

$$X_\alpha = (\sigma_1, \dots, \sigma_N)$$

$$\sigma_j = \begin{cases} +1 \\ -1 \end{cases}$$

Hamiltonian

$$H = - \frac{J}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

↑  
Nearest-neighbor summation.

Metropolis.

Choose a spin at random and  
independently flip it,

$$\sigma_j \rightarrow \sigma'_j = -\sigma_j$$

The resulting change in energy  
is

$$\Delta E = + \sigma_j \sum_{i \in \{j\}} \sigma_i$$

↑  
Neighbors on a

Square lattice

If  $\Delta E = 0$ , accept the movement.

If  $\Delta E > 0$ , generate an  $\eta \in [0, 1]$

- random #.

Compare with  $w = e^{-\Delta E / T}$ .

If  $\eta \leq w \Rightarrow$  accept

$\eta > w \Rightarrow$  reject.

---

A remark to Speed up algorithm:

For each attempted update,

generate a random number  $\eta$ .

Accept if  $\eta \leq w$

Reject if  $\eta > w$ .

If  $\Delta E < 0$ ,  $w > 1$ , so that we still  
always accept.

In order to avoid if - statements  
in the code, the update may  
be done as follows:

$$\sigma_j = (2 * \text{max}(0, \text{int}(1 + r - w)) - 1) * \delta_j$$

$w = e^{-\Delta E / T}$

A hand-drawn graph on grid paper showing a sigmoidal curve that starts near zero, passes through 0.5 at the center, and approaches 1.0 as x increases. The curve is labeled "random #".

Keep a table  
of these  
numbers.

In connection with spin systems,  
the Monte Carlo method gives  
us sample configurations that  
follow Boltzmann statistics,

$$P_{\alpha} \propto e^{-E_{\alpha} / T}$$

Our aim in statistical physics  
is to calculate the partition  
function.

$$Z = \sum_{\{G\}} e^{-H(G)/T} = e^{-F/T}$$

Free energy.

For example, average energy is  
given by

$$\langle E \rangle = \frac{1}{Z} \sum_{\{G\}} H(G) e^{-H(G)/T}$$

$$= - T^2 \frac{d}{dT} \ln Z.$$

Rather than summing over all configurations, we may sum over all energies:

$$Z_1 = \sum_{\{g\}} e^{-H(g)/T} = \sum_E g(E) e^{-E/T}$$

### Density of states.

(In a continuous system, the partition function is the Laplace transformed of the density of states,

$$Z(T) = \int_0^{\infty} dE g(E) e^{-E/T}$$

Why not sample this rather than the Boltzmann weight?

The idea is now to use the Metropolis algorithm to generate samples with probability proportional to  $g(E)$ , but without knowing  $g(E)$  beforehand.

### The Wang-Landau algorithm

We wish to construct a Markov chain in energy space.

### The ellhopolis algorithm:

Given  $p_a$ :

Fractional probabilities for

Markov chain:

$$P_{\alpha\beta} = T_{\alpha\beta} \min\left(1, \frac{p_\beta}{p_\alpha}\right)$$

Probability to choose state  $\beta$   
as final state while being  
in state  $\alpha$ .

The probability is uniform.

Hence, if we make a histogram  
over states we have tried, it  
should be uniform.

The density of states is the  
number of microscopic states  
with the same energy  $E$ .