多体問題の計算科学

Computational Science for Many-body problems

2023.5.16

#6: 拡張アンサンブル法によるモンテカルロ計算

Extended Ensemble Method for Monte Carlo Methods

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

Today

Classical

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

Quantum

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

Today’s contents

- MD
  - Control temperature and pressures
    - Velocity scaling and the Nosé-Hoover method
    - Andersen's method for pressure
- Extended ensemble methods
  - Back ground
  - Extended ensemble methods using information of the density of states
  - Another extended ensemble: Replica exchange method

Contents

- ~~Basics of MD simulation~~
  - ~~Newton equation, the purpose of MD simulation~~
  - ~~Examples of numerical integrations~~
- ~~NVE ensemble: standard MD simulation~~
  - ~~Symplectic integral~~
- Control temperature and pressures
  - Velocity scaling and the Nosé-Hoover method
  - Andersen's method for pressure

Control temperature

Temperature control: velocity scaling

The most simplest method for temperature setting: **Velocity Scaling**

(L. V. Woodcock, Chem. Phys. Lett. **10** ,257 (1971).)

Total kinetic energy: $K = \sum_i \frac{\boldsymbol{p}_i^2}{2m_i}$

Under the canonical (NVT) ensemble

$$\langle K \rangle = \frac{3}{2} N k_B T$$ (Equipartition of energy in 3d)

➡ Define effective temperature of a snapshot:

$$T_{\text{eff}} \equiv \frac{2K}{3Nk_B}$$

Rescale velocities every time step as

$$\boldsymbol{p}_i' = \boldsymbol{p}_i \sqrt{\frac{T}{T_{\text{eff}}}} \quad \Rightarrow \quad K' = \frac{3}{2} N k_B T$$

Results of the velocity scaling

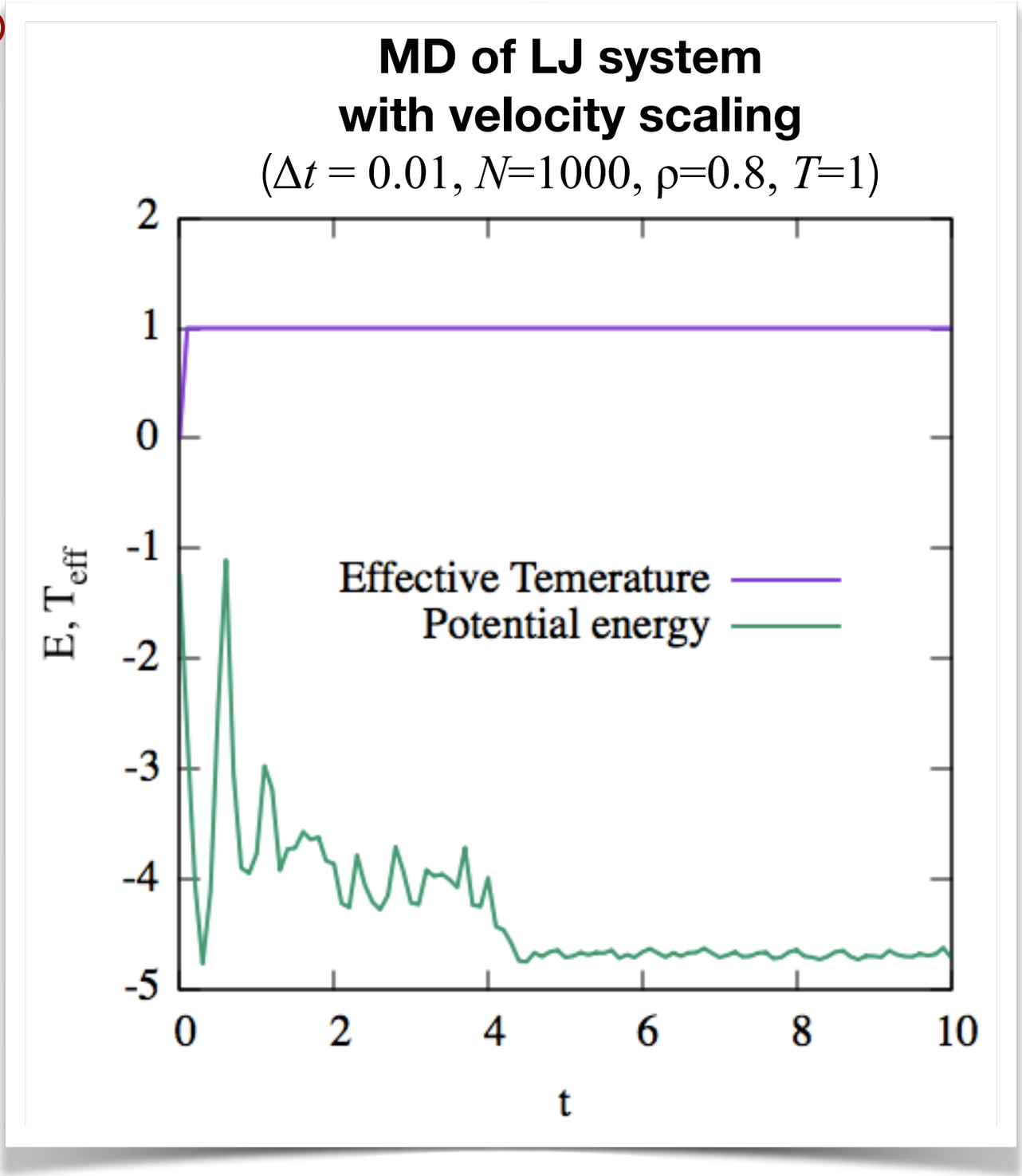
Total kinetic energy is artificially fixed to

$$K = \frac{3}{2} N k_B T$$

Under velocity scaling dynamics, the trajectories do not necessarily obey the canonical ensemble.

However,

- We can use it for an initialization for NVE ensemble.
- Position fluctuation *could be* effectively similar to that of NVT ensemble.



Temperature control: Langevin dynamics

Langevin dynamics

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i(\{\boldsymbol{q}_i\}) \underline{- \gamma \boldsymbol{p}_i} + \underline{\boldsymbol{R}_i}$$

Dissipation

Random force

(Gaussian white noise)

$$\langle \boldsymbol{R}_i(t) \rangle = \boldsymbol{0}$$

$$\langle \boldsymbol{R}_i(0) \boldsymbol{R}_j(t) \rangle = 2D_i \delta_{ij} \delta(t)$$

Long-time average of Langevin dynamics becomes
the canonical ensemble with temperature T,
if random forces satisfy the relation

$$D_i = \frac{k_B T}{m_i \gamma}$$

Einstein relation

Fluctuation-dissipation theorem

Temperature control: Nosé thermostad

Nose thermostad S. Nosé, Mol. Phys., **52**, 255 (1984). S. Nosé, J. Chem. Phys., **81**, 511 (1984).

Extended Hamiltonian System with a "heat bath"

$$\mathcal{H}_N = \sum_i \frac{(\boldsymbol{p}_i')^2}{2m_i s^2} + V(\{\boldsymbol{q}_i\}) + \frac{P_s^2}{2Q} + gk_BT\ln s$$

Original Hamiltonian with scaled momentum

$$\mathcal{H}\left(\left\{\frac{\boldsymbol{p}_i'}{s}\right\}, \{\boldsymbol{q}_i\}\right)$$

Heat-bath

s: scale factor for time

$$t' = st$$
$$\boldsymbol{p}_i' = s\boldsymbol{p}_i$$

Canonical equation (along t')

$$\frac{d\boldsymbol{p}_i'}{dt'} = -\frac{\partial V}{\partial \boldsymbol{q}_i} = \boldsymbol{F}_i(\{\boldsymbol{q}_i\}) \qquad \frac{dP_s}{dt'} = \frac{1}{s}\left(\sum_i \frac{(\boldsymbol{p}_i')^2}{m_i s^2} - gk_BT\right)$$

$$\frac{d\boldsymbol{q}_i}{dt'} = \frac{\boldsymbol{p}_i'}{m_i s^2} \qquad \frac{ds}{dt'} = \frac{P_s}{Q}$$

Temperature control: Nosé-Hoover method

Nosé-Hoover dynamics

Real-time dynamics with $\zeta = \dfrac{ds}{dt'}$ (W. G. Hoover, Phys. Rev. A, **31**, 1695 (1985).)

$$\boldsymbol{p}_i = \frac{\boldsymbol{p}_i'}{s} \qquad t = \frac{t'}{s}$$

$$\frac{d\boldsymbol{q}_i}{dt} = \frac{\boldsymbol{p}_i}{m_i}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i(\{\boldsymbol{q}_i\}) - \zeta \boldsymbol{p}_i$$

$$\frac{d\zeta}{dt} = \frac{gk_B}{Q}\left[\frac{1}{gk_B}\sum_i \frac{\boldsymbol{p}_i^2}{2m_i} - T\right] = \frac{1}{\tau^2}\left[T_{\mathrm{eff}} - T\right]$$

$g = 3N$ (# of DOF)

$\tau^2 = \dfrac{Q}{gk_B}$ (characteristic time scale)

New degree of freedom represents viscosity: ζ

➡ It changes the sign depending on the difference between the effective temperature and the aimed temperature.

(It also accelerates the velocity if $T_{\mathrm{eff}} < T$)

* This dynamics is not symplectic. ➡ Symplectic version: Nosé-Poincare method

S. D. Bond, *et.al.* J. Comp. Phys. **151**, 114 (1999)

Nosé-Hoover dynamics becomes NVT ensemble

Short proof:

(Based on Hisashi Okumura's review paper,
"分子動力学シミュレーションにおける温度・圧力制御")

$$\mathcal{H}_N = \mathcal{H}\left(\left\{\frac{\boldsymbol{p}'_i}{s}\right\}, \{\boldsymbol{q}_i\}\right) + \frac{P_s^2}{2Q} + gk_BT\ln s$$

MD on (q, p',t') dynamics yields NVE ensemble of H_N

$$\lim_{\tau'\to\infty}\frac{1}{\tau'}\int_0^{\tau'} dt' O(\{\frac{\boldsymbol{p}'_i}{s}\},\{\boldsymbol{q}_i\}) = \frac{\int d\boldsymbol{p}'_i d\boldsymbol{q}_i dP_s ds O(\{\frac{\boldsymbol{p}'_i}{s}\},\{\boldsymbol{q}_i\})\delta(E-\mathcal{H}_N)}{\int d\boldsymbol{p}'_i d\boldsymbol{q}_i dP_s ds \delta(E-\mathcal{H}_N)}$$

$$= \frac{\int d\boldsymbol{p}_i d\boldsymbol{q}_i dP_s ds s^{3N} O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\})\delta(E-\mathcal{H}-\frac{P^2}{2Q}-gk_BT\ln s)}{\int d\boldsymbol{p}_i d\boldsymbol{q}_i dP_s ds s^{3N}\delta(E-\mathcal{H}-\frac{P^2}{2Q}-gk_BT\ln s)}$$

s^{3N} comes from $\boldsymbol{p}'_i = s\boldsymbol{p}_i$

from $$\int ds s^{3N}\delta(E-\mathcal{H}-\frac{P^2}{2Q}-gk_BT\ln s) = \frac{1}{gk_BT}e^{-\frac{3N+1}{gk_BT}(\mathcal{H}+\frac{P^2}{2Q}-E)}$$

$$= \frac{\int d\boldsymbol{p}_i d\boldsymbol{q}_i O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\})e^{-\frac{3N+1}{gk_BT}\mathcal{H}}}{\int d\boldsymbol{p}_i d\boldsymbol{q}_i e^{-\frac{3N+1}{gk_BT}\mathcal{H}}}$$

$$\delta(f(x)) = \frac{\delta(x-x_0)}{|f'(x_0)|} \quad (f(x_0)=0)$$

Canonical ensemble if $g = 3N+1$

Nosé-Hoover dynamics becomes NVT ensemble 2

Time average on ***t*** :

$$\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau} dt O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\}) = \lim_{\tau\to\infty}\frac{\tau'}{\tau}\frac{1}{\tau'}\int_0^{\tau'} dt' \frac{O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\})}{s}$$

from $\boxed{\tau = \int_0^{\tau'} \frac{1}{s} dt'}$

$$= \frac{\lim_{\tau'\to\infty}\frac{1}{\tau'}\int_0^{\tau'} dt' \frac{O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\})}{s}}{\lim_{\tau'\to\infty}\frac{1}{\tau'}\int_0^{\tau'} dt' \frac{1}{s}}$$

$$= \frac{\int d\boldsymbol{p}_i d\boldsymbol{q}_i O(\{\boldsymbol{p}_i\},\{\boldsymbol{q}_i\}) e^{-\frac{3N}{gk_BT}\mathcal{H}}}{\int d\boldsymbol{p}_i d\boldsymbol{q}_i e^{-\frac{3N}{gk_BT}\mathcal{H}}}$$

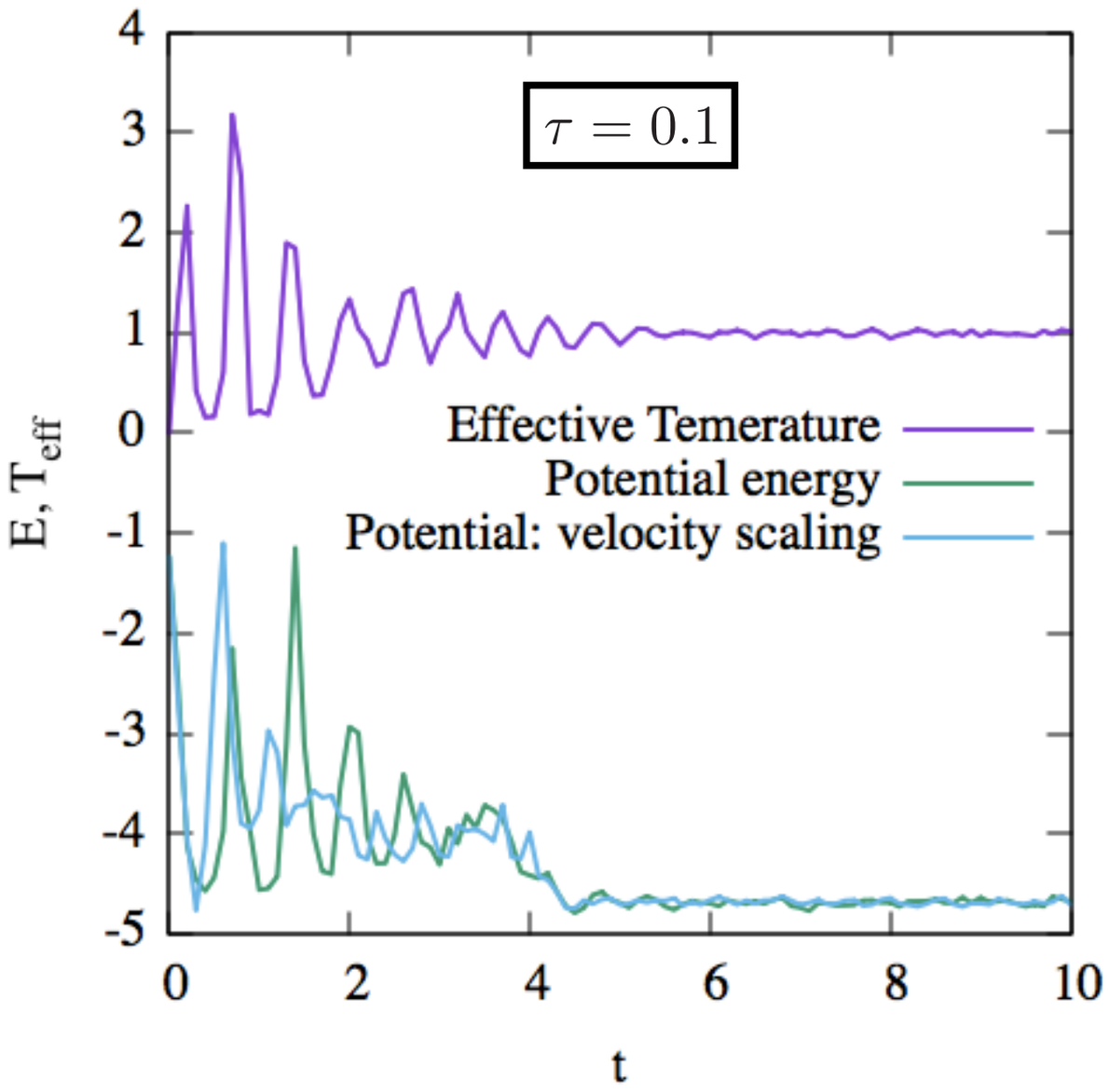
Canonical ensemble if $g = 3N$

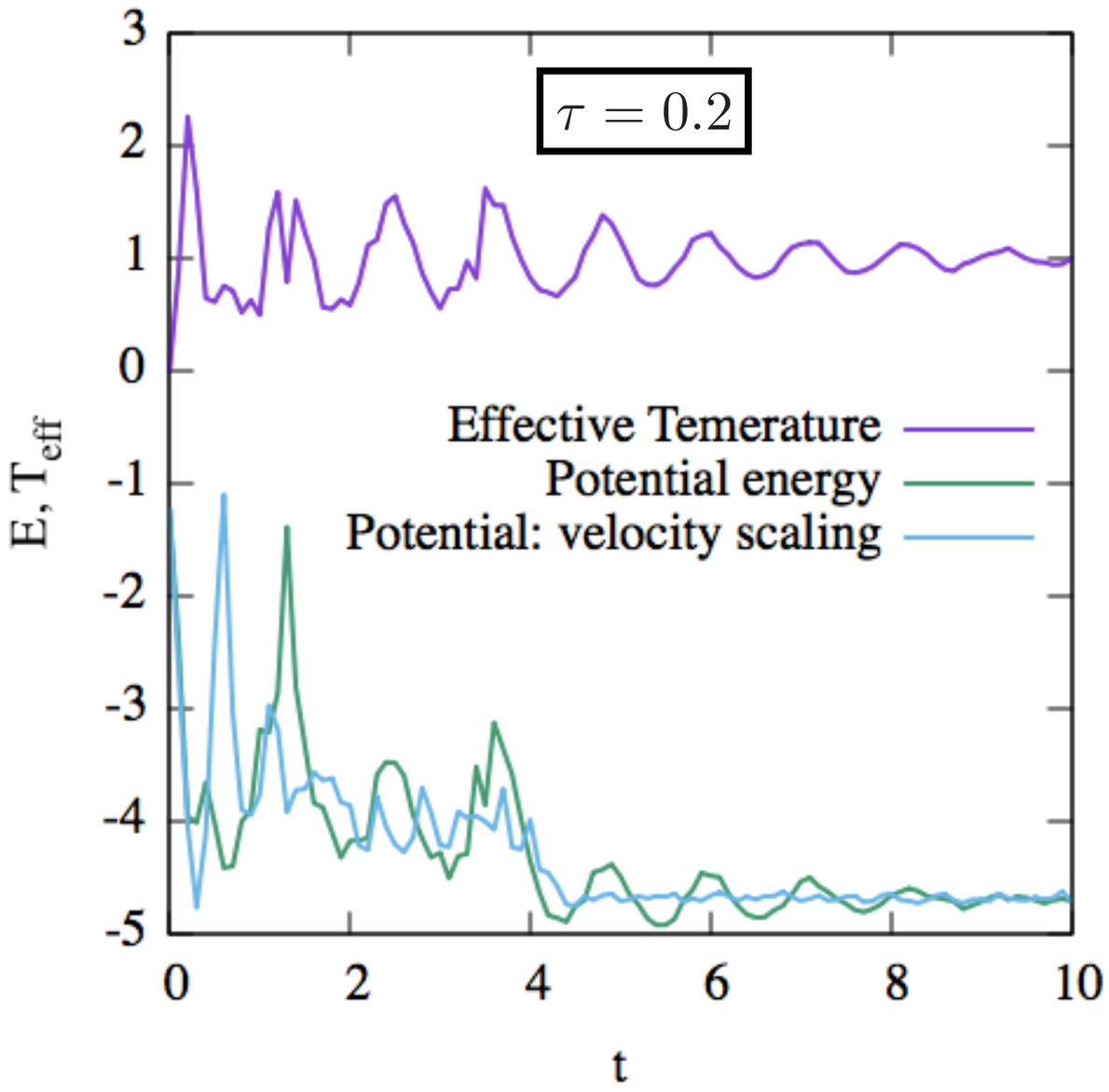
Results of the Nose-Hoover dynamics

- Temperature behaves like damped oscillation.
  - Period is related to τ (or Q)
- Potential energy converges almost same value with that of velocity scaling.

MD of LJ system

($\Delta t = 0.01$, N=1000, ρ=0.8, T=1)





Control pressure (will be skipped)

Pressure control: Andersen method

H. C. Andersen, J. Chem. Phys. **72** (1980) 2384.

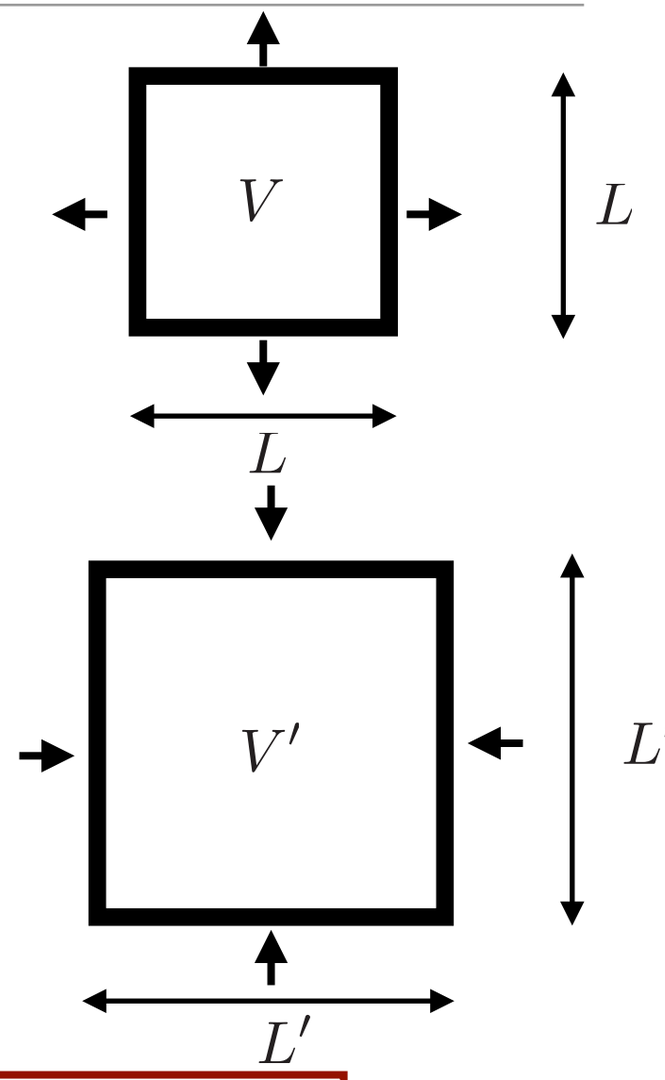
Extended Hamiltonian System with a "piston"

$$\mathcal{H}_A = \sum_i \frac{\tilde{\boldsymbol{p}}_i^2}{2m_i V^{\frac{2}{3}}} + V_p(\{V^{\frac{1}{3}}\tilde{\boldsymbol{q}}_i\}) + \frac{P_V^2}{2M} + PV$$

Original Hamiltonian with scaled coordinate and momentum

Piston

$$\tilde{\boldsymbol{q}}_i = V^{-\frac{1}{3}}\boldsymbol{q}_i$$
$$\tilde{\boldsymbol{p}}_i = V^{\frac{1}{3}}\boldsymbol{p}_i$$



Canonical equation

$$\frac{d\tilde{\boldsymbol{q}}_i}{dt} = \frac{\tilde{\boldsymbol{p}}_i}{m_i V^{\frac{2}{3}}} \qquad \frac{dV}{dt} = \frac{P_V}{M}$$

$$\frac{d\tilde{\boldsymbol{p}}_i}{dt} = V^{\frac{1}{3}}\boldsymbol{F}_i(\{V^{\frac{1}{3}}\tilde{\boldsymbol{q}}_i\}) \qquad \frac{dP_V}{dt} = \frac{1}{3V}\sum_i \left[\frac{\tilde{\boldsymbol{p}}_i{}^2}{m_i V^{\frac{2}{3}}} + \boldsymbol{F}_i \cdot (V^{\frac{1}{3}}\tilde{\boldsymbol{q}}_i)\right] - P$$

Pressure control: Andersen method

H. C. Andersen, J. Chem. Phys. **72** (1980) 2384.

In original coordinates

$$\frac{d\boldsymbol{q}_i}{dt} = \frac{\boldsymbol{p}_i}{m_i} + \frac{\dot{V}}{3V}\boldsymbol{q}_i \qquad \frac{dV}{dt} = \frac{P_V}{M}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i - \frac{\dot{V}}{3V}\boldsymbol{p}_i \qquad \frac{dP_V}{dt} = \underline{\frac{1}{3V}\sum_i \left[\frac{\boldsymbol{p}_i^2}{m_i} + \boldsymbol{F}_i \cdot \boldsymbol{q}_i\right]} - P$$

P_{eff} :virial theorem

$$= P_{\mathrm{eff}} - P$$

New degree of freedom controls the pressure like a piston.

P_{v} changes the sign depending on the difference between the effective pressure and the aimed pressure.

Andersen method gives us “approximate” NPH ensemble.

H = Enthalpy

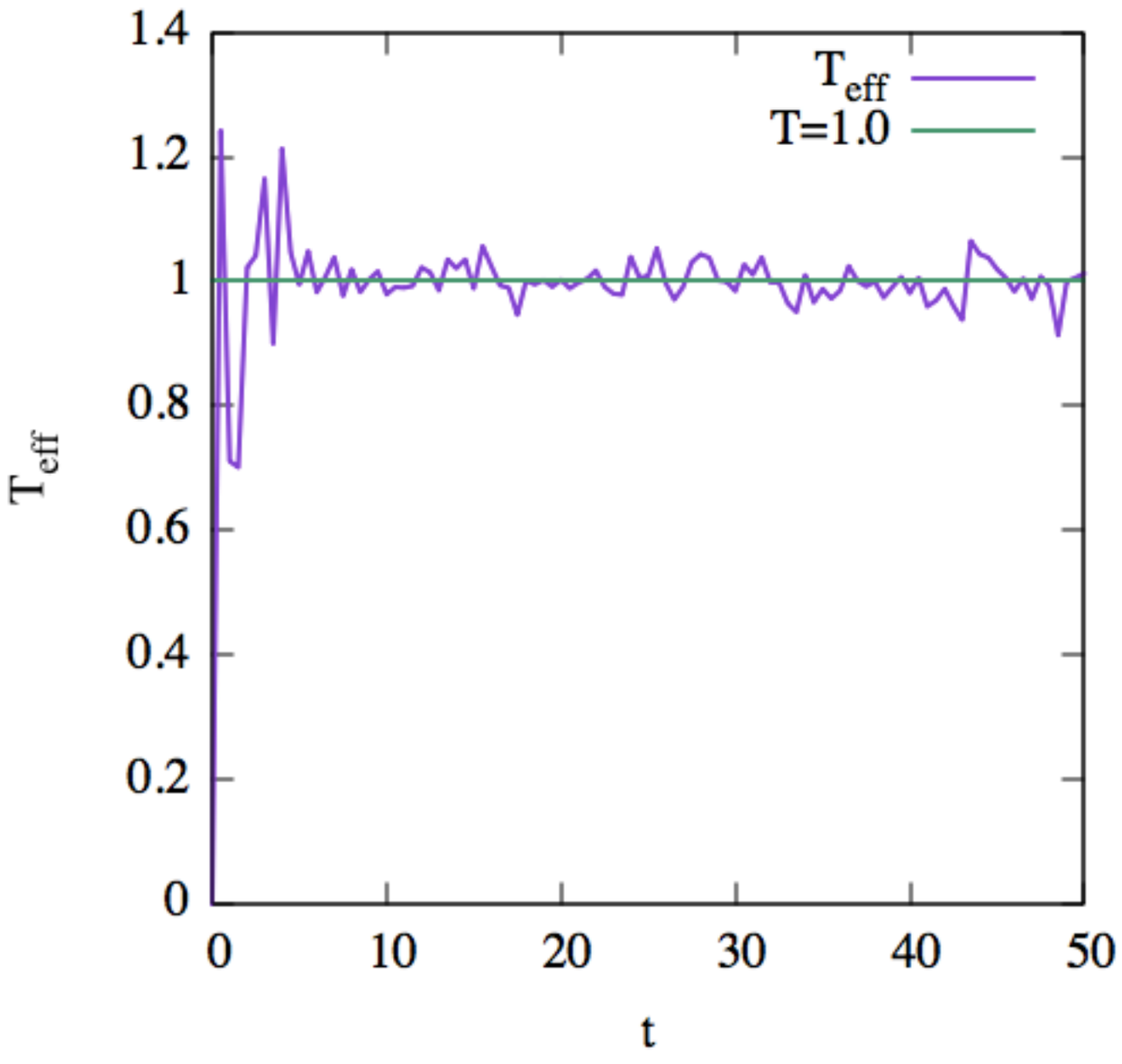
NPT ensemble

MD of LJ system

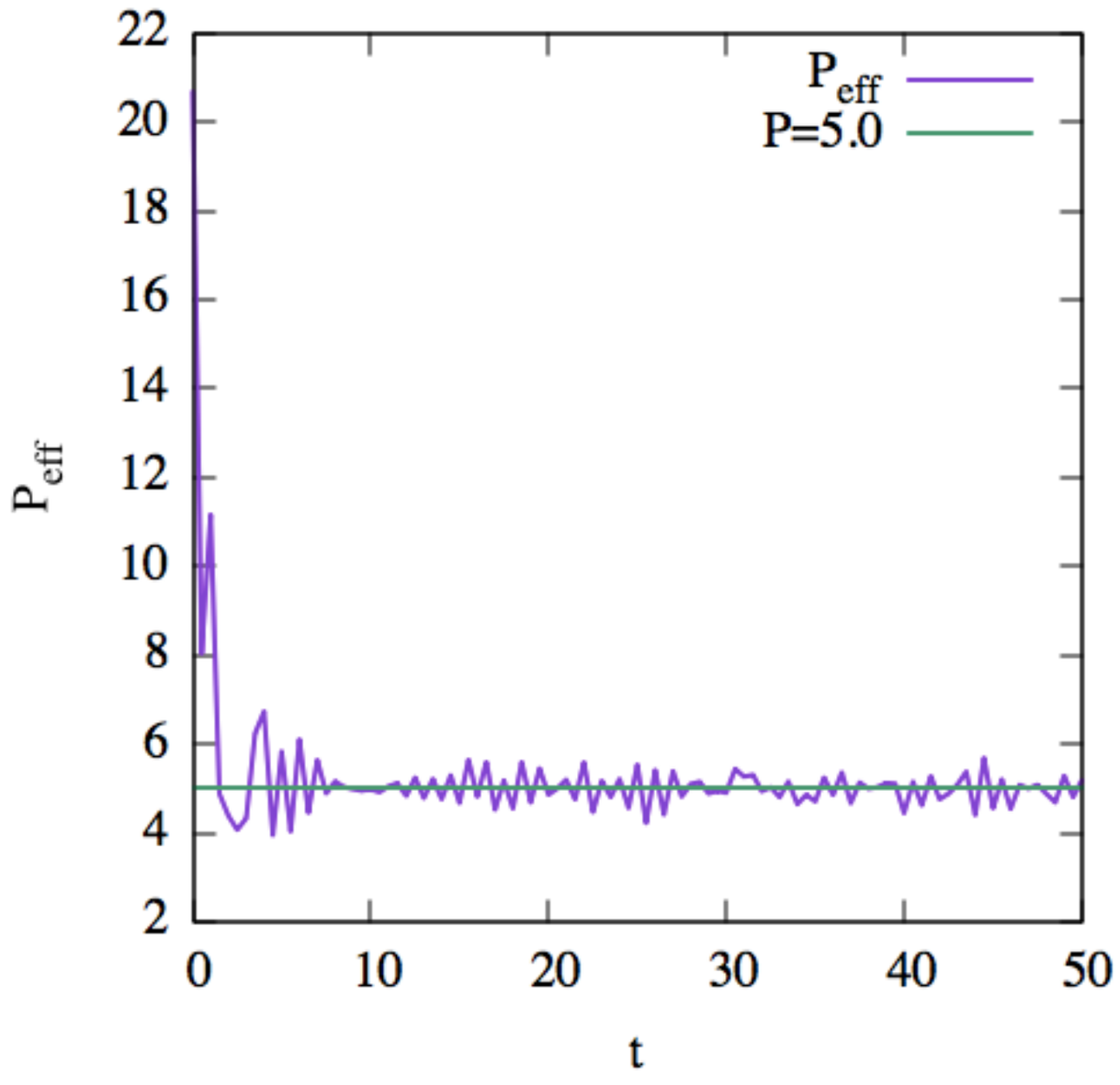
($\Delta t = 0.005$, N=1000, T=1, P=5)

By combining temperature and pressure controls,
we can obtain NPT ensemble. *e.g.* Nosé-Andersen method

Temperature



Pressure



Exercise: MD simulation of LJ particles(not a report)

Let's try MD simulation of LJ particles with NVE, NVT, and NPT ensembles.

- In NVE simulation (e.g. by Verlet method),
  see the conservation of the total energy.
- By using, velocity scaling or Nose-Hoover thermostat,
  try to control temperature.
- By combining temperature control and pressure control
  try to simulate NPT ensemble.

To perform these exercise, you may use,

- Your own code
- LAMMPS
  - http://lammps.sandia.gov
- MDACP (for NVE simulation.)
  - http://mdacp.sourceforge.net/index.html
- My sample codes for jupyter notebook.
  - To run the sample code you need
    - numpy, and numba (numba is used for speed up)

References (books)

- “Computational Physics”, J. Thijssen, Cambridge University Press.
  （「計算物理学」J.M.ティッセン著、松田和典他訳、シュプリンガー・フェアラーク東京.
- 「分子シミュレーション」上田顯著、裳華房.

Extended Ensemble method for Monte Carlo Methods

Contents

- Back ground
  - Density of states and the histogram method
- Extended ensemble methods using information of the density of states
  - Multi Canonical Method
  - Wang-Landau method
- Another extended ensemble: Replica exchange method

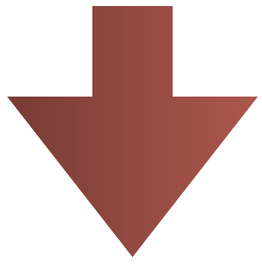
Back ground

Extended ensemble = general ensemble

In conventional MC or MD simulation:

We try to estimate expectation values under
"physically meaningful" ensembles.

NVE, NVT, NPT, …



Even if an ensemble is not directly connected to any physical systems, we can use is to enhance the efficiency of numerical calculations (MC, MD) for interested physical systems.

Large relaxation time in standard MC and MD

- Critical phenomena
  - $\tau \sim L^z$ with standard algorithm (critical slowing down)
  - z can be significantly reduced by using "global update"
- First order phase transition, Glass transition (structural glass, spin glass), protein foldings,
  - $\tau \sim \exp(\Delta E/T)$ or $\exp(\Delta E/|T\text{-}T_c|)$; Note $\Delta E \propto L^d$ $(or\ L^{d\text{-}1})$!
  - Exponential can be reduce to polynomial by using extended ensemble methods.

Density of state and histogram method

Origin of exponentially long relaxation time

Partition function of the canonical ensemble

$$Z = \int d\Gamma e^{-\beta \mathcal{H}(\Gamma)} = \int dE \underline{\rho(E)} e^{-\beta E} = \int dE e^{-\underline{\beta F(E)}}$$

Density of states

"Free energy"

$$F(E) \equiv E - k_B T \log \rho(E)$$

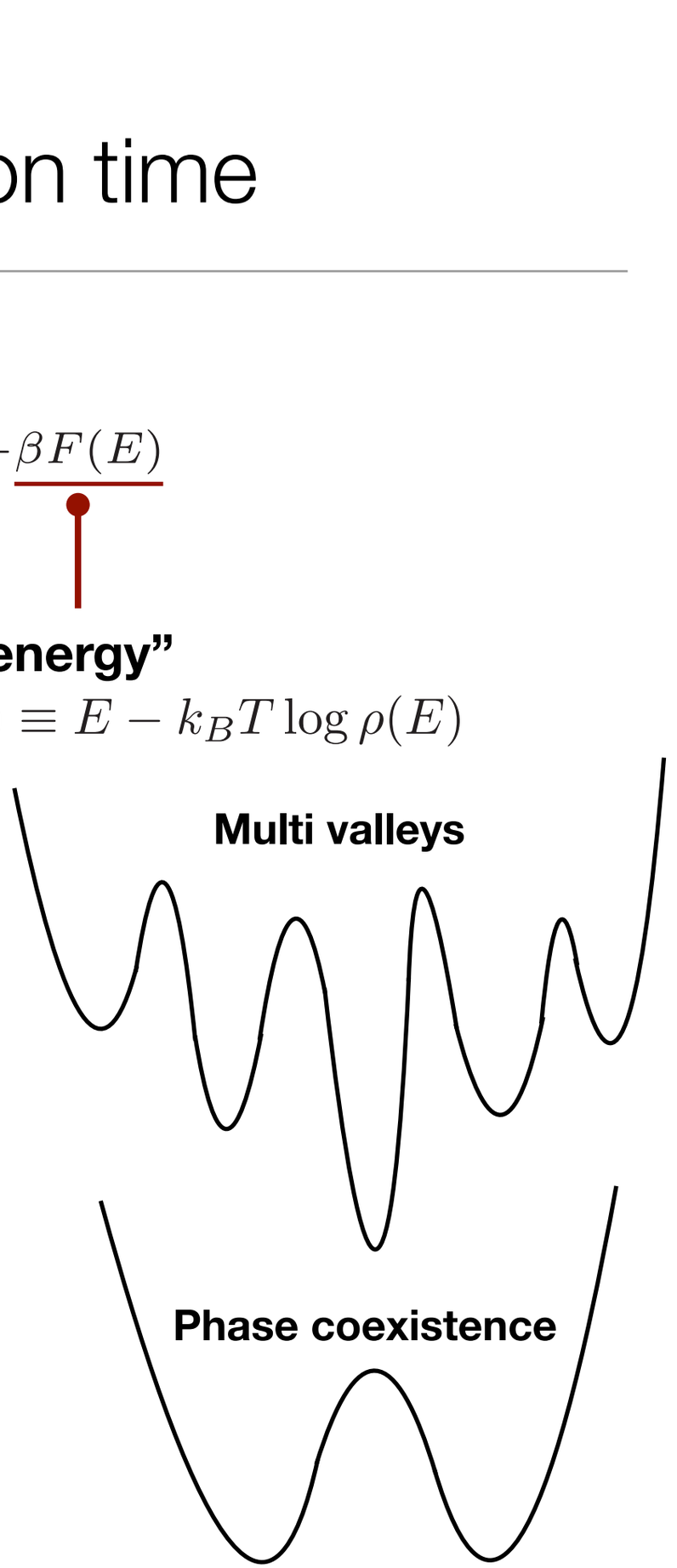
Probability distribution for energy

$$P(E) = \frac{1}{Z} e^{-\beta F(E)}$$

Note! Free energy is extensive: $F(E) \propto N$

- "Transition probability" is proportional to the exponential of Free-energy difference: exp(-ΔF/T)
- Usual algorithm of MC (and MD) changes the state (or the energy) gradually.

If there are local minima, the relaxation time could be exponentially large as the size is increased.



Density of states

$$Z = \int d\Gamma e^{-\beta \mathcal{H}(\Gamma)} = \int dE \rho(E) e^{-\beta E}$$
$$= \int dE \int dM \rho(E, M) e^{-\beta E}$$

$\int d\Gamma$ ~O(N)-dimensional integral

$\int dE$ ~1-dimensional

$\int dE \int dM$ ~2-dimensional

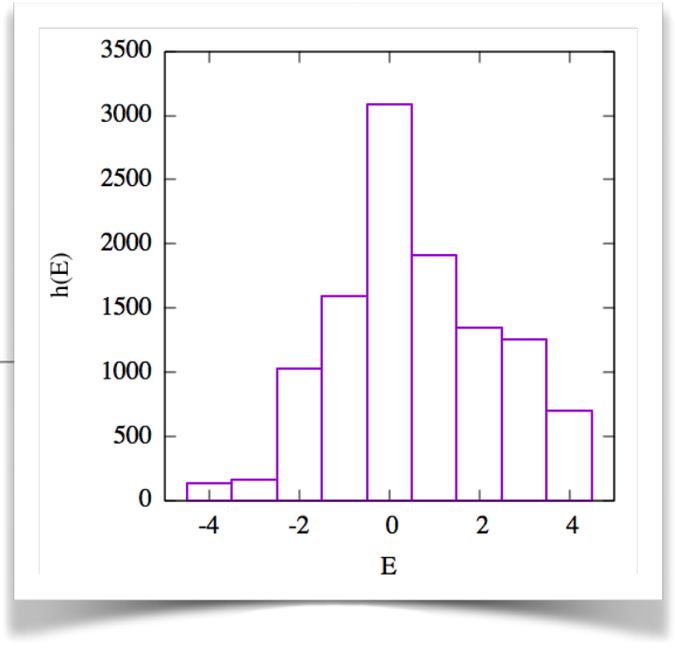
- If we know the exact $\rho(E)$(or $\rho(E, M)$), the calculation of partition function is reduced to 1 or (a few) -dimensional integral.
- Even if we only know an approximate density of states,

$$\tilde{\rho}(E) \simeq \rho(E)$$

we can improve the sampling efficiency by using its information.

- Histogram method
- Multi canonical method
- Wang-Landau method

Energy Histogram



Energy histogram:

In MC or MD calculations

$h(E_i)$:# of samples (snap shots) with energy in

$$E_i - \Delta E/2 \leq E < E_i + \Delta E/2$$

$$\Rightarrow \quad P(E)\Delta E \simeq \frac{1}{N_h} h(E)$$

Total # of samples

$$N_h \equiv \sum_i h(E_i)$$

e.*g.* NVT ensemble:

$$P(E) = \frac{1}{Z(\beta)} \rho(E) e^{-\beta E} \quad \Rightarrow \quad \rho(E) \simeq \frac{Z(\beta)}{N_h \Delta E} h(E) e^{\beta E}$$

We can calculate (approximate) density of states from usual MC or MD simulations!

Because we don't know the partition function,
DOS is determined up to the proportional coefficient.

Histogram method (reweighting method)

Energy expectation value of different temperatures

$$\langle E \rangle_{\beta'} = \frac{\int dE \rho(E) E e^{-\beta' E}}{\int dE \rho(E) e^{-\beta' E}} \simeq \frac{\sum_i E_i h(E_i) e^{-(\beta'-\beta)E_i}}{\sum_i h(E_i) e^{-(\beta'-\beta)E_i}}$$

Any expectation values can also be calculated by the histogram method.

$$\langle O \rangle_{\beta'} \simeq \frac{\sum_i O(E_i) h(E_i) e^{-(\beta'-\beta)E_i}}{\sum_i h(E_i) e^{-(\beta'-\beta)E_i}}$$

$$\rho(E) \simeq \frac{Z(\beta)}{N_h \Delta E} h(E) e^{\beta E}$$

Average at energy E_i

$$O(E_i) \equiv \sum_{E(\Gamma_j) \in E_i} O(\Gamma_j)$$

Limitation of histogram method

Reweighted histogram becomes
less accurate
when T' is far from the original T.

"Tail" of the original histogram has only small # of snapshots.→large noise

Central limit theorem

Width of energy distribution: $\propto \sqrt{N}$

Average of energy: $\propto N$

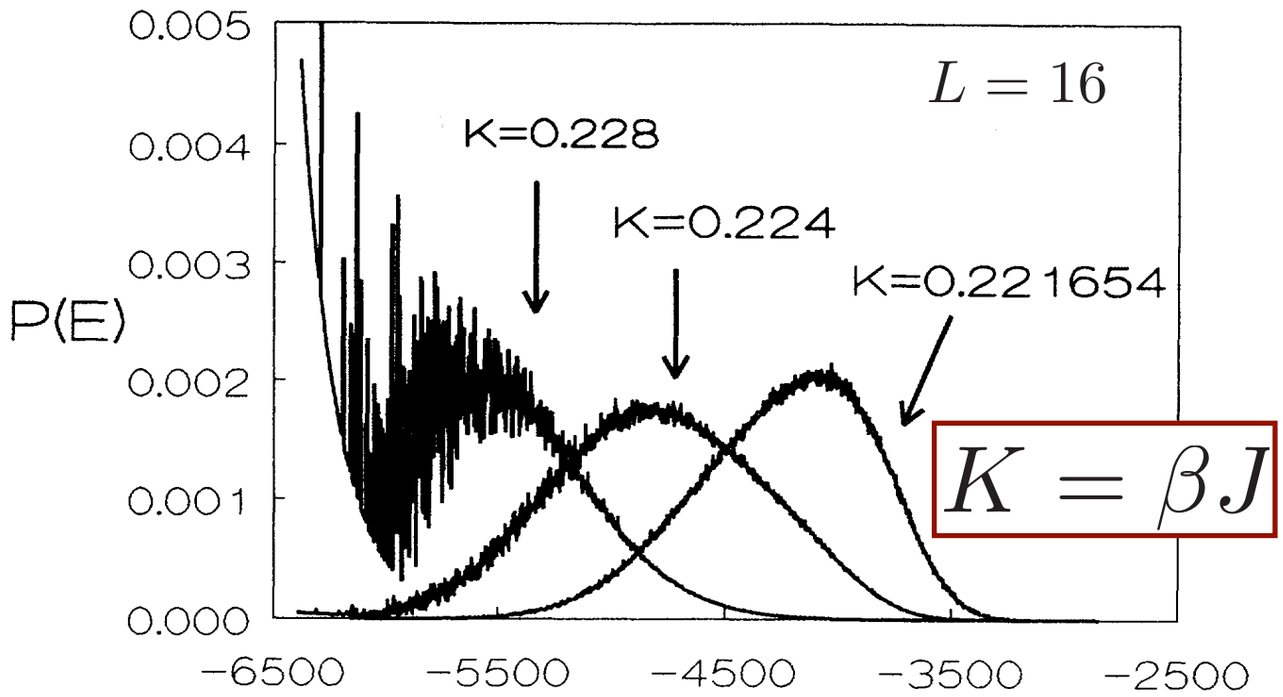
Distribution becomes narrower as *N* is increased!

Reliable temperature region for reweighting:

$$\Delta T \propto \frac{1}{\sqrt{N}}$$

Energy distribution of 3d-Ising model

A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991)



MC simulation at K=0.221654

Reweighting to
K=0.224 and K=0.228

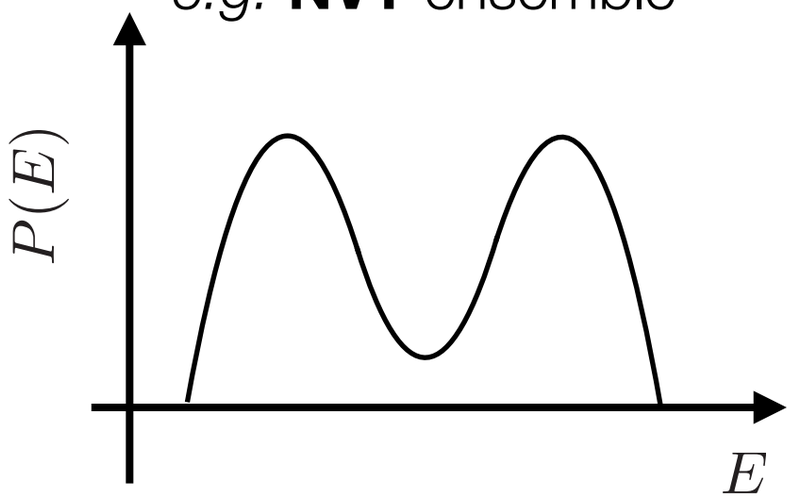
Multi Canonical methods

Idea of Multi-Canonical method

B.A. Berg and T. Neuhaus (1992)

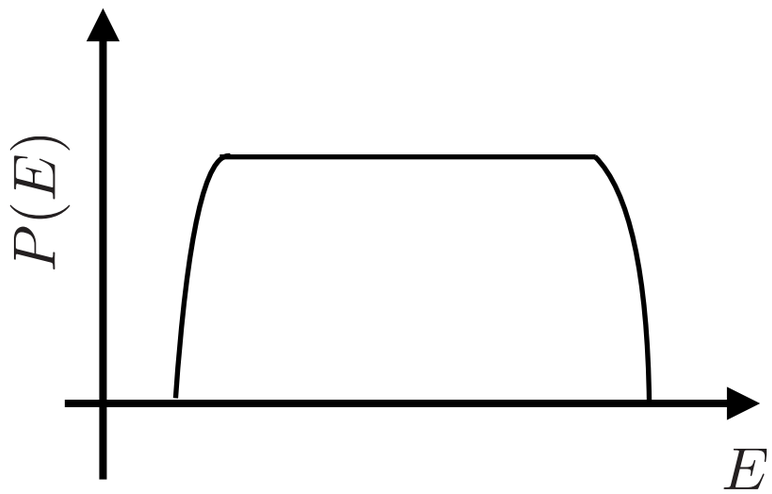
If we can prepare a special ensemble
where the energy distribution is “flat”,
we can efficiently sample all relevant states.

e.g. **NVT** ensemble



$$P(E) \propto \rho(E) e^{-\beta E}$$

“special” ensemble



$$\tilde{P}(E) \propto \rho(E) e^{-S(E)} = \text{const.}$$

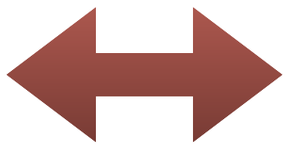
Special ensemble is related to log of DOS!

$$S(E) = \log \rho(E)$$

How to obtain the special ensemble?

Special ensemble is log of DOS!

$$S(E) = \log \rho(E)$$



DOS is unknown!

We can obtain $S(E)$ approximately by iterative calculations.

“Sketch” of an iterative algorithm:

1. Run MC simulation on a high temperature and calculate energy histogram.

$$h(E) \sim \rho(E) e^{-\beta E}$$

2. Based on the energy histogram, extract approximate $S(E)$.

$$S^0(E) = \beta E + \log h(E)$$

3. **Loop** n
    1. Run MC simulation under $S^{(n)}(E)$ and calculate histogram $h^{(n)}(E)$
    2. Calculate next $S^{(n+1)}(E)$ as

$$S^{(n+1)}(E) = S^{(n)}(E) + \log h^{(n)}(E)$$

How to obtain the special ensemble?

3. **Loop** n
   1. Run MC simulation under $S^{(n)}(E)$ and calculate histogram $h^{(n)}(E)$
   2. Calculate next $S^{(n+1)}(E)$ as

$$S^{(n+1)}(E) = S^{(n)}(E) + \log h^{(n)}(E)$$

- The histogram $h^{(n)}(E)$ is expected to be $h^{(n)}(E) \sim \rho(E)e^{-S^{(n)}(E)}$
- When $S^{(n)}(E)$ becomes close to $log\, \rho(E)$, the histogram becomes almost flat.

→ We can efficiently sample the histogram and DOS.

- By using accurate $S^{(n)}(E)$ we can calculate expectations values under the canonical ensemble by using reweighting technique.

$$\langle O \rangle_\beta = \frac{\int dE O(E)\rho(E)e^{-S(E)}e^{-\beta E+S(E)}}{\int dE \rho(E)e^{-S(E)}e^{-\beta E+S(E)}} = \frac{\langle Oe^{-\beta E+S(E)}\rangle_S}{\langle e^{-\beta E+S(E)}\rangle_S}$$

Detailed algorithm (will be skipped)

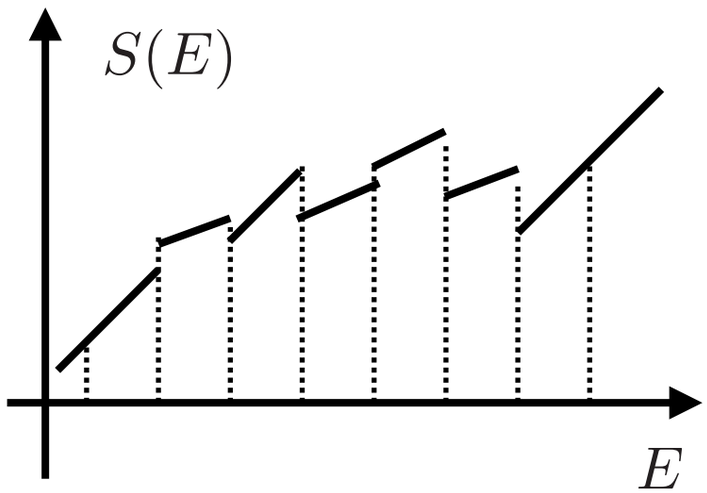
B.A. Berg, Nucl. Phys. B (Proc. Suple.) **63**A-C, 982 (1998)

Suppose $S(E)$ looks like: $S(E) = \beta(E)E - \alpha(E)$

(Energy dependent temperature)

$$S(E) \simeq \beta_i E - \alpha_i$$

for $E_i - \Delta E/2 \leq E \leq E_i + \Delta E/2$



In a specific interval, we want to optimize β and α,
i.e. $P(E)$ becomes flat.

By defining $\beta_i \equiv \dfrac{S(E_{i+1}) - S(E_i)}{\Delta E}$

$$\alpha_{i-1} = \alpha_i + (\beta_{i-1} - \beta_i)E_i$$

We fix $\alpha_{i_{max}} = 0$

Detailed algorithm (will be skipped)

B.A. Berg, Nucl. Phys. B (Proc. Suple.) **63**A-C, 982 (1998)

Iteration :how to determine next β and α

In order to make the histogram flat, $S^{(n+1)}(E) = S^{(n)}(E) + \log h^{(n)}(E)$

$$\tilde{\beta}_i^{(n+1)} = \beta_i^{(n)} + \log \frac{h_{i+1}^{(n)}}{h_i^{(n)}}$$

This estimator could be suffered from large statistical error

Gradual change from the previous β

$$\beta_i^{(n+1)} = (1 - c_i)\beta_i^{(n)} + c_i \tilde{\beta}_i^{(n+1)}$$

*For optimal c_i , see the reference

α is calculated from β

$$\alpha_{i-1}^{(n+1)} = \alpha_i^{(n+1)} + (\beta_{i-1}^{(n+1)} - \beta_i^{(n+1)})E_i$$

Example of application

q-state Potts model on the square lattice

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{S_i, S_j} \qquad S_i = 0, 1, 2, \cdots, q-1$$

Phase transition at

$$T_c/J = \frac{1}{\log(1+\sqrt{q})}$$

$q = 2$: Equivalent to Ising model

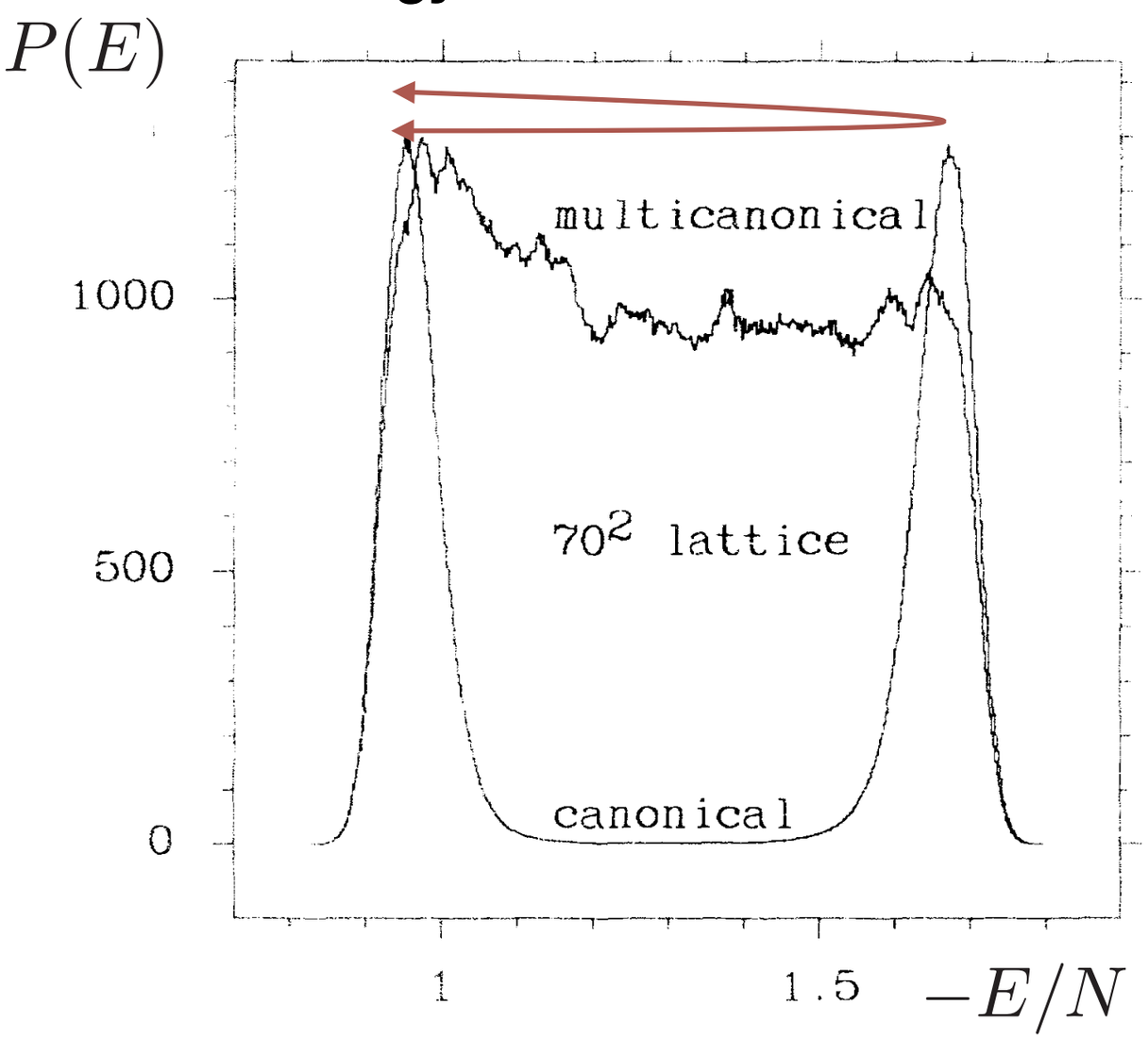
$q \leq 4$: Continuous phase transition

$q > 5$: 1st order phase transition

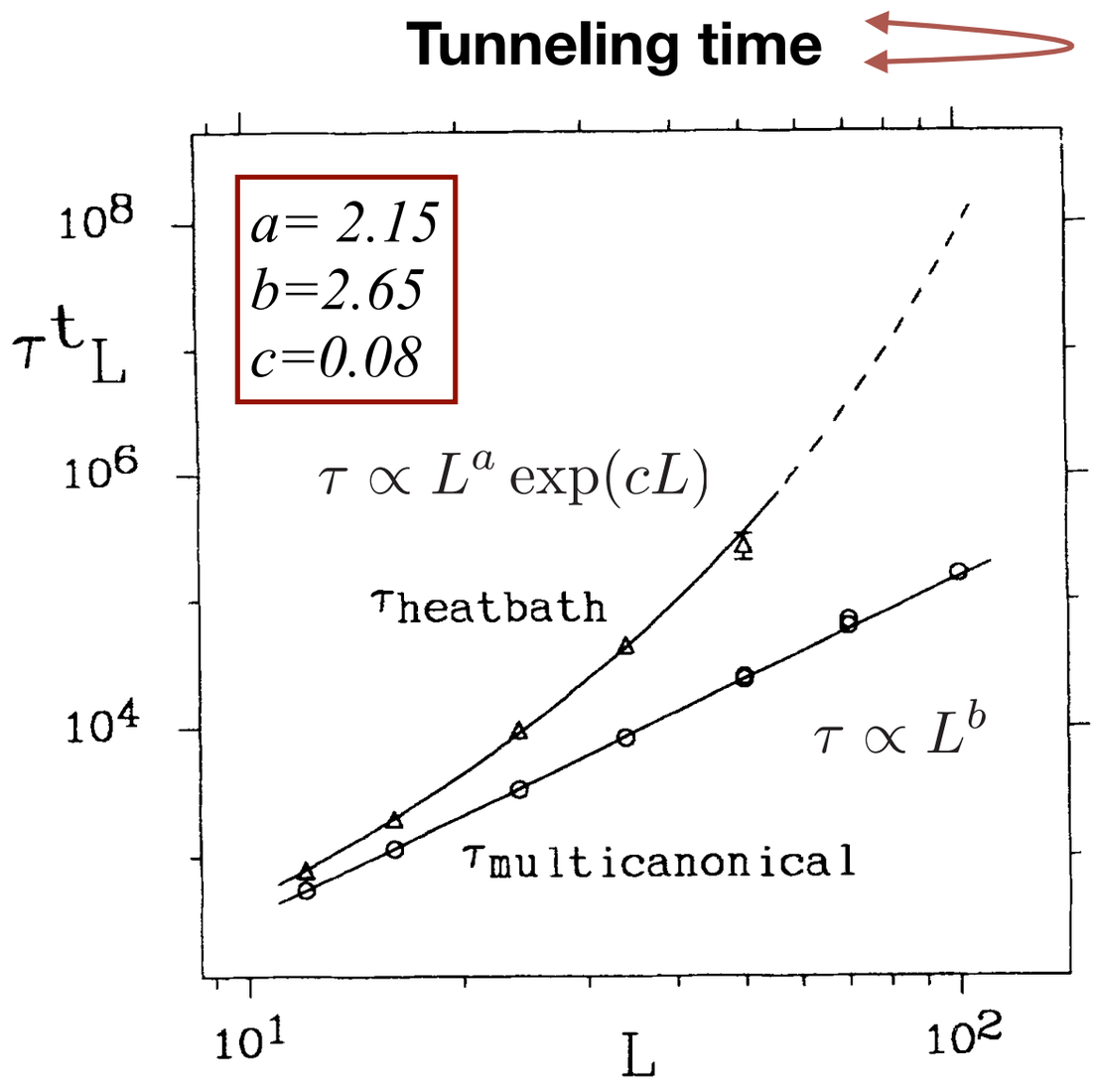
Multi Canonical method for q=10 Potts model

B.A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992)

Energy distribution around Tc



Tunneling time



By Multi canonical method, the tunneling time is reduced to the power of L!

Wang-Landau method

Need to update

Wang-Landau method

F. Wang and D. P. Landau (2001)

Another method to obtain the density of state:

Random walk on the energy space

Markov Chain Monte Carlo with the transition probability

$$W_{\Gamma\to\Gamma'} = \min\left(\frac{g(E(\Gamma))}{g(E(\Gamma'))}, 1\right)$$

$g(E)$:estimate of DOS

→ Its steady state is

$$P(\Gamma) \propto \frac{1}{g(E(\Gamma))}$$

The energy distribution (histogram) :

$$P(E)dE = P(\Gamma)d\Gamma = P(\Gamma)\rho(E)dE \propto \frac{\rho(E)}{g(E)}dE$$

if $g(E) = \rho(E)$ → This MCMC gives us a completely flat histogram!

Wang-Landau method:update of g(E)

F. Wang and D. P. Landau (2001)

Initially, we don't know DOS. → Set an initial guess, e.g. $g(E) = 1$

Along MCMC, we update $g(E)$ of the $E(\Gamma)$ as

$$g_{new}(E) = g(E) \times f \qquad (\log g_{new}(E) = \log g(E) + \log f)$$

*Note after N step, g(E) changes like

$$g_{new}(E) \sim g(E) f^{N \frac{\rho(E)}{g(E)}}$$

g(E) increases when $g(E) < \rho(E)$ for $f > 1$.

If the multiplication factor is "gradually" reduced to $f = 1$,

$g(E)$ eventually converges to $\rho(E)$.

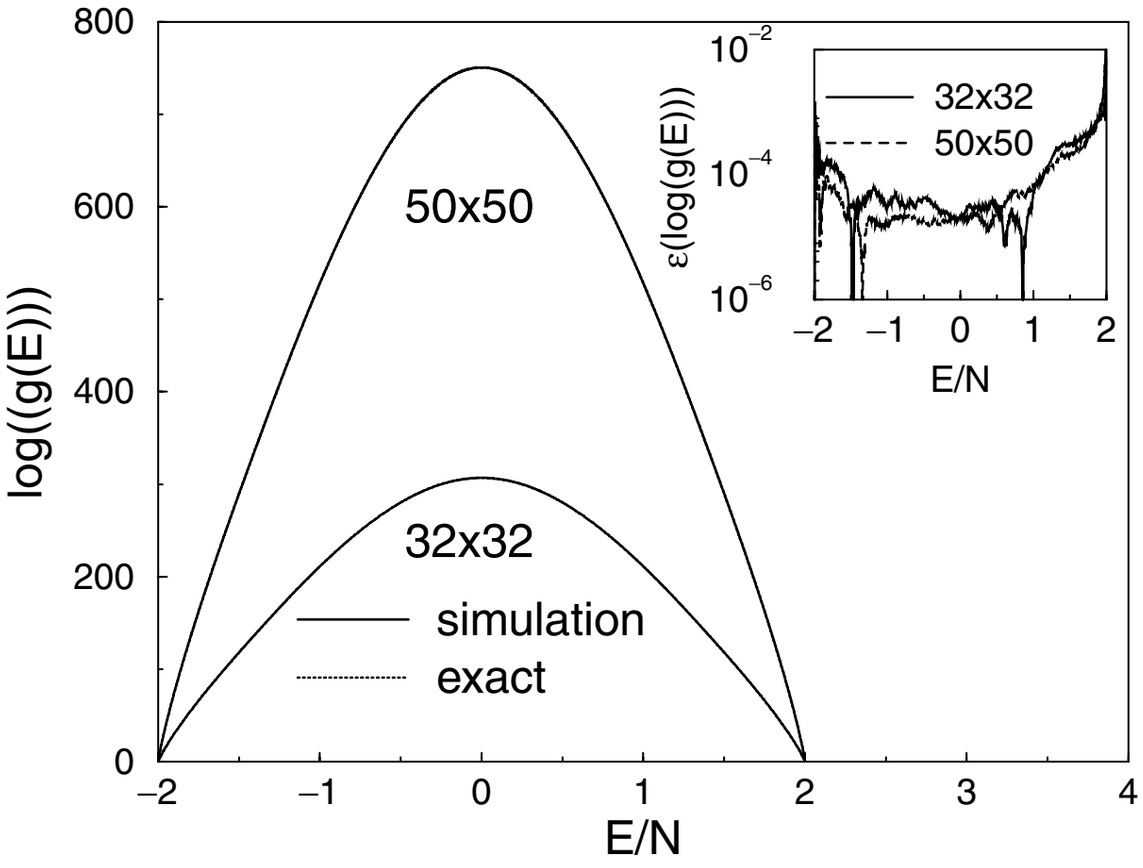
"gradual" change of f :

1. Initially $f = f_0$ (e.g. $f_0 = e^1$)
2. Loop i
   - If (the histogram $h(E)$ becomes "flat"?)
     - Then, we decrease f_i as
       $f_{i+1} = (f_i)^x$ (e.g. $x = 1/2$),
       and reset the histogram.
3. Repeat until f_i becomes enough small (e.g. $f \sim \exp(10^{-8})$)

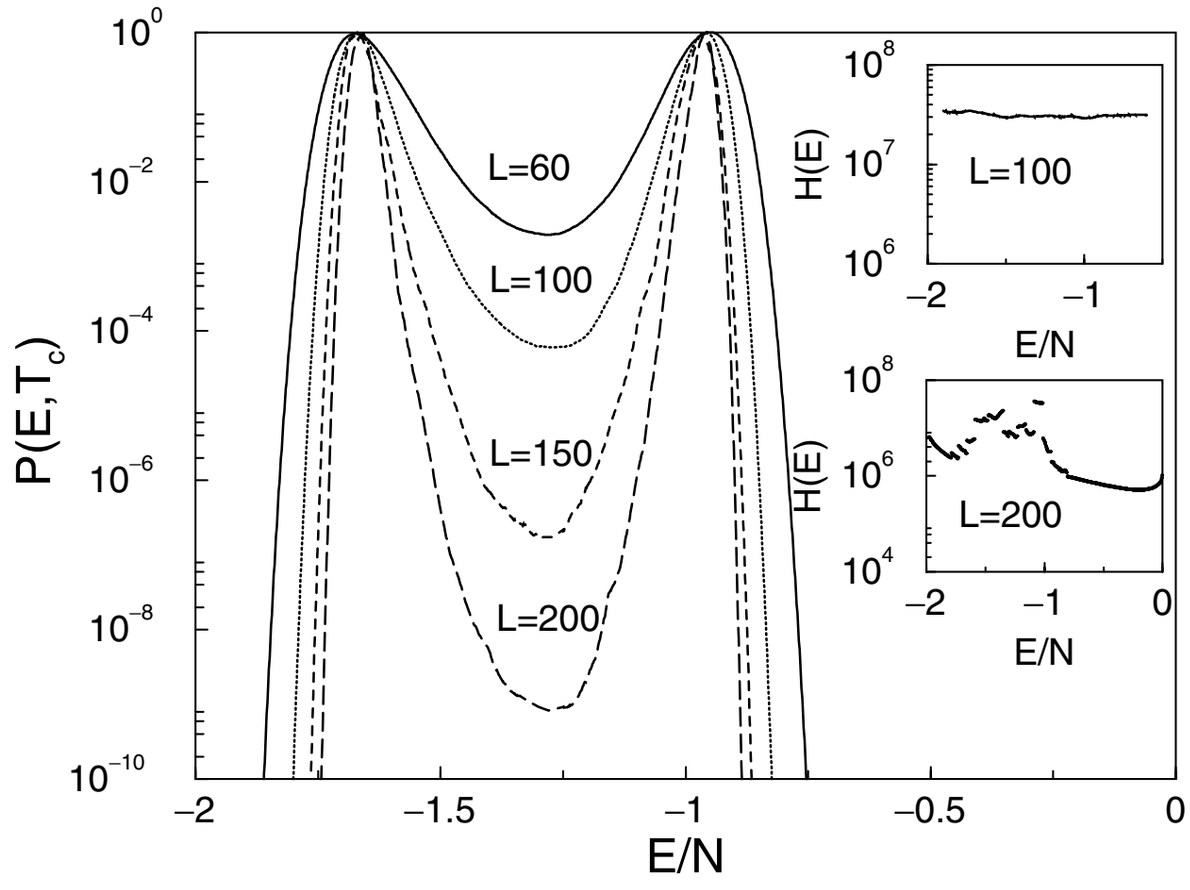
Power of Wang-Landau method

F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001)

Density of state of 2D-Ising model



Density of state of q=10 Potts model



We can obtain very accurate density of state by Wang-Landau method!

Replica Exchange method

K.Hukushim and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996).

Replica exchange (parallel tempering)

A different type of extended ensemble:

Usual MC or MD considers one parameter and one realization:

$$T,\ \Gamma = \{S_i\}, \{\boldsymbol{q}_i, \boldsymbol{p}_i\}$$

Replica exchange method considers
multiple parameters together with multiple realizations:

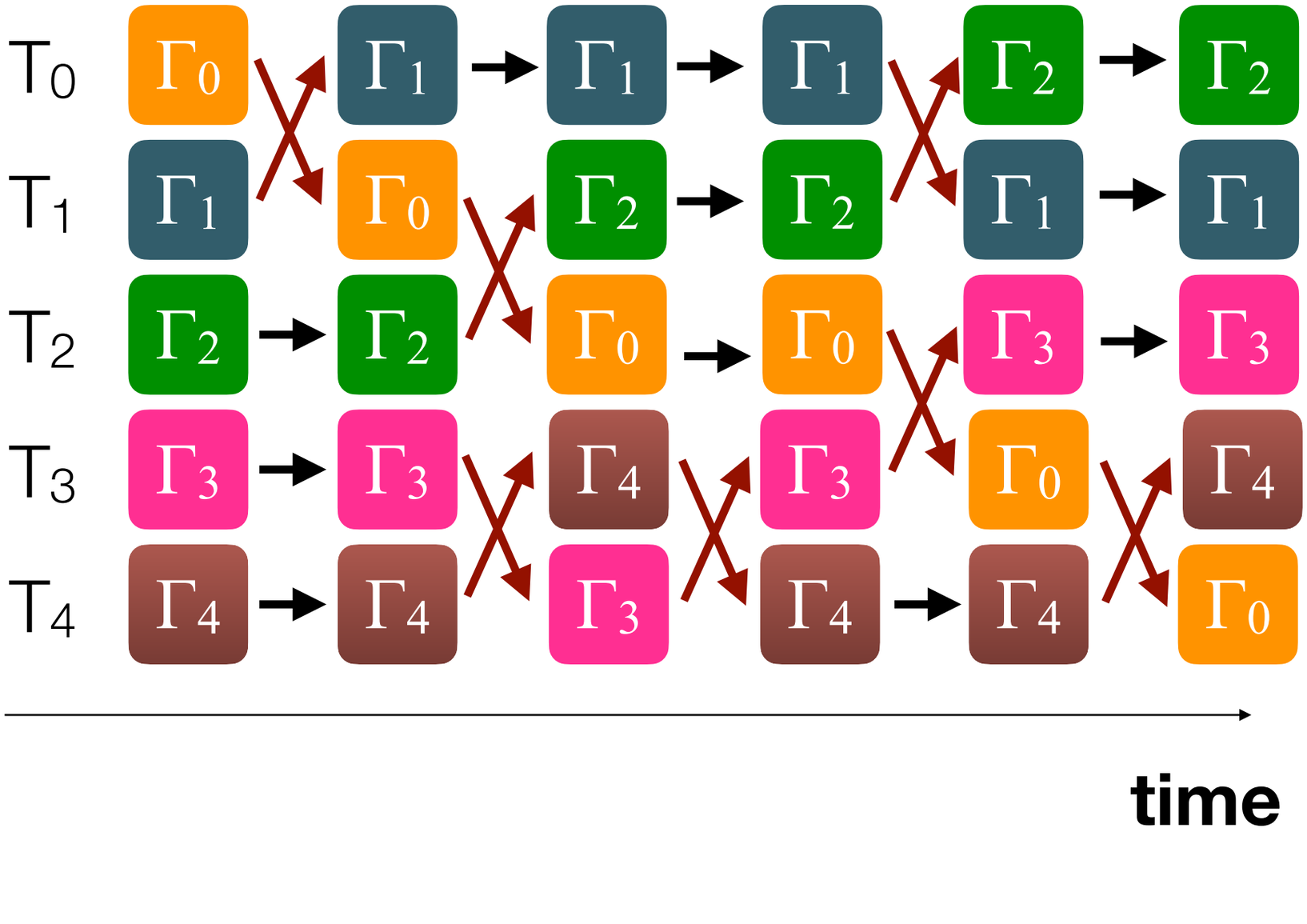
$$\{T_0, T_1, \cdots, T_M\},\ \{\Gamma_0, \Gamma_1, \cdots, \Gamma_M\},$$

Try to sample "(M+1)-dimensional" joint-distribution

$$P(\Gamma_0, \Gamma_1, \cdots, \Gamma_M; T_0, T_1, \cdots, T_M)$$

“Replica exchange”

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

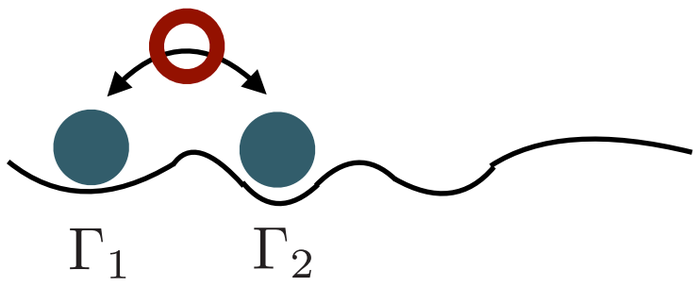


Purpose of replica exchange

Free energy landscape depends on the parameter

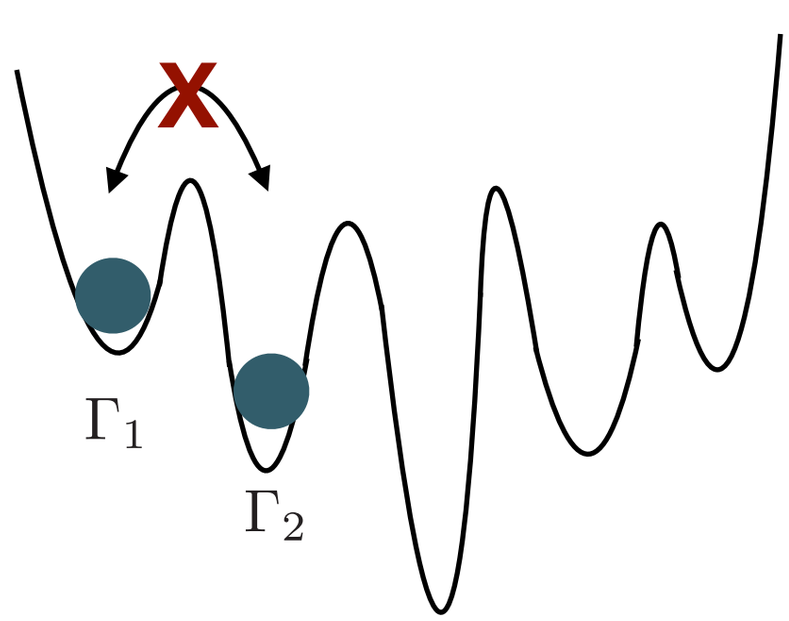
High temperature:T_h

Γ easily moves to other points!



Low temperature:T_l

Γ hardly moves to other minima!



Make a pass like:

$$\{\Gamma_1, T_l\} \rightarrow \{\Gamma_1, T_h\} \rightarrow \{\Gamma_2, T_h\} \rightarrow \{\Gamma_2, T_l\}$$

low **high** **high** **low**

* Parameter is not necessary a temperature.

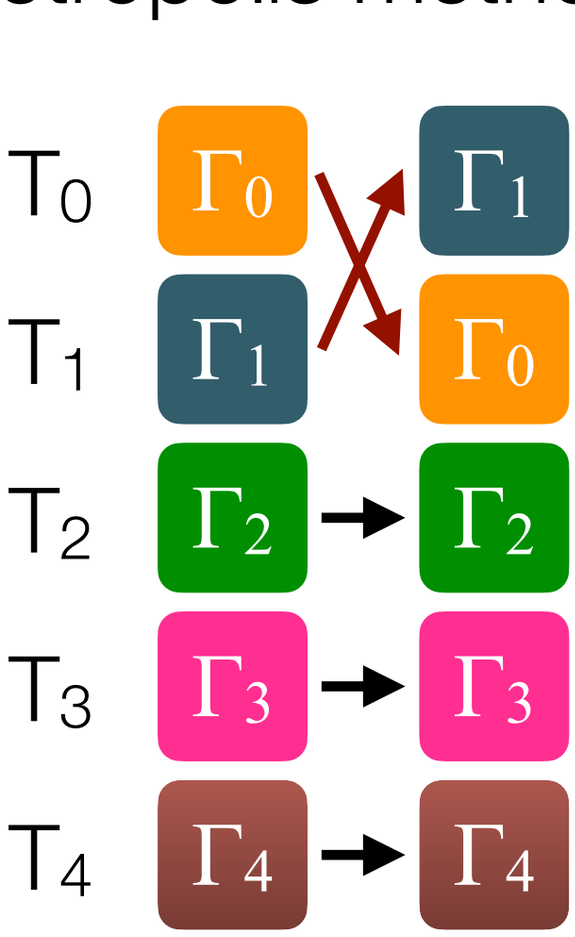
Markov Chain Monte Carlo for Replica Exchange

Target steady state distribution:

$$P(\Gamma_0, \Gamma_1, \cdots, \Gamma_M; T_0, T_1, \cdots, T_M) \propto e^{-\sum_i^M \beta_i E_i}$$

$$E_i \equiv \mathcal{H}(\Gamma_i)$$

Metropolis method:



$\mathcal{T}$ **:sequence of temperatures**

$$\mathcal{T} = \{T_1, T_0, T_2, \cdots\}$$

$$\{T_0, \Gamma_0\}, \{T_1, \Gamma_1\} \to \{T_1, \Gamma_0\}, \{T_0, \Gamma_1\}$$

$$\mathcal{T}_{01} \qquad\qquad \mathcal{T}_{10}$$

Transition probability

$$W_{\mathcal{T}_{01} \to \mathcal{T}_{10}} = \min\left(1, \frac{P(\{\Gamma_i\}; \mathcal{T}_{10})}{P(\{\Gamma_i\}; \mathcal{T}_{01})}\right)$$

$$\frac{P(\{\Gamma_i\}; \mathcal{T}_{10})}{P(\{\Gamma_i\}; \mathcal{T}_{01})} = \frac{e^{-\beta_1 E_0 - \beta_0 E_1}}{e^{-\beta_0 E_0 - \beta_1 E_1}}$$

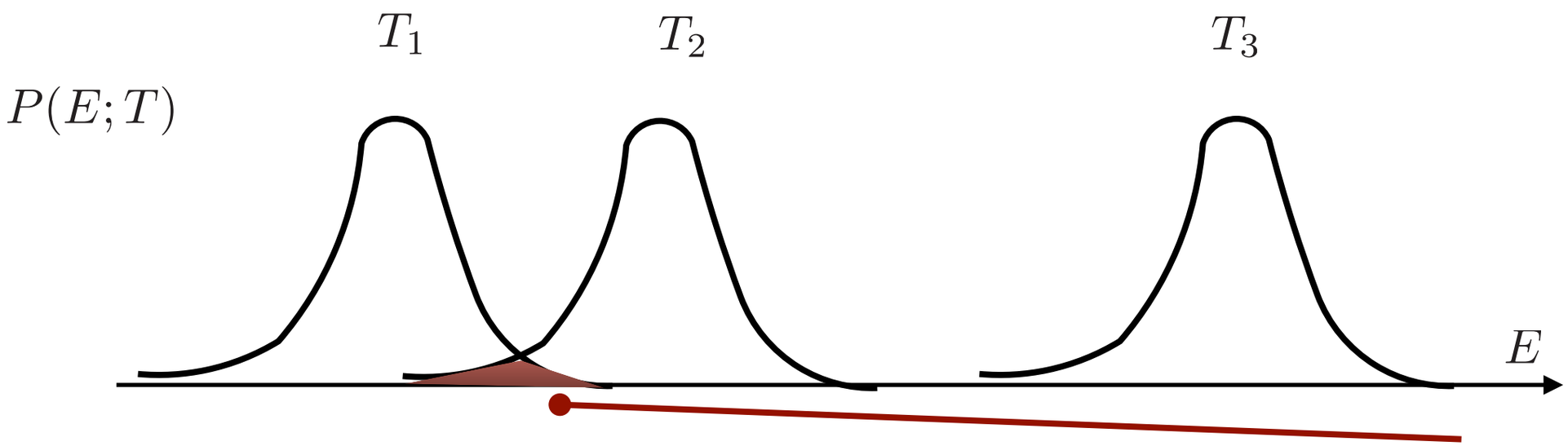
$$= e^{(\beta_0 - \beta_1)(E_0 - E_1)}$$

Select of temperature sequence

$$\frac{P(\{\Gamma_i\};\mathcal{T}_{10})}{P(\{\Gamma_i\};\mathcal{T}_{01})} = e^{(\beta_0-\beta_1)(E_0-E_1)} = \frac{P(E_1;T_0)P(E_0;T_1)}{P(E_0;T_0)P(E_1;T_1)}$$

Energy distribution at T

$P(E;T)$



Almost all exchange occurs the energy region of “overlap”.

$\{\Gamma_1, T_1\}, \{\Gamma_2, T_2\} \rightarrow \{\Gamma_1, T_2\}, \{\Gamma_2, T_1\}$:acceptable!

$\{\Gamma_2, T_2\}, \{\Gamma_3, T_3\} \rightarrow \{\Gamma_2, T_3\}, \{\Gamma_3, T_2\}$:almost rejected!

For efficient exchange, we have to choose a sequence of temperatures so that the energy distributions have finite overlap!

Usually we only exchange the nearest neighbor pairs of temperatures

Select of temperature sequence: Example

Suppose $C = \dfrac{dE}{dT} = \text{const.}$

$$\frac{P(\{\Gamma_i\}; \mathcal{T}_{10})}{P(\{\Gamma_i\}; \mathcal{T}_{01})} = e^{(\beta_0 - \beta_1)(E_0 - E_1)}$$

➡ Temperature sequence satisfying almost "flat" transition probability

$$(\beta_i - \beta_{i+1})(E_i - E_{i+1}) = \text{const.}$$

$$\Leftrightarrow \quad C\frac{(T_{i+1} - T_i)^2}{T_{i+1}T_i} = \text{const.}$$

$$\Rightarrow \quad T_{i+1} = \alpha T_i \quad \textbf{:Temperatures are geometric sequence!}$$

$$\alpha \sim 1 + O(1/\sqrt{C})$$

Important notice:

Heat capacity C is an extensive quantity: $C \sim O(N)$

➡ In order to keep finite overwrap, we need to increase temperature point M as

$$M \propto \sqrt{N} \qquad (T_{max} = T_M = \alpha^M T_{min})$$

Relaxation time of the replica exchange

In order to confirm the equilibration of the whole system,
usually we need two criterions.

1. The correlation time at the highest temperature is sufficiently short,
   e.g. $\tau=O(1)$

   → If a replica visits the highest temperature, it can easily change its state Γ.

2. All replicas make several (~O(10)) round trips between
   the lowest and the highest temperatures

   → The ensemble at the lower temperature is in the equilibrium.

The second part determines the relaxation time of the method.

$$\tau_{\mathrm{RE}} \sim \text{round trip time}$$

* If the replica exchange is an random walk:

$$\text{round trip time} \propto M^2$$

Summary of replica exchange

Algorithm:

1. Make a temperature set $\{T_1, T_2, \ldots, T_M\}$
2. Loop n
   (1) Do MC or MD for M replicas: $\{\Gamma_1, \Gamma_2, \ldots \Gamma_M; T_1, T_2, \ldots, T_M\}$
   (2) Calculate the energies of replicas
   (3) Try replica exchange based on, e.g. Metropolis method
   - Usually we alternatively try replica exchange such as
     even n; $\{1\leftrightarrow2\},\{3\leftrightarrow4\},\{5\leftrightarrow6\},\ldots$
     odd n; $\{2\leftrightarrow3\},\{4\leftrightarrow5\},\{6\leftrightarrow7\},\ldots$
     Note: each exchange trial is independent
   (4) Observe the quantities for $\{\Gamma_1, \Gamma_2, \ldots \Gamma_M; T_1, T_2, \ldots, T_M\}$

If we already have a MC or MD programs,
it is very easy to introduce the replica exchange method!

Next week (5/23)

Classical

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

Quantum

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