gamma = \{\boldsymbol{r}_i, \boldsymbol{p}_i\}$ → N-particles= $2dN$ dimension

Variety of models: variety of interacting potentials

Hard sphere

$$V(\boldsymbol{r}_i - \boldsymbol{r}_j) = \begin{cases} 0 & (r > r_c) \\ \infty & (r \leq r_c) \end{cases} \qquad r = |\boldsymbol{r}_i - \boldsymbol{r}_j|$$

$V(r)$

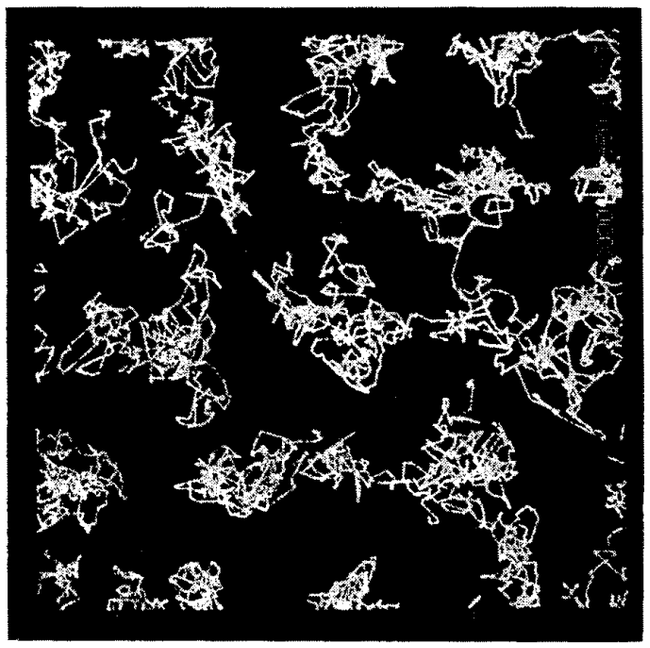


The first application of molecular dynamics

Alder and Wainwright, J. Chem. Phys. **27**, 1208 (1957);**31**, 459 (1959)

- Event driven molecular dynamics simulation

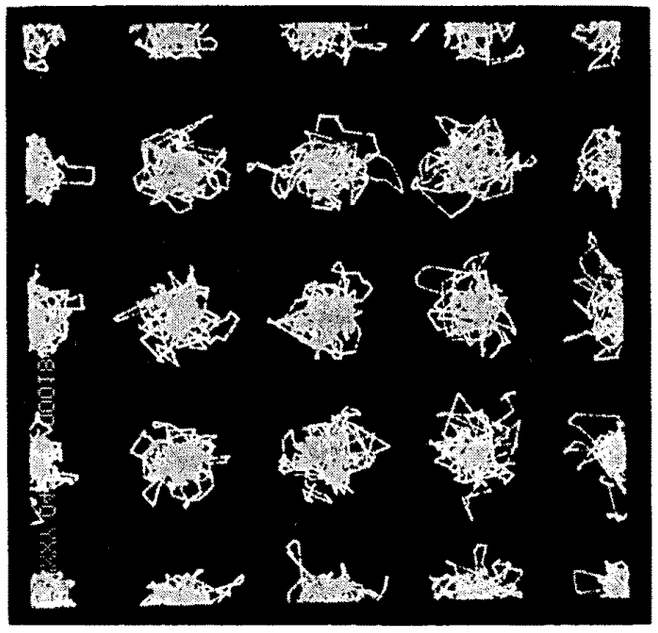
Fluid



Phase transition

(Alder transition)

Crystal

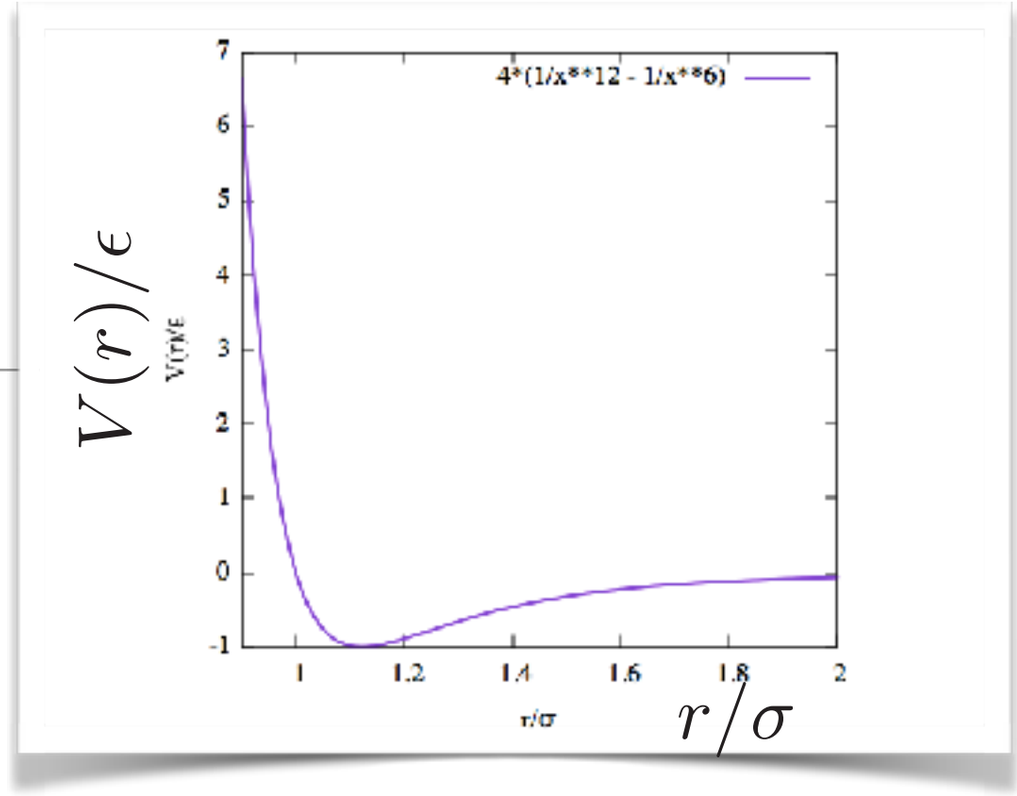


32 particle system

Lennard-Jones potential

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

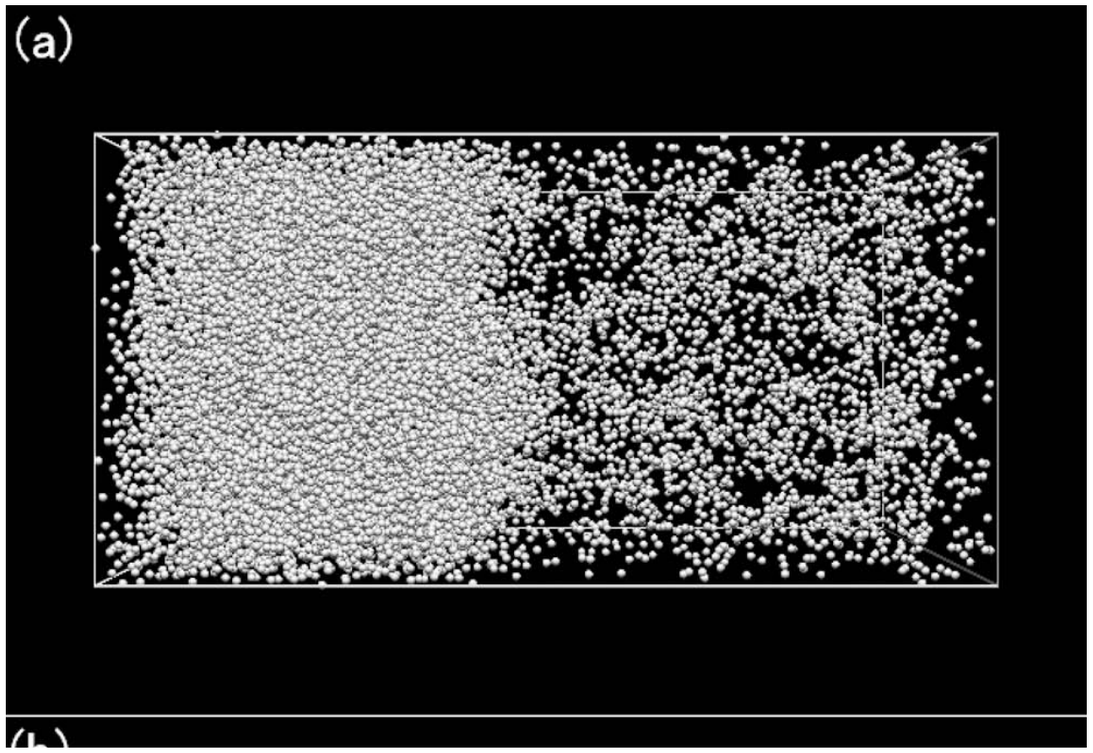
Model potential for noble gas (Ar, …)



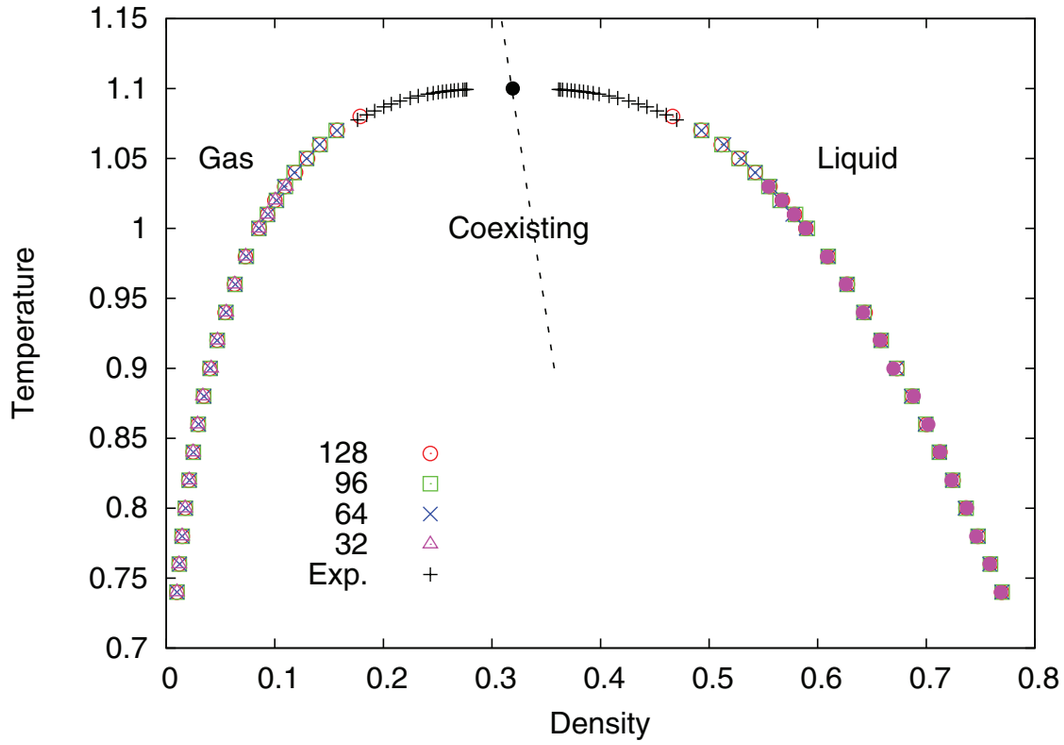
Recent simulation: H. Watanabe et al, J. Chem. Phys. **136**, 204102 (2012).

(~1,000,000 particles)

Gas-Liquid coexistence



Phase diagram



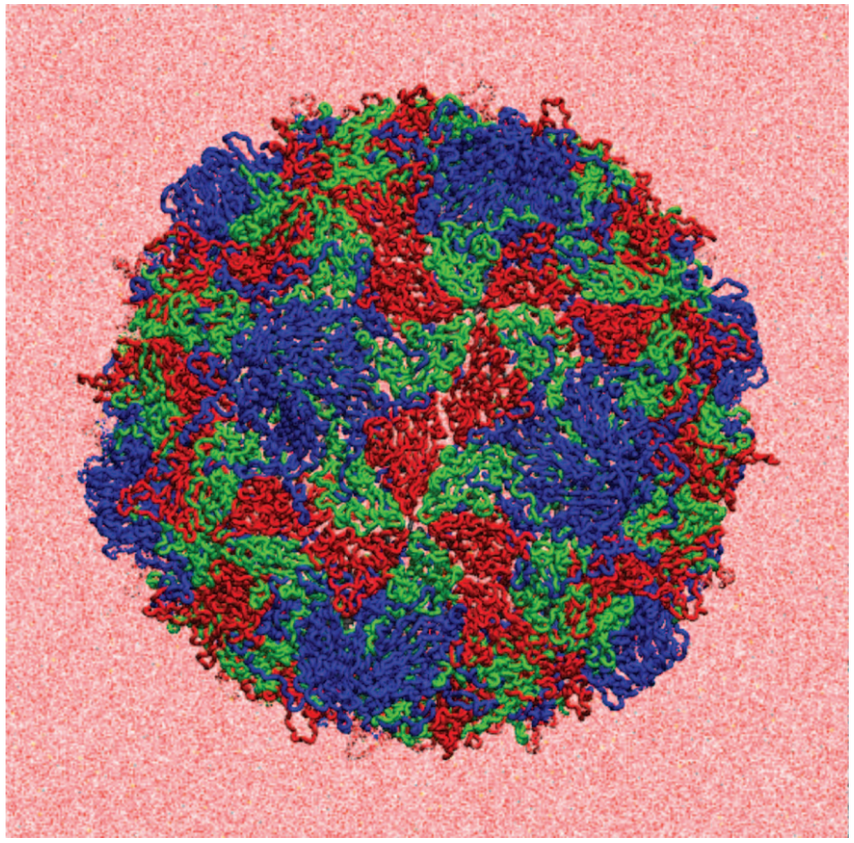
Complex systems

Eg. Poliovirus capsid in electrolyte solution（電解質溶液）

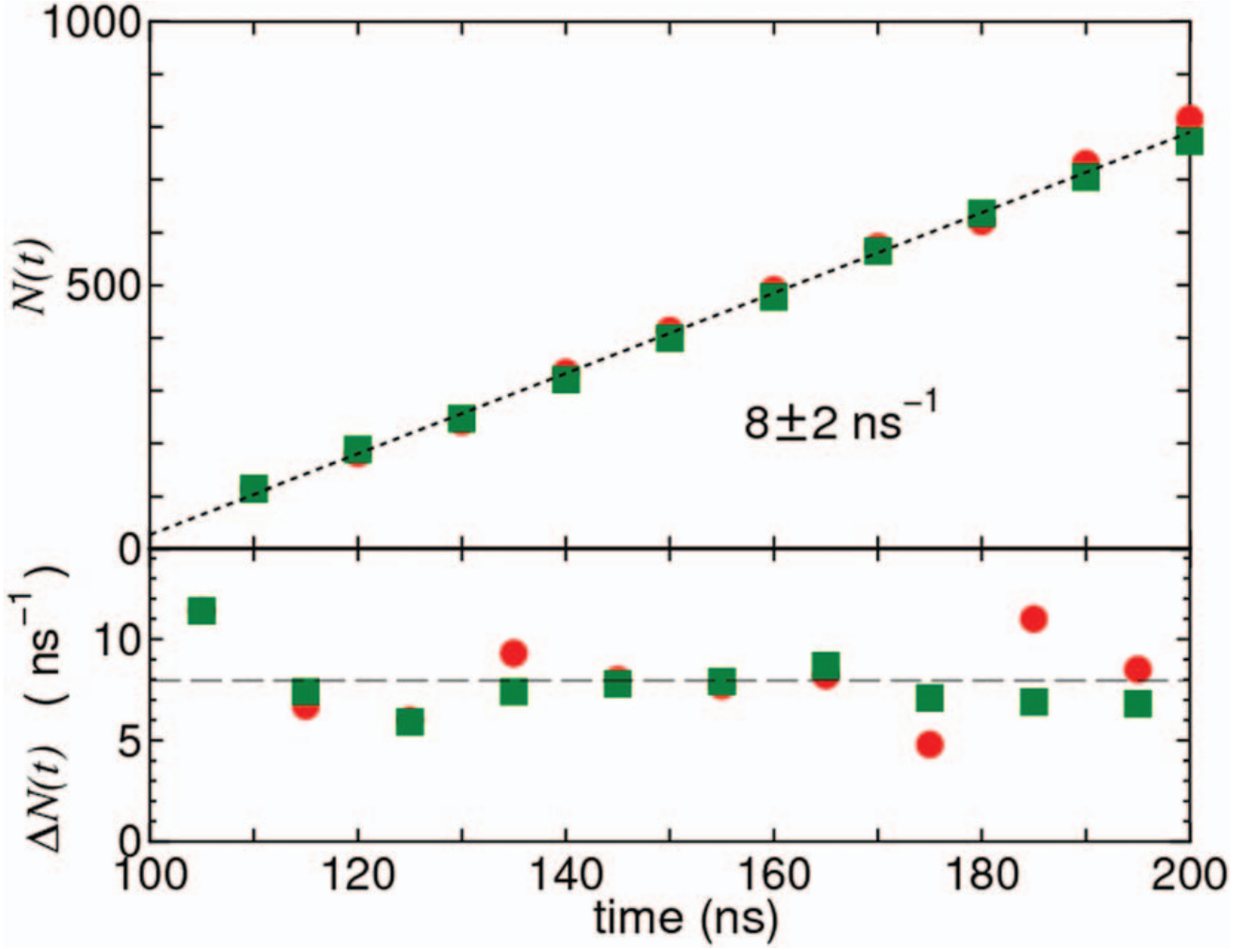
Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

Long-range coulomb interaction

Poliovirus capsid



Dynamics of water molecules



Computational science for (classical) statistical models

Statistical mechanics: Ensemble

Statistical mechanics:

Connect microscopic models to macroscopic observable

Example: Ising model

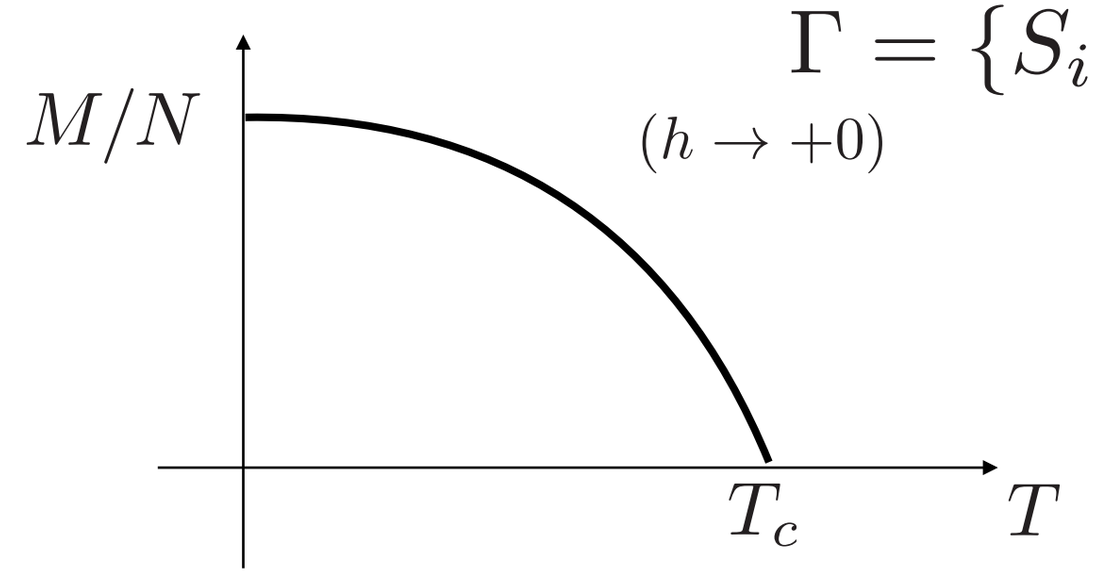
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \qquad (S_i = \pm 1 = \uparrow, \downarrow)$$

Canonical ensemble (NVT-ensemble)：

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

Example: magnetization at T:

$$M(T) = \left\langle \sum_i S_i \right\rangle_T = \sum_\Gamma \sum_i S_i P(\Gamma; T)$$



Statistical mechanics: important ensembles

Micro Canonical ensemble (NVE-ensemble)：

$$P(\Gamma; E) \propto \sum_{\Gamma} \delta(E - \mathcal{H}(\Gamma))$$

E: energy

NPT-ensemble：

$$P(\Gamma; P, T) \propto \int dV e^{-\beta PV} \sum_{\Gamma(V)} e^{-\beta \mathcal{H}(\Gamma)}$$

P: pressure
V: volume

$$\beta = \frac{1}{k_B T}$$

Grand Canonical ensemble (μVT-ensemble)：

$$P(\Gamma; \mu, T) \propto \sum_{N} \frac{1}{N!} e^{\beta \mu N} \sum_{\Gamma(N)} e^{-\beta \mathcal{H}(\Gamma)}$$

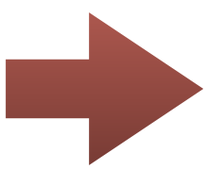
μ: chemical potential

General ensemble：

- Not necessarily related to thermal equilibrium
- But, it may represent a steady state of a certain physical system
  - Non-equilibrium steady state

Computational science for statistical models

Purpose of computational science



Calculate ensemble averages numerically

Two types of approaches

- Evaluate ensemble average as a “time average”
  based on a special dynamics
  - Monte Carlo (MC) , Molecular Dynamics (MD)
  - Target of this lecture
- Calculate partition function directly
  - Transfer matrix method, Tensor network method
  - It will be treated partly in “計算科学における情報圧縮 (A-term)”

Long time average

Long time average for ensemble average

States depending on time

$$\Gamma(t) = \{q_i(t), p_i(t)\}, \{S_i(t)\}, \cdots$$

Long time average

$$\langle \hat{O} \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T \hat{O}(\Gamma(t)) dt$$

$$= \lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} \hat{O}(\Gamma(t))$$

$\hat{O}(\Gamma)$: Observable such as Energy, magnetization, momentum, force, ...

If we can find a good dynamics which satisfies

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \hat{O}(\Gamma(t)) = \int d\Gamma P(\Gamma)$$

(Time average coincides with an ensemble average.)

We can calculate **ensemble averages** through **dynamical simulations**.

Typical dynamics:

- Molecular dynamics:

  Dynamics of Γ obeys a differential equation (Newtonian equation).

$$\frac{d}{dt}\begin{bmatrix} q_i \\ p_i \end{bmatrix} = \begin{bmatrix} \partial\mathcal{H}/\partial p_i \\ -\partial\mathcal{H}/\partial q_i \end{bmatrix}$$

  → The Hamiltonian is constant of the motion.
  The long time average gives us
  an average over **micro canonical ensemble.**

- Markov Chain Monte Carlo:

  Dynamics of Γ obeys a master equation.

$$\rho_{t+1}(\Gamma) - \rho_t(\Gamma) = \sum_{\Gamma'} W_{\Gamma'\to\Gamma}\rho_t(\Gamma') - \sum_{\Gamma'} W_{\Gamma\to\Gamma'}\rho_t(\Gamma)$$

  $\rho_t(\Gamma)$:probability distribution

  $W_{\Gamma\to\Gamma'}$:transition probability

  → The long time average gives us
  a variety of ensemble averages
  depending on W.

Time Correlation and relaxation time

Time correlation function

$$C_{AB}(t) \equiv \langle \hat{A}(0)\hat{B}(t)\rangle - \langle \hat{A}\rangle\langle \hat{B}\rangle$$

Auto correlation function

$$C_{AA}(t) \equiv \langle \hat{A}(0)\hat{A}(t)\rangle - \langle \hat{A}\rangle^2$$

***Average over initial states**

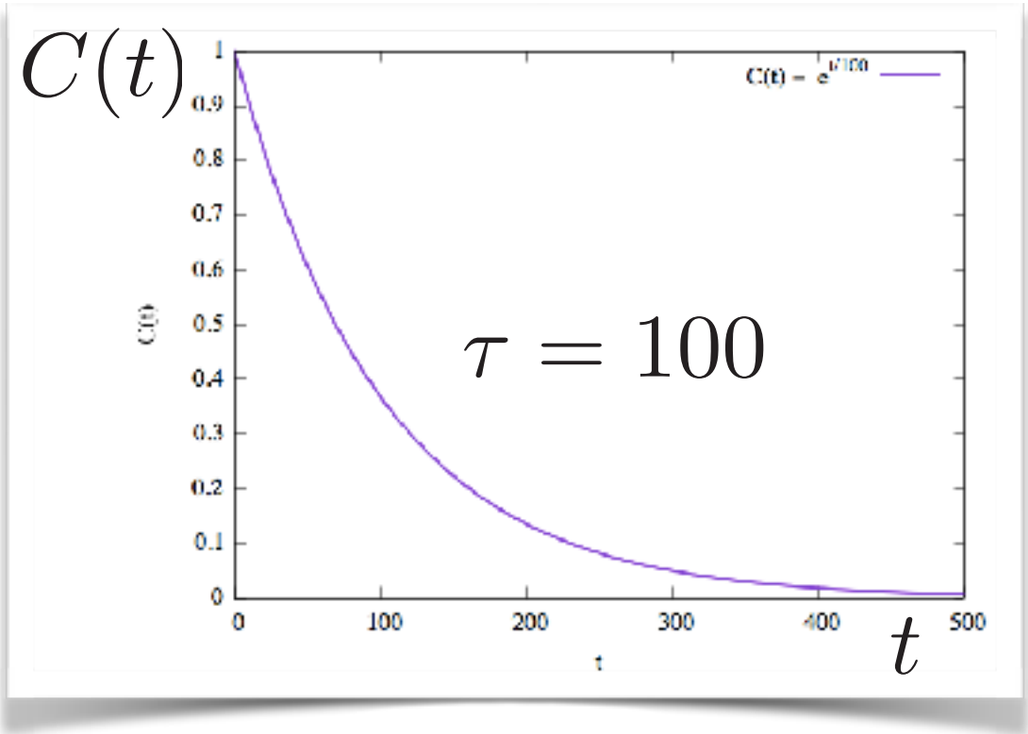
$$\langle \hat{O}(t)\rangle = \int d\Gamma \hat{O}(\Gamma(0))P(\Gamma(0))$$

(It is different from the time average.)

Typical asymptotic behavior

$C_{AA}(t) \sim e^{-t/\tau_A}$ exponential decay

Relaxation time: τ_A



Relaxation time and sampling

Error due to finite number of sampling

$$\bar{A} \equiv \frac{1}{T}\sum_{t=1}^{T} \hat{A}(\Gamma(t))$$

$\langle \cdots \rangle$:average over trajectories (initial condition)

Standard error: $\epsilon^2 = \langle \bar{A}^2 \rangle - \langle \bar{A} \rangle^2$

$$\epsilon^2 = \left\langle \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=1}^{T} A_{t_1}A_{t_2} \right\rangle - \left\langle \frac{1}{T}\sum_{t=1}^{T} A_t \right\rangle$$

$$= \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=2}^{T} C_{AA}(|t_2 - t_1|)$$

$$C_{AA}(\Delta t) \sim C_{AA}(0)e^{-\Delta t/\tau}$$

$$\Delta t = |t_2 - t_1|$$

$$= \frac{1}{T^2}\sum_{\Delta t=1}^{T-1} 2(T-\Delta t)C_{AA}(\Delta t) + \frac{C_{AA}(0)}{T}$$

$$\underset{T\to\infty}{\sim} \frac{1+2\tau}{T}C_{AA}(0) \quad \Rightarrow \quad \epsilon \propto \sqrt{\frac{1+2\tau}{T}}$$

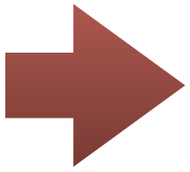
In order to reduce the error, we want to reduce τ.

Phenomena with large relaxation time

- Critical phenomena
  - $\tau \sim (T\text{-}T_c)^{-\nu z}$ with standard algorithm (critical slowing down)
  - z can be significantly reduced by using "**global update**"
- Glass transition (structural glass, spin glass), protein folding, first order phase transitions
  - $\tau \sim \exp(a/T)$ or $\exp(a/|T\text{-}T_c|)$
  - Exponential can be reduce to polynomial by using **extended ensemble methods**.

Information for future exercises

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



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

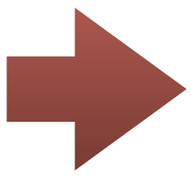
Q. Are you familiar with running python codes?

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

Instead, I will prepare a FAQ site for these python code.

- **In addition, we will provide informations of open source softwares related to the topics.**

Some of them run, at least, on ECCS with default configurations.



I recommend you to get ECCS account to test them, including the above python codes.

(ECCS = Educational Campus-wide Computing System)

Next week

Classical

1st: Introduction

2nd: Difficulties in many-body problems

3rd: Classical statistical models and numerical simulation

4th: Classical Monte Carlo method and its applications

5th: Molecular dynamics simulation and its applications

6th: Extended ensemble method for Monte Carlo methods

Quantum

7th: Quantum statistical models and numerical simulation

8th: Quantum Monte Carlo methods

9th: Applications of quantum Monte Carlo methods

10th: Quantum many-body problems and huge sparse matrices

11th: Krylov subspace methods and its applications

12th: Sparse matrices and quantum statistical mechanics

13th: Parallelized algorithm in many-body problems