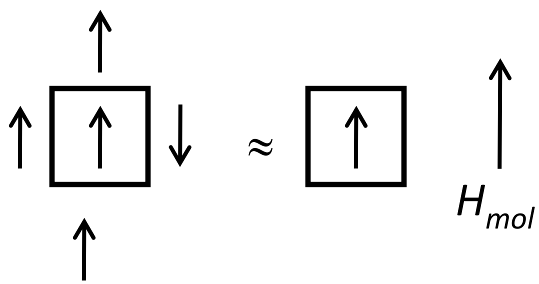
Mean field theory

focus on one spin

assume neighboring spins apply an average field



$$E_v = -\mu H \sum s_i - \frac{1}{2}\sum_{i,j} J_{ij} s_i s_j \qquad J_{ij} = J, \;\; i, j \;\; \text{nearest neighbors}$$

$$-\frac{2E_v}{2s_i} = \mu H + \sum_j J_{ij} s_j \qquad\qquad 0 \quad \text{otherwise}$$

$$\mu H_i = \mu H + \sum_j J_{ij} s_j$$

$$\langle H_i \rangle = H + \sum J_{ij} \langle s_j \rangle / \mu$$

$$= H + Jz \langle s_i \rangle / \mu, \qquad z = \text{ \# nearest neighbors}$$

$$\langle s_1 \rangle \approx \frac{\sum_{s_1=\pm 1} s_1 \left(e^{\beta\mu(H+\Delta H)s_1} \right)}{\sum_{s_1=\pm 1} \left(e^{\beta\mu(H+\Delta H)s_1} \right)}, \qquad \Delta H = Jz \langle s_1 \rangle / \mu$$

$$m = \tanh\left(\beta\mu H + \beta zJm\right)$$

$$m = \frac{\langle M \rangle}{N\mu} = \frac{\sum \mu s_i}{N\mu} = \langle s_i \rangle = \langle s_1 \rangle$$

Consider $H = 0$, there is a non zero solution to the eq. $m = \tanh\left(\beta zJm\right)$

if $\beta Jz > 1$ $\longrightarrow$ $T_c = \dfrac{2JD}{k}$

for $T < T_c$ the solution is $\beta = \dfrac{1}{2Jzm}\ell n\left(\dfrac{1+m}{1-m}\right)$

MFT predicts (incorrectly) phase trans. In 1-D

	MFT	*exact*
$2D$	$T_c = 4J/k$	$T_c = 2.3J/k$
	$T_c = 7J/k$	$T_c = 4J/k$

MFT neglects fluctuations

can be refined

Actually is correct in four dimensions

Renormalization Group theory (1971, Wilson)

illustrated 1D Ising problem

$$Q = \sum_{s_1,\ldots s_N=\pm 1} e^{K(\ldots+s_1 s_2+s_2 s_3+\ldots)}, \quad K = J/kT$$

$$Q = \sum e^{K(s_1 s_2+s_2 s_3)} e^{K(s_3 s_4+s_4 s_5)} \ldots$$

Now sum over even #'d spins

consider 4 spins

$$e^{K(s_1 s_2+s_2 s_3+s_3 s_4+s_4 s_1)}$$

$$= e^{K(s_1 s_2+s_2 s_3)} e^{K(s_3 s_4+s_4 s_1)}$$

$$= e^{K(s_1+s_3)} e^{K(s_3 s_4+s_4 s_1)}$$

$$+ e^{-K(s_1+s_3)} e^{K(s_3 s_4+s_4 s_1)}$$

$$= \left[e^{K(s_1+s_3)} + e^{-K(s_1+s_3)} \right] * \left[e^{K(s_3+s_1)} + e^{-K(s_3+s_1)} \right]$$

Rewrite as a partition function for a lattice with *N/2* spins (with a new *K*)

If we can do this, we can repeat the strategy $\rightarrow$ recursion relation and solve the problem.

we want

$$e^{K(s+s')} + e^{-K(s+s')} = f(K)e^{K'ss'}$$

s and *s'* = 1 or -1 $\longrightarrow$ $e^{2K} + e^{-2K} = f(K)e^{K'}$

s, s' of opposite sign $\longrightarrow$ $2 = f(K)e^{-K'}$

2 eqns in 2 unknowns

Write $\ell n Q = N g(K)$

$$Q(K,N) = f(K)^{N/2} Q(K', N/2)$$

$$\ell n Q(K,N) = \frac{N}{2} \ell n f(K) + \ell n Q\left(K', \frac{N}{2}\right)$$

Want $\ell n Q = N g(K)$

$$g(K) = \frac{1}{2} \ell n f(K) + \frac{1}{2} g(K')$$

$$g(K') = 2g(K) - \ell n\left[2\sqrt{\cosh(2K)}\right]$$

---

alternatively

$$K = \frac{1}{2}\cosh^{-1}\left(e^{2K'}\right)$$

$$g(K) = \frac{1}{2} g(K') + \frac{1}{2}\ell n 2 + \frac{K'}{2}$$

take *K' = 1* – spin coupling negligible

$$Q(0.1, N) \approx Q(0, N) = 2^N$$

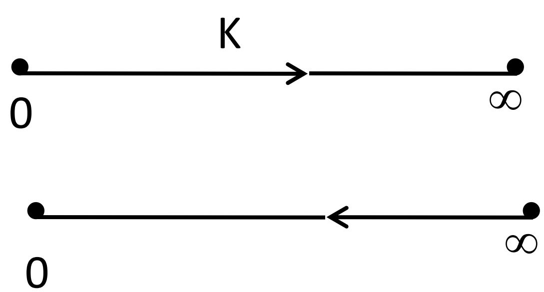
$$g(.01) \approx \ell n2$$

$$K = 0.1003334$$

$$g(K) = 0.698147$$

$$K = 0.3274$$

$$g(K) = 0.745814 \quad \left[g(K) exact = 0.745827 \right]$$

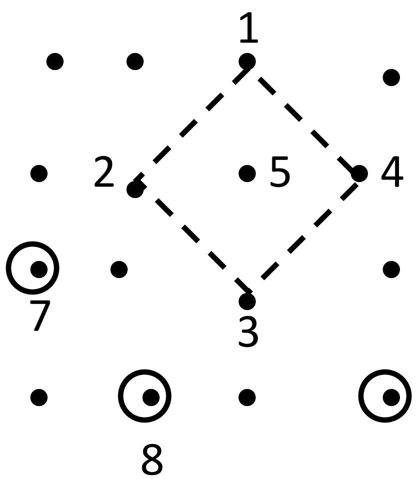


can start near 0 and $\rightarrow \infty$
can start large *K* and $\rightarrow \infty$

No phase transition

RG for 2D Ising model

Sum over ½ the spins as shown.



$$Q = \sum \left[e^{K(s_1+s_2+s_3+s_4)} + e^{-K(s_1+s_2+s_3+s_4)} \right]$$
$$x \left[e^{K(s_2+s_3+s_7+s_8)} + e^{-K(s_2+s_3+s_7+s_8)} \right]$$
$$\ldots$$

$$e^{K(s_1+s_2+s_3+s_4)} + e^{-K(s_1+s_2+s_3+s_4)}$$
$$= \underbrace{f(K)e^{\left[N/2K_1(s_1s_2+s_2s_3+s_3s_4+s_4s_1)\right.}}_{\text{what we would like}}{}^{\left.+K_2(s_1s_3+s_2s_4)+K_3s_1s_2s_3s_4\right]}$$

what we would like

but four choices
$$s_1 = s_2 = s_3 = s_4 = \pm 1$$
$$s_1 = s_2 = s_3 = -s_4 = \pm 1$$
$$s_1 = s_2 = -s_3 = -s_4 = \pm 1$$
$$s_1 = -s_2 = s_3 = -s_4 = \pm 1$$

$$K_1 = \frac{1}{4}\ell n\ \cosh(4K)$$

$$K_2 = \frac{1}{8}\ell n\ \cosh 4K$$

$$K_3 = \frac{1}{8}\ell n\ \cosh 4K - \frac{1}{2}\ell n\ \cosh 2K$$

$$f(K) = 2\left[cpsj(2K)\right]^{1/2}\left[\cosh(4K)\right]^{1/8}$$

$$Q = \sum_{N_{spins}} e^{K\sum' s_i s_j} = \left[f(K)\right]^{N/2}\sum_{N/2_{spns}} e^{\left[K_1\sum_{ij}' s_i s_j + K_2\sum_{\ell,m}'' s_\ell s_m + K_3\sum_{pqrt} s_p s_q s_r s_t\right]}$$

(" means next nearest neighbor)

remove degrees of freedom
$\rightarrow$ more complicated interactions

Not of correct form for RG

Set $K_2 = 0, K_3 = 0$

$$Q(K,N) = [f(K)]^{N/2} Q(K_1, N/2)$$

$$K_1 = \frac{1}{4} \ell n \cosh(4K)$$

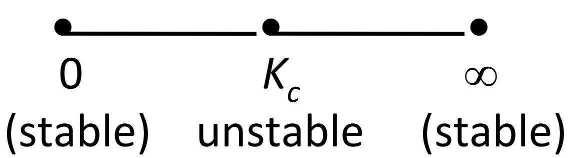
same as for 1D $\rightarrow$ no phase transition

Improved theories introduce approximations to K_2

get $K' = \frac{3}{8} \ell n \cosh(4K)$

non-trivial fixed point $K_c = \frac{3}{8} \ell n \cosh(4K_c)$

$K_c = 0.50698$



gives critical exponents of C_v and M/N
very close to exact values

Metropolis Monte Carlo Approach

trajectory	s_1	s_2	s_3	s_4	…
v_1	1	1	-1	1	…
v_2	1	-1	-1	1	…
v_3	-1	-1	-1	1	…
v_4	1	-1	1	-1	…

…………

$$\langle G \rangle = \frac{1}{T}\sum_{t=1}^{T} G_{v_t},$$ where T = # steps

How can we generate such a trajectory?

20 x 20 2D Ising model $\rightarrow$ $2^{400} > 10^{100}$ configurations

Can get good results sampling 10^6 of these

But need to choose configurations in a clever way choose some configuration

$$v \qquad (\ldots,1,-1,1,1,\ldots)$$

randomly choose a site and flip the spin

$$v' \quad \rightarrow \quad (\ldots,1,1,1,1,\ldots)$$

$$\Delta E_{vv'} = E_{v'} - E_v$$

if $\Delta E \leq 0,$ accept

if $\Delta E > 0,$ generate random # *x* on [0, 1]

accept if $e^{-\beta \Delta E}$ if $\geq x$

otherwise reject

low probability of accepting moves with large > in energy!

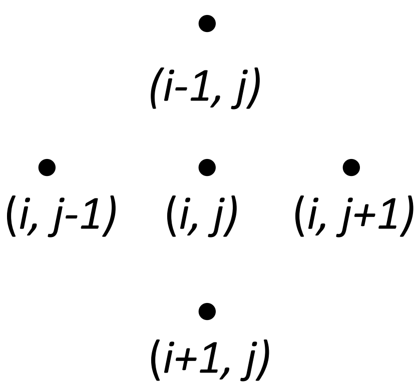
In running Monte Carlo on 2D Ising problem

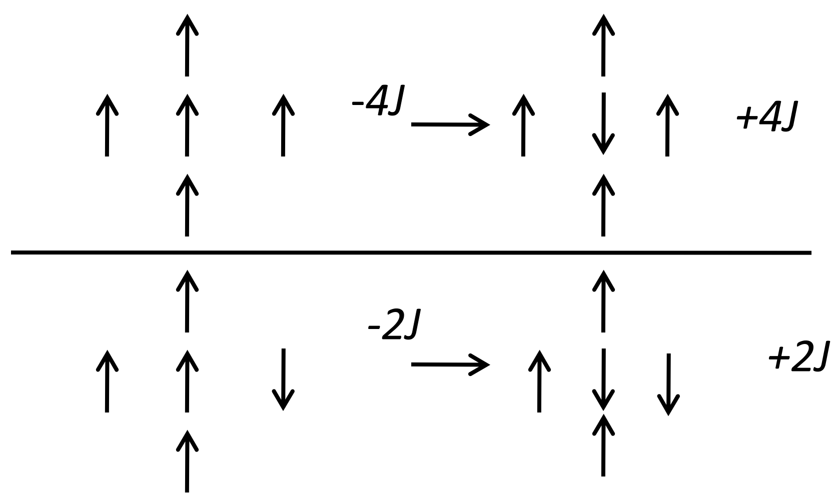
(1) can choose spin sites at random or sweep through the lattice

(2) in computing E_{new} only need to evaluate interactions with 4 neighbors of flipped spin

$$E_{new} = E_{old} + \Delta E$$

so very little computer time for updating energy





$$e^{-\beta \Delta E}$$

2D Ising model $\Delta E = \pm 8J,\ 4J,\ 0$

so can calculate these exponents once, before loops, greatly reducing computer time

Can calculate magnetization, $\langle E \rangle$, $\langle E^2 \rangle$, correlation functions, etc. on the fly or store the trajectory and do post simulation analysis

Metropolis Monte Carlo is not limited to single spin flips (or single particle moves)

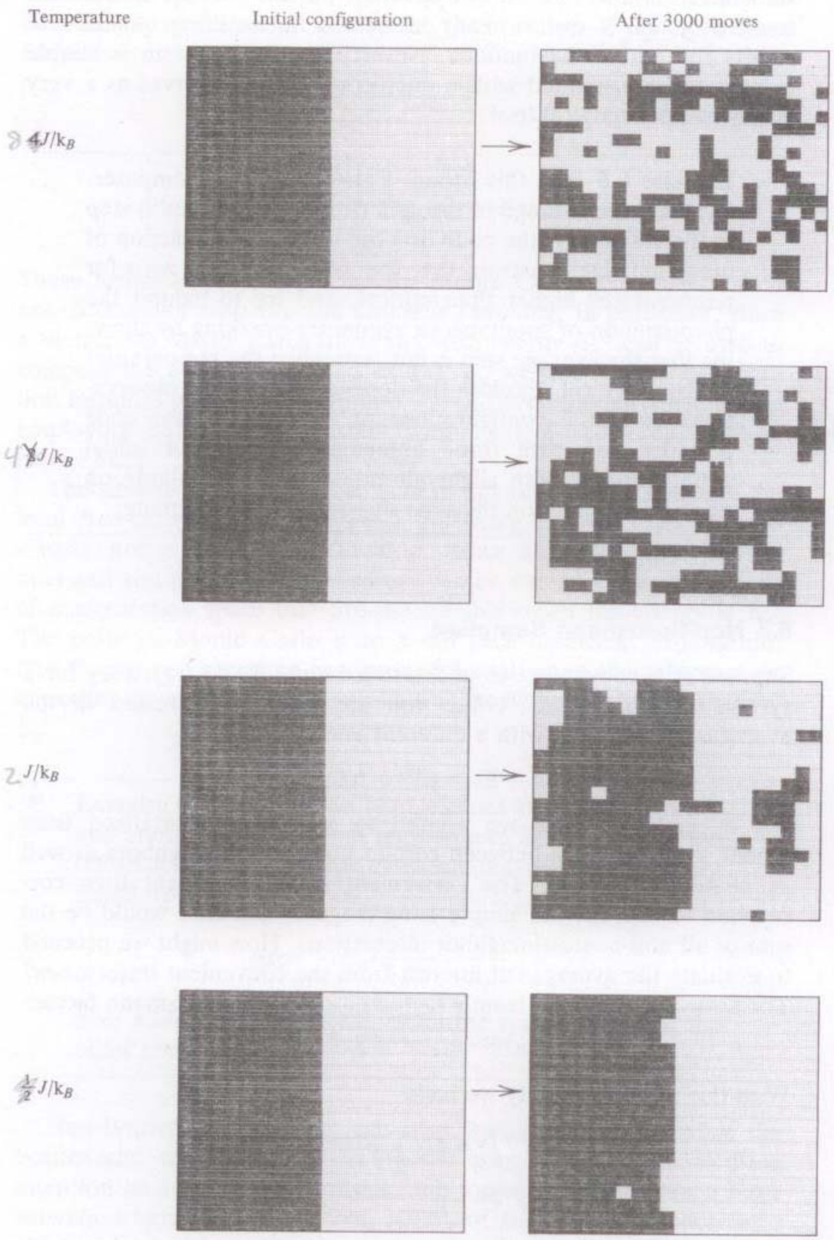
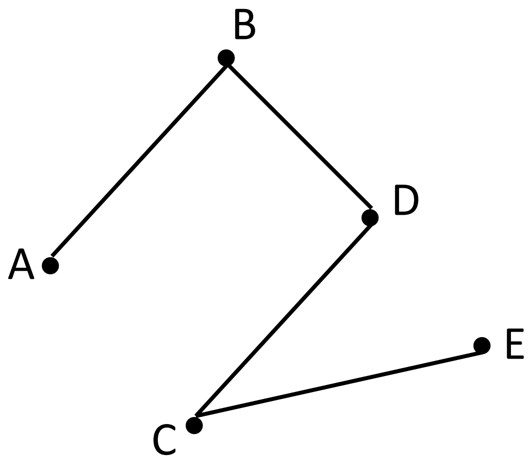


Fig. 6.3. Configurations in a Monte Carlo trajectory of a 20 × 20 Ising model.

from Chandler

Simulated annealing Monte Carlo optimization



traveling salesperson problem given a set of cities, what is the path a salesperson must follow to visits each city once but traveling the shortest distance?

key $e^{-\Delta L/T}$ where ΔL is the change in the path length

e.g., $L_{old} = AB + BD + DC + CE$

$L_{new} = AB + BD + DE + EC$

start with high T_1 (high)
go to lower T_2
loop until T very low

In general, start from multiple initial guesses

Non-Boltzmann sampling

suppose you sample with $E_v^{(0)}$ but you are really interested in $E_v = E_v^{(0)} + \Delta E_v$

e.g., $E_v^{(0)}$ has *NN* interactions
E_v includes non-*NN* interactions as well

$$e^{-\beta E_v} = e^{-\beta E_v^{(0)}} e^{-\beta \Delta E_v}$$

$$Q = \sum_v e^{-\beta E_v} = Q_0 \frac{\sum_v e^{-\beta E_v^{(0)}} e^{-\beta \Delta E_v}}{Q_0} = Q_0 \left\langle e^{-\beta \Delta E_v} \right\rangle_0 \quad \leftarrow$$

average wrt $E_v^{(0)}$ energies

$$\left\langle G \right\rangle = \frac{1}{Q} \sum_v G_v e^{-\beta E_v}$$

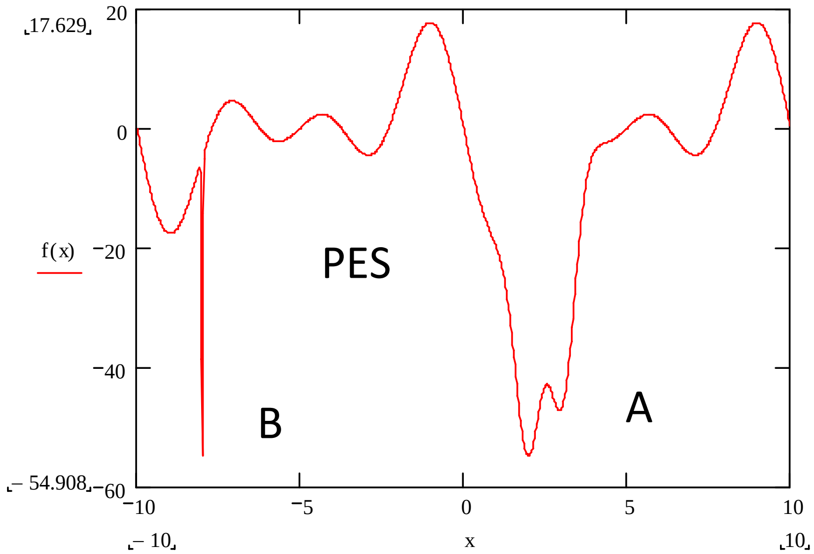
$$= \frac{Q_0}{Q} \frac{\sum G_v e^{-\beta E_v}}{Q_0} = \frac{Q_0}{Q} \left\langle G_v e^{-\beta \Delta E_v} \right\rangle_0$$

$$= \frac{\left\langle G_v e^{-\beta E_v} \right\rangle_0}{\left\langle e^{-\beta \Delta E_v} \right\rangle_0}$$

Non-Boltzmann sampling

most useful when the $E_v^{(0)}$ trajectory is close to the E_v trajectory

Can also use a simulation at T to calculate properties at T', can help solve quasiergodicity problems



A MC simulation at low T starting in region A will not access region B due to the high barrier

So, could consider a modified surface with the large barrier removed (similar to the E^v, $E_v^{(0)}$ approach described above)

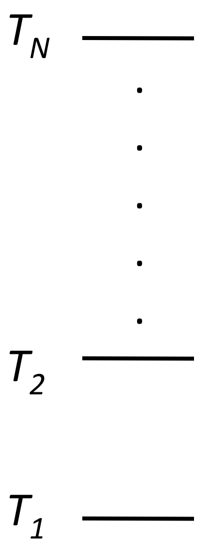
Or could run an MC at high T and use this distribution to sample at low T.

Parallel tempering (replica exchange)

run Monte Carlo simulations in parallel
for several different temperatures

- most of the time do standard Metropolis moves

- occasionally attempt exchanges of configurations at adjacent *T*′s.



At high T, the swaps of configurations between replicas, allows moves between potential wells

Umbrella sampling – designed to sample rare events

$$E_v^{(0)} = E_v + W_v$$

$W_v = 0$ for the configurations of interest

W_v large for all other configurations

consider $\tilde{A}(M)$ for the Ising problem

$$e^{-\beta \tilde{A}(M)} = \sum_v \Delta\left(M - \mu \sum s_i\right) e^{-\beta E_v}$$

$$e^{-\beta \tilde{A}(M)} \propto P(M) = \left\langle \Delta\left(M - \mu \sum s_i\right)\right\rangle$$

sum over states for which magnetization = *M*

P(*M*) is the probability of observing the magnetization *M*

if $kT / J \approx 1$ states with *M = 0* inadequately sampled

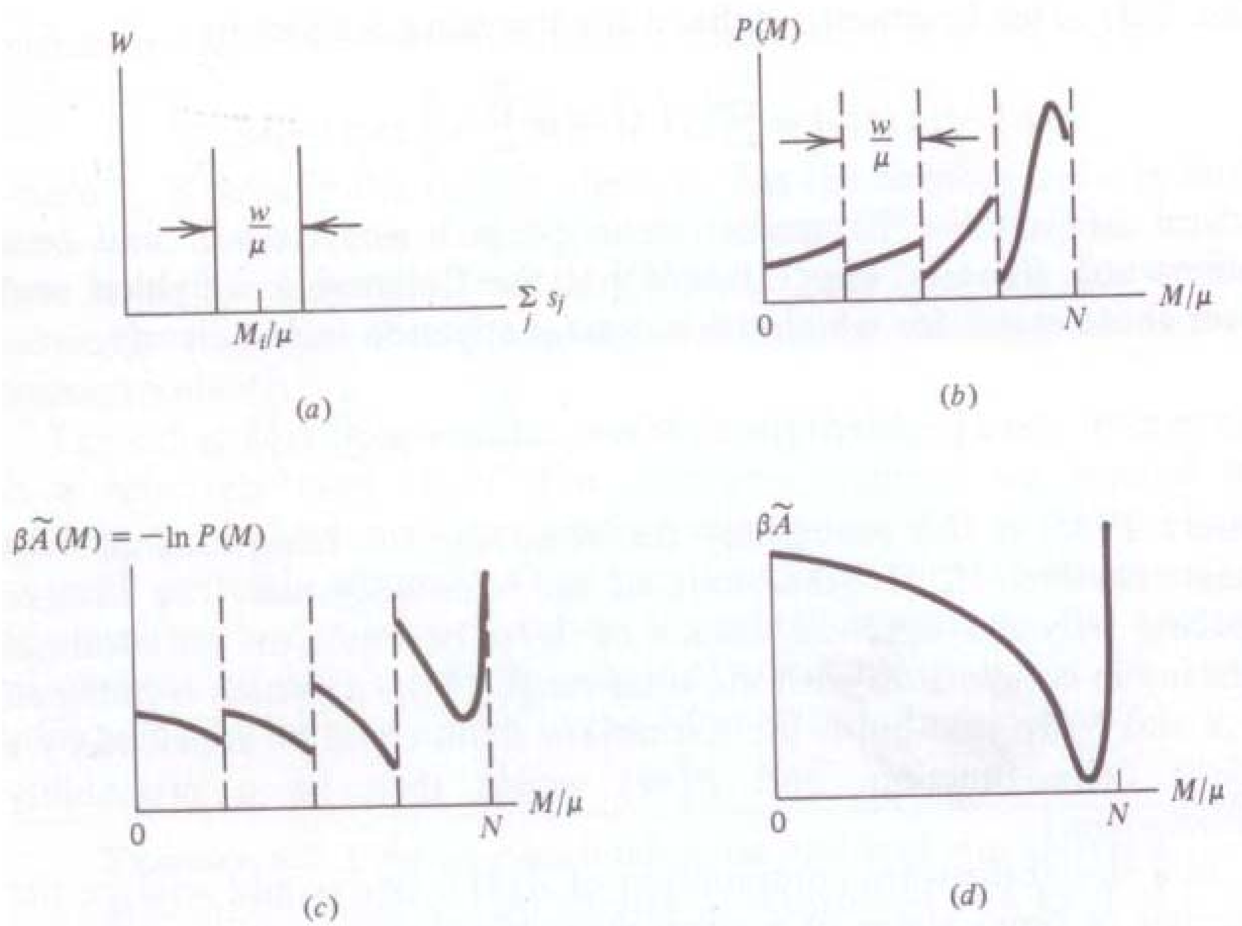
solved with umbrella sampling

$$W_v = 0,\ M_i - \frac{w}{2} \le \mu \sum s_j \le M_i + \frac{w}{2}$$

∞, otherwise

requires $\frac{N\mu}{w}$ simulations

Total possible range $2\mu N$, with each window being $2w$ wide



There is a 2nd minimum at negative *M/μ*

Application of umbrella sampling to the Ising problem.(from Chandler)