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The applications of Ising Model in statistical thermodynamics and quantum mechanics - A review -

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Abstract

This article provides a review on the theory of Ising model and its applications in statistical thermodynamics and quantum mechanics. Ising model has been created by the German physicist Ernst Ising to mathematically model ferromagnetism in statistical mechanics. It consists of discrete variables that knowns as magnetic dipole moments of atomic spins that can be found in either +1 or -1 state. The spins are distributed in a lattice geometry and interacting with each neighbour spin causing variant structural phases. Ising model provides the phase transition in a simplified model. The two-dimensional square lattice orientation od spin is considered to be the smelliest phase transition model

Keywords: A. Ising Model; Hamiltonian; Quantum Annealing; Lattice.

INTRODUCTION

There is this natural connection between what is computationally hard and what's physically difficult to solve" P. Wittek. The Ising Model is a statistical model that can help make this connection. Magnetism is a class of physical phenomena that are mediated by magnetic fields. Magnetism is one aspect of the combined electromagnetic force. It refers to physical phenomena arising from the force caused by magnets, objects that produce fields that attract or

repel other objects. Magnetism is an inherently quantum phenomena. All materials experience magnetism, some more strongly than others. Permanent magnets, made from materials such as iron, experience the strongest effects, known as ferromagnetism (Figure.1). With rare exception, this is the only form of magnetism strong enough to be felt by people. The fact of interacting of the particles with each other make it difficult to solve models in statistical mechanics as well as relativistic quantum field theory. However, the Ising model is a suitable example of a statistical model in this framework, as it captures all main effects and interactions between variable [1-3].

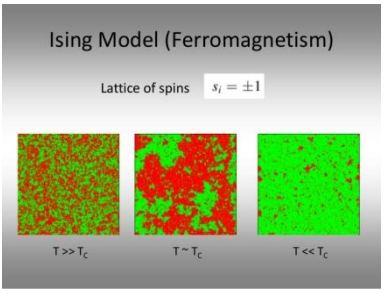


Figure 1: Lattice structure of Ising Model

The Ising Model does not correspond to an actual physical system. It is represented by a lattice structure where its sides are in either -1 or +1. The Ising model is applied in multiple physical systems such as: Magnets, alloys, and lattice gas. If we consider a magnet, we will find that each site represents a spin in the material. Each spin acts as a minimized magnet. If all spins are aligned, then the entire lattice will act as a big magnet. If we add more magnets to this system, we can sum up their pairwise interaction to get the total energy. The total energy of the system is called the Hamiltonian (Figure.2).

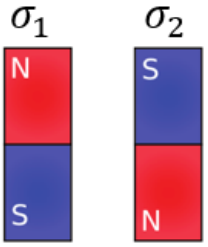
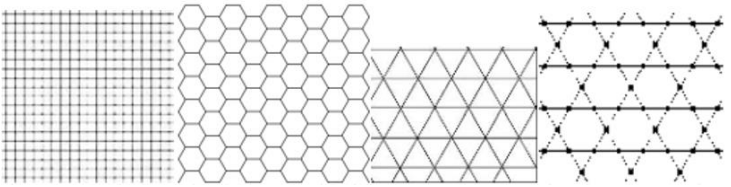


Figure 2: Hamiltonian in the Ising Model

One type of Hamiltonian in the Ising model is the external field, in which the external magnetic field (h) split the energies of the spin-down and spin-up states such that one will be higher in energy and the other one is the lower. Size of (h) shows the strength of the field while the sign tells whether it is filliped up or down. The total contribution of the individual spin fields is the sum of all sites. Since each spin has a unique mini magnetic field an interaction between the neighbouring spins could take place.

For a lattice of N sites with a spin S at both site following the two possibilities of -1 and +1. A configuration is defined by orientations of the spin all N sites (Figure.3).



Square Lattice *Hexagonal Lattice* *Triangular lattice* *Kagone Lattice*

Figure.3: Different orientations lattice structures

Theoretical suggestions and exemplifications of quantum annealing (Figure.4) made by various groups over the past decade [4-7] have stimulated considerable interest in understanding the mechanism of quantum annealing better. A theoretical discussion of the relative merits of classical annealing and quantum annealing is therefore desirable. Quantum Annealing repeats the transition (the annealing) over and over again. Having collected a number of samples, we pick the spin configuration with the lowest energy as our solution. There is no guarantee that this is the ground state. Si represents the spin within the lattice site. The interaction energy is then defined as:

$$E_I\{S_i\} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_{i=1}^{N} B_i S_i$$

Where I represent the Ising model. A factor of 2 has been absorbed into J_{ij} and we set $g\mu B = 1$ in the last term. <I,J> means nearest neighbour pairs of spins [8,9]. So <I,J> is the same as <J,I> is the exchange constant; it sets the energy scale. For simplicity, one sets J_{ij} equal to a constant J. If J > 0, then the spins want to be aligned

parallel to one another, and we say that the interaction is ferromagnetic. Example (3 magnets):

-0.0 (1, 1, 1)
-2.0 (1, 1, -1)
-0.0 (1, -1, 1)
2.0 (1, -1, -1)
2.0 (-1, 1, 1)
-0.0 (-1, 1, -1)
-2.0 (-1, -1, 1)
-0.0 (-1, -1, -1)

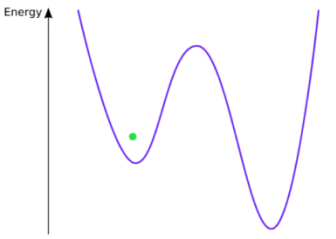


Figure 4: Quantum Annealing

If J < 0, then the spins want to be antiparallel to one another, and we say that the interaction is antiferromagnetic. If J_{ij} is a random number and can either be positive or negative, then we have what is called a spin glass. For simplicity we will set Jij = J > 0 and study the ferromagnetic Ising model. The last term represents the coupling of the spins to an external magnetic field B. The spins are assumed to lie along the z-axis as is the magnetic field B~ = Bzˆ. The spins lower their energy by aligning parallel to the field. I put Bi to indicate the possibility that the field could vary from spin to spin. If the field Bi is random, this is called the random field Ising model. We will assume a constant uniform magnetic field so that Bi = B > 0. So, the interaction energy becomes:

$$E_I\{S_i\} = -J\sum_{\langle i,j\rangle} S_i S_j - B\sum_{i=1}^{N} S_i$$

The partition function is given by:

$$Z = \sum_{s_1=-1}^{+1}\sum_{s_2=-1}^{+1}\cdots\sum_{s_N=-1}^{+1} e^{-\beta E_I\{S_i\}}$$

Ising models are often examined without an external field interacting with the lattice, that is, $h = 0$ for all j in the lattice Λ. Using this simplification, the Hamiltonian becomes:

$$H(\sigma) = -\sum_{\langle i\ j\rangle} J_{ij}\sigma_i\sigma_j$$

In quantum mechanics, the Hamiltonian is not a function of variables, but of operators. We will simulate what it means in a quantum circuit.

The Pauli spin matrices denotes the 2×2 identity operator [10]. The operator that replicates the effect of what we have seen in the classical case is the Pauli-Z matrix, defined as

$$\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \sigma^z \,|\, 0\rangle = (+1)\ |\, 0\rangle \qquad \sigma^z \,|\, 1\rangle = (-1)\,|\, 1\rangle$$

We need to add a term that does not commute with the rest of the terms. A transverse field is such, which is an on-site interaction just like the external field.

$$H = -\sum_{<i,j>} J_{ij}\sigma_i^Z\sigma_j^Z \ - \sum_i h_i\sigma_i^Z \ - \sum_i g_i\sigma_i^X$$

We are naturally interested in finding the lowest energy configuration. However, we cannot use some gradient-based method to find it, since the variables are binary, plus the optimization landscape is nonconvex. The Ising model can be mapped into several other models. Creating a solid analytical approach based on statistics from theories and experiments is essential for all engineering applications such as aerospace engineering [11-16]. Two of the famous applications are the lattice gas and the binary alloy. The term lattice gas was first used by Yang and Lee [17] in 1952 from their research on a model gas known earlier. To clarify the concept of lattice gas, consider a lattice of volume V and a collection of N particles, where N < V . The particles are placed on the vertices of the lattice such that not more than one particle can occupy a given site, and only particles on nearest-neighbour lattice sites interact. Therefore, we consider here the following potential energy between two atoms if they are on the same site the potential energy equal to $+\infty$, if the two atoms are nearest neighbours the potential energy equal to $-\varepsilon_0$,

otherwise equal to zero. The interaction potential between two lattice sites i and j is given by:

$$V(|\vec{r}_i - \vec{r}_j|)$$

$$V(r) = \begin{cases} \infty & (r = 0) \\ -\varepsilon_o & (r = a) \\ 0 & \text{otherwise} \end{cases}$$

The interaction energy is

$$E_G\{n\} = -\varepsilon_o \sum_{\langle i,j \rangle} n_i n_j$$

A binary alloy is a solid consisting of 2 different types of atoms. For example, ß–brass is a body-centred cubic lattice made up of Zn and Cu atoms. At T = 0, the lattice is completely ordered, and a copper atom is surrounded by zinc atoms and vice-versa. However, at non-zero temperatures the zinc and copper atoms can exchange places. Above a critical temperature of T = 742 K, the Zn and Cu atoms are thoroughly mixed so that the probability of finding a Zn atom on given site is 1/2. Similarly, the probability of finding a Cu atom on given site is 1/2. To model a binary alloy, one starts with a lattice of N sites, and two different types of atoms, A and B. Each site has only one atom so that NA + NB = N. The occupation of each site is given by:

$$n_i = \begin{cases} 1 & \text{if site i is occupied by atom A} \\ 0 & \text{if site i is occupied by atom B} \end{cases}$$

Monte Carlo methods for numerical simulation

This method is based on the concept of single-spin-flip dynamics, which states that in each transition, we will only change one of the spin sites on the lattice. By using single- spin-flip dynamics, we can get from any state to any other state by flipping each site that differs between the two states one at a time [18-21]. The algorithm first chooses selection probabilities g(μ, ν), which represent the probability that state ν is selected by the algorithm out of all states, given that we are in state μ. It then uses acceptance probabilities A(μ, ν) so that detailed balance is satisfied. If the new state ν is accepted, then we move to that state and repeat with selecting a new state and deciding to accept it. If ν is not accepted, then we stay in μ. This process is repeated until some stopping criteria is met, which for the Ising model

is often when the lattice becomes ferromagnetic, meaning all the sites point in the same direction.

Second order phase transition

Magnetic moments (Figure 5) are permanent dipole moments within the atom which are made up from electrons' angular momentum and spin. Electrons inside atoms contribute magnetic moments from their own angular momentum and from their orbital momentum around the nucleus. Magnetic moments from the nucleus are insignificant in contrast to magnetic moments from electrons. Thermal contribution will result in higher energy electrons causing disruption to their order and alignment between dipoles to be destroyed. Ferromagnetic, paramagnetic, ferrimagnetic and antiferromagnetic materials have different structures of intrinsic magnetic moments [21-24]. It is at a material's specific Curie temperature where they change properties. The transition from antiferromagnetic to paramagnetic (or vice versa) occurs at the Néel temperature which is analogous to Curie temperature.

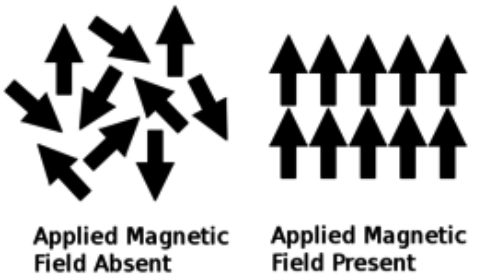


Figure 5: Magnetic fields within the atom

Summary

The theory behind Ising model and applications of Ising model in statistical thermodynamics and quantum mechanics were reviewed in this paper. Ising model first introduced by the German physicist Ernst Ising to mathematically model ferromagnetism in statistical mechanics. It consists of discrete variables that knowns as magnetic dipole moments of atomic spins that can be found in either +1 or -1 state. The spins are distributed in a lattice geometry and interacting with each neighbour spin causing variant structural phases. Ising model provides the phase transition in a simplified model. The two-

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