

Computational Science for many-body problems

- This class is from 15:10 to 16:40 (90 min.)
- The recording of the 1st lecture has been uploaded on ITC-LMS.
 - We will also upload the recordings of the following lectures on ITC-LMS

古典統計力学模型と数値計算

Classical Statistical Models and Numerical Simulation

理学系研究科 大久保毅

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Today

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: Quantum lattice models and numerical simulation

8th: Quantum Monte Carlo methods

9th: Applications of quantum Monte Carlo methods

10th: Linear algebra of large and sparse matrices for
quantum many-body problems

11th: Krylov subspace methods and their applications to
quantum many-body problems

12th: Large sparse matrices, and quantum statistical mechanics

13th: Parallelization for many-body problems

Background of the lecturer

大久保 豪 (OKUBO Tsuyoshi)

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Research:

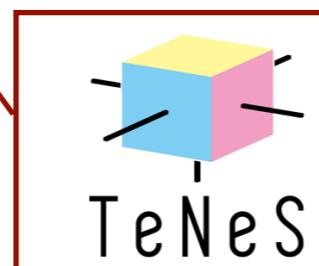
Statistical Physics, Condensed matter physics, Magnetism,
(Computational Physics)

- 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



Massively parallel tensor network solver

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

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?

Q. Which is more difficult, quantum or classical?

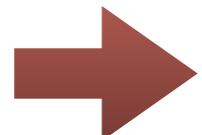
Many-body problems: Quantum or Classical?

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 necessarily based on quantum mechanics

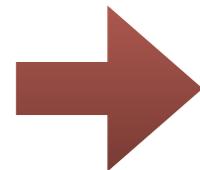
- Percolation, covering, packing, ...
- Stochastic process, dynamical system (力学系) , ..
- Critical phenomena (臨界現象)
- ...

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.

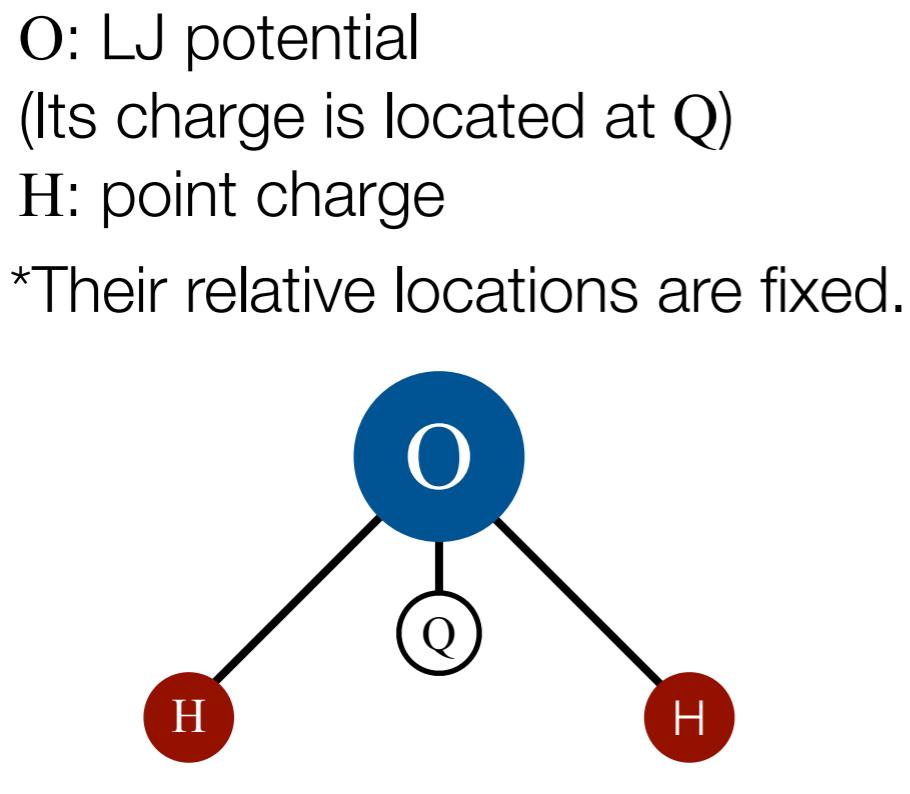
Approximated two-body interactions between classical particles:

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

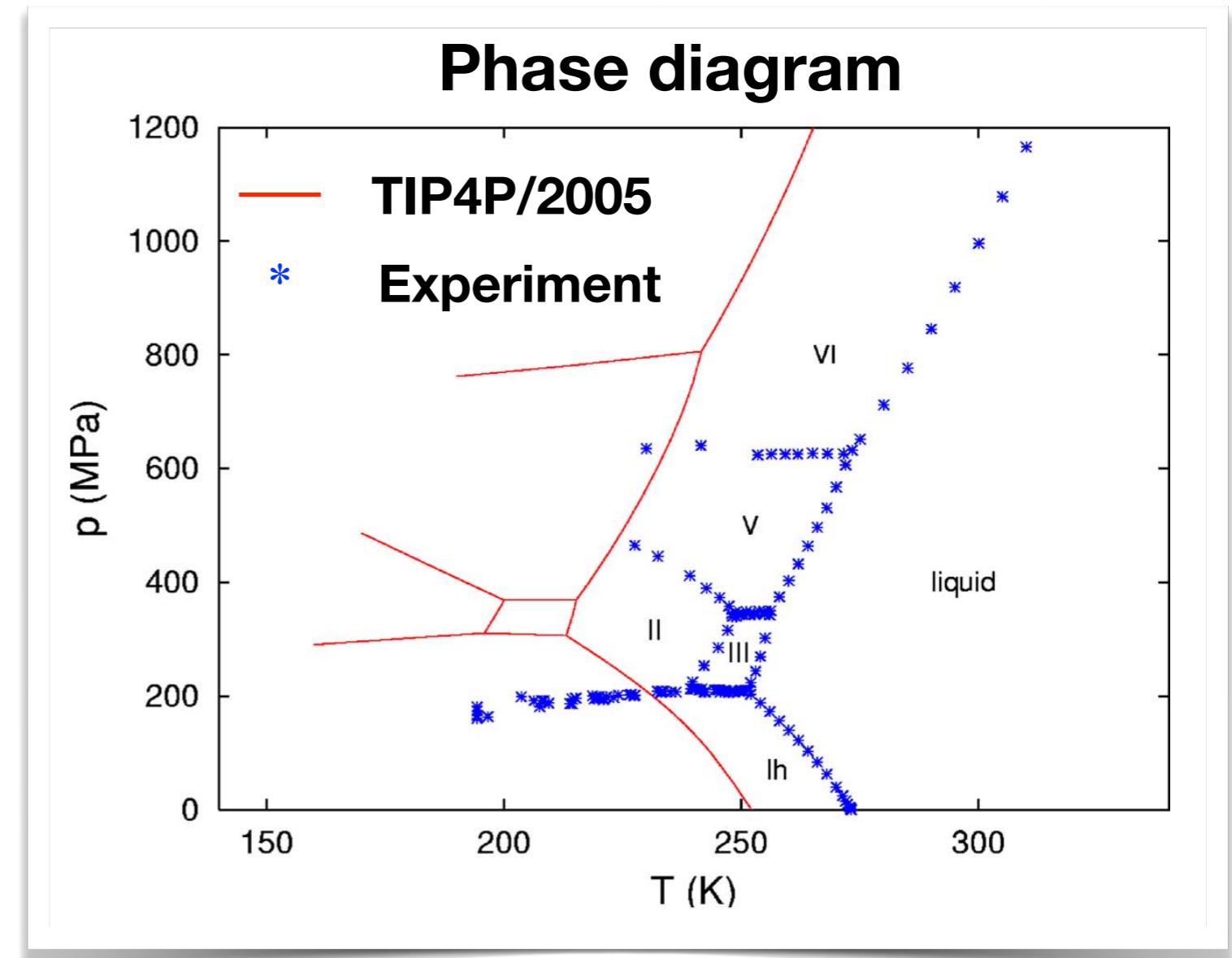
Example: water (H_2O)

For H_2O , there are lots of effective potentials

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



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

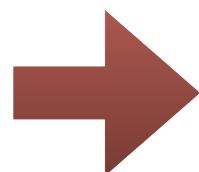


Classical problems as an approximation: magnetism

(Electron) spins: “Quantum” degree of freedom

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

$$S=1/2, 1, 3/2, \dots$$



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

Iron (Fe): Ferromagnet (強磁性体)

Below the Curie temperature $T_c \approx 1043$ 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 $T_c \approx 2.054$ 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 : $\xi \sim |T - T_c|^{-\nu}$

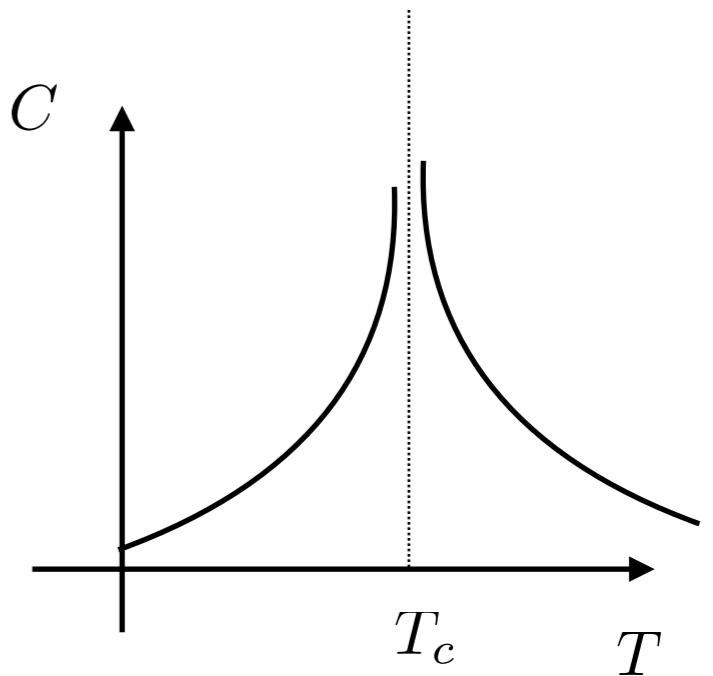
Specific heat : $C \sim |T - T_c|^{-\alpha}$

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

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

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

= **Critical exponent**



Pure classical problems: Critical phenomena

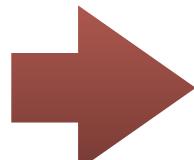
Universality

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

Ising model: the order parameter has Z_2 symmetry

<i>Ising systems</i>	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 ₃ Al ₅ O 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
 - 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

Target of studies: Static or Dynamic

Static properties:

Physical properties **independent on time**.

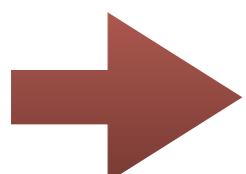
(free) energy, specific heat, (static) susceptibilities, ...

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 (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

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

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).

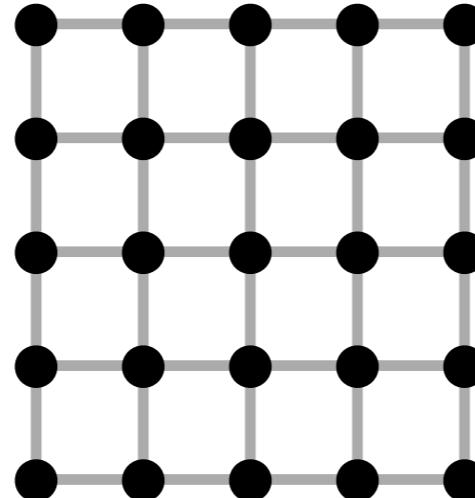
Lattice

1D



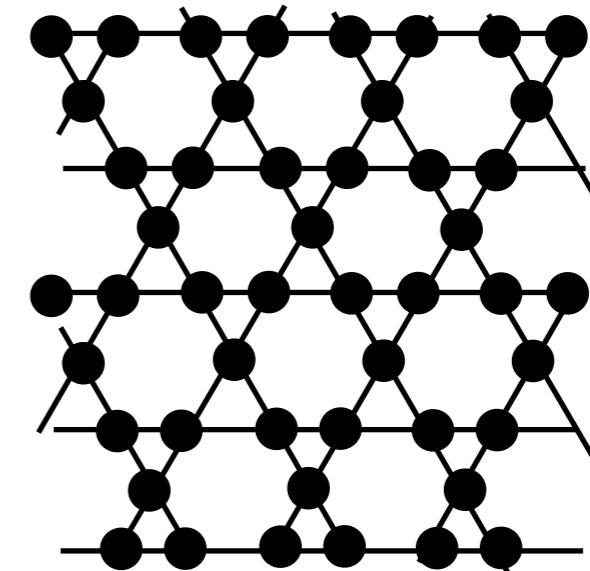
2D

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

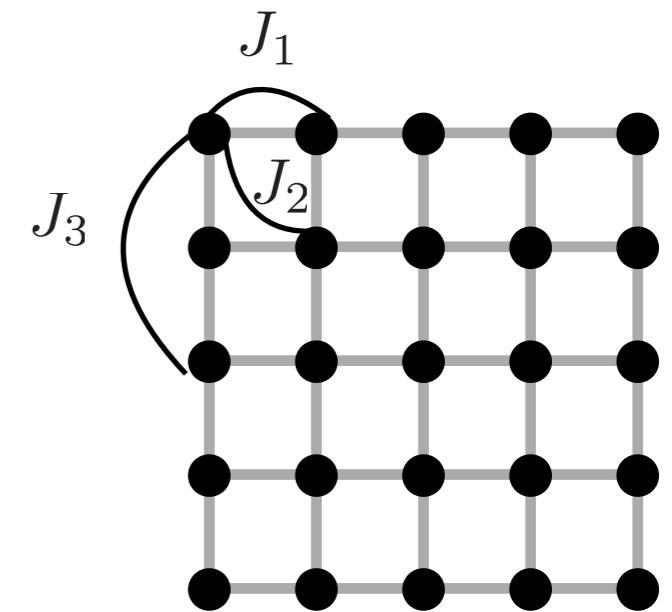
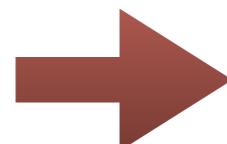
$$D \sum_i (S_i^z)^2 + E \sum_i [(S_i^x)^2 - (S_i^y)^2]$$

$D \rightarrow +\infty$: XY spins

$D \rightarrow -\infty$: Ising spins

Dzyaloshinskii-Moriya interaction

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

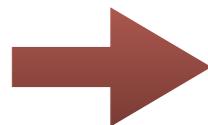


A lot of “novel” magnetism
appears even in classical
spin system

Topological Z_2 vortex

Classical **antiferromagnetic** Heisenberg model
on triangular lattice

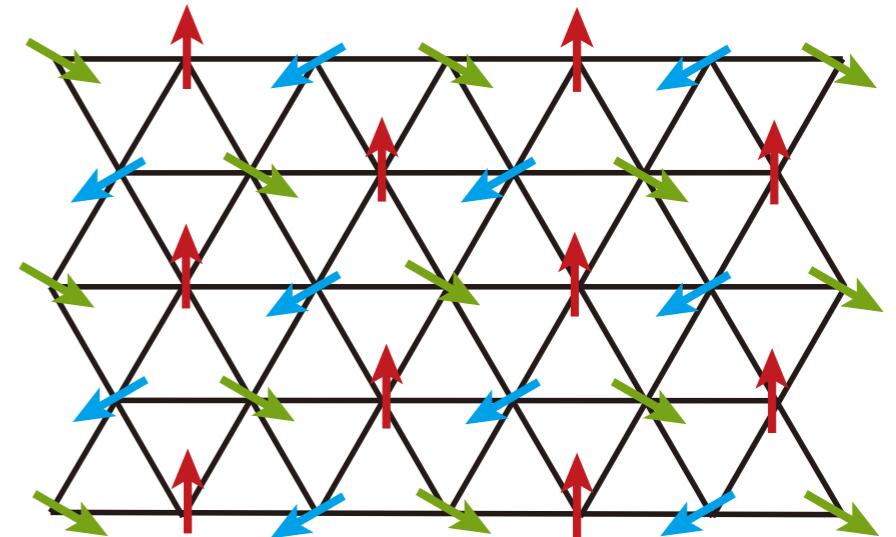
local 120° structure has **$SO(3)$** symmetry



Topological excitation
“ Z_2 vortex”



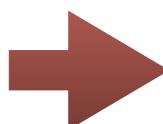
120° structure



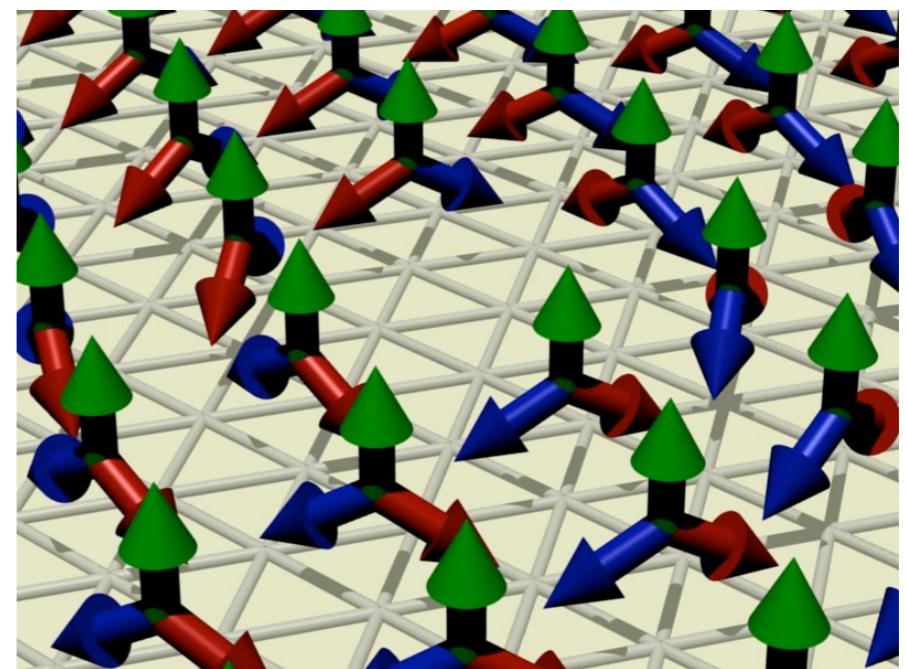
It is characterize by Z_2 value
“exist” or “not-exist”

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

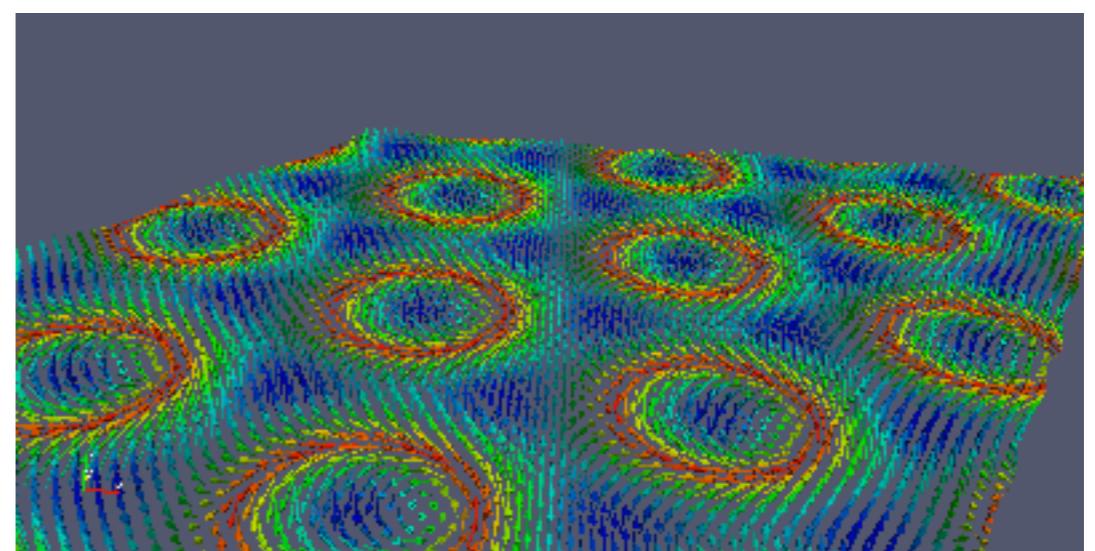
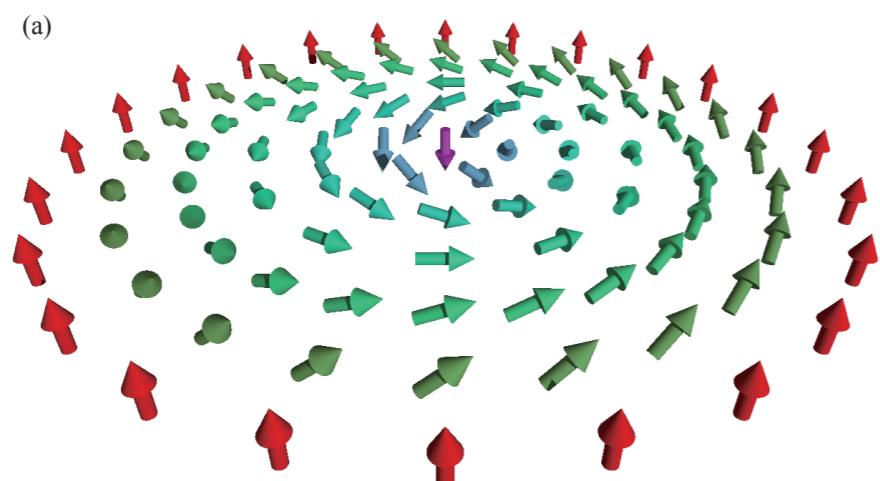
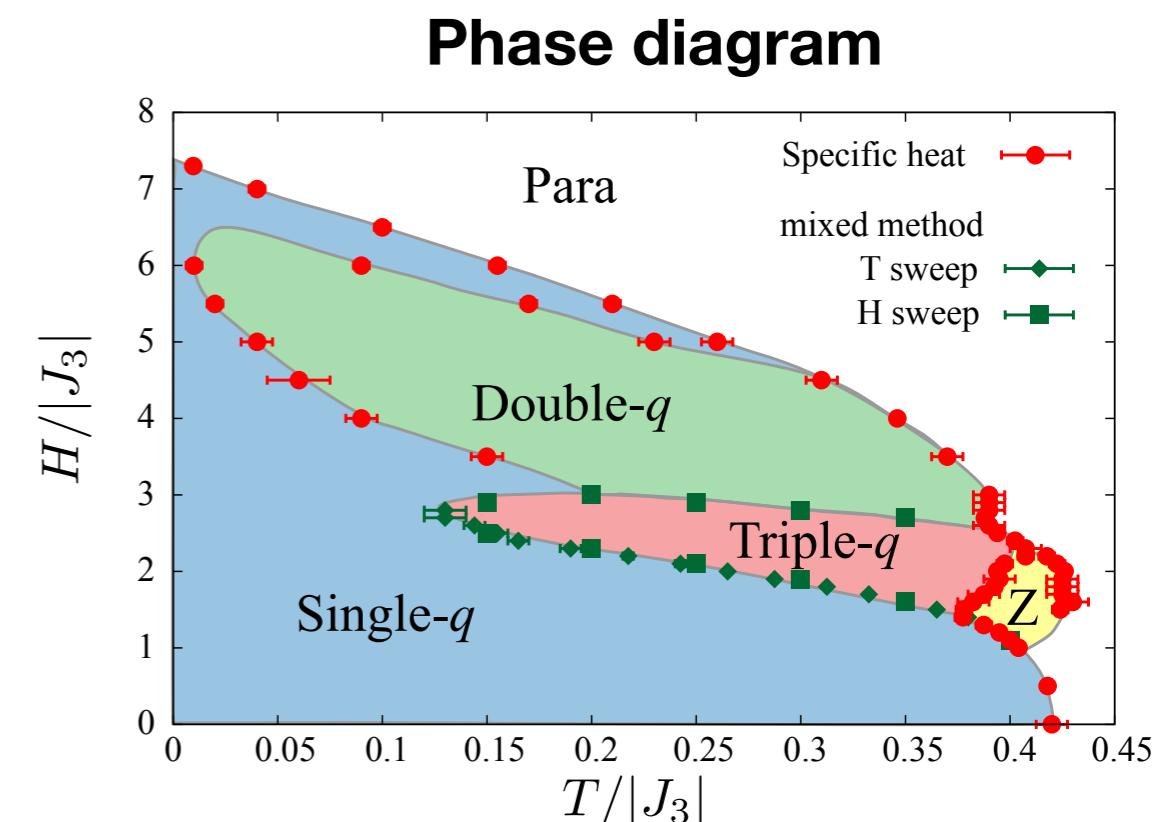
T. Okubo et al Phys. Rev. Lett. **108**, 017206 (2012).

Classical **antiferromagnetic** Heisenberg model
on triangular lattice under magnetic fields

By considering J_1 and J_2 (or J_3) interaction
(effective model for NiGa_2S_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

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

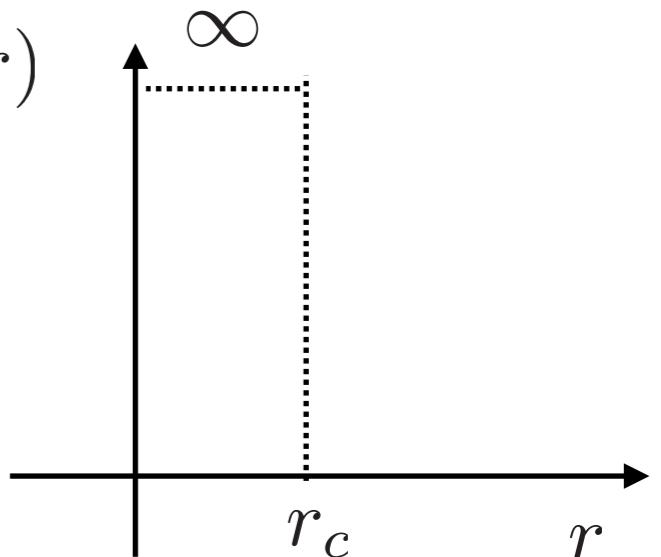
Kinetic Energy: $\frac{p_i^2}{2m_i}$

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

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

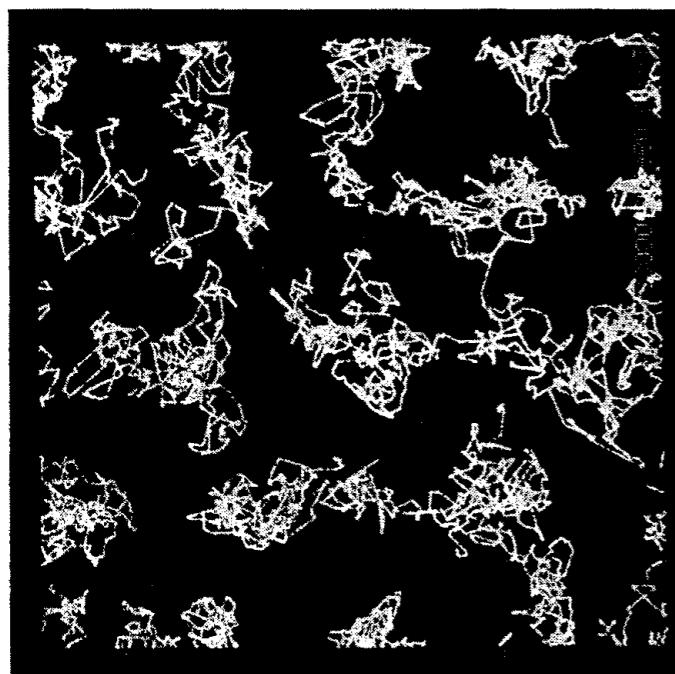


The first application of molecular dynamics

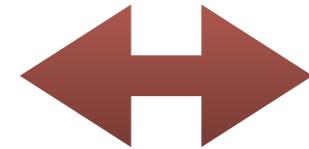
Alder and Wainwright, J. Chem. Phys. **27**, 1208 (1957); **31**, 459 (1959)

- Event driven molecular dynamics simulation

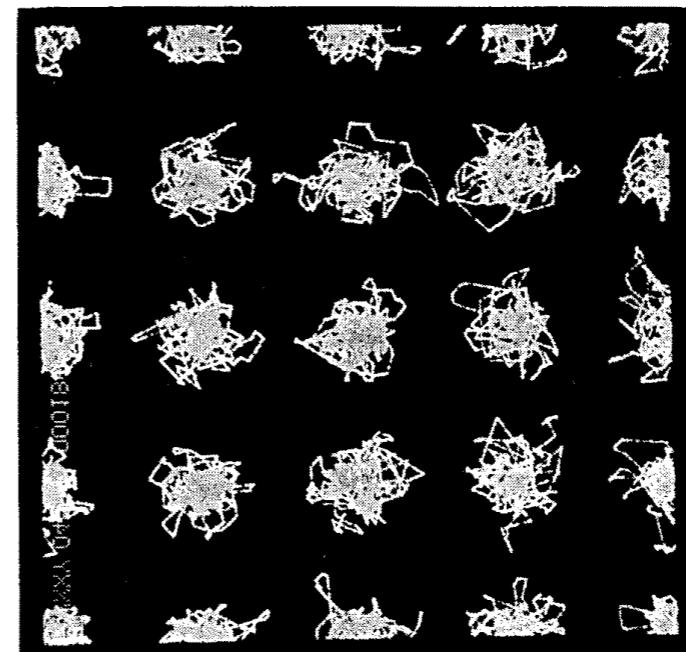
Fluid



Phase transition
(Alder transition)



Crystal



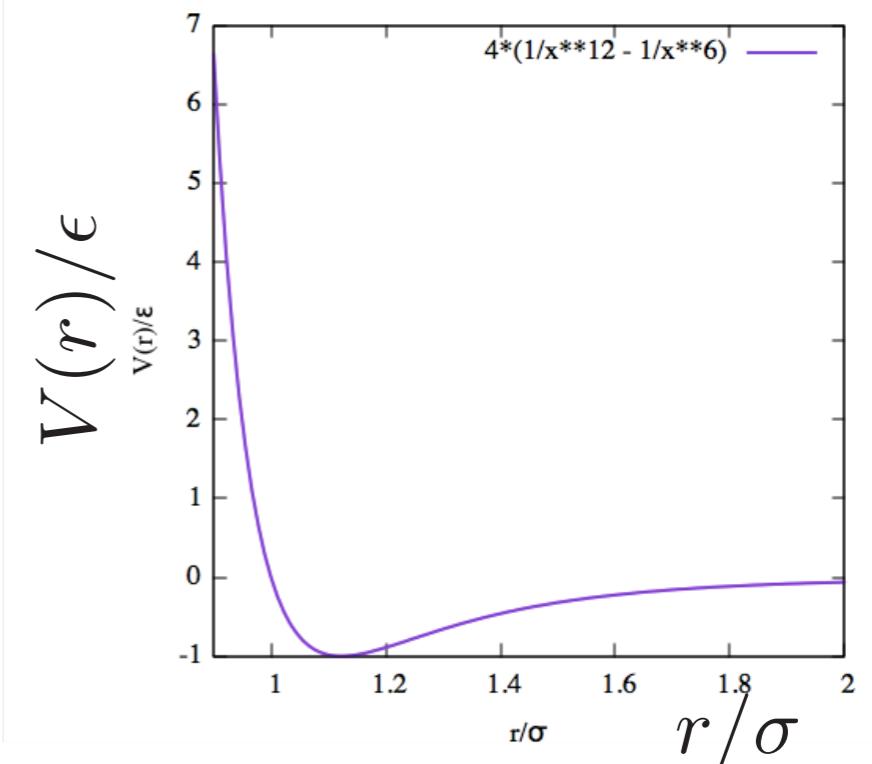
32 particle system

Lennard-Jones potential

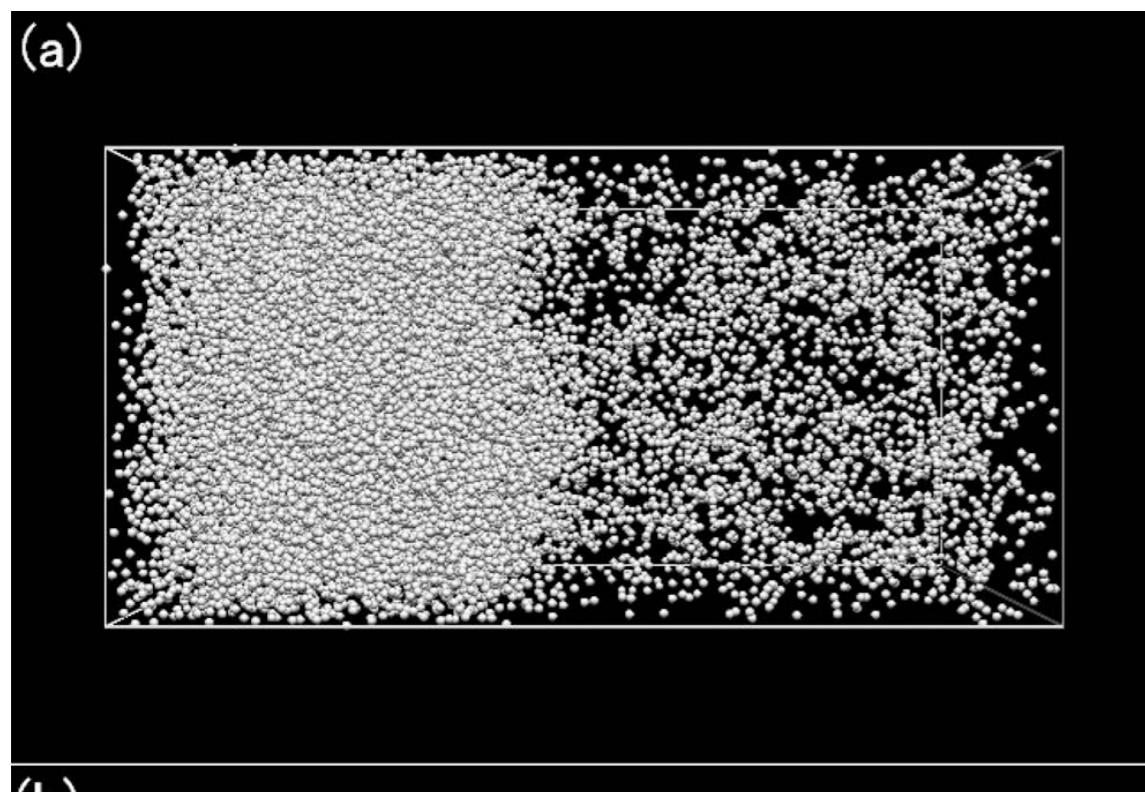
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

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

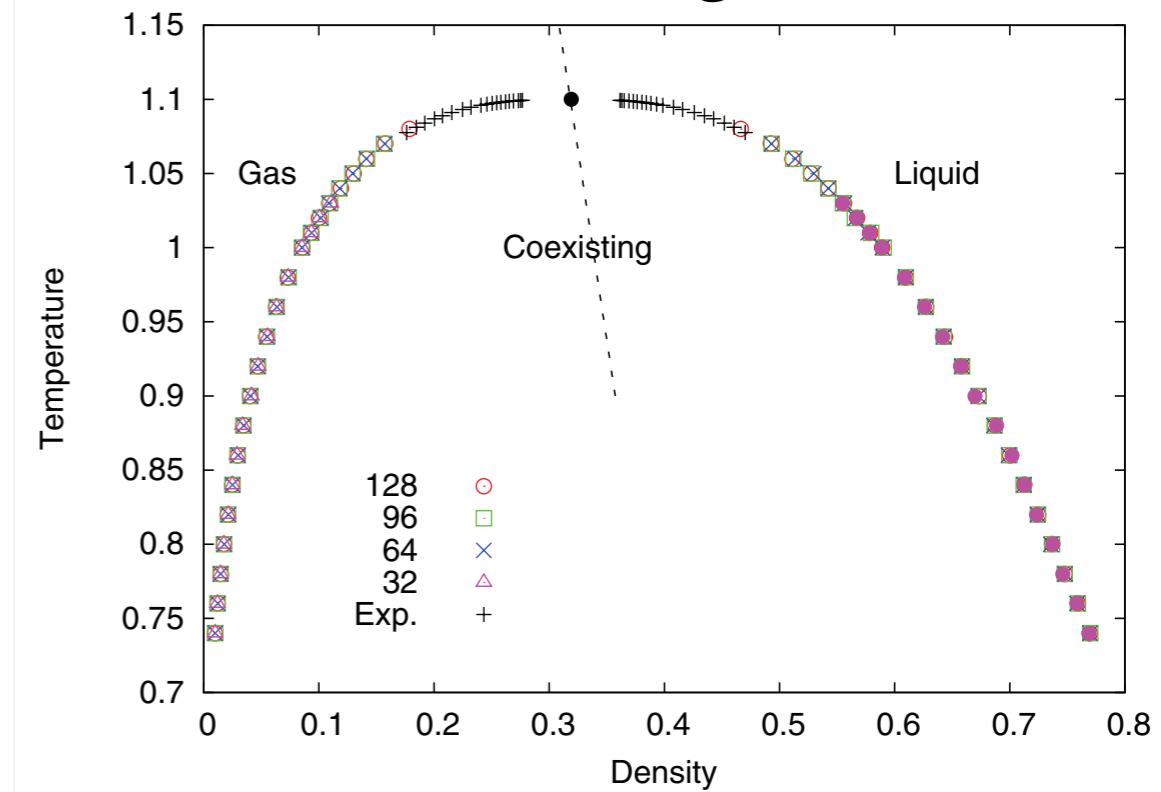
Recent simulation: H. Watanabe et al, J. Chem. Phys. **136**, 204102 (2012).
(~1,000,000 particles)



Gas-Liquid coexistence



Phase diagram

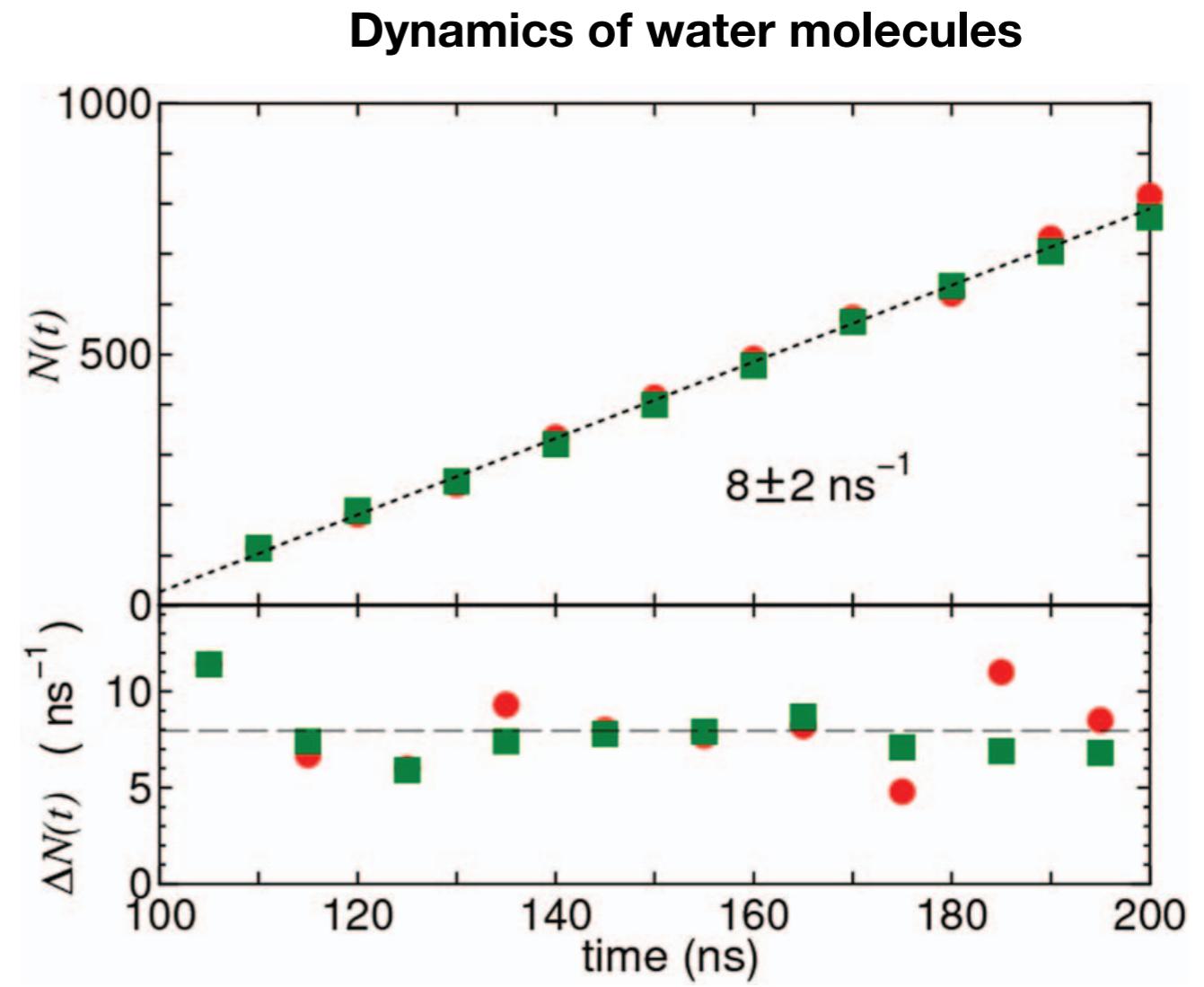
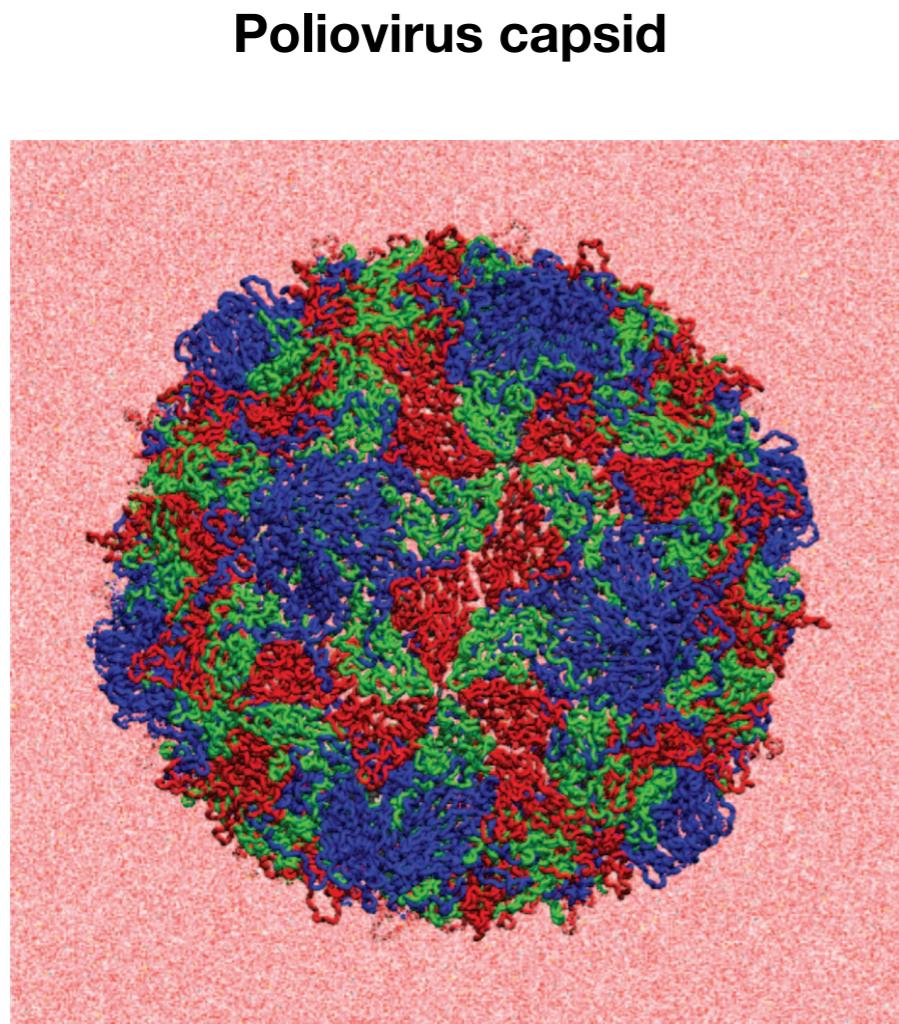


Complex systems

Poliovirus capsid in electrolyte solution (電解質溶液)

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

Long-range coulomb interaction

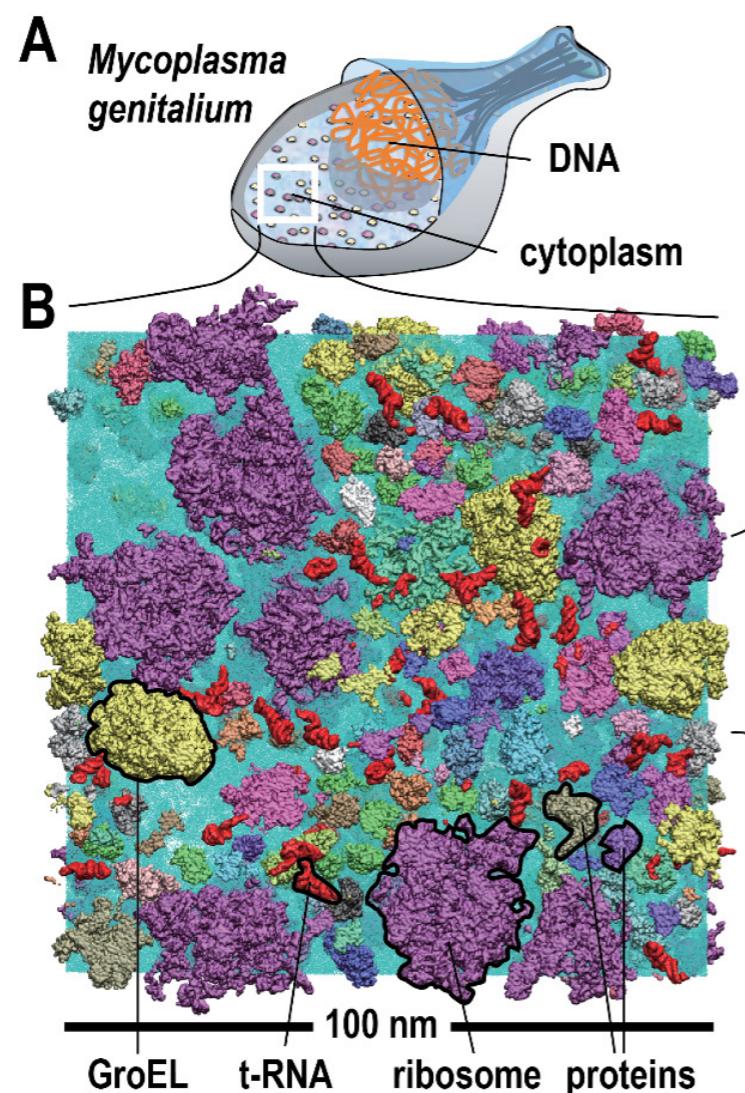


Complex systems

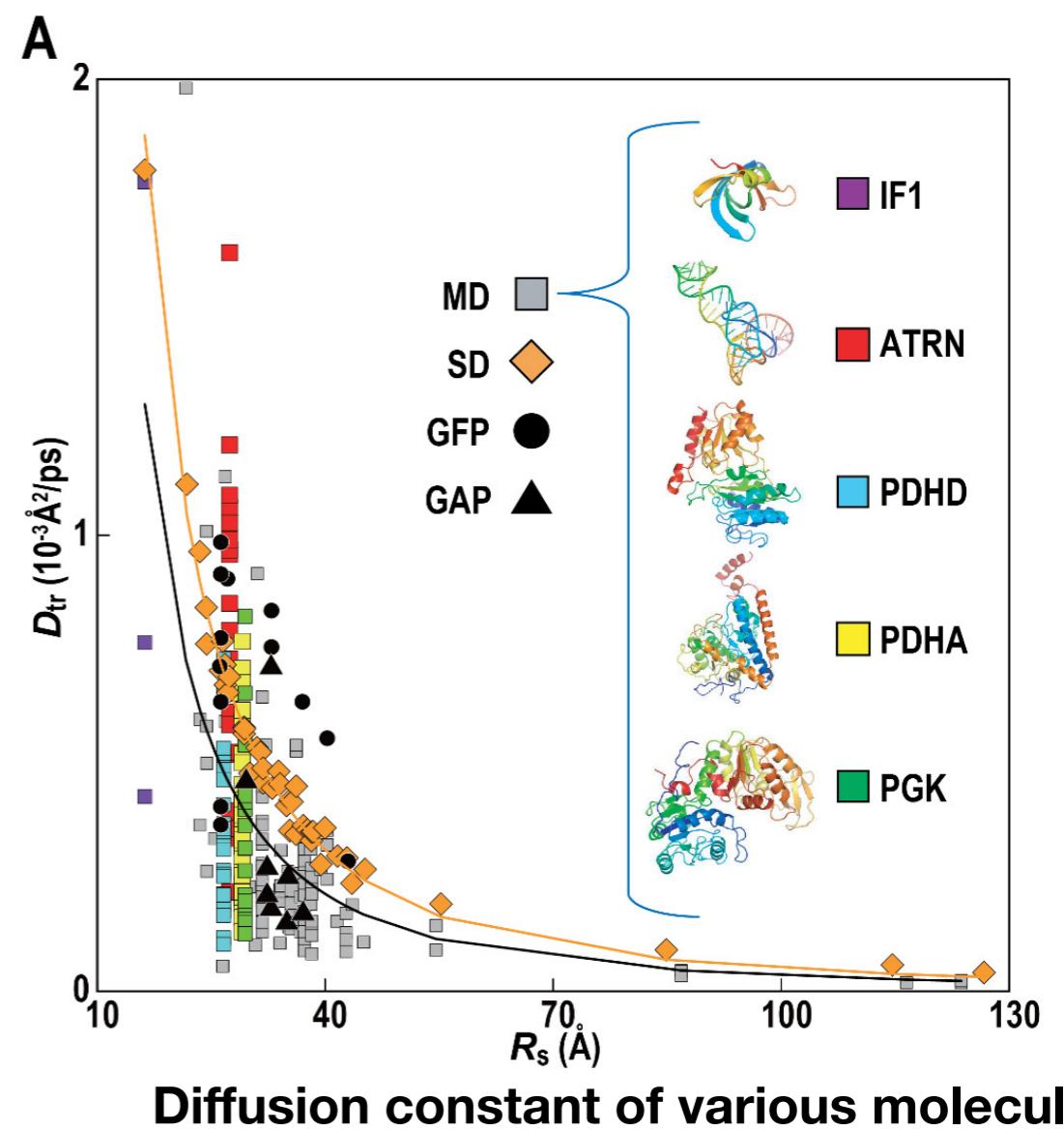
Atomistic model of bacterial cytoplasm (バクテリアの細胞質)

→ **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

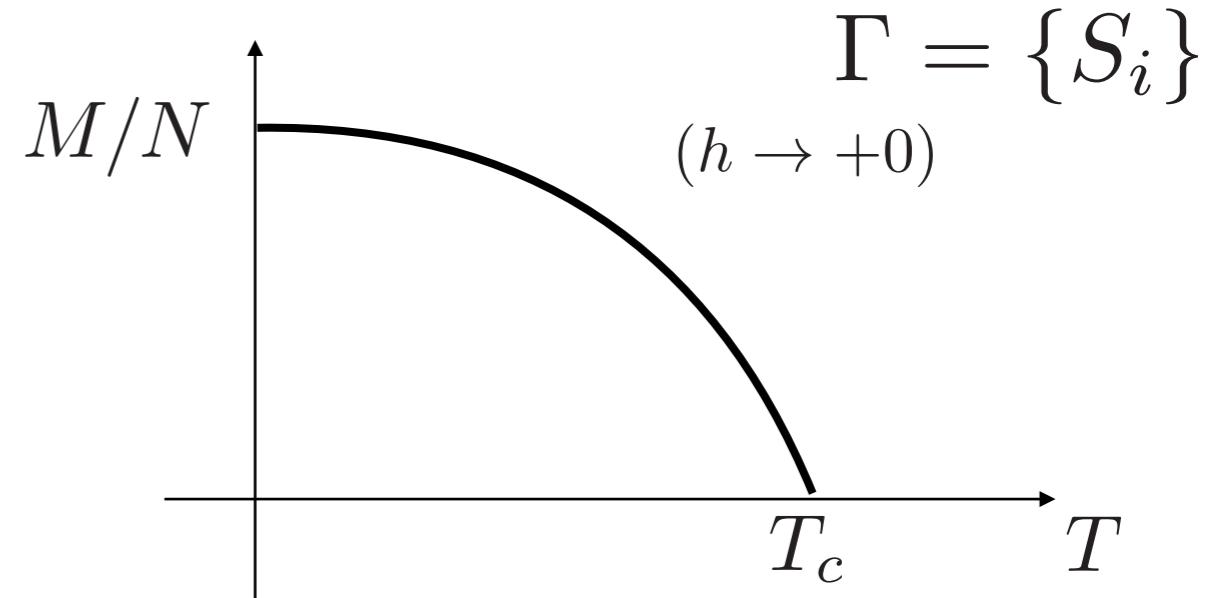
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \quad (S_i = \pm 1 = \uparrow, \downarrow)$$

**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

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 (μ VT-ensemble) :

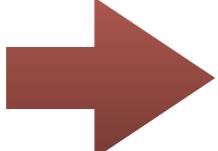
$$P(\Gamma; \mu, T) \propto \sum_N \frac{1}{N!} e^{\beta \mu N} \sum_{\Gamma(N)} e^{-\beta \mathcal{H}(\Gamma)} \quad \mu: \text{chemical potential}$$

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

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 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**.

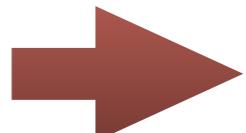
- Markov Chain Monte Carlo:

Dynamics of Γ obeys a 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

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

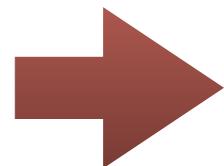
*Average over initial states

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

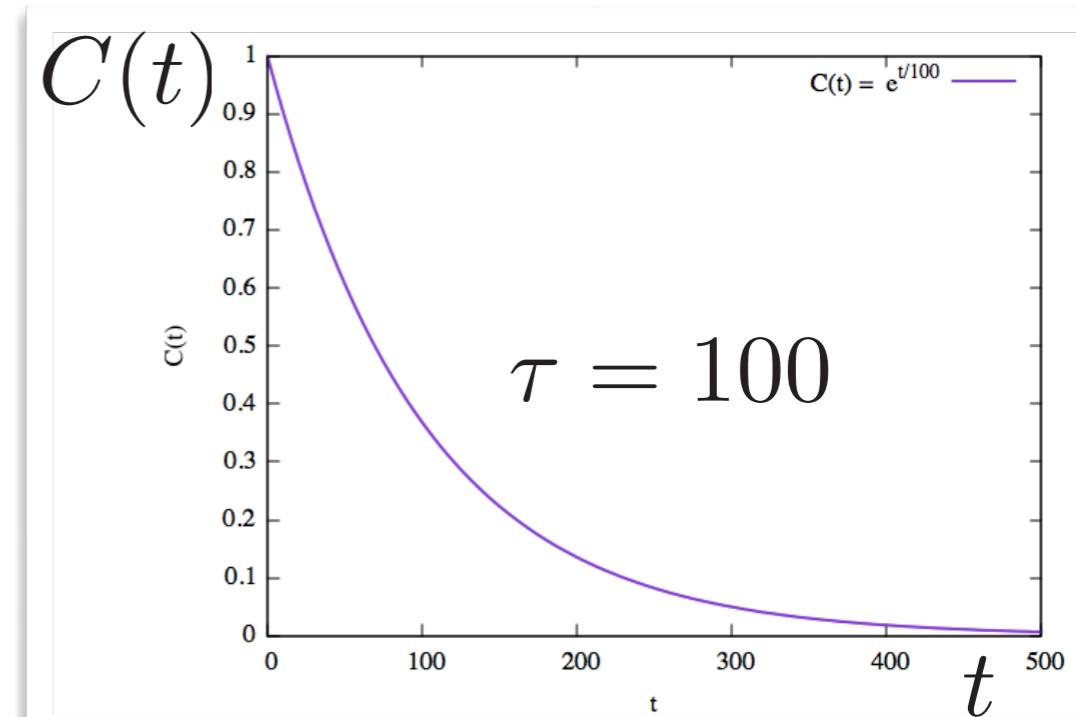
(It is different from the time average.)

Typical asymptotic behavior

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



Relaxation time: τ_A



Relaxation time and sampling

Error due to finite number of sampling

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

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

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

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

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

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

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

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

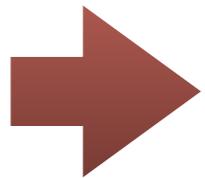
In order to reduce the error, we want to reduce τ .

Phenomena with large relaxation time

- 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**.

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".

Next (4/26)

- 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: Quantum lattice models and numerical simulation
- 8th: Quantum Monte Carlo methods
- 9th: Applications of quantum Monte Carlo methods
- 10th: Linear algebra of large and sparse matrices for quantum many-body problems
- 11th: Krylov subspace methods and their applications to quantum many-body problems
- 12th: Large sparse matrices, and quantum statistical mechanics
- 13th: Parallelization for many-body problems