

# Lec9

- Recap: Statistical Mechanics
- Ising model
- Monte Carlo methods

# Many degrees of freedom

- Want to understand systems with very many degrees of freedom
- No need/want to solve all dynamical equations. Want only *time averages* of quantities averaged over all degrees of freedom.
- By *ergodic* hypothesis can generate these averages by averaging over all *microstates* of system with a certain probability

Probability of finding the system in some state with energy  $E$  at temperature  $T$  is given by  $e^{-\frac{E}{kT}}$

k – Boltzmann's constant  
 $1.38 \times 10^{-23} m^2 kgs^{-2} K^{-1}$

# Statistical Mechanics

- The calculation of averaged quantities such as energy, temperature, pressure in terms of averaging over probability distributions is called *Statistical Mechanics*.
- In detail (the average of) any quantity  $Q$  is given by:

$$\langle Q \rangle = \frac{1}{\mathcal{N}} \int \prod_i^N dx_i dp_i Q(x_i, p_i) e^{-E(x_i, p_i)/kT}$$

- This is a big integral! It cannot be done analytically.
- Typically Monte Carlo methods are used to evaluate it approximately. Natural to use importance sampling with  $e^{-E/kT}$  the probability distribution.

# Recap - Importance Sampling

## MC

To evaluate the integral  $I = \int_a^b dx p(x) f(x)$

$$I \sim \frac{b-a}{N} \sum_{i=1}^N f(x_i)$$

where  $x_i$  drawn from distribution  $p(x)$

i.e number of points in range  $x \rightarrow x + dx$  is  $p(x)dx$

$p(x)$  should be *normalized* -  $\int dx p(x) = 1$

How to draw numbers from distribution  $p(x)$  ?

# Importance Sampling

Metropolis algorithm:

- Start from some point  $x_0$ . Generate new point randomly eg

$$x_i \rightarrow x_{trial} = x_i + 2b(r - 0.5)$$

- Calculate  $\omega = \frac{p(x_{trial})}{p(x_i)}$
- Compare to random number. If  $r < \omega$  accept new pt  $x_i$
- Otherwise try again.

# Variations

- Methods work when integrals replaced by sums (and just as necessary!). Eg Ising model.

- When many dof carry out importance sampling for each integral/sum. eg

$$x_i \rightarrow x_i + \delta x; y_i \rightarrow y_i + \delta y; z_i \rightarrow z_i + \delta z \dots$$

- Alternative way of describing things: we are *updating* each dof using a Metropolis algorithm. Eg Ising.
- Procedure *guarantees* we end up sampling points in the configuration space with probability  $p(x, y, z, )$

# Wrinkles for Stat Mech

- Here  $p = e^{-E/kT}$
- So  $\omega = e^{-\frac{\Delta E}{kT}}$  is probability for accepting the update Metropolis move
- Notice. Can calculate change in energy by a *local* calculation since interactions are local.
- Interpretation. In general system evolves towards states with lower energy. But occasionally can undergo *thermal fluctuation* to higher energy state. Characteristic of systems in *thermal equilibrium*

## Simple example – Ising Model

- Consider magnetic materials – at atomic level these consist of stationary magnetic dipoles or spins which form lattice.
- Spins can point up or down (N or S) and in a ferromagnet the energy of the system is lowered if neighboring spins point in same direction.
- 2D Ising model : replace spins by variable  $s_i = \pm 1$  living on sites of 2D lattice with energy given by

$$E = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i$$

## Simulation details

- Go thru 'spins' one by one on lattice.
- Try to update (here flip from up to down or vice versa)
- Accept/reject using Metropolis test  $e^{-\delta E/kT}$
- Once equilibrium is reached – measure observables by simple averaging on set of configs generated by Monte Carlo
- eg.  $\langle Q \rangle = \frac{1}{N} \sum_{\text{config } C} Q(C)$  with statistical error that varies as  $1/\sqrt{N}$  for  $N$  configs

# Basic observations

2 regimes:

- $T > T_c$ . Average spin (magnetization) is zero
- $T < T_c$  Average spin is non-zero (permanent magnetization)
- Phase transition at  $T = T_c$ . At this point *fluctuations in average spin  $\chi$  get large*

$$\chi = \frac{1}{L^2} (\langle M^2 \rangle - \langle M \rangle^2)$$

- On  $L \times L$  lattice at  $T = T_c$  this  $\chi \sim L^{\frac{\gamma}{\nu}}$

# Critical exponents

- Exponent  $\gamma$ ,  $\nu$  termed critical exponents.
- Universal: don't depend on details of interactions - just dimension, symmetry, ...
- Measure using MC (also other methods)
- Where do divergences come from ?

# Critical Phenomena

- The underlying reason for this universality is that the critical system exhibits very long range correlations between individual molecular constituents. The distance over which these correlations take place is called the correlation length  $\xi \rightarrow \infty$ .
- This washes out details on scale of lattice spacing. correlation function:

$$\langle s_0 s_i \rangle \sim e^{-i/\xi}$$