LCP

group 8

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1 Ising Model

In the standard assumptions, particles with a certain spin (up or down) are located on the N nodes of a lattice (sites) and interact with their nearest neighbours, i.e. those particles with whom they share an edge (bond). For simplicity, spin up is identified with a value $s_i = +1$, spin down is $s_i = -1$ (spins are measured in units of $\hbar/2$). The Hamiltonian of a given configuration S is given by

$$H(S) = -\sum_{<ij>} J_{ij} s_i s_j - H \sum_i s_i$$

The first term is a summation over all pairs of interacting spins; if the behaviour of the material is ferromagnetic $J_{ij} > 0$ and concordant spins give a negative contribution to the Hamiltonian. The lowest energy level is associated with all spins concordant. So far, the Hamiltonian has Z_2 symmetry, and spontaneous magnetization cannot arise:

$$M = \frac{1}{N} \sum_{i=1}^{N} s_i = 0$$

With N being the amount of sites. For square lattice one simply replaces N by L^2 where L is the lattice length.
If one adds the second term, which is simply the potential energy due to an external magnetic field B, this explicitly breaks the Z_2 symmetry. Even if one does not consider this term, two remarkable facts arise: as the number of sites $N \to \infty$ there is spontaneous symmetry breaking; if the temperature is above T_C(Curie temperature) the behaviour of the model is paramagnetic. These facts can be explained using the canonical ensemble of statistical mechanics. Every configuration is given a probability:

$$P(S) = \frac{e^{-\beta H(S)}}{Z}$$

with $\beta = \frac{1}{k_B T}$ and Z the partition function. The configuration with the minimum Hamiltonian, i.e. the equilibrium one, is also the most likely. By making use of mean-field arguments and simplifying assumptions, one can get a self-consistent equation:

$$< S >= tanh(\beta J < S >)$$

The Ising model may be studied on a generic graph. We are interested in networks whose degree distribution is a power law:

$$p_k = CK^{-\gamma}$$

p_k is the probability mass that a node has degree k, C is a normalization constant and γ is called "power law parameter" and controls the slope of the power law.

2 Partition Function

Let us recall the definition of the partition function:

$$Z = \sum_n e^{-\beta E_n}$$

where E is the total energy of the system and consider the energy eigenstates

$$\widehat{H}|n\rangle = E_n|n\rangle$$

yielding

$$Z = \sum_n e^{-\beta E_n} = Tr(e^{-\beta \widehat{H}})$$

and we know that

$$\widetilde{H} = -\beta \widehat{H}$$

consequently

$$Z = Tr(e^{\widetilde{H}})$$

3 Magnetic Susceptibility and Specific Heat

Another interesting quantity is the magnetic susceptibility χ. This quantity is related to the equilibrium fluctuations of magnetization

$$\chi = \beta(\langle M^2 \rangle - \langle M \rangle^2)$$

Near the critical temperature T_c, several physical properties obey a power law dependence on $\mid T - T_c \mid$. Critical exponents are commonly labelled $\alpha, \beta, \gamma, ...$ for $T < T_c$, each corresponding to a specific physical quantity.For $T > T_c$, the exponents are commonly accompanied by a prime. The exponents describe phase transitions of these quantities usually near a critical temperature T_c.So magnetic susceptibility can be written as

$$\chi_M \sim\mid 1-\frac{T}{T_c}\mid^{-\gamma}$$

The specific heat can be written as

$$C_H \sim\mid 1-\frac{T}{T_c}\mid^{-\alpha}$$

α and γ are critical exponents.The dimension of space is very important in phase transitions. Critical exponents fall into different universality classes depending upon both, the space dimension and on the system degrees of freedom.
For a magnetic system, the second exponent, β, is the easiest to conceptualise. β, corresponding to the order parameter of the system, which in a magnetic system is the magnetisation. Thus, what β describes is the behaviour when the system spontaneously magnetises. Assuming no external magnetic field

$$M \sim\mid 1-\frac{T}{T_c}\mid^{\beta}$$

The value for β was found to be $\beta = 1/8$ for the 2D Ising model.

4 Metropolis

Monte Carlo simulations of the Ising model are performed through the Metropolis Algorithm (MA). In principle we could construct all the possible states the system can access $\{n\}$ $((S))$ and their energies $E(H(S))$. With that information, we could construct the partition function and recover all the thermodynamics of the system. However there are 2^N possible states the system can access, so it is impractical to follow this path for large systems that obey $N >> 1$. This problem is solved by designing a Markov chain (or transition matrix) in such way that its stationary distribution is the desired distribution. MAs belong to a more general class of algorithms, Monte Carlo Markov Chains (MCMCs), which are used when the probability distribution of the Monte Carlo inputs is unknown. The stationary distribution is:

$$P(S) = \frac{1}{Z}e^{-\beta H(S)}$$

In our case,the partition function Z is a summation over 2^N terms and cannot be computed even if the graph is small. The idea of MCMCs is to sample such a probability distribution by making use of an ergodic Markov Chain. But what is a Markov chain? It is one type of stochastic process. It is an evolution in time that is not determinist, but there is a transition probability from the current state to a new state.(A Markov chain satisfies that the probability distribution of the next state depends only on the current state.) The MA satisfies the detailed balance condition (needed for ergodicity) in such a way that Z cancels out. In practice, one takes a starting configuration S with Hamiltonian $H(S)$

and modifies it, such as to obtain S' with $H(S')$. Then, the probability to accept the new configuration is

$$P(S \to S') = min\{1, e^{-\beta[H(S')-H(S)]}\}$$

If $H(S'^{)} < H(S)$ the new configuration is accepted with certainty: this is a step towards the equilibrium state (which is just the most likely in statistical mechanics). If $H(S'^{)} > H(S)$ the new configuration may be accepted: this should prevent the system to get stuck in local minima. The key term in previous is β: if β is high, T is low and it is less likely that higher energy configurations will be accepted; if β is low, T is high (there is a lot of noise) and almost any new configuration is accepted. Intuitively, in the first case the system will rush towards the equilibrium state; in the latter case it will just "wander around" the phase space.

5 Phase Transition

Second order phase transitions are also seen in magnetic systems, such as the Curie point in ferromagnets,which separates the paramagnetic phase from the ferromagnetic one. That means that below the Curie temperature, the system presents spontaneous magnetization in absence of an external magnetic field, whereas above it, the system is not magnetized and only responds when an external magnetic field is applied. It is our goal to illustrate what happens in second-order transitions and how do the thermodynamic properties of the systems behave.