

多体問題の計算科学

Computational Science for Many-body problems

2023.4.11

#2: 古典統計力学模型と数値計算

Classical Statistical Models and Numerical Simulation

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

# Today

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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

# Outline

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- 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?

Q. Which is more difficult, quantum or classical?

# Many-body problems: Quantum or Classical?

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Two types of classical many-body problems

## 1. Approximation of quantum problems

Nature: Elementary particles obey quantum mechanics.

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



Classical mechanics is **an approximation**.

## 2. Pure classical problems

Classical problems not necessary based on quantum mechanics

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

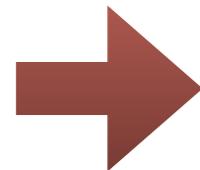
# Classical problems as an approximation: molecules

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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:

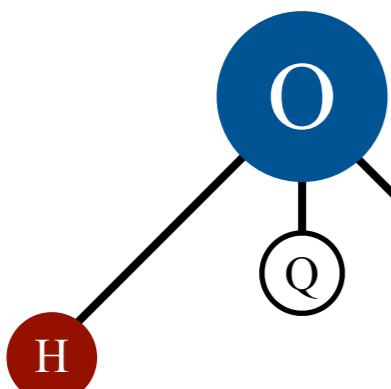
- Lennard-Jones potential for noble gas
- Effective potential for water
- .....

# Example: water ( $\text{H}_2\text{O}$ )

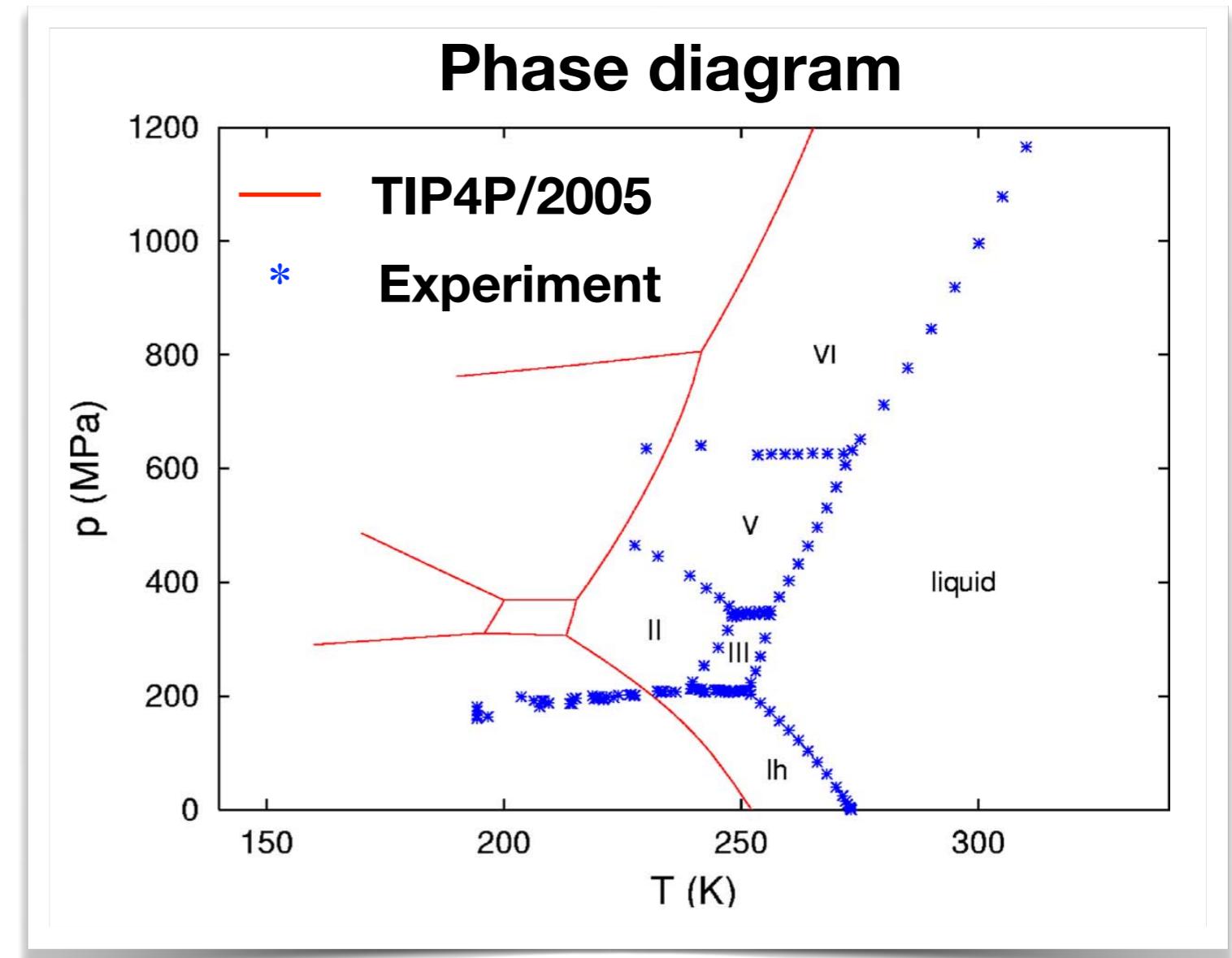
For  $\text{H}_2\text{O}$ , there are lots of effective potentials

Example: TIP4P/2005 (J. L. F. Abascal 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!



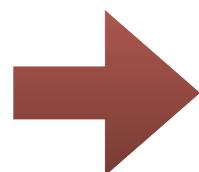
# Classical problems as an approximation: magnetism

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(Electron) spins: “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
- ....

# Example: ferromagnetism

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Iron (Fe): Ferromagnet (強磁性体)

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



The simplest approximation of the ferromagnets:

## Classical Heisenberg model

$$\mathcal{H} = - \sum_{(i,j)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Heisenberg spin:  $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$

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

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

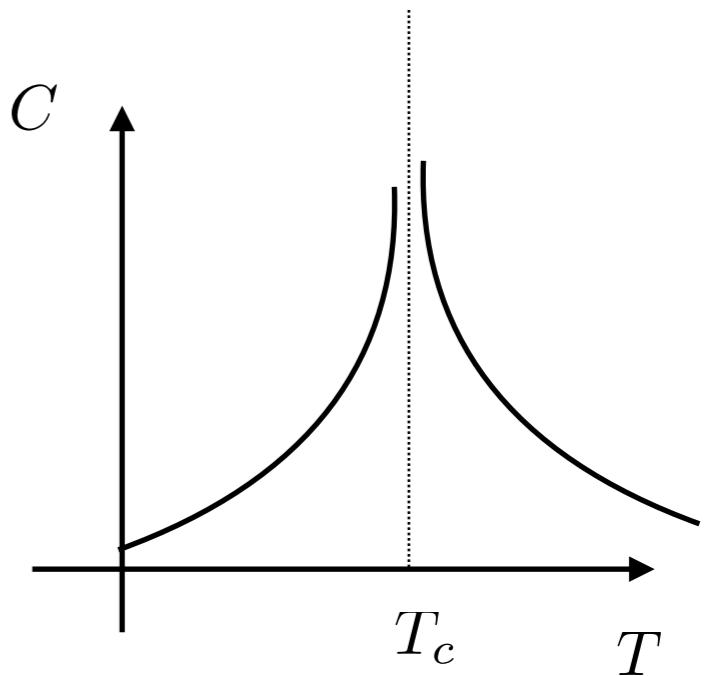
Specific heat :  $C \sim |T - T_c|^{-\alpha}$

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

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

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

= **Critical exponent**



# Pure classical problems: Critical phenomena

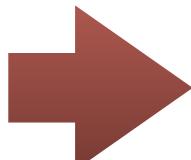
Universality

Critical exponents depend only on  
**symmetries** and **spacial dimensions**.

Ising model: the order parameter has  $Z_2$  symmetry

<i>Ising systems</i>	$\alpha$	$\beta$	$\gamma$	$\nu$	$\eta$
2D-Ising(exact)	0	$1/8=0.125$	$7/4=1.75$	$1/2=0.5$	0
Fe film <sup>a</sup>	N/A	$0.13\pm0.02$	$1.74\pm0.05$	N/A	N/A
3D-Ising <sup>b</sup>	*0.10994	*0.3264	*1.23719	0.63002(10)	0.03627(10)
Dy <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> <sup>c,d</sup>	$0.12\pm0.03$	$0.26\pm0.02$	$1.16\pm0.04$	$0.61\pm0.02$	N/A
LJ(model liquid) <sup>e</sup>	*0.11	0.3285(7)	*1.2	0.63(4)	*0.1
Xe <sup>f</sup>	$0.110\pm0.003$	$0.325\pm0.002$	$1.241\pm0.002$	$0.630\pm0.002$	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

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- Percolation problem
  - Physics of Bingo game
  - Models of infectious diseases, e.g. SIR model, on graphs
- Sphere packing
  - What is the densest packing in a box?
  - Packing structure of poly-disperse systems?
- Stochastic process
  - Dynamics of financial trades
  - Dynamics of population, society, ...

Targets of this lecture (classical part)

# Target of studies: Static or Dynamic

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## Static properties:

Physical properties **independent on time**.

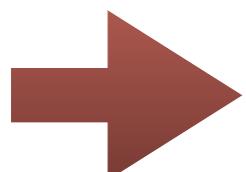
(free) energy, specific heat, (static) susceptibilities, ...

## 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

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Equilibrium system:

Systems are **described by thermodynamics**

Non-Equilibrium system:

Systems are **not** described by thermodynamics

**Steady state (定常状態) :**

Its physical quantities are **independent of time.**

**Non-steady state (非定常状態) :**

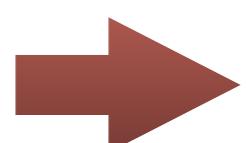
Its physical quantities depend on time.

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

# Target of my lecture

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Steady state of classical system (**not necessarily in equilibrium**)

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

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

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

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

# Examples of classical statistical models

# Statistical mechanical models:

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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).

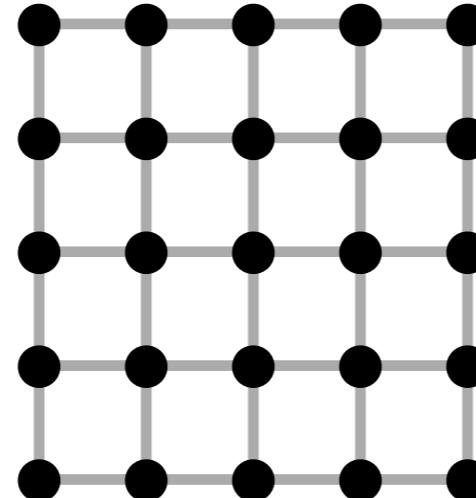
## Lattice

1D



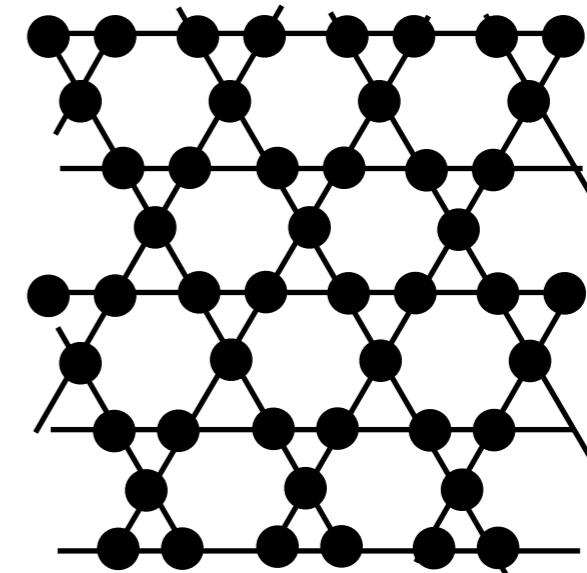
2D

Square lattice



Chain

Kagome lattice



3D

Simple cubic, FCC lattice, BCC lattice, ...

# Classical spin degree of freedom

- Spin:**
1.  $S \rightarrow \infty$  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

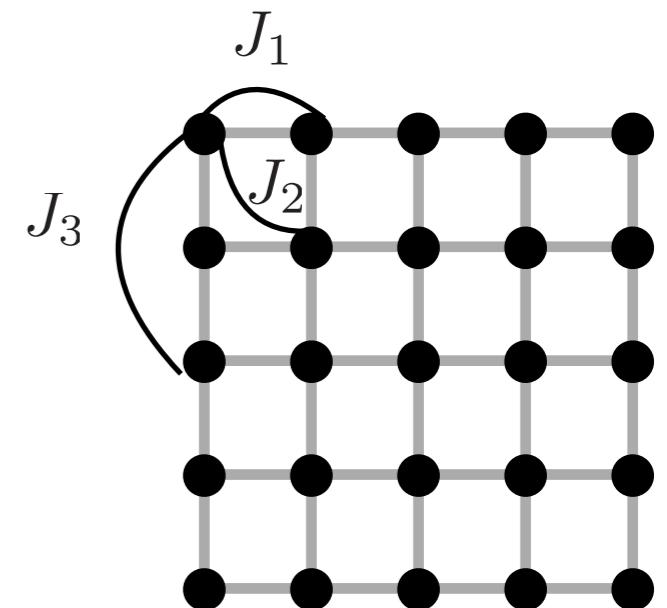
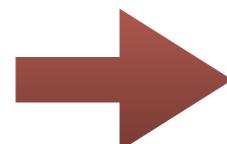
$$D \sum_i (S_i^z)^2 + E \sum_i [(S_i^x)^2 - (S_i^y)^2]$$

$D \rightarrow +\infty$  : XY spins

$D \rightarrow -\infty$  : Ising spins

Dzyaloshinskii-Moriya interaction

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

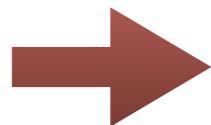


A lot of “novel” magnetism  
appears even in classical  
spin system

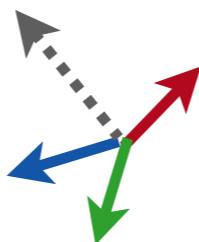
# Topological $Z_2$ vortex

Classical **antiferromagnetic** Heisenberg model  
on triangular lattice

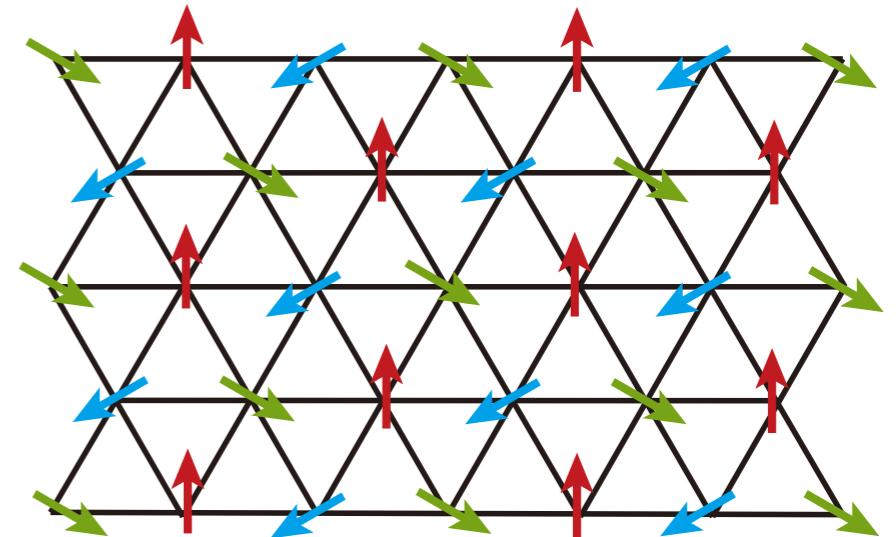
local  $120^\circ$  structure has  **$SO(3)$**  symmetry



Topological excitation  
“ $Z_2$  vortex”



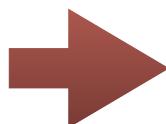
$120^\circ$  structure



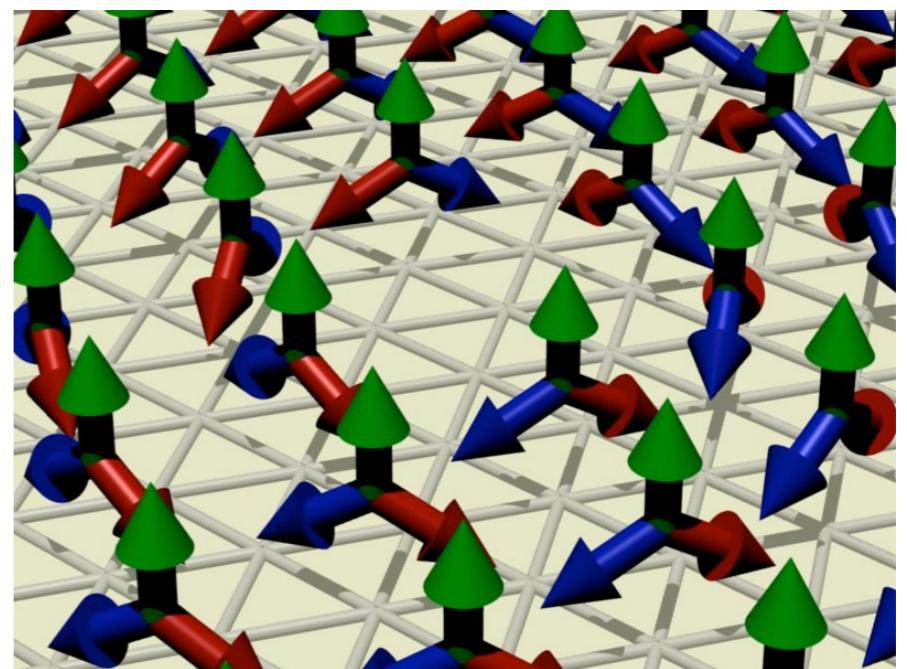
It is characterize by  $Z_2$  value  
“exist” or “not-exist”

Possible phase transition with respect to  
binding-unbinding of  $Z_2$  vortex

H. Kawamura and S. Miyashita (1984)



My research project using  
Monte Carlo simulation using **supercomputer**



# Example: Magnetic skyrmion

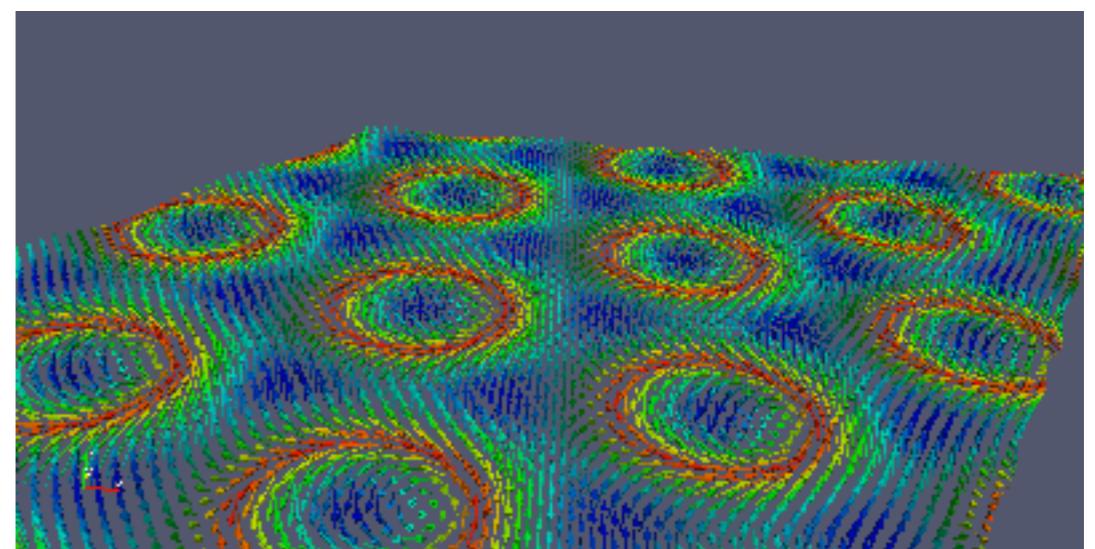
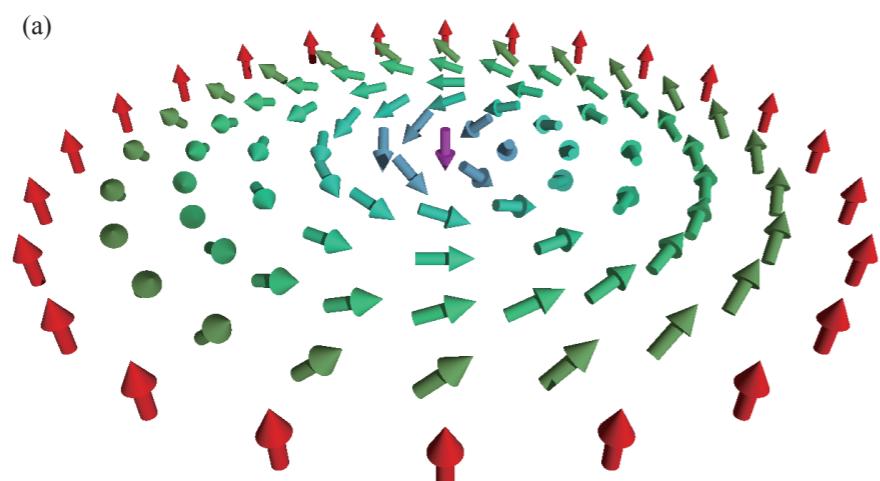
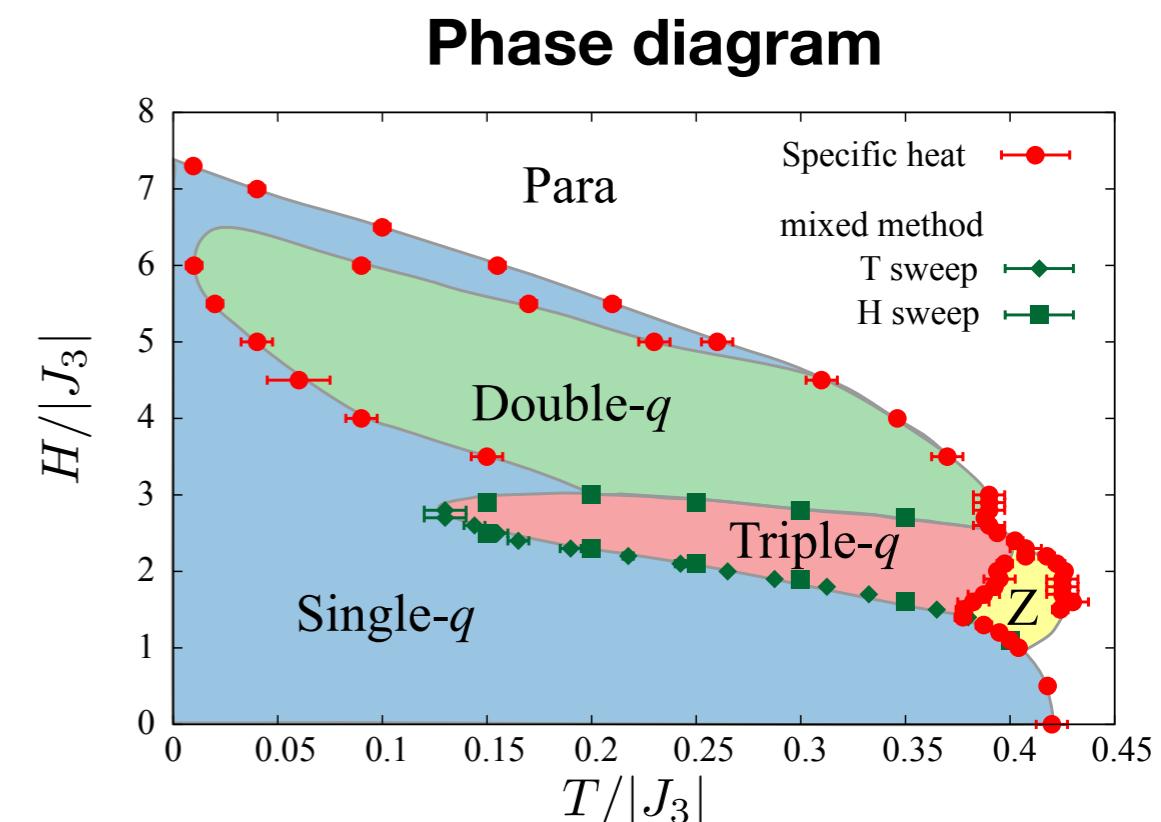
T. Okubo et al Phys. Rev. Lett. **108**, 017206 (2012).

Classical antiferromagnetic Heisenberg model  
on triangular lattice under magnetic fields

By considering  $J_1$  and  $J_2$  (or  $J_3$ ) interaction  
(effective model for  $\text{NiGa}_2\text{S}_4$ )

→ Novel multiple- $q$  states are stabilized  
One of them is identical with  
**“magnetic skyrmion lattice”**

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



# Particle systems

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Particle systems:

Particles moving in continuous space by interacting each other.

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

Two components in Hamiltonian

Interaction potential:  $V(\mathbf{r}_i - \mathbf{r}_j)$

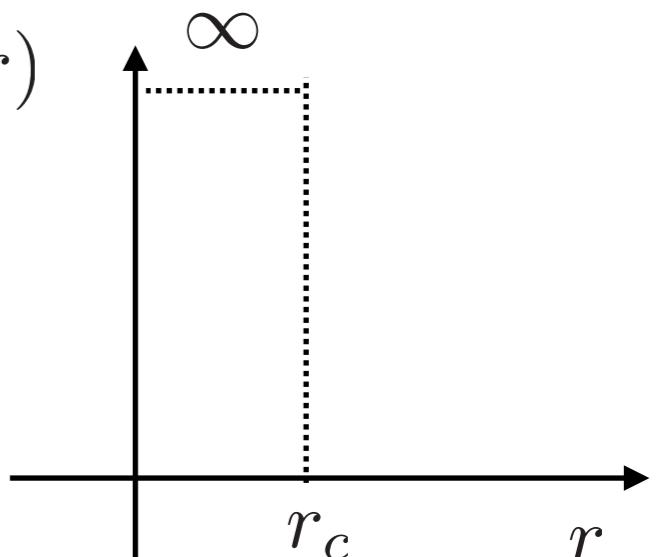
Kinetic Energy:  $\frac{p_i^2}{2m_i}$

Phase space:  $\Gamma = \{\mathbf{r}_i, \mathbf{p}_i\} \rightarrow N\text{-particles} = 2dN \text{ dimension}$

Variety of models: variety of interaction potentials

# Hard sphere

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

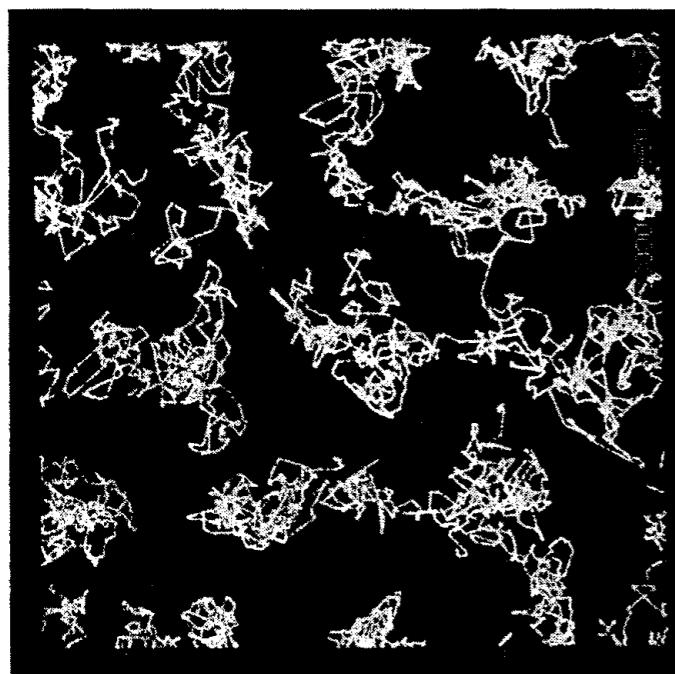


The first application of molecular dynamics

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

- Event driven molecular dynamics simulation

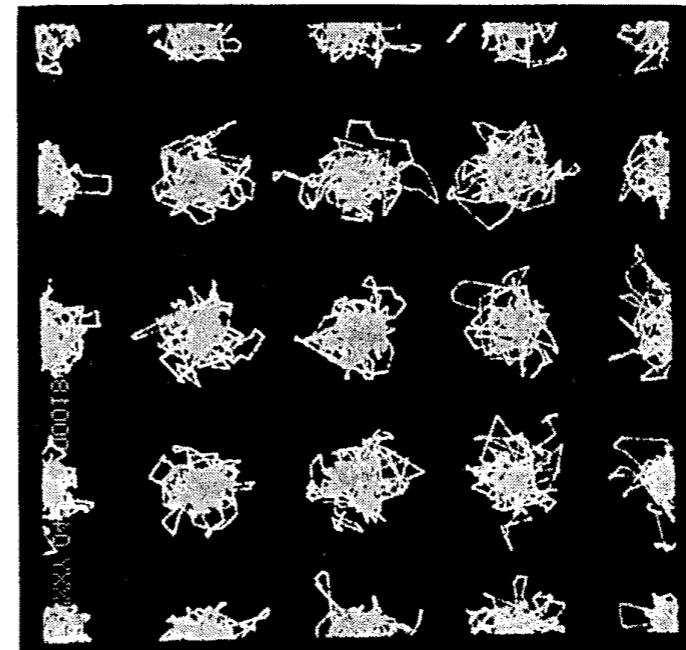
Fluid



Phase transition  
(Alder transition)



Crystal



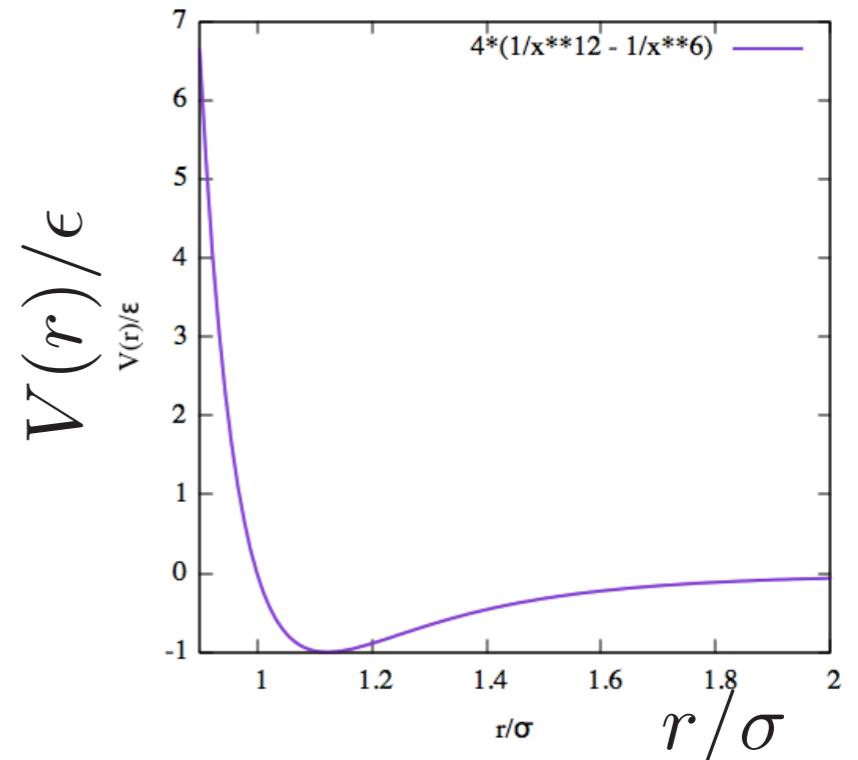
**32 particle system**

# Lennard-Jones potential

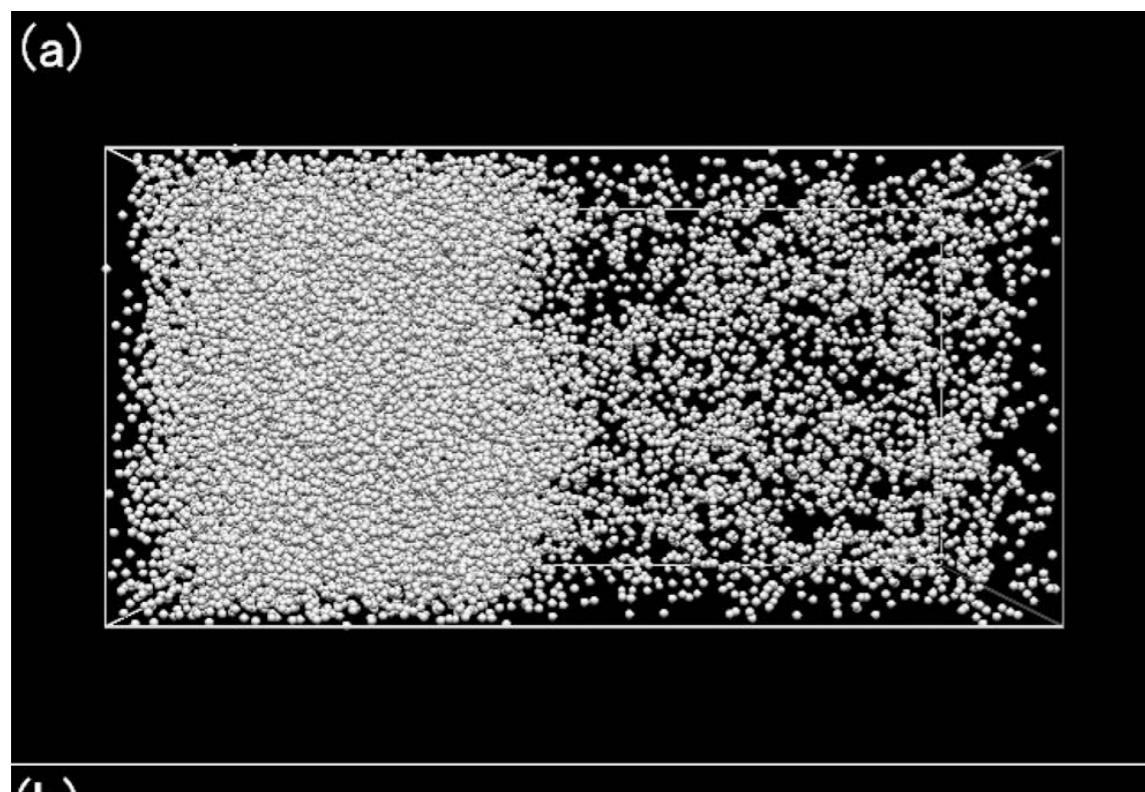
$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

Model potential for noble gas (Ar, ...)

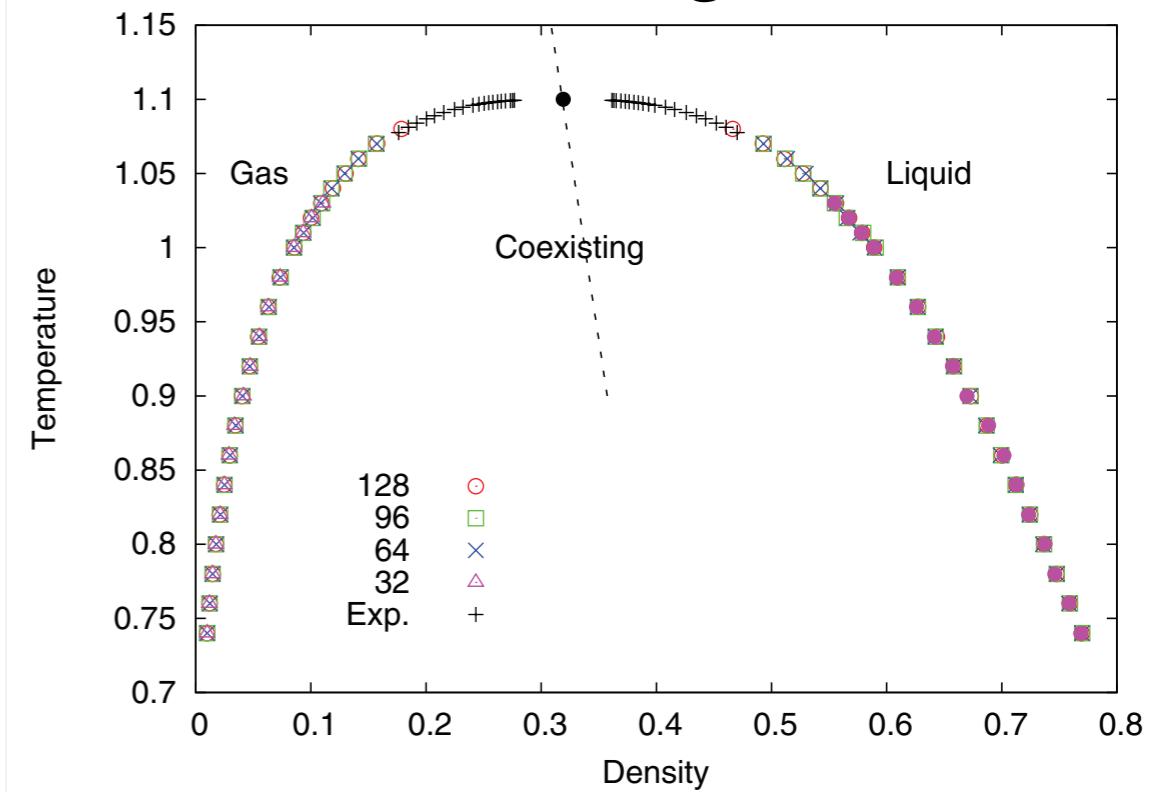
Recent simulation: H. Watanabe et al, J. Chem. Phys. **136**, 204102 (2012).  
(~1,000,000 particles)



## Gas-Liquid coexistence



## Phase diagram

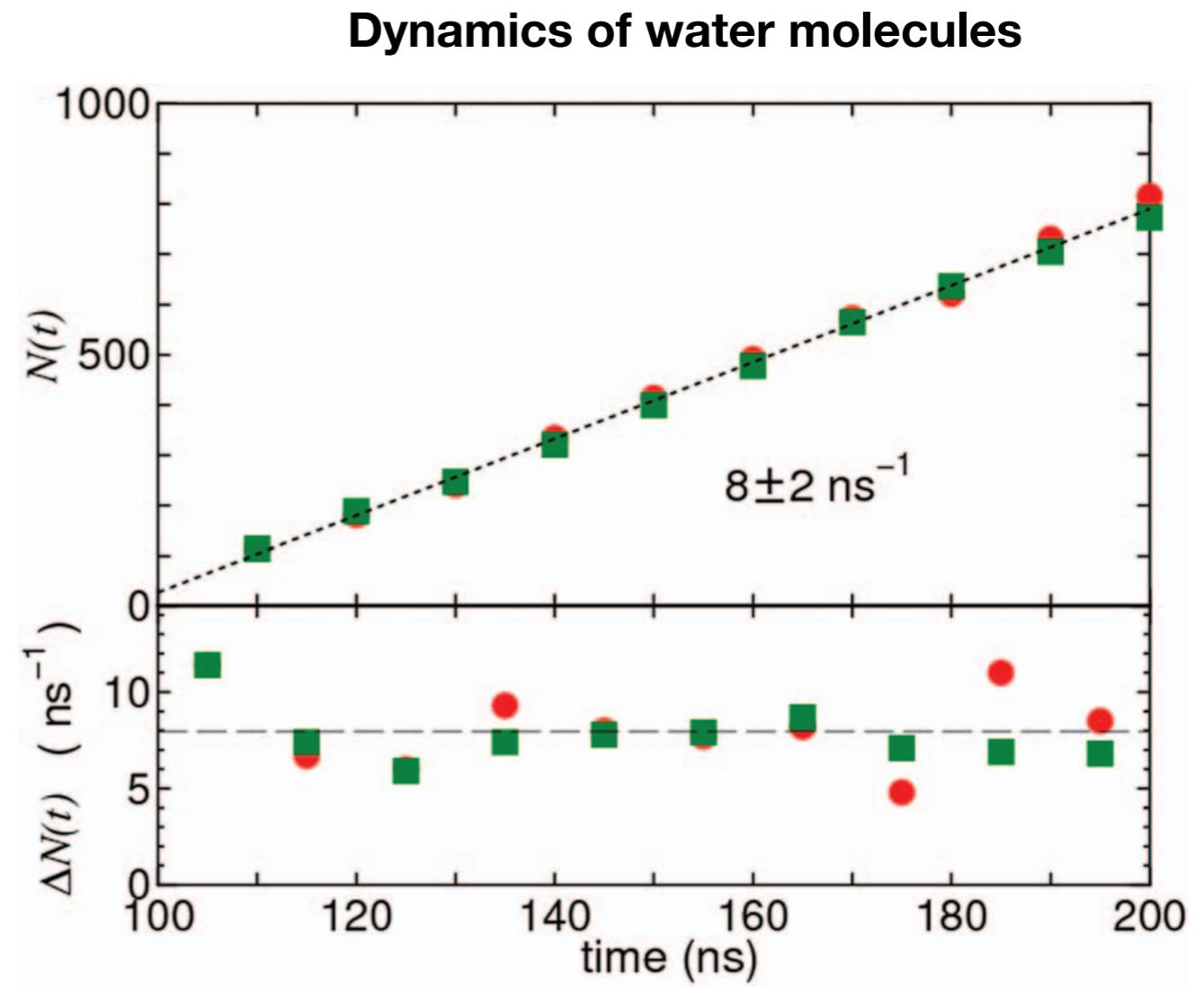
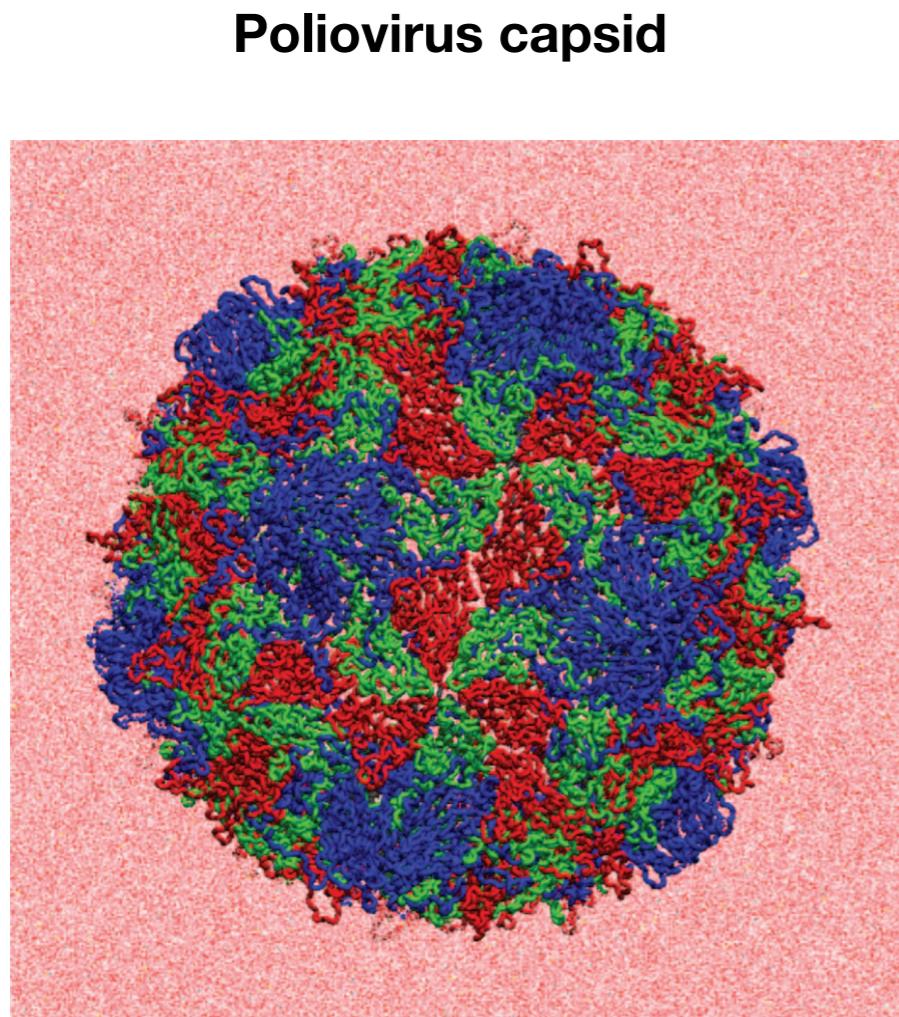


# Complex systems

## Poliovirus capsid in electrolyte solution (電解質溶液)

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

Long-range coulomb interaction

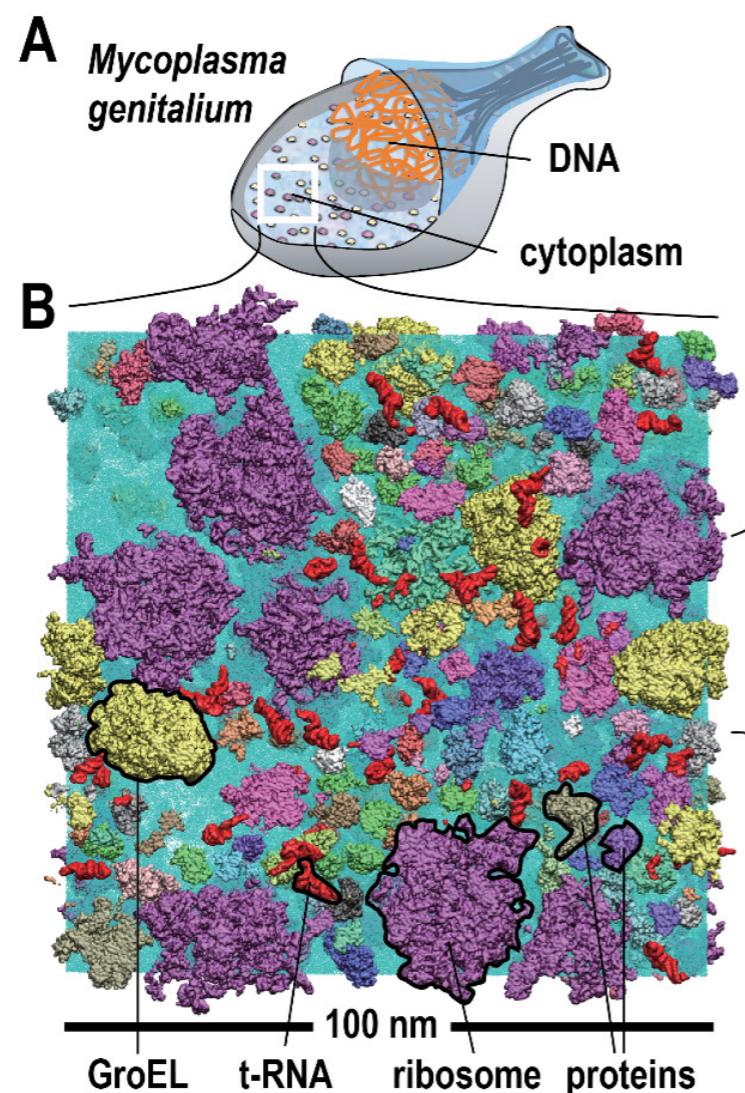


# Complex systems

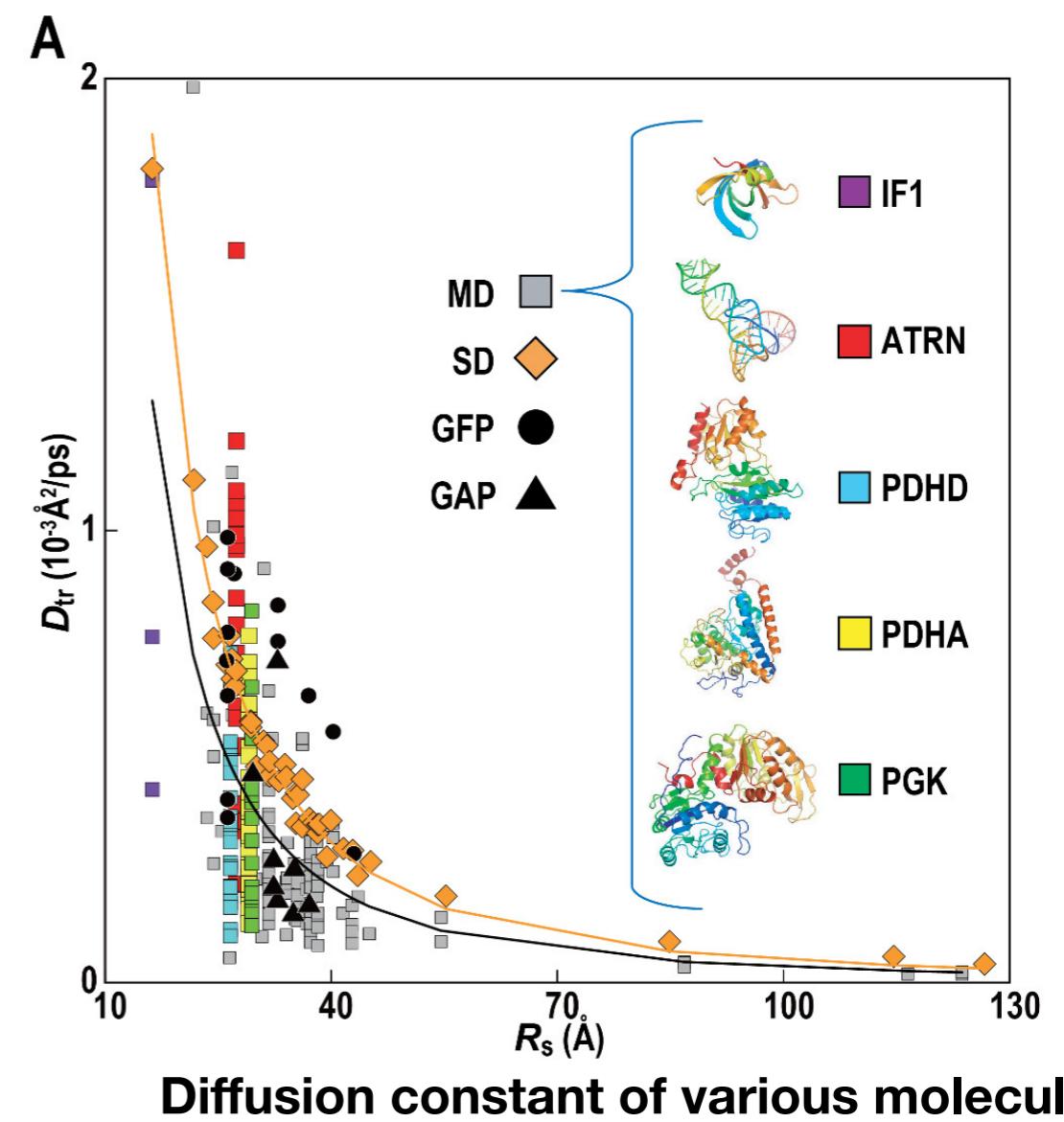
Atomistic model of bacterial cytoplasm (バクテリアの細胞質)

→ **100 million atoms**

I. Yu, et al., *elife* 5, e19274 (2016).



Diffusion constant of various molecules



Computational science for (classical) statistical models

# Statistical mechanics: Ensemble

Statistical mechanics:

Connect microscopic models to macroscopic observable

Example: Ising model

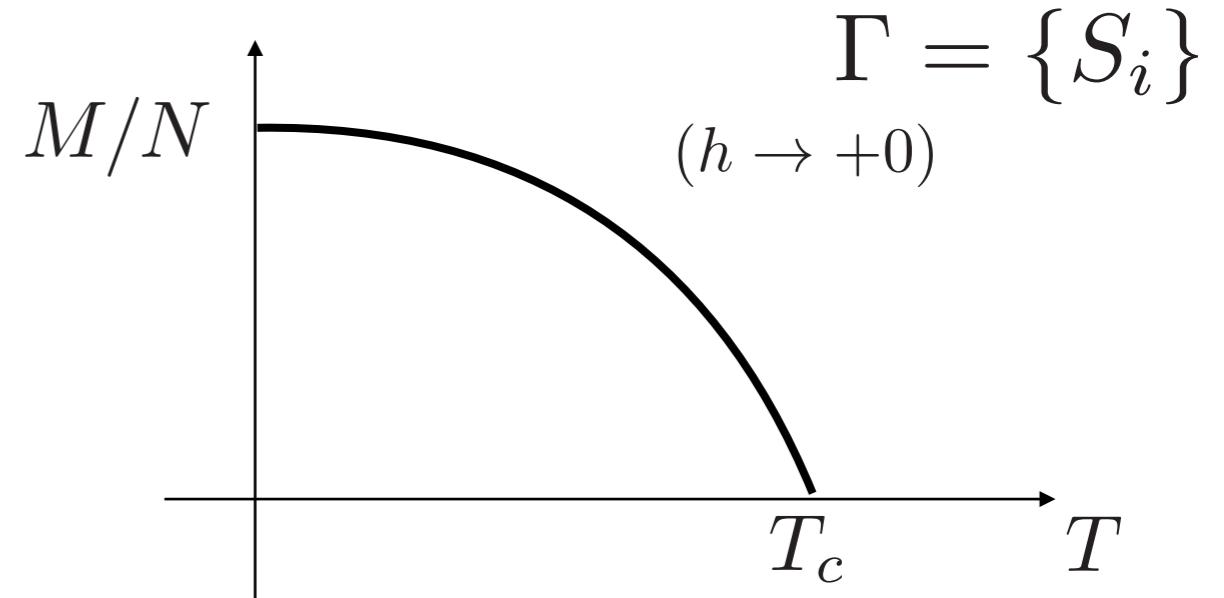
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \quad (S_i = \pm 1 = \uparrow, \downarrow)$$

**Canonical ensemble  
(NVT-ensemble) :**

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

Example: magnetization at  $T$ :

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



# Statistical mechanics: important ensembles

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## **Micro Canonical ensemble (NVE-ensemble) :**

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

## **NPT-ensemble :**

$$P(\Gamma; P, T) \propto \int dV e^{-\beta PV} \sum_{\Gamma(V)} e^{-\beta \mathcal{H}(\Gamma)} \quad \begin{array}{l} P: \text{pressure} \\ V: \text{volume} \end{array} \quad \beta = \frac{1}{k_B T}$$

## **Grand Canonical ensemble ( $\mu$ VT-ensemble) :**

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

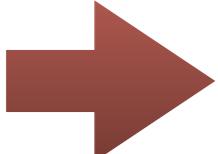
## **General ensemble :**

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

# Computational science for statistical models

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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  
“Information compression in computational science and quantum computings” (A semester)

Long time average

# Long time average for ensemble average

States depending on time

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

## Long time average

$$\begin{aligned}\langle \hat{O} \rangle &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \hat{O}(\Gamma(t)) dt \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=1}^T \hat{O}(\Gamma(t))\end{aligned}$$

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

If we can find a good dynamics which satisfies

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

(Time average coincides with an ensemble average.)

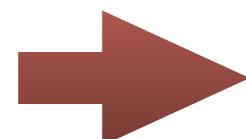
We can calculate **ensemble averages** through **dynamical simulations**.

# Typical dynamics:

- Molecular dynamics:

Dynamics of  $\Gamma$  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**.

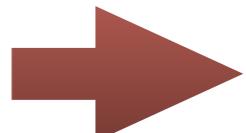
- Markov Chain Monte Carlo:

Dynamics of  $\Gamma$  obeys a stochastic process represented by master equation.

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

$\rho_t(\Gamma)$  :probability distribution

$W_{\Gamma \rightarrow \Gamma'}$  :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

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

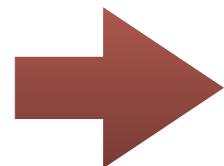
\*Average over initial states

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

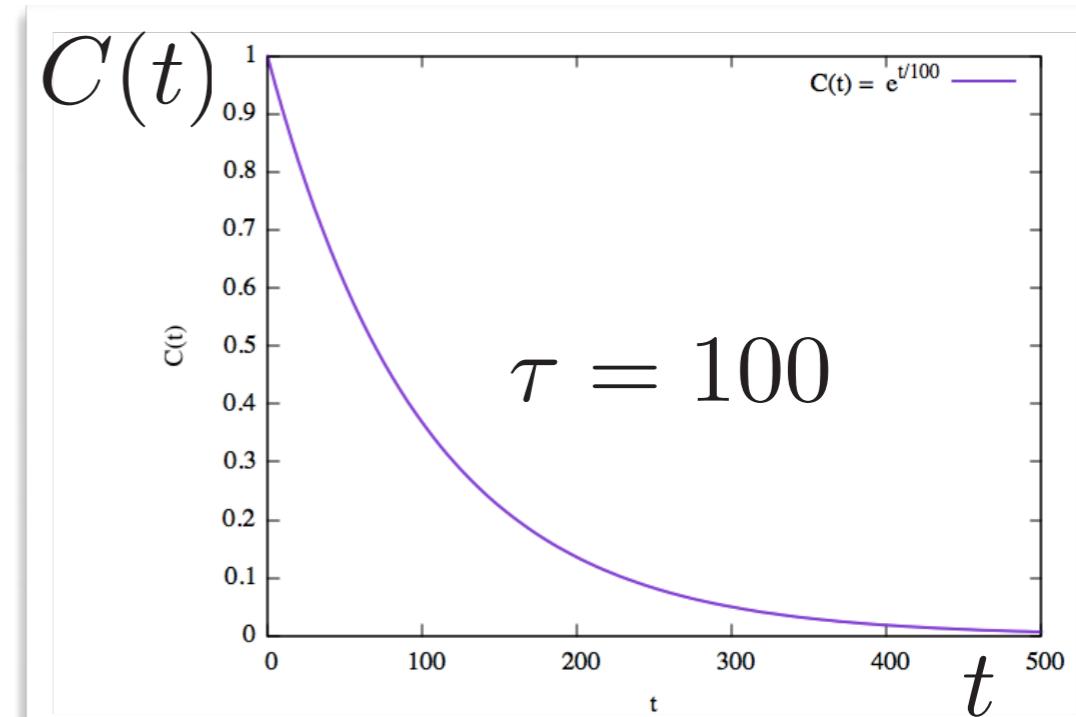
(It is different from the time average.)

Typical asymptotic behavior

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



Relaxation time:  $\tau_A$



# Relaxation time and sampling

Error due to finite number of sampling

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

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

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

$$\begin{aligned}\epsilon^2 &= \left\langle \frac{1}{T^2} \sum_{t_1=1}^T \sum_{t_2=1}^T A_{t_1} A_{t_2} \right\rangle - \left\langle \frac{1}{T} \sum_{t=1}^T A_t \right\rangle^2 \\ &= \frac{1}{T^2} \sum_{t_1=1}^T \sum_{t_2=1}^T C_{AA}(|t_2 - t_1|) \\ &= \frac{1}{T^2} \sum_{\Delta_t=1}^{T-1} 2(T - \Delta_t) C_{AA}(\Delta t) + \frac{C_{AA}(0)}{T}\end{aligned}$$

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

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

$$1 \ll \tau \ll T$$

$$T \xrightarrow{\sim} \frac{1+2\tau}{T} C_{AA}(0) \quad \rightarrow \quad \epsilon \propto \sqrt{\frac{1+2\tau}{T}}$$

In order to reduce the error, we want to reduce  $\tau$ .

# Phenomena with large relaxation time

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- Critical phenomena
  - $\tau \sim (T-T_c)^{-\nu z}$  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  $\exp(a/|T-T_c|)$
  - Exponential can be reduce to polynomial by using **extended ensemble methods**.

# Next week (4/25)

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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