Stat mech is the area of physics that deals with connecting microscopic details of a system to macroscopic thermodynamic quantities, eg

$$\sum \frac{1}{2} m_i v_i^2 = \frac{3}{2} kT \quad \text{(for monoratomic system).}$$

For any arbitrary microscopic quantity q, stat mech tells us that the macroscopic "expectation value" $\langle q \rangle$ is given from the weighted sum

$$\langle q \rangle = \frac{\sum_{\text{states}} q^s e^{-\beta E_s}}{\sum_s e^{-\beta E_s}} \equiv \frac{\sum e^{-\beta E_s}}{Z} \quad \beta = \frac{1}{kT}$$

$Z \leftarrow$ partition function.

That is, states contribute with a weight proportional to $e^{-\beta E_s}$, so $E_s \gg 0$ contributes little, $E_s \ll$ contributes a lot! Ie, favor low energy states, but T "balances" the game.

Suppose we want to calculate an average quantity for the "Ising model" ...

Monte Carlo Method

In stat mech, our goal is typically to evaluate an average thermodynamic property. In the canonical ensemble, this is given by $\beta = \frac{1}{kT}$

$$\langle q \rangle = \frac{\sum_s q_s e^{-\beta E_s}}{\sum_s e^{-\beta E_s}}$$

where we sum over all states $\{s\}$

What if we want to numerically evaluate this for a system that cannot be analytically solved?

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eg: Consider a spin system on a $10 \times 10 \times 10$ lattice (3-D). If we allow for both interaction with a field, and interactions between spins, cannot solve analytically. If we try to enumerate states -- 2 states for each spin, we have 2^{1000} states! $\approx 10^{300}$!

Typical simulation can only sample $\approx 10^{10}$ states... or 1 state in 10^{290}!! Bad sampling!

How does nature work? Nature does not bother sampling all states! Observed value is dominated by most probable states -- so if we can figure out which states to sample, we could get an average much more easily!

eg: the gas molecules in a room never go to one side

MC 2

approach: we want to sample states $\{s\}$ from a probability dist $p(s_i)$. Then have

$$q_N = \frac{\sum_{i=1}^{N} q(s_i)\, e^{-\beta E(s_i)}\, p^{-1}(s_i)}{\sum_{i=1}^{N} e^{-\beta E(s_i)}\, p^{-1}(s_i)}$$

($p^{-1}(s_i)$: removes bias)

for $N \to \infty$, we sample all states & $q_N \to \langle q \rangle$

the problem: How do we choose $p(s_i)$ so that $q_N \to \langle q \rangle$ is for N "relatively small" — ie, how do we choose the important states!

resolution: we know $p(E) = e^{-\beta E}/Z$, ie the system samples states according to Boltzman distribution

So let's pick states the same way!

$$\Rightarrow p(s_i) = e^{-\beta E(s_i)}/Z$$

$$\Rightarrow q_N = \frac{\sum_{i=1}^{N} q(s_i)\, e^{-\beta E(s_i)}\, Z/e^{-\beta E(s_i)}}{\sum_{i=1}^{N} e^{-\beta E(s_i)}\, Z/e^{-\beta E(s_i)}} = \frac{\sum_{i=1}^{N} q(s_i)}{\sum_{i=1}^{N} 1} = \frac{1}{N}\sum_{i=1}^{N} q(s_i)$$

OK, so we know what probability to pick states with, but HOW do we actually pick those states? If we do it at random, we do no better!

(Does not matter how if we enumerate all states, but have to be careful when sampling a limited amount of phase space).

Markov Process is a mechanism that takes a system from state $s \to s'$. Must satisfy:

1. Does not depend on prior history, only states s & s'
2. Time invariant
3. $\sum_{s'} P(s \to s') = 1$; note that $s' = s$ is allowed (i.e. system can stay in initial state)

Detailed Balance: the rate of transitions into & out of the state s must be equal

$$\sum_{s'} p(s)\, P(s \to s') = \sum_{s'} p(s')\, P(s' \to s)$$

↑ transitions out of s ↖ transitions into s.

There are many ways to satisfy this condition. A simple way is

$$p(s)\, P(s \to s') = p(s')\, P(s' \to s)$$

$$\Rightarrow \quad \frac{P(s \to s')}{P(s' \to s)} = \frac{p(s')}{p(s)}$$

recall that $p(s) = e^{-\beta E(s)}/Z$

$$= \frac{e^{-\beta E(s')}}{e^{-\beta E(s)}}$$

$$= e^{-\beta (E(s') - E(s))}$$

In other words, the probability of going to a new state is the Boltzman factor of the energy change!

so almost there, we know what $\frac{P(s\to s')}{P(s'\to s)}$ is,

but we still must make a choice for $P(s\to s')$.

The Metropolis algorithm recognizes that system like to go to lower energy. Hence Metropolis chooses

$P(s\to s') = 1$ if $E(s') - E(s) < 0$ ie new state is lower energy.

since $\frac{P(s\to s')}{P(s'\to s)} = e^{-\beta(E(s')-E(s))}$, for $E(s') - E(s) < 0$

$$P(s'\to s) = e^{+\beta(E(s') - E(s))}.$$

$$\rightsquigarrow \boxed{P(s\to s') = \begin{cases} 1 & \text{if } \delta E \le 0 \\ e^{-\beta\delta E} & \text{if } \delta E > 0 \end{cases}}$$ Metropolis Monte Carlo Algorithm.

So we always accept moves that lower energy, & accept moves that raise energy according to Boltzmann probability!

Not Unique! We made choices

① $p(s)\,P(s\to s') = p(s')\,P(s'\to s)$ to satisfy detailed balance

② $p(s) = e^{-\beta E(s)}/Z$

③ $P(s\to s')$ according to Metropolis

Other algorithms possible!

Metropolis Algorithm for the Potts Model

Potts Model: The energy/Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \left(1 - \delta(s_i, s_j)\right)$$

J = coupling strength between spins

s_i = ~~state~~ state of spin i; $s_i \in [0, q-1]$ & $s \in \mathbb{Z}$

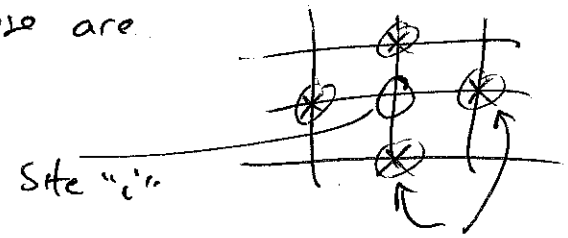
$\delta(s_i, s_j)$ = Kronecker δ-fctn, ie

$$\delta(s_i, s_j) = \begin{cases} 1 & s_i = s_j \\ 0 & s_i \neq s_j \end{cases} \Rightarrow$$

Spins want to be in the same state! Lower energy!

The sum $\sum_{\langle ij \rangle}$ is restricted to nearest neighbors $i \neq j$.

On a 2-D square-lattice, these are



The thermodynamic properties of this model can be exactly analytically solved on a 2-D square-lattice, but the solution method is beyond the scope of this course. The important result is that there is a temperature T_c where this model has a phase-transition to a spontaneously magnetized state.

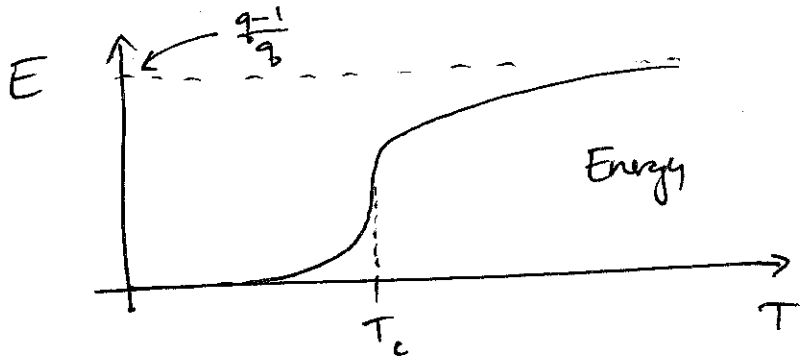
In other words, at high T, thermal excitations overwhelm the energetic desire for spins to be in the same state. In this case, the fraction of spins in each state, which we call the magnetization $M(T > T_c) = \frac{1}{q}$.

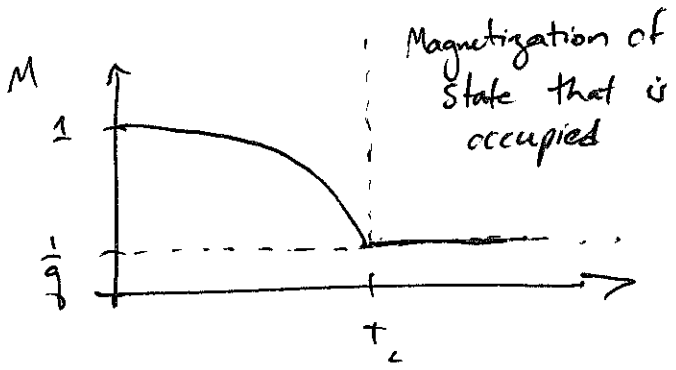
For $T < T_c$, the system will start to be dominated by 1 of the q states (note: we do not know which one, since they are all identical). In this case, as $T \to 0$, the magnetization of one state, that is the fraction in that state will approach 1, while the occupancy of all other states $\to 0$.

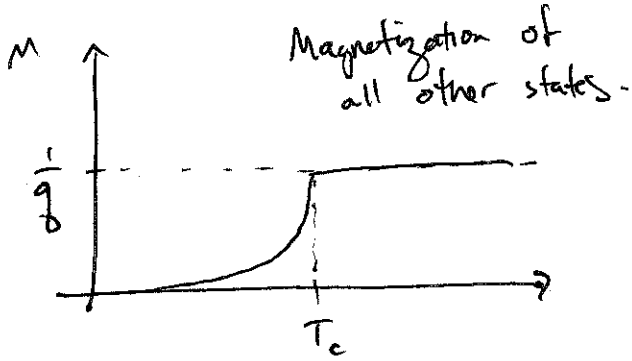
In units where Boltzmann's constant $k_B = 1$,

$$T_c = \frac{1}{\ln(1+\sqrt{q})}$$

$q = 4$
$T_c = 0.910$







How do we implement this in MONTE CARLO? (2D square-lattice)

(1) Create a collection of $M \times N$ spins with random values (or read a pre-determined configuration)

(2) Select a spin & calculate the change of energy if

$$s_i \to (s_i + \Delta s) \bmod q = s_i^{new}$$

↑ modulus!

eg: $0 \bmod 2 = 0$, $1 \bmod 2 = 1$, $2 \bmod 2 = 0$, $3 \bmod 2 = 1$ } just the remainder of a division

where $\Delta s \in [0, q-1]$ on $\mathbb{Z}$

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

(sums over j restricted to nearest neighbors.)

$$= J \left[\sum_j (1 - \delta(s_{new}, s_j)) - \sum_j (1 - \delta(s_i, s_j)) \right]$$

$$= J \sum_j \left(\delta(s_i, s_j) - \delta(s_{new}, s_j) \right)$$

(3) If $\Delta E \leq 0$, accept the move, ie set $s_i = s_{new}$

If $\Delta E > 0$, accept with probability $e^{-\beta \Delta E}$ $(\beta = 1/kT)$

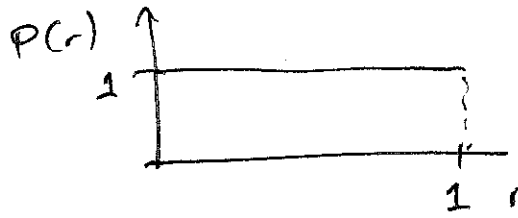
(more on this in a moment....)

(4) After some number of ~~up~~ updates, evaluate the energy and the fraction of spins in each state.

(5) Return to step 2.

Q: How do we accept a move with probability $e^{-\beta \Delta E}$?

① Pick a uniformly distributed random number $r \in [0, 1)$

ie 

You can use the pseudo-random number generator erand48 for this

② If $r \leq e^{-\beta \Delta E}$ accept

$r > e^{-\beta \Delta E}$ reject.

$(\beta = 1/kT)$