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 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 computational science and this lecture
- Examples of classical statistical models
- Computational science for (classical) statistical models
  - Statistical ensembles
  - Numerical calculation for ensemble average
    - 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

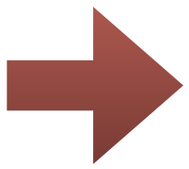
- Percolation, covering, packing, …
- Stochastic process, “dynamical” system, ..
- Critical phenomena
- …

Classical problems as an approximation: molecules

Interaction of molecules:

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

For accurate treatment, we need to consider quantum mechanics



However, we can approximate the system as a set of "classical" point particles

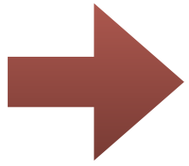
- Lennard-Jones potential for noble gas
- Effective potential for water
- ….

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
- ….

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

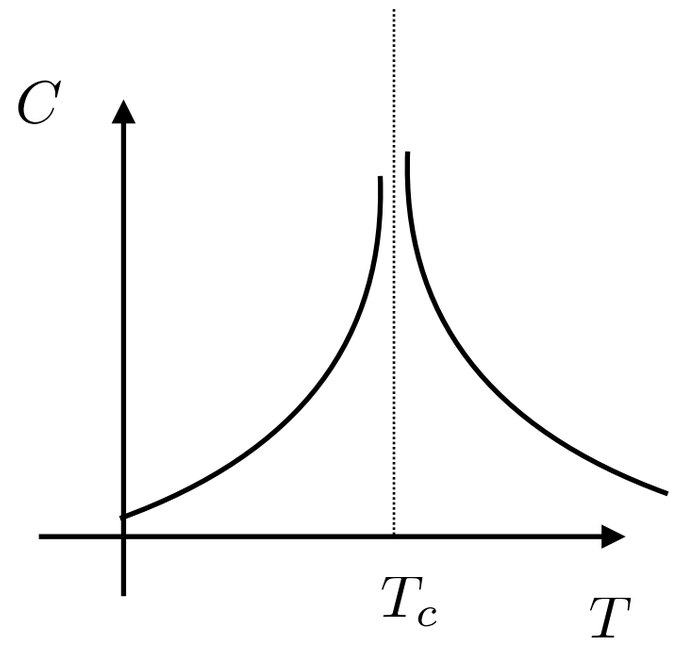
Specific heat : $C \sim |T - T_c|^{-\alpha}$

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 studies: Static or Dynamics

Static properties:

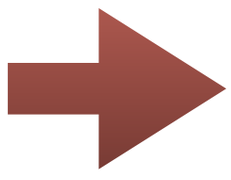
Physical properties independent on time

(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

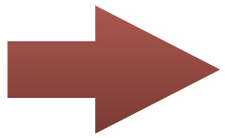
Non-steady state:

Its physical quantities are depends 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 $P(\Gamma)$

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

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

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

- 3rd: Classical statistical models and numerical simulation
- 4th: Classical Monte Carlo method and its applications
- 5th: Molecular dynamics and its applications
- 6th: Extended ensemble method for Monte Carlo methods

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
  - 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, 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 and interact each other

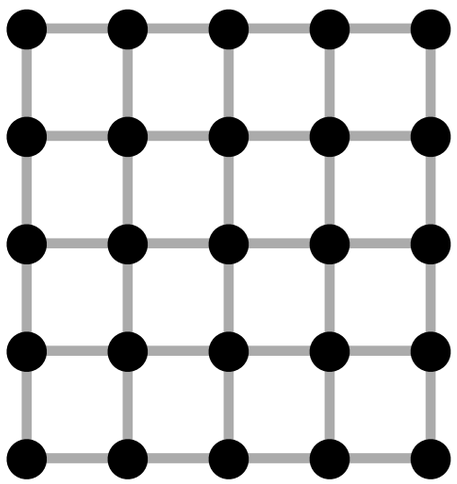
Lattice

1D

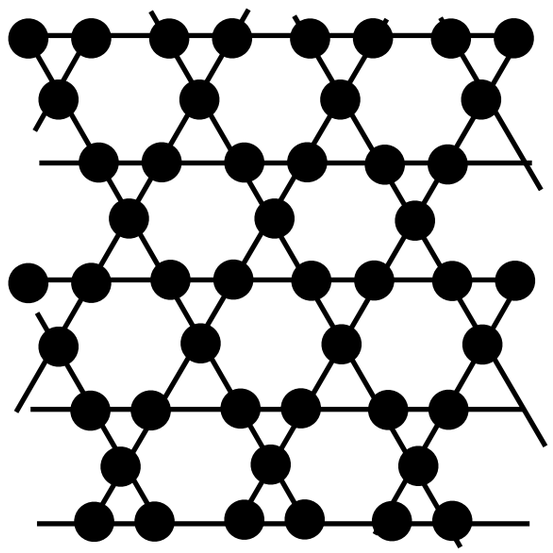
Chain

2D

Square lattice



Kagame lattice



3D simple cubic, FCC lattice, BCC lattice, …

Classical spin degree of freedom

Classical spin:
1. $S \to \infty$ limit of quantum spin
2. simple degree of freedom reflecting symmetry

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

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

A lot of magnetism can be understand through classical Heisenberg spin

2. Ising spin $S_i = \pm 1 = \uparrow, \downarrow$
   - Strong easy axis anisotropy
   - Representing underlying Z_2 symmetry

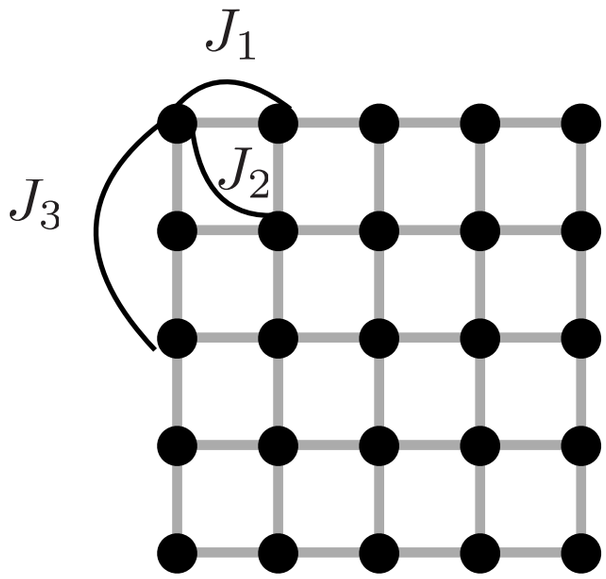
3. XY spin $S_i = (S_i^x, S_i^y)$ Two component unit vector: $(S_i^x)^2 + (S_i^y)^2 = 1$
   - Strong easy plane anisotropy
   - Representing underlying U(1) symmetry

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

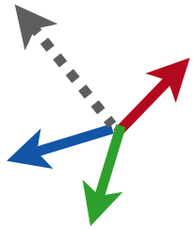
$$\sum_{\langle i,j \rangle} \vec{D} \cdot (S_i \times S_j)$$

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

Topological Z_2 vortex

Classical antiferromagnetic Heisenberg model
on triangular lattice

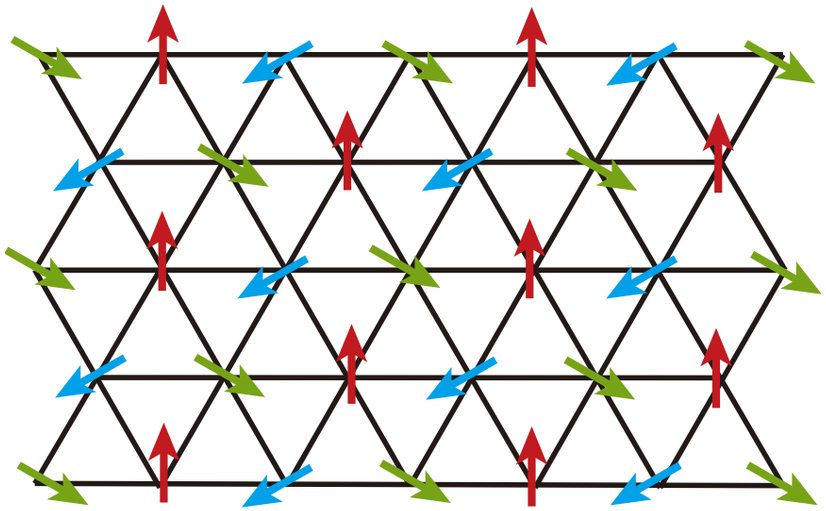
local 120° structure has SO(3) symmetry



Topological excitation

"Z_2 vortex"

120° structure

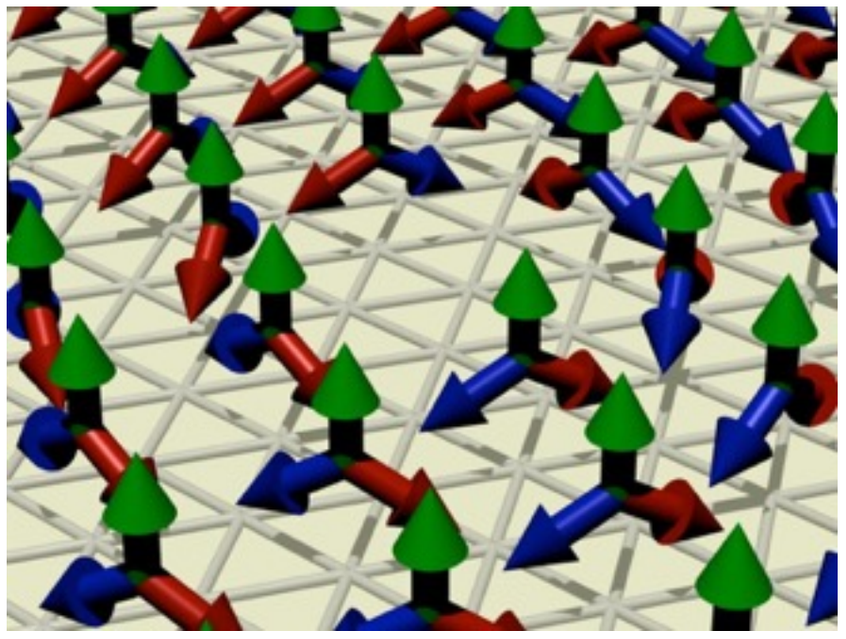


It is characterize by Z_2 value
"exist" or "not-exist"

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

H. Kawamura and S. Miyashita (1984)

My search project using
Monte Carlo simulation using K-computer



Magnetic skyrmion

Classical antiferromagnetic Heisenberg model on triangular lattice under magnetic fields

By considering J_1 and J_2 (or J_3) interaction

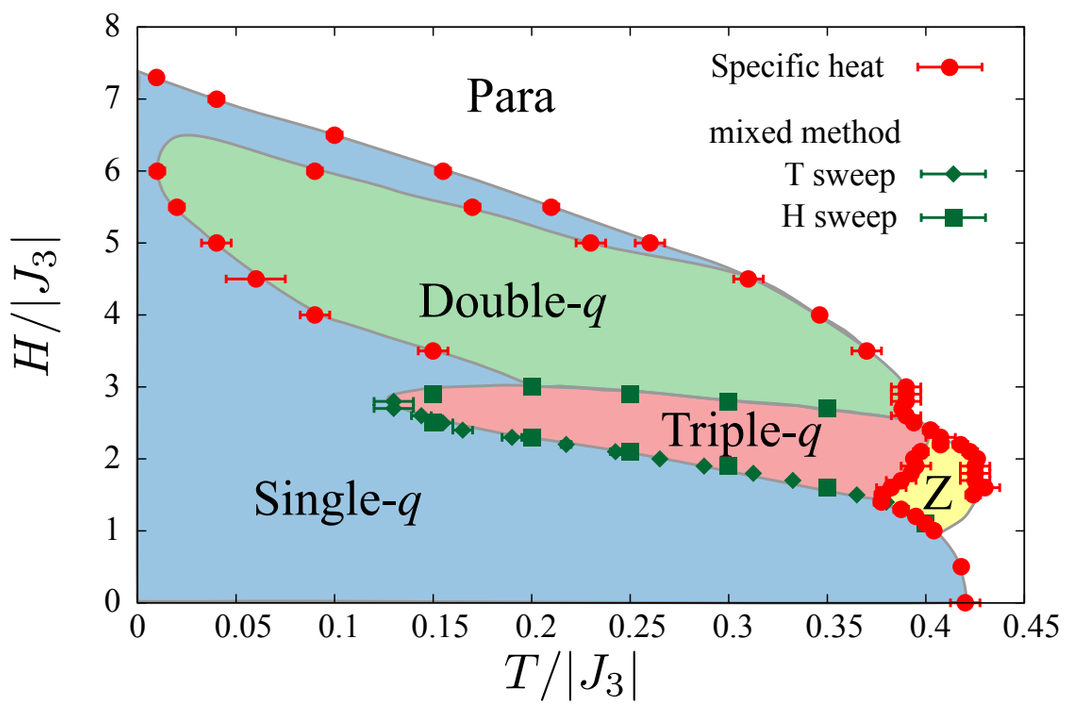
(effective model for $NiGa_2S_4$)

→ Novel multiple-q states are stabilized

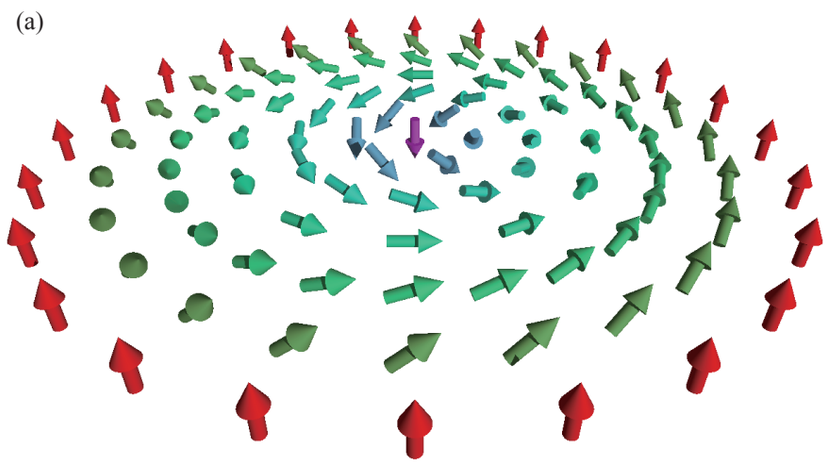
One of them is identical with "magnetic skyrmion"

This has been also investigated by Monte Calro simulation

Phase diagram



Magnetic skyemion



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

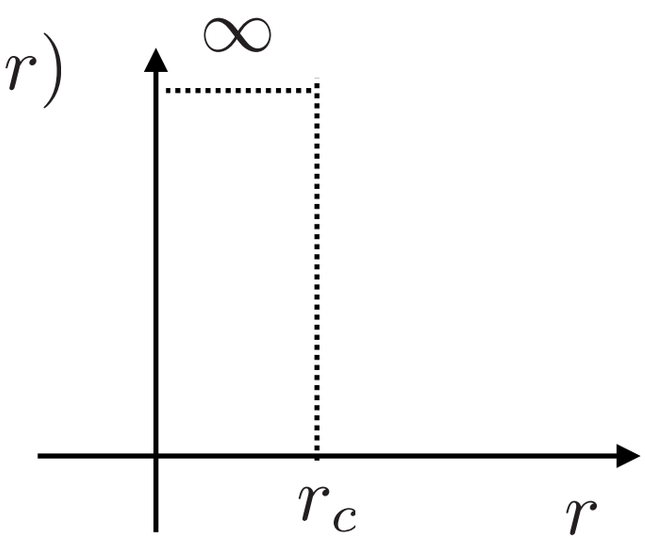
Kinetic Energy: $\dfrac{p_i^2}{2m_i}$

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

Variety of models: variety of interacting potentials

Hard sphere

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

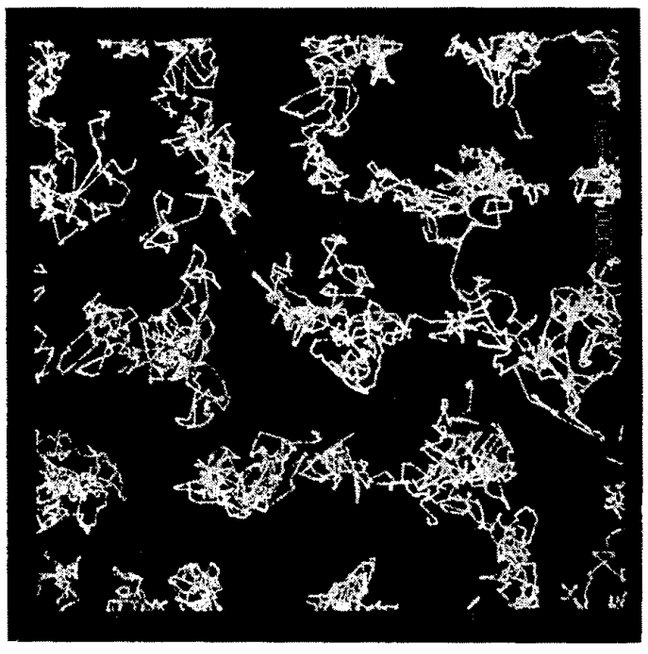


The first application of molecular dynamics

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

- Event driven molecular dynamics simulation

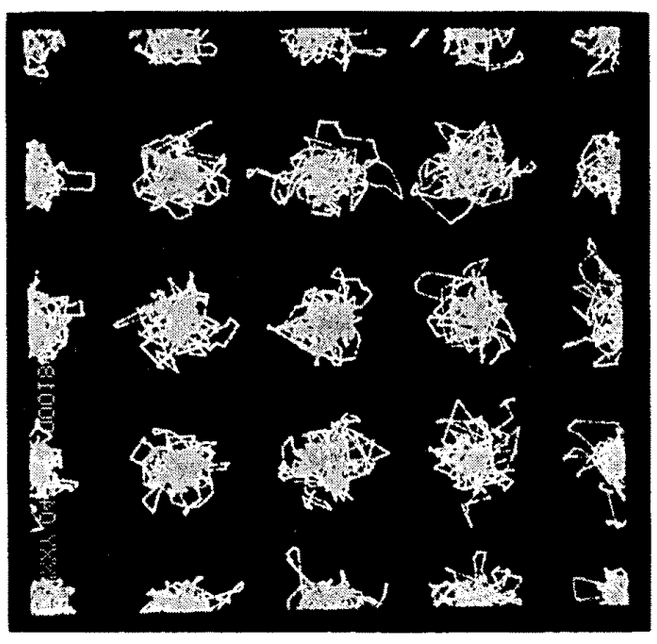
Fluid



Phase transition

(Alder transition)

Crystal

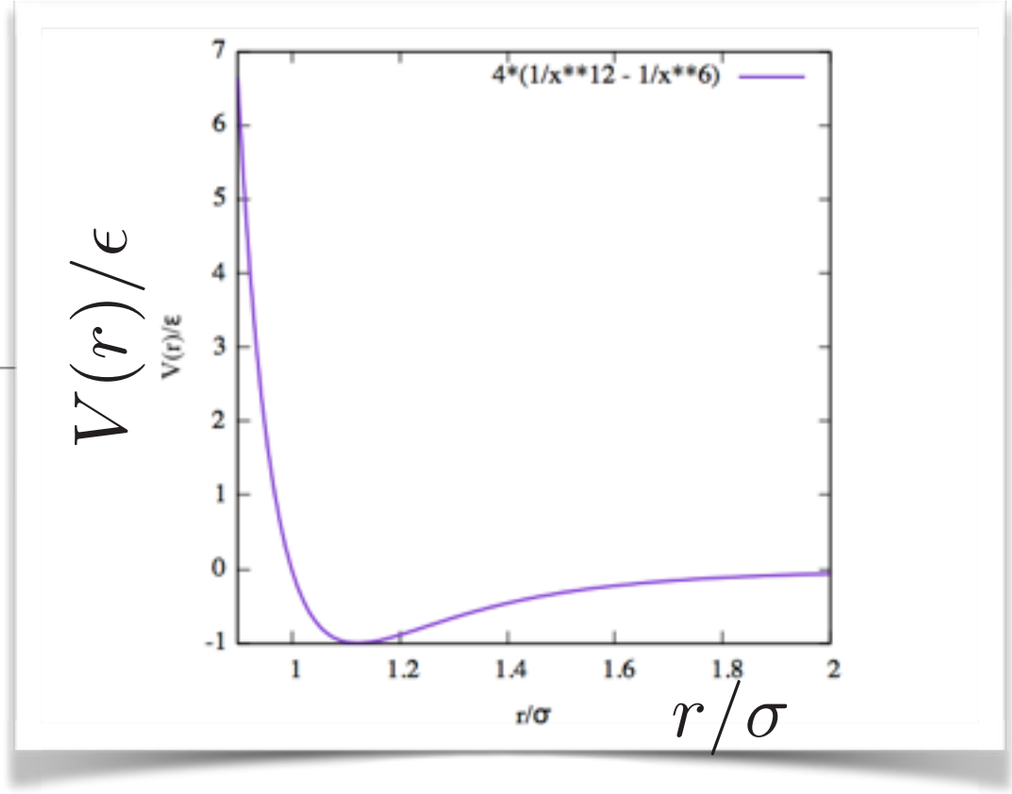


32 particle system

Lennard-Jones potential

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

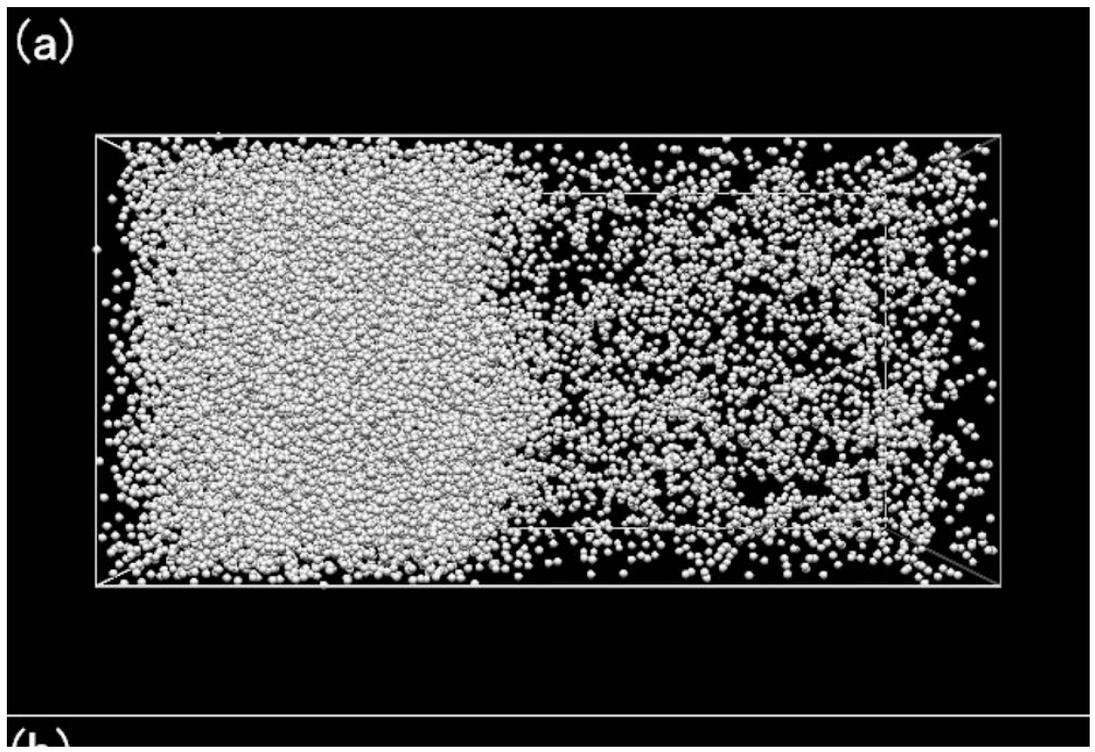
Model potential for noble gas (Ar, …)



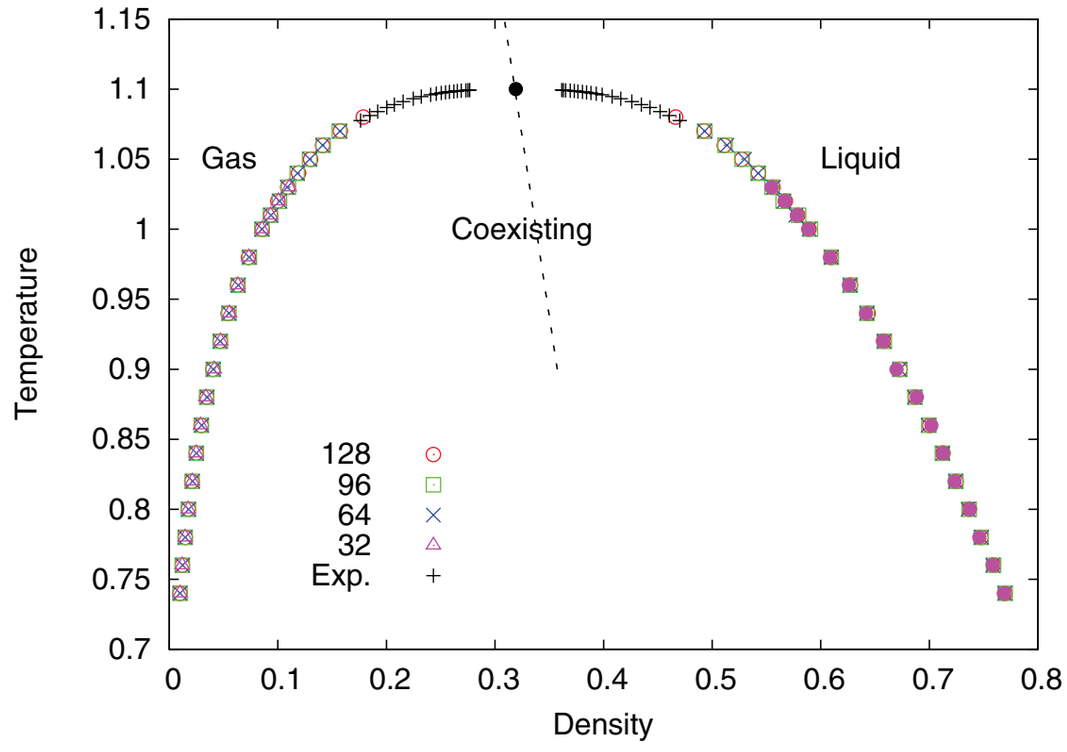
Recent simulation: H. Watanabe et al, J. Chem. Phys. **136**, 204102 (2012).

(~1,000,000 particles)

Gas-Liquid coexistence



Phase diagram



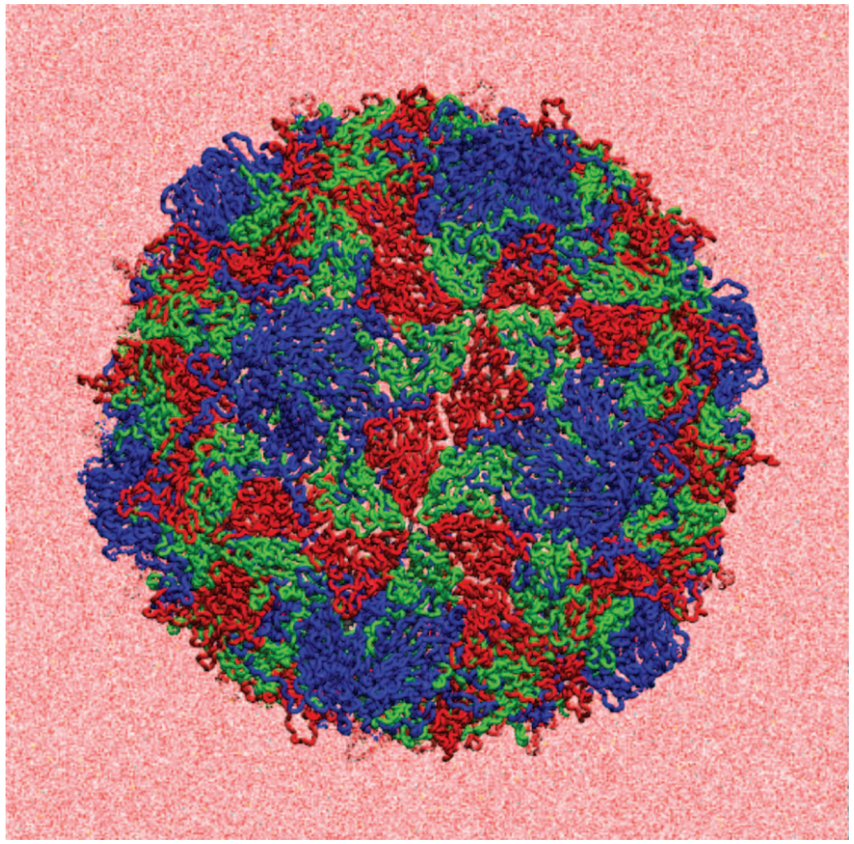
Complex systems

Eg. Poliovirus capsid in electrolyte solution

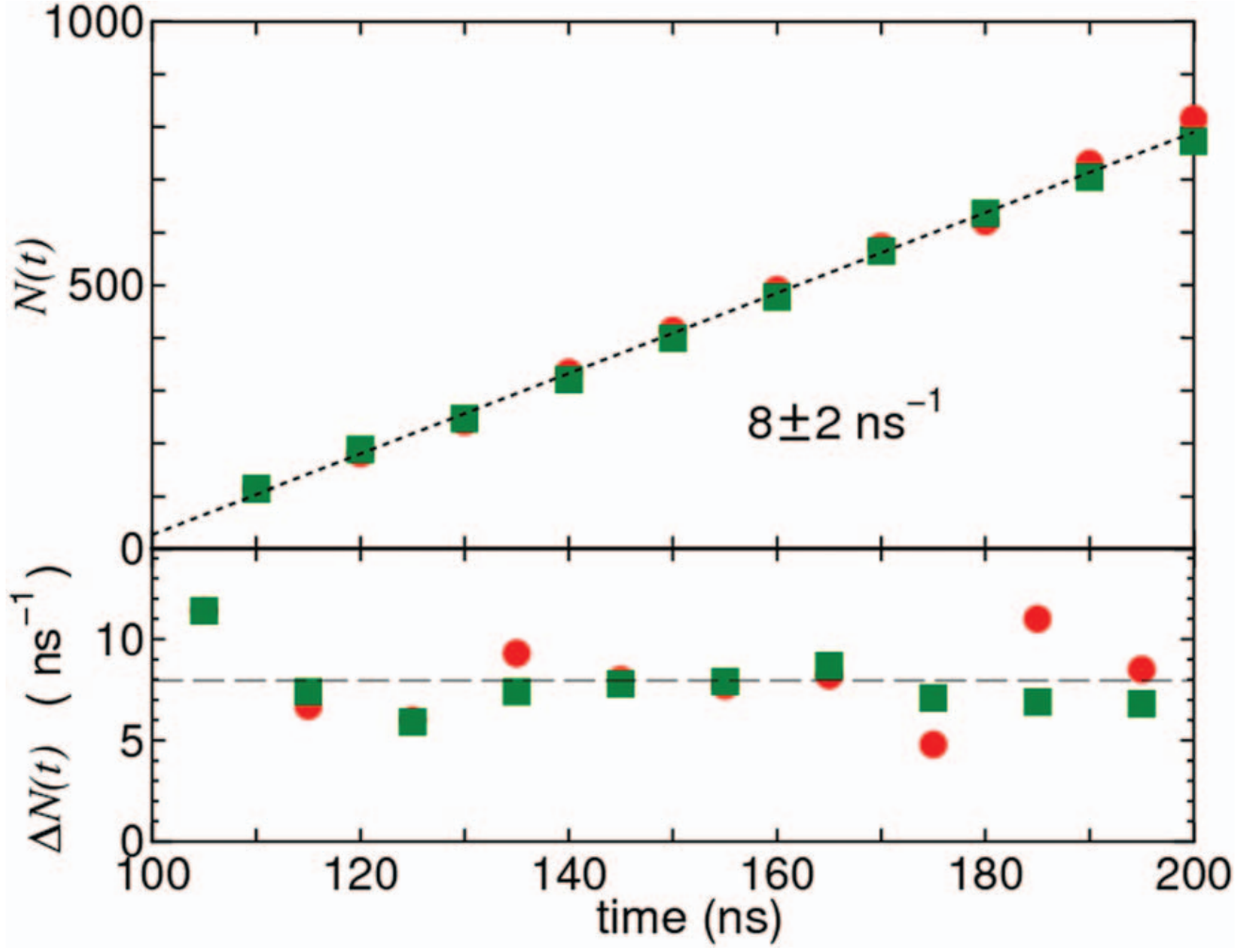
Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

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

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

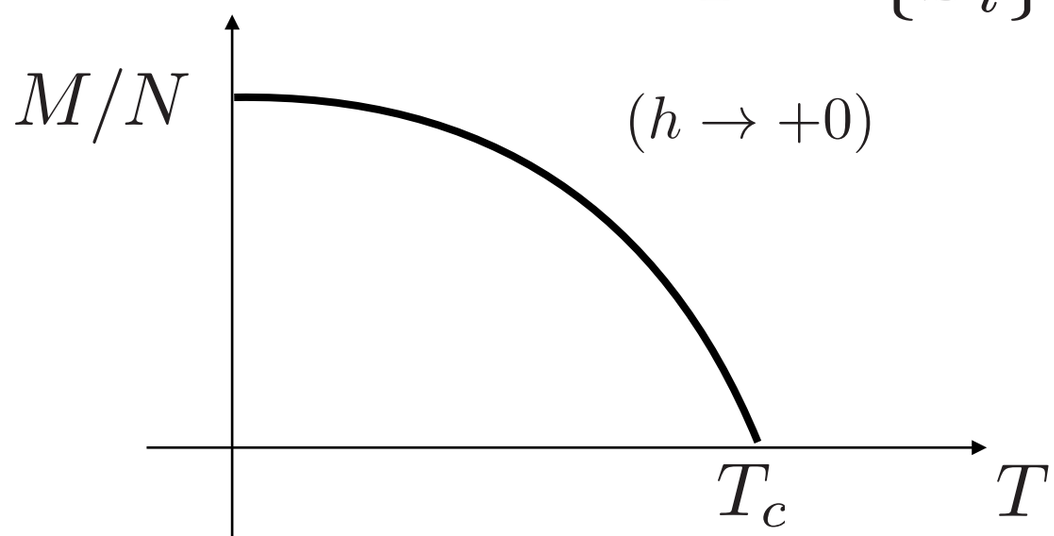
Canonical ensemble (NVT-ensemble) :

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

Magnetization at T:

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

$$\Gamma = \{S_i\}$$



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)：

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

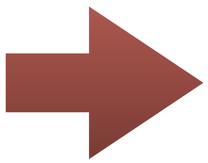
μ: chemical potential

General ensemble：

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

Computational science for statistical models

Purpose of computational science for statistical models



Calculate ensemble averages numerically

Two types of approaches

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

Time average for ensemble average

States depending on time

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

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

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

Molecular dynamics:

Dynamics of Γ obeys a differential equation (Newton equation)

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

Monte Carlo:

$\rho_t(\Gamma)$:probability distribution

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

Dynamics of Γ obeys a master equation

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

Time Correlation and relaxation time

Time correlation function

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

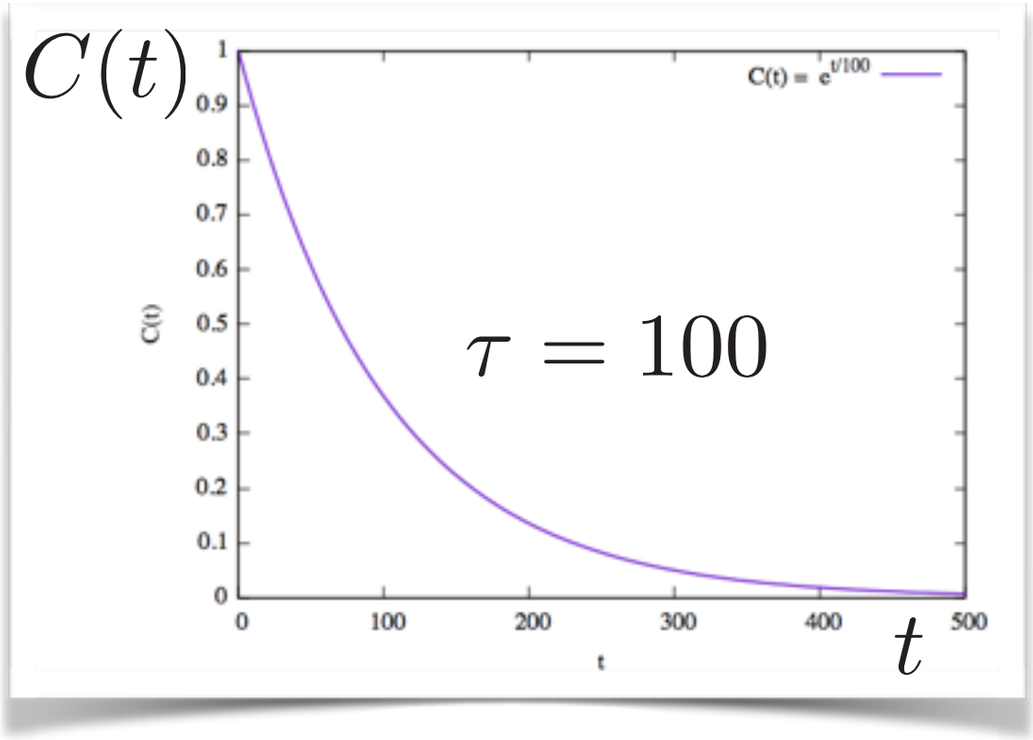
Auto correlation function

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

Typical asymptotic behavior

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

Relaxation time: τ_A



Relaxation time determines efficiency of sampling

smaller τ → higer efficiency

lager τ → lower efficiency

Error estimation

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

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

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

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

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

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 transition
  - $\tau \sim \exp(a/T)$ or $\exp(-a/|T\text{-}T_c|)$
  - Exponential can be reduce to polynomial by using extended ensemble methods

Next week

Classical

第１回：　物理学における多体問題
第２回：　多体問題における困難
第３回：　古典統計力学模型と数値計算
第４回：　古典モンテカルロ法とその応用
(Classical Monte Carlo method and its applications)
第５回：　分子動力学法とその応用
第６回：　拡張アンサンブル法によるモンテカルロ計算

Quantum

第７回：　量子統計力学模型と数値計算
第８回：　量子モンテカルロ法
第９回：　量子モンテカルロ法の応用
第１０回：　量子多体問題と巨大な疎行列の線形代数
第１１回：　クリロフ部分空間法の量子多体問題への応用
第１２回：　巨大な疎行列と量子統計力学
第１３回：　多体問題の並列計算アルゴリズム