Optimized statistical ensembles

for slowly equilibrating classical and quantum systems

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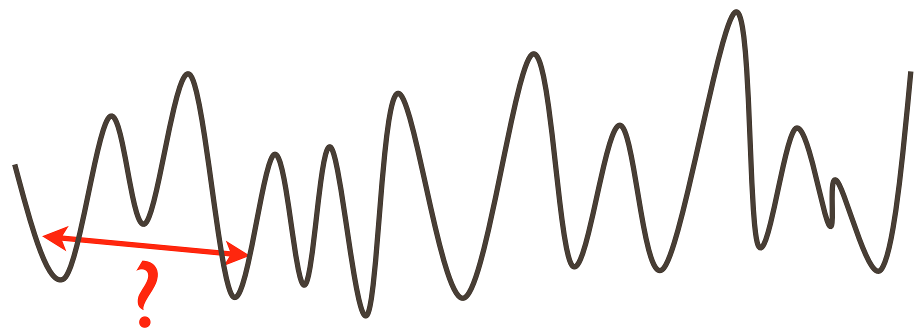
Motivation

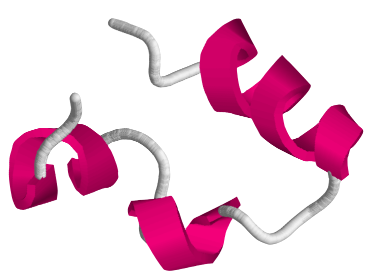
Many interesting phenomena in complex many-body systems
arise only in the presence of

- **multiple energy scales**
- **complex energy landscapes**
- **slow equilibration**

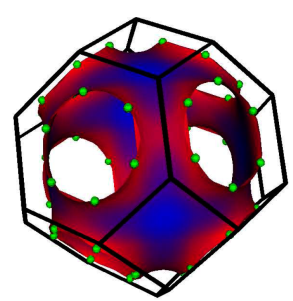


critical behavior

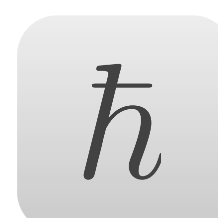
folding of proteins



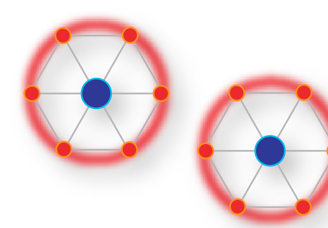
frustrated magnets



quantum systems

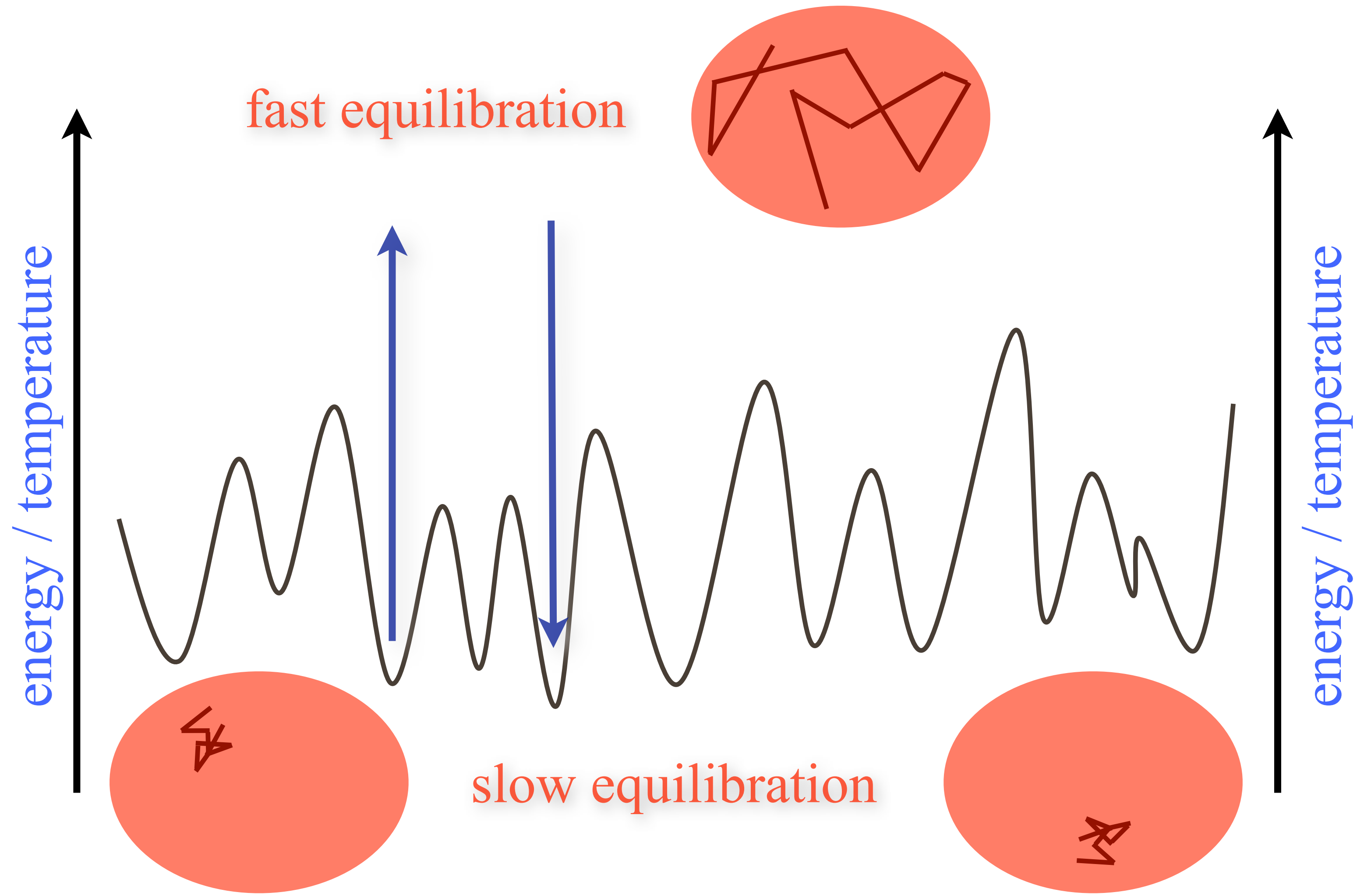


dense liquids



Random walks in energy/temperature

Random walk in temperature space increases equilibration.

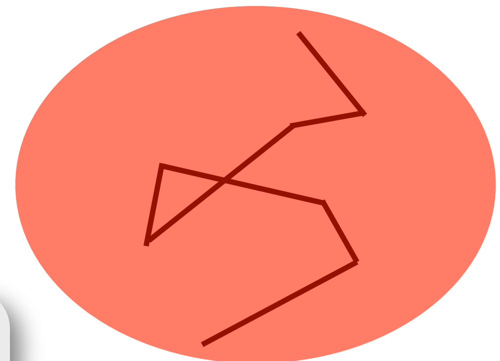


Simulation of Markov chains

Monte Carlo, parallel tempering, replica exchange molecular dynamics

- Sample configurations in **phase space**

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_i \longrightarrow c_{i+1} \longrightarrow \ldots$$



Metropolis algorithm (1953)

propose a (small) change to a configuration

$$\underbrace{\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow}_{c_i} \longrightarrow \underbrace{\uparrow\uparrow\uparrow\uparrow\Downarrow\uparrow\uparrow\uparrow}_{c_j}$$

accept/reject the update with probability

$$p_{acc} = \min\left(1, \frac{w(c_j)}{w(c_i)}\right)$$

How do we choose these weights?

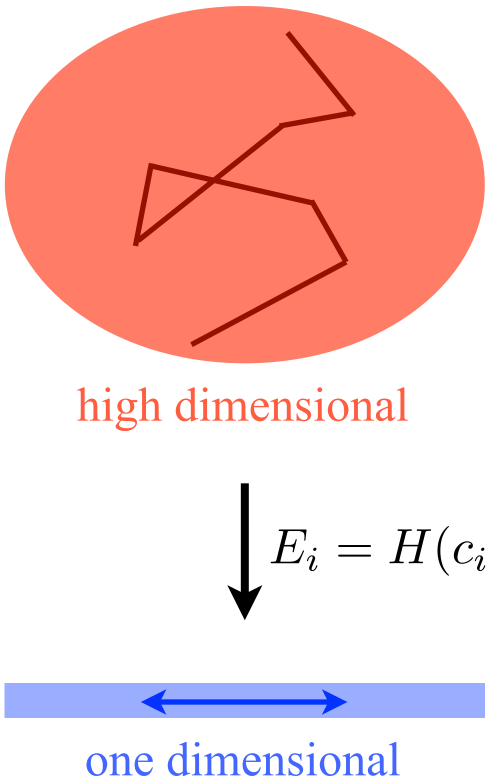
Statistical ensembles

- Sample configurations in **phase space**

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_i \longrightarrow c_{i+1} \longrightarrow \ldots$$

- Project onto random walk in **energy space**

$$E_1 \longrightarrow E_2 \longrightarrow \ldots \longrightarrow E_i \longrightarrow E_{i+1} \longrightarrow \ldots$$



- We define a **statistical ensemble**

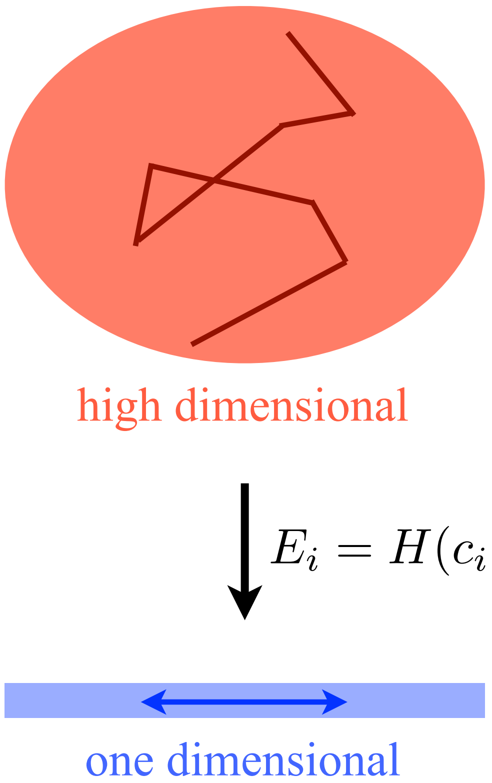
$$w(c_i) = w(E_i) = \exp(-\beta E_i)$$

$$p_{acc}(E_1 \to E_2) = \min\left(1, \frac{w(E_2)}{w(E_1)}\right) = \min\left(1, \exp(-\beta \Delta E)\right)$$

Statistical ensembles

- Sample configurations in **phase space**

$$c_1 \rightarrow c_2 \rightarrow \ldots \rightarrow c_i \rightarrow c_{i+1} \rightarrow \ldots$$



- Project onto random walk in **energy space**

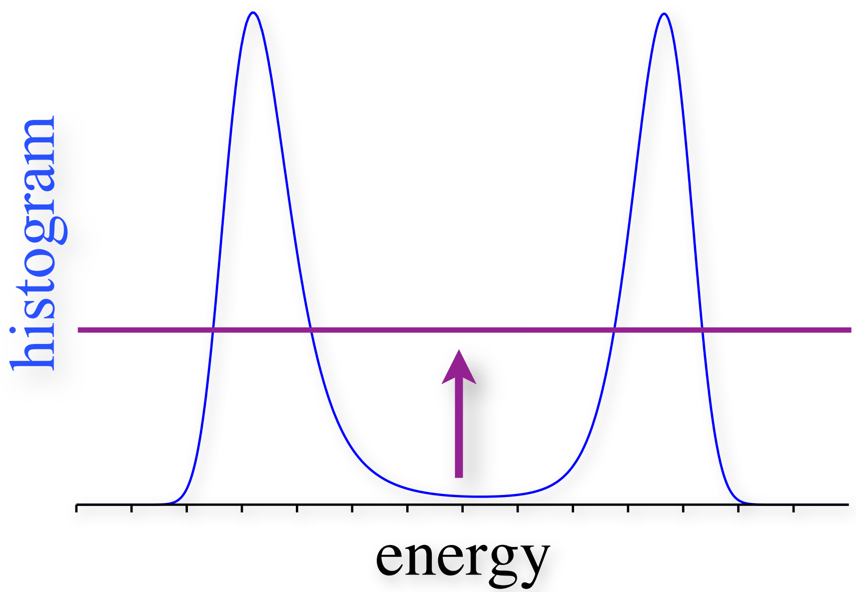
$$E_1 \rightarrow E_2 \rightarrow \ldots \rightarrow E_i \rightarrow E_{i+1} \rightarrow \ldots$$

- **Phase space:** The simulated system does a biased, but **Markovian** random walk.

- **Energy space:** The projected random walk is **non-Markovian**, as memory is stored in the system's configuration.

Extended ensemble simulations

- **Broaden the sampled energy space**, e.g. by sampling a flat histogram.



$$w(E) = \exp(-\beta E)$$

$$w(E) = 1/g(E)$$

density of states

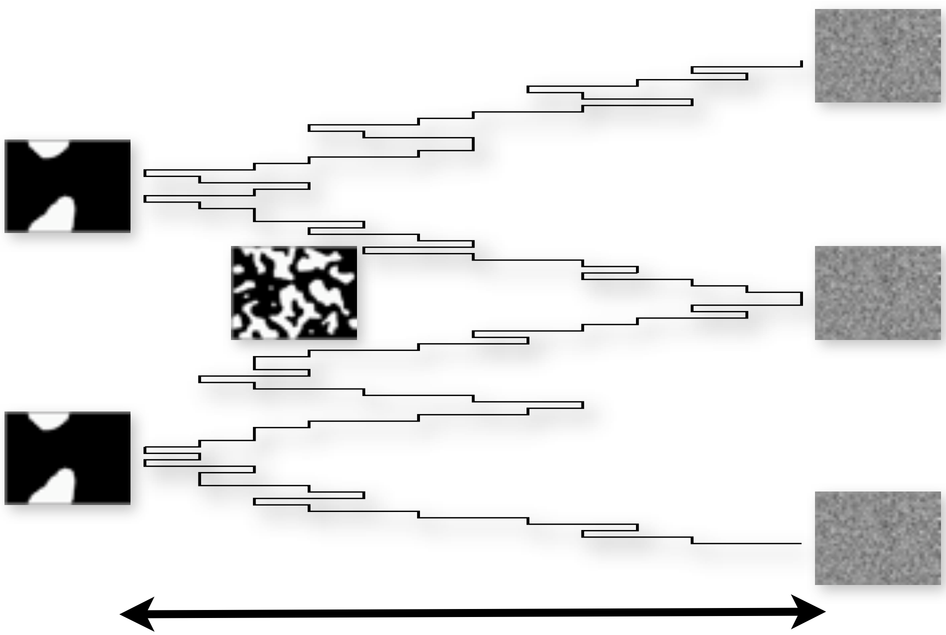
$$n_w(E) = w(E)\, g(E)$$

histogram

weight / ensemble

Multicanonical simulations, Berg & Neuhaus
Wang-Landau algorithm

How well does this work?

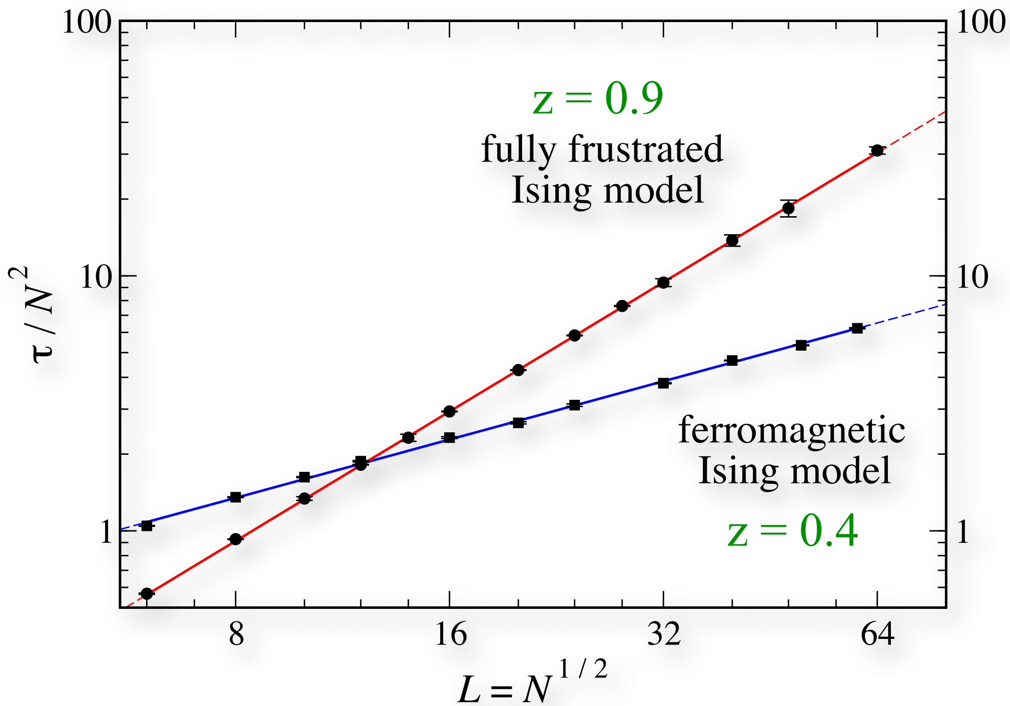


$$E \sim N$$

The energy range scales like N.

$$\tau \sim N^2$$

The round-trip time should scale like N^2.



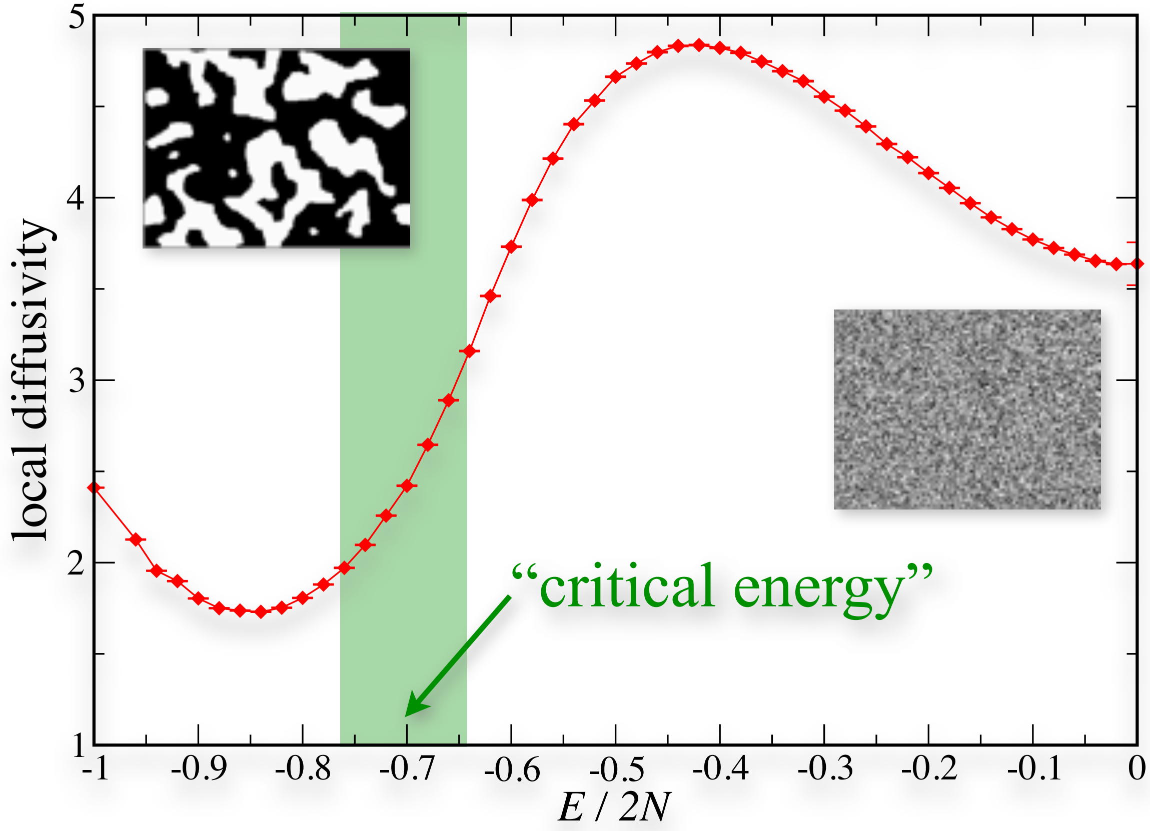
Flat-histogram sampling

$$\tau \sim N^{2+z}$$

Critical slowing down.

The problem: local diffusivity not constant

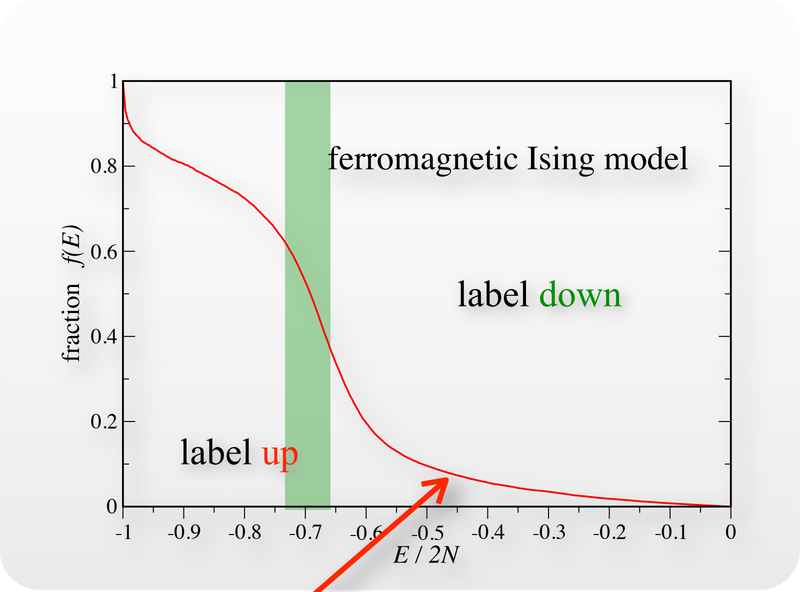
$$D(E, t_D) = \langle [E(t) - E(t + t_D)]^2 \rangle / t_D$$



- The **local diffusivity** is **NOT** independent of the energy.

Optimizing the ensemble

Measure the **current** in the energy interval



local diffusivity

$$j = D(E)\, n_w(E)\, \frac{df}{dE}$$

current

histogram

derivative of fraction

Determine the **local diffusivity**.

Maximize current by varying histogram/ensemble.

Phys. Rev. E **70**, 046701 (2004).

Optimizing the ensemble (cont'd)

Optimal histogram turns out to be

$$n_w^{(opt)}(E) \propto \frac{1}{\sqrt{D(E)}}$$

Ensemble optimization algorithm

Feedback the local diffusivity

optimized ensemble

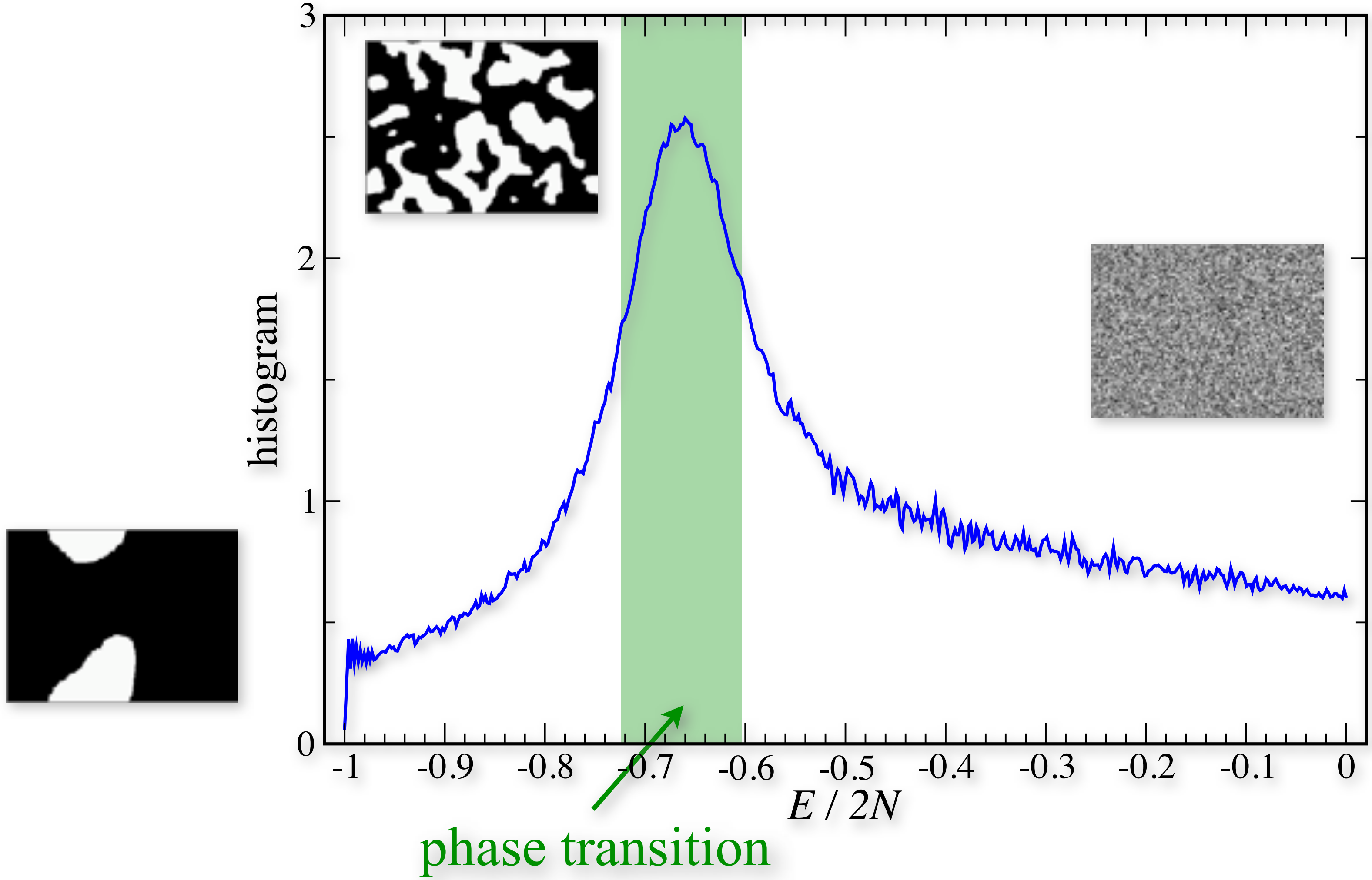
$$w'(E) \propto w(E) \cdot \sqrt{\frac{df}{dE} \cdot \frac{1}{n_w(E)}}$$

original ensemble

and **iterate** feedback until convergence.

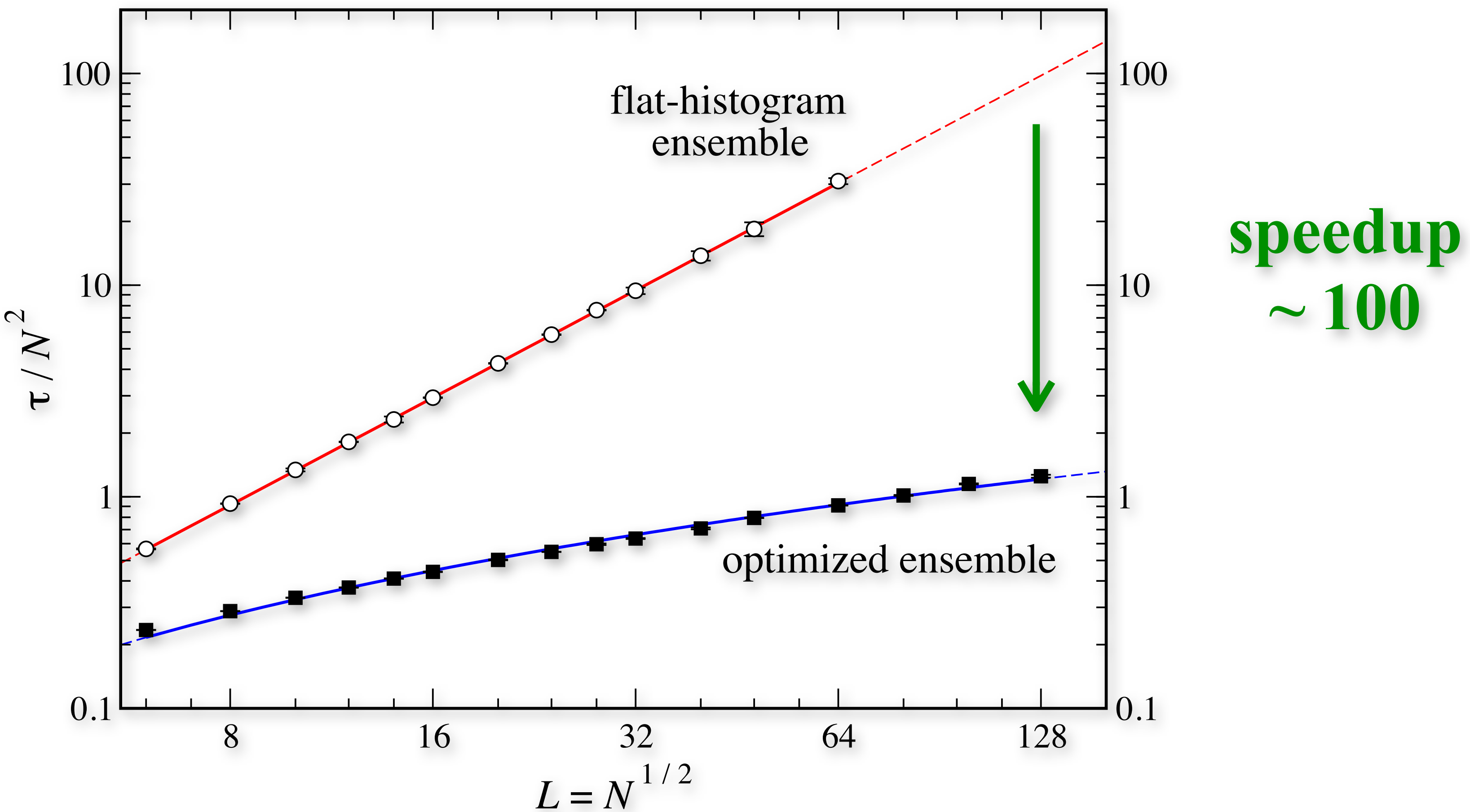
Phys. Rev. E **70**, 046701 (2004).

Optimized histogram



- **Feedback reallocates resources** towards the critical energy.

Performance of optimized ensemble

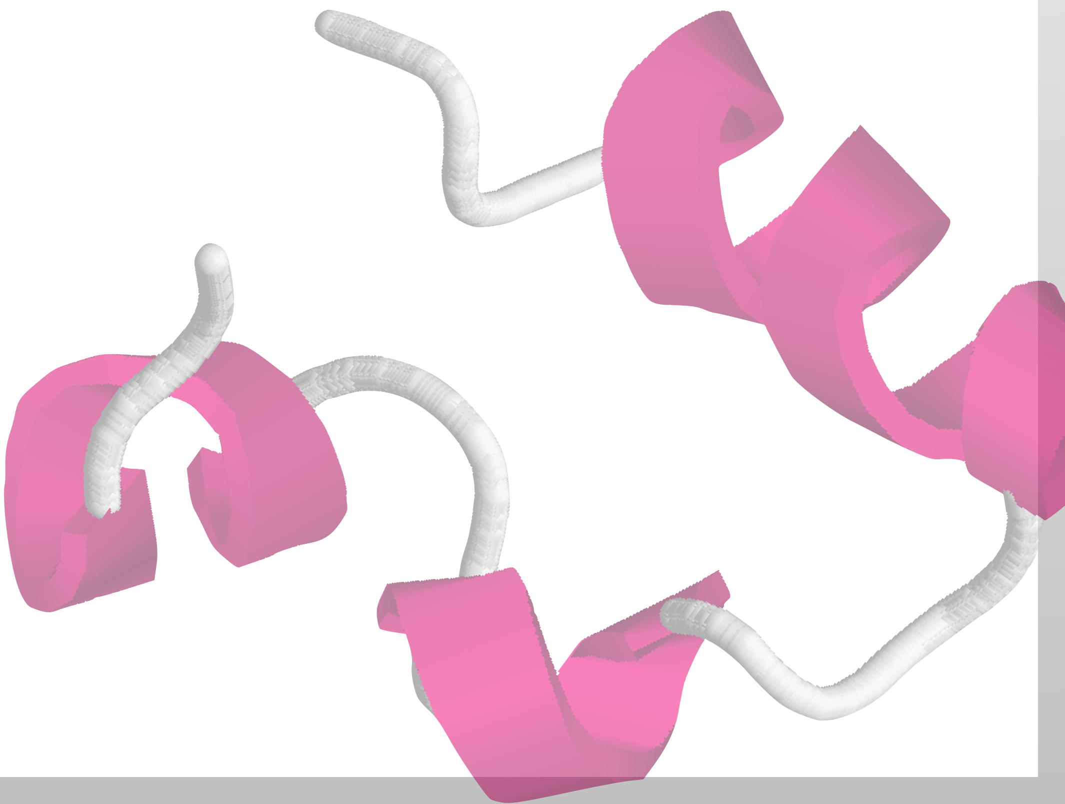


The round-trip times scale like $O\left([N \log N]^2\right)$.

Example

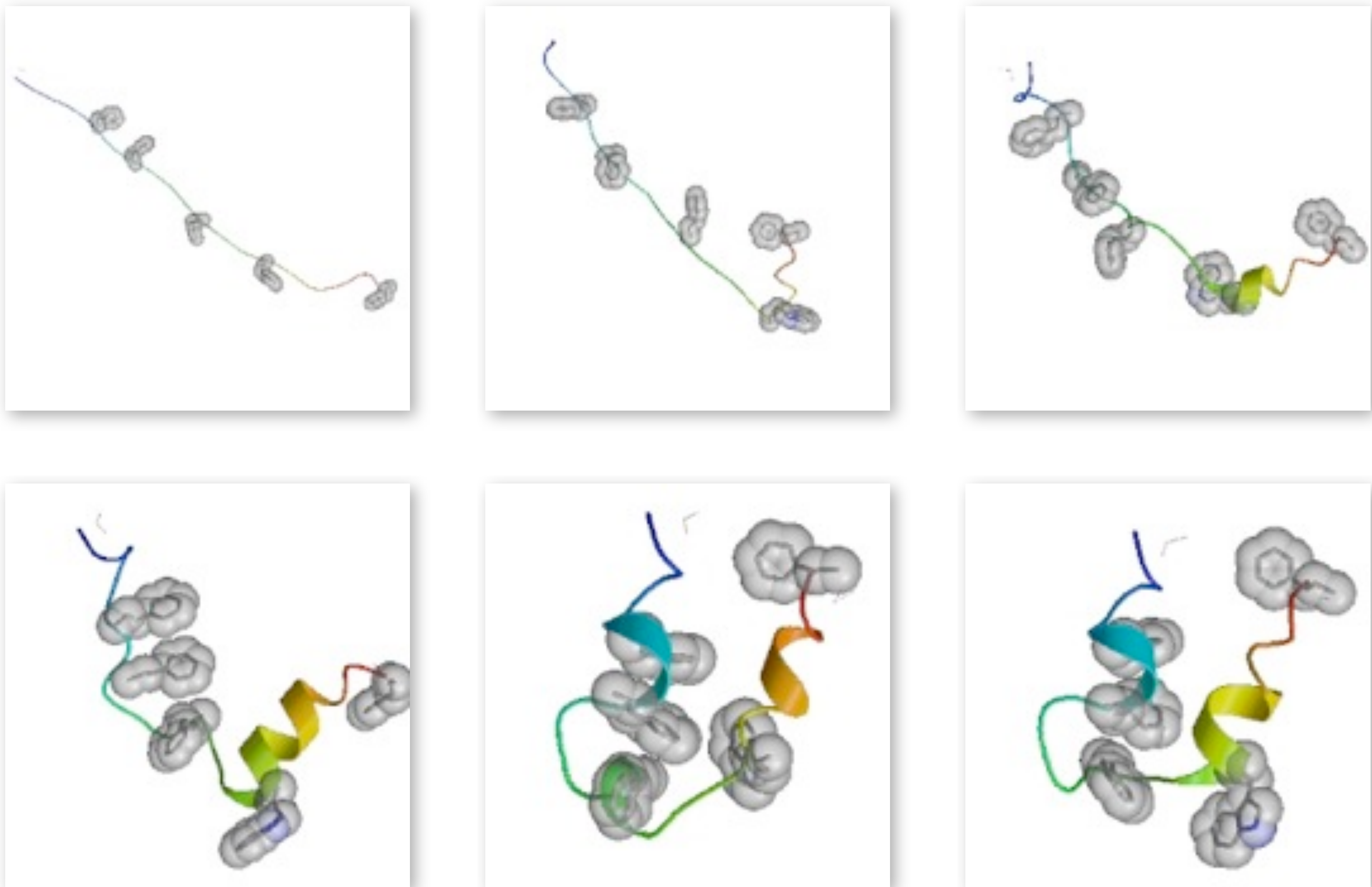
Folding of a (small) protein

ST, M. Troyer, U.H.E. Hansmann
J. Chem. Phys. **124**, 174903 (2006).



A small protein: HP-36

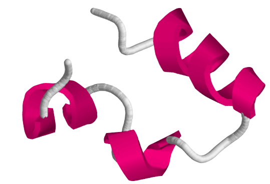
The chicken villin headpiece



folding@home project

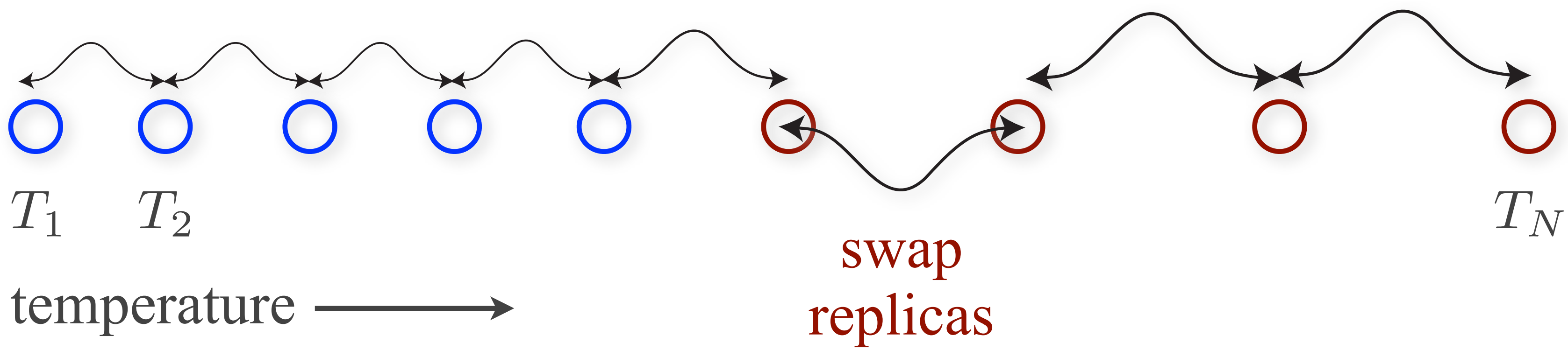
folding time: 4.3 microseconds

Parallel tempering



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

Simulate **multiple replicas** of the system at various temperatures.

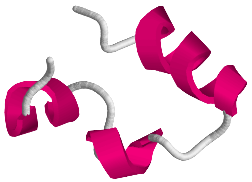


$$p(E_i, T_i \rightarrow E_{i+1}, T_{i+1}) = \min(1, \exp(\Delta\beta\Delta E))$$

Single replica performs **random walk** in temperature space.

How do we choose the temperature points?

Ensemble optimization



Feedback algorithm

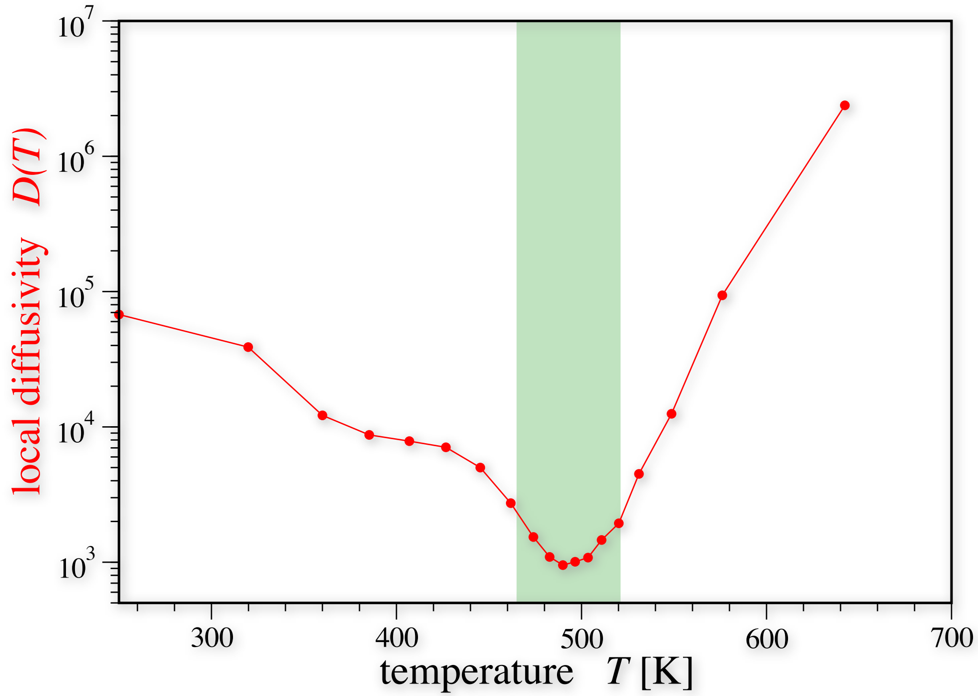
Measure **local diffusivity** $D(T)$ of current in temperature space.

Optimal choice of temperatures

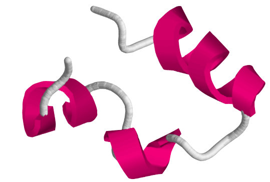
$$\boxed{\eta^{\mathrm{opt}}(T)} \sim \frac{1}{\sqrt{D(T)}}$$

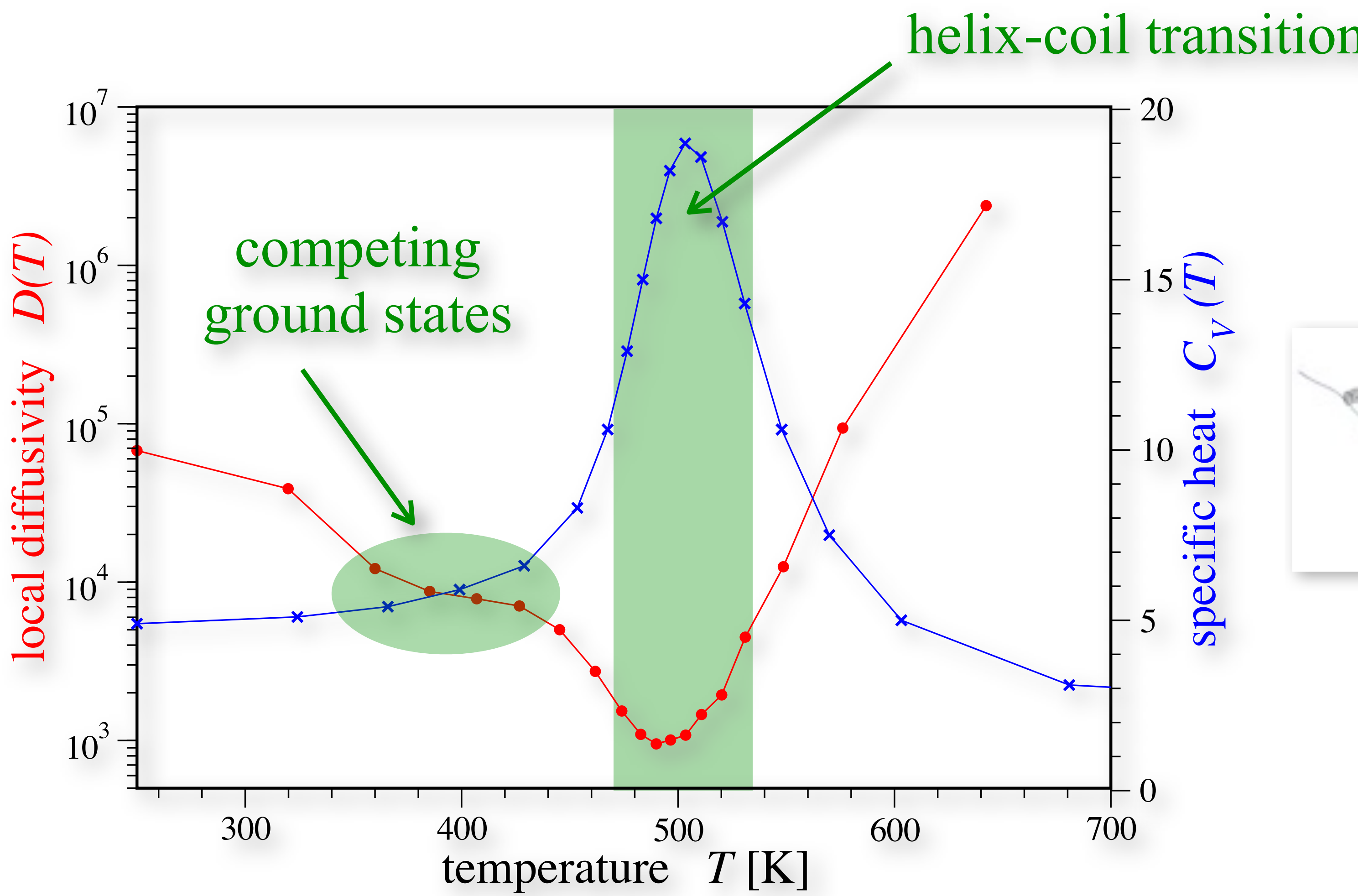
density of T-points

Iterate feedback of diffusivity.



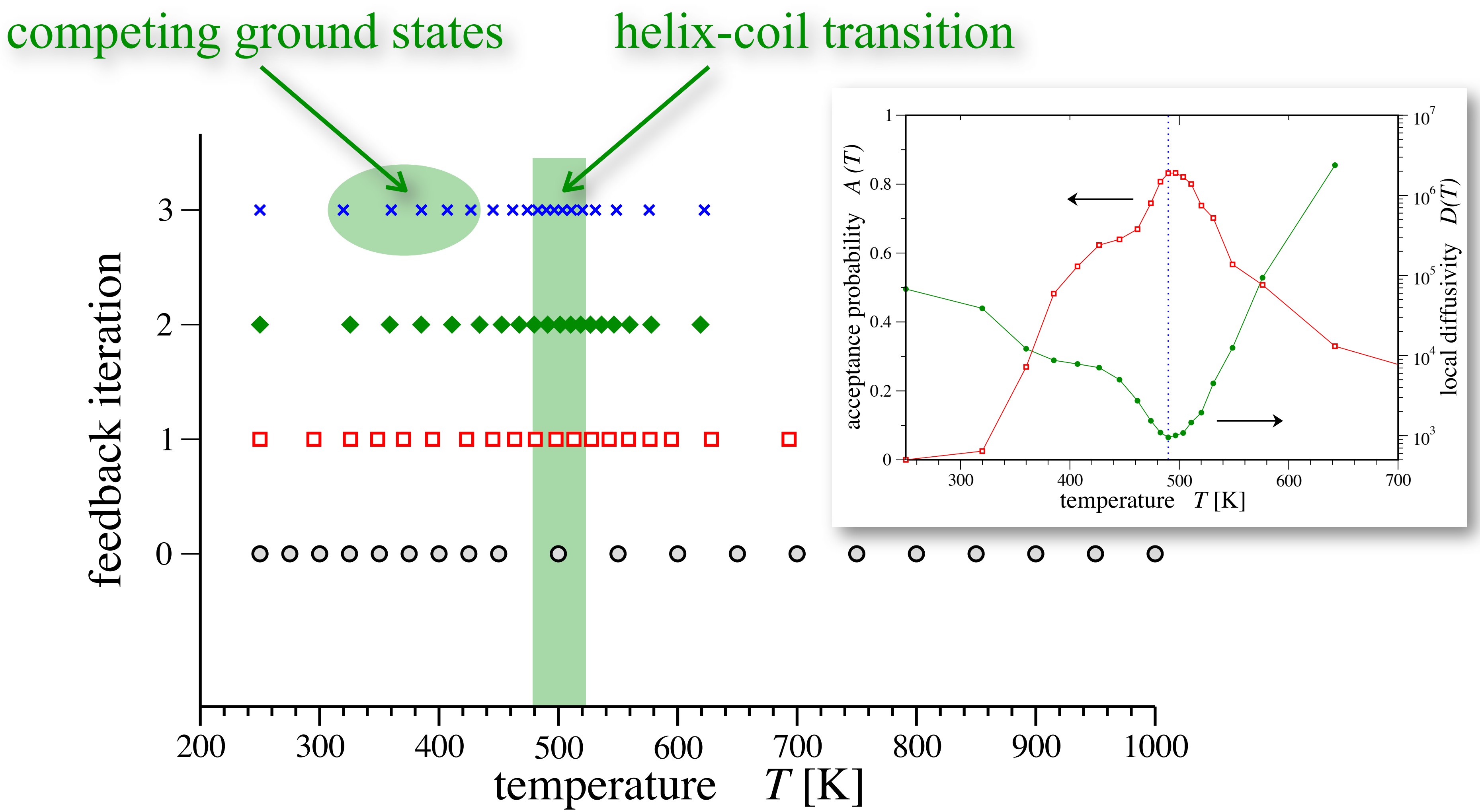
Random walk in temperature





- **Multiple temperature scales** are revealed by the local diffusivity.

Optimized temperature sets



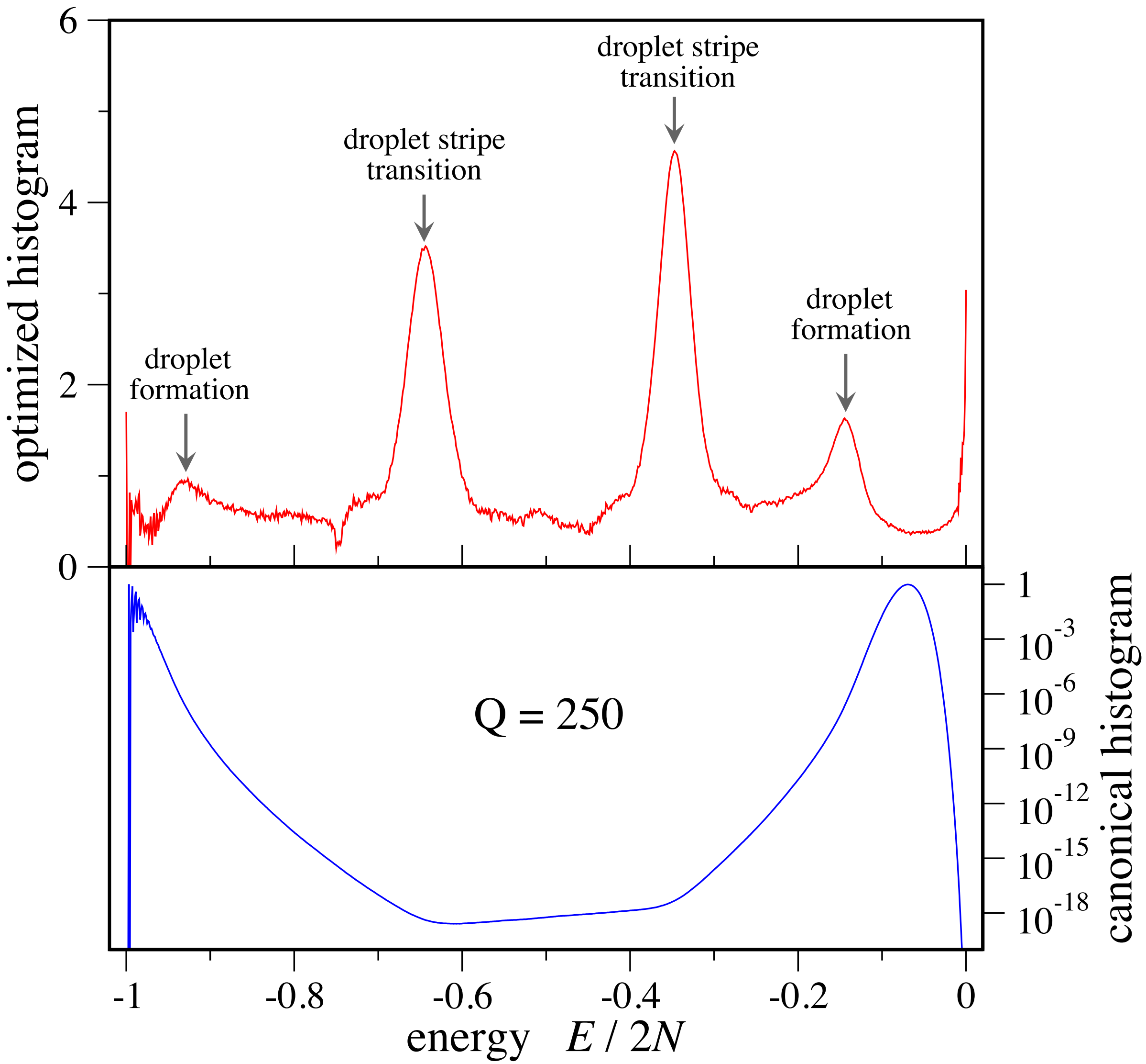
- Feedback reallocates resources towards the relevant temperature scales.

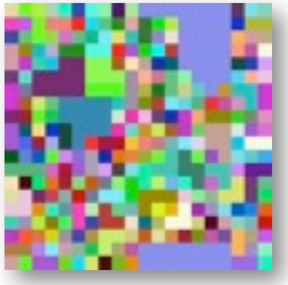
Example

Strong first-order transitions

B. Bauer, E. Gull, ST, M. Troyer, and D.A. Huse
J. Stat. Mech. P01020 (2010).

The large-Q Potts model





droplet formation

droplet stripe transition

droplet formation

Example

Quantum systems

S. Wessel, N. Stoop, E. Gull, ST, M. Troyer
J. Stat. Mech. P12005 (2007).

Quantum systems

$\hbar$

Reconsider the high-temperature series expansion

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}\,(-H)^n = \sum_{n=0}^{\infty} \boxed{g(n)}\, \beta^n$$

coefficients
"density of states"

We can define a broad-histogram **ensemble in the expansion order**.

M. Troyer, S. Wessel & F. Alet, PRL **90**, 120201 (2003).

Stochastic series expansion (SSE) samples these coefficients

$n \to 0$

high temperatures

?

$\langle n \rangle \propto \beta N$

$n \to \infty$

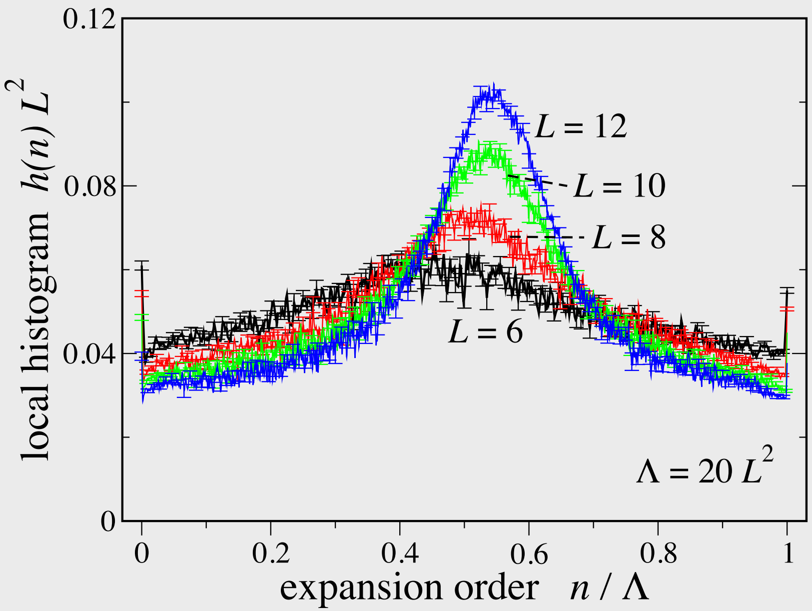
low temperatures

Examples

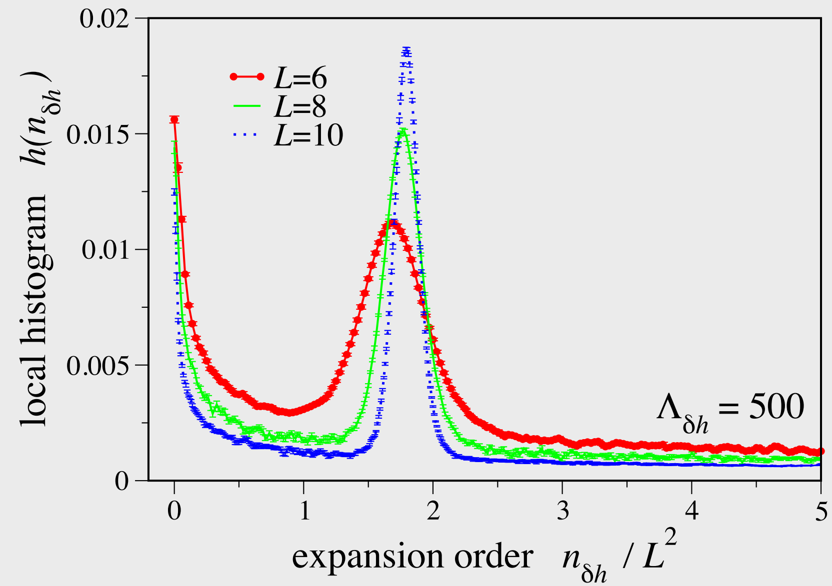
Thermal first-order transition

hard-core bosons
with next-nearest neighbor repulsion

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V_2 \sum_{\langle\langle i,k \rangle\rangle} n_i n_k - \mu \sum_i n_i$$



Spin-flop transition

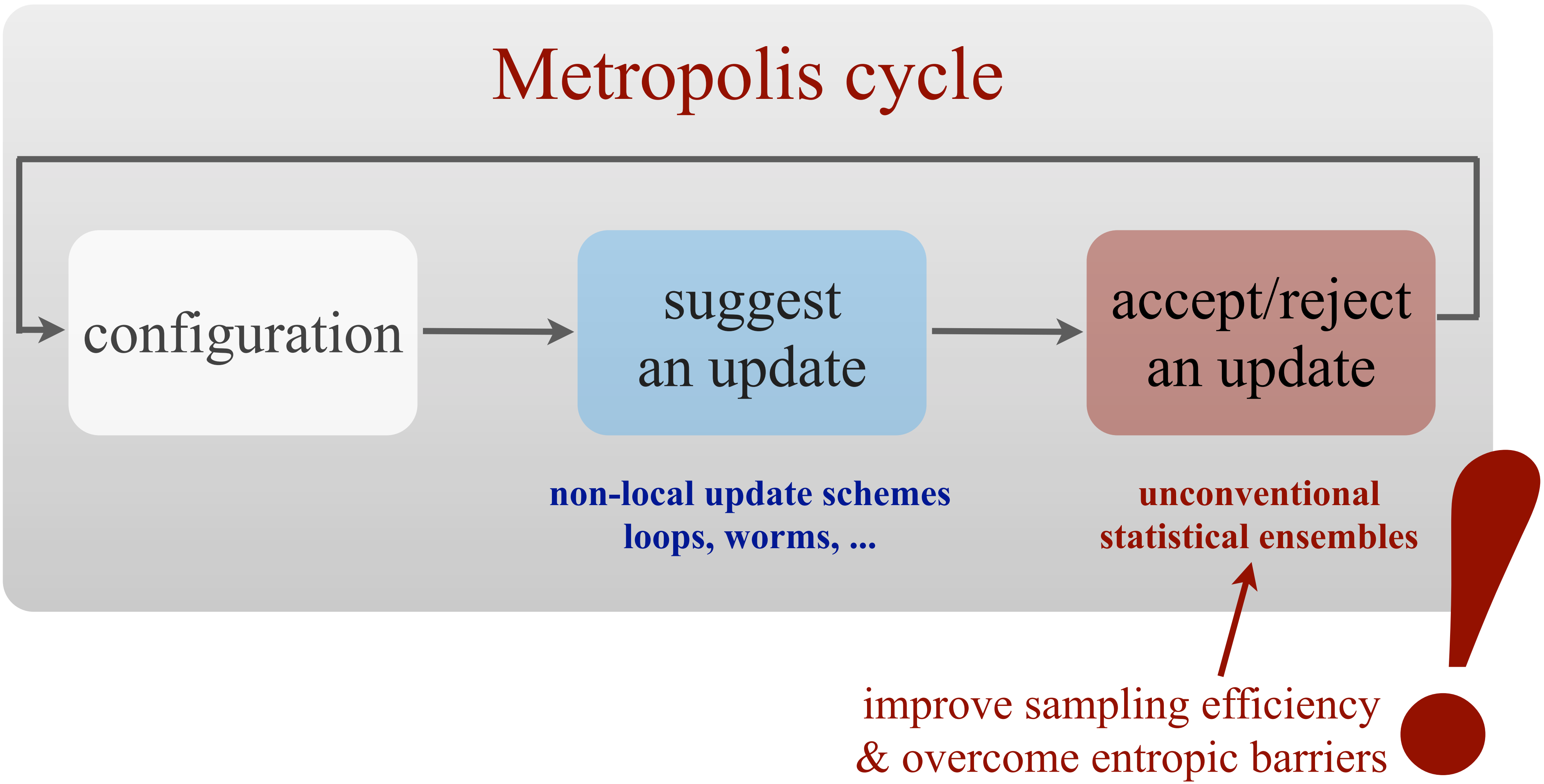


spin-1/2 XXZ model in a magnetic field

$$H = J \sum_{<i,j>} \left[S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right]$$

$$-h \sum_i S_i^z$$

Summary



Phys. Rev. E **70**, 046701 (2004).
J. Chem. Phys. **124**, 174903 (2006).