Lec10

- Many degrees of freeedom - statistical physics
- Phase transitions, critical phenomena
- Magnetic systems - Ising model
- Mean field theory, correlations

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 $1.38 \times 10^{-23} m^2 kg s^{-2} K$

Statistical Mechanics

- The calculation of averaged quantitives such as energy, temperature, pressure in terms of averaging over probability distributions is called Statistical Mechanics.

- In detail any quantity such as energy is given by:

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

- This is a big integral! To do it numerically must use Monte Carlo methods.

- Furthermore, since integrand is zero for almost all (x_i, p_i) must use importance sampling using $e^{-E/kT}$.

Simple example – Ising Model

- Can use these methods to study molecular systems – complementary to molecular dynamics simulations considered earlier. But easier ...

- 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

$$E = -J \sum_{<ij>} s_i s_j$$

Even simpler system

- The Ising model is still very complicated to solve exactly.

- Warm up consider a single spin in an external magnetic field $E = -Hs$ Using statistical mechanics mean spin is given by

$$< s >= \frac{\sum_{s=\pm 1} s e^{-Hs/kT}}{\sum_s e^{-Hs/kT}}$$

leading to

$$< s >= \tanh\left(H/kT\right)$$

Mean field approximation

Go back to original 2D Ising system. Replace the sum over nearest neigbor spins by the interaction with an effective magnetic field.

$$-J\sum_j\sum_i s_i s_j \rightarrow -4J < s > \sum_i s_i$$

Now solve the equation

$$< s >= \tanh\left(-4J < s > /kT\right)$$

Graphically: see 2 solns:

- $T > T_c$ $< s >= 0$
- $T < T_c$ 2 solns. One with $< s >\neq 0$

Numerical Solution

Use *bisection* algorithm to solve for $< s >$.
eg. To solve equation $f(x) = 0$ find 2 points x_1 and x_2 at which f has opposite sign.
Root lies somewhere between
Examine the midpoint $(x_1 + x_2)/2$ and hence determine new interval to search.
Note: interesting region close to $kT/J = kT_c/J = 4$.

Close to the transition ...

For small $< s >$ use approx

$$\tanh x = x - x^3/3$$

Find

$$< s >= \sqrt{\frac{3}{T}\left(\frac{kT}{4J}\right)^3}\,(T_c - T)^{\frac{1}{2}}$$

Power laws.
Implies $\chi =< M^2 > - < M >^2 = \frac{\partial < s >}{\partial T}$ diverges as $T \to T_c$!

Phase transitions

- Ising system can exist in two phases $< S >= 0$ - magnetized and $< S >\neq 0$ – unmagnetized.

- Controlled by temperature.

- Close to T_c system exhibits power law behavior.

- Many examples of systems exist with several phases characterized by macroscopic state eg

  – Solid-liquid transition at some critical T_c

  – Percolation, p_c

Critical exponents

While mean field theory is usually quantitatively wrong the basic idea of critical exponents describing behavior near phase transitions is right.

- Eg. Specific Heat C, Magnetization M, Magnetic susceptibility χ

$$
\begin{aligned}
C &\sim (T - T_c)^{-\alpha} \, \alpha = 0 \\
M &\sim (T - T_c)^{\beta} \, \beta = \frac{1}{8} \\
\chi &\sim (T - T_C)^{-\gamma} \, \gamma = \frac{15}{8}
\end{aligned}
$$

Critical Phenomena

- Close to the phase transition ($T \sim T_c$) the system exhibits critical behavior eg. specific heat $C \sim (T - T_c)^{-\alpha}$

- The *critical exponent* α is *universal* - it is the same for many different materials.

- 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 $\xi \to \infty$.

- This washes out details on scale of lattice spacing. correlation function:

$$< s_0 s_i > \sim e^{-i/\xi}$$

Monte Carlo

- Use a simple algorithm to move from state i to state j. Note: integration pt x_i in simple case is now a point in state space $s_i, i = 1 \dots N$

- Design that algorithm to ensure that after some iterations the probability of any state occuring is just $e^{-E/kT}$. Thus new integration pt/config selected according to $e^{-\Delta E/kT}$.

- Measure observables by simple averaging over this set of states. Yields eg. $< M >= \frac{1}{N}\sum_{\text{configC}} M(C)$ with statistical error that varies as $1/\sqrt{N}$ for N states

Phase transitions in Ising model

- Simplest case - two dimensions.

- Find for $T = T_c = 2.269$ fluctuations in M have a peak.

- $M \sim 0$ for $T > T_c$. $M = 0$ for $T < T_c$

- Close to T_c, $\chi \sim (T - T_C)^{1.875}$ in 2 dimensions. $M \sim (T - T_C)^{0.5}$