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Bragg-Williams theory of phase transition: Ising Concept

Physics

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ABSTRACT

In this article, we study the phase transition of system from Non-ferromagnetic to ferromagnetic phase within the Bragg-Williams approximation. This is the Second order phase transition around the transition temperature, in this type of transition, the state of the body changes continuously with some kind of change in the symmetry of the lattice. We discuss that in the Bragg-Williams theory this transition is well captured. The Ising concept (model) include discrete variables that represent by one of two states either +1 or -1. The spins are arranged in a graph, like a lattice, allowing each spin to interact with its neighbors. This concept use for the identification of different order phase transitions, as a simplified concept of reality. The two-dimensional ising concept for a square lattice is one of the simplest statistical models to illustrate the phase transition.

1. INTRODUCTION

By the behavior of the order parameter around the transition temperature phase transition is classified. The order parameter for ferromagnetic transitions is the magnetization and for water vapour transition it is density. Order parameter means the order with-in the given system. Order is lost among the spins at high temperature for magnetic system. As a result average value of the order parameter is to be zero. An order sets in as we down the temperature to the critical temperature and, the order parameter is non-zero under this temperature. The nature of the phase transition can be characterized with the help of order parameter. The average value of a generic order parameter symbolized by < >. The change in < > is discontinuous for a first order phase transition around the critical temperature while for a system undergoing second order phase transition it changes continuously. Few quantities like entropy are discontinuous around the first order transition point, besides order parameter it also should be mentioned. In between the crossing over from one phase to the other latent heat(L) is present that is whyproperty of <α> change around critical temperature.

The motive behind this article is to study about the phase transition of system from Non-ferromagnetic to ferromagnetic phase. The Ising model which has immense impact in understanding and explaining phase transition.

The order parameter is remains constant where the Mean-Field theory is approximation. Spatial fluctuation is neglected by us within the system. The first approach taken by researchers to predict the phase diagrams using mean field theory as it leads to results may differ from actual value most of the times . One of the best approaches for explaining phase transition is the Landau's mean field theory approach from various formulations of mean field theory.

2. ISING CONCEPT AND BRAGG-WILLIUM THEORY

One of the simplest methods to capture the phase diagram is Ising Model (Concept) which is being used especially for Non-ferromagnetic to ferromagnetic transition. This model has been designed to examine the behavior of substances with molecules having a magnetic moment. The assumption of this model is signifies isotropic interaction prevails among adjacent molecules, the

An array of N fixed points called lattice sites is considered in the system, it forms an n-dimensional periodic lattice (n= 1,2....). With a spin variable Si (i=1 ,2,.....N) that is either +1 or -1 signifies spin up or spin down states correspondingly Connected with each lattice site. the coupling can be done only between the two adjacent neighbor spins. Hence Ising Hamiltonian can be written as

$$HI\,(si) = -\epsilon\sum si\,sj - H\sum si = E\ \text{(Total Energy)}$$

The event $\epsilon > 0$ parallels to ferromagnetism. The energy E inclined to be minimum For stable equilibrium, Consequently, the spontaneous configuration of least energy totaly polarized configuration in this all the Ising spins are indicated in the same way. In equation (1) the sum over (i, j) constants N/2 terms where is the number of adjacent neighbours of any given site (coordination number of lattice) like in BCC =6.

The partition function is

$$Q = \sum\sum \ldots\ldots \sum e^{-\beta EI(s)}$$

where each si ranges independently over the values +1 or -1. Hence there are 2N terms in the summation. All thermodynamic parameter like internal energy, heat capacity, entropy Helmholtz free energy etc. calculated with the help of Q but it is extremely difficult. Many approximate used to solve this; one of them is the Bragg-Williams approximation.

Bragg-Williams theory

The Ising Hamiltonian or total energy of the Configuration is

$$E_I(s_i) = -\epsilon\sum_{(i,j)} s_i s_j - H\sum s_i \qquad (2)$$

Bragg and Williams assumed that the distribution of spins is at random.Let us focus our attention to the magnetic moment of the system just described. One expects the total magnetic moment is proportional to the total number of up spins (N_{up} or N+) and down spins (N_{down} or N-). Assuming the total number of sites as $N = N_{up} + N^{down}$, we expect

N+ / N = Probability of finding the spin up

N-/N= Probability of finding the spin down

3Total Ising energy is

$$EI = -\epsilon\gamma N/2[(N+/N)^2 + (N-/N)^2 - 2N+N-/N^2] - H(N+ --) \qquad (3)$$

Total magnetic moment is M=(N+ - –)

$$M/N = 2N+/N - 1 = m$$

$$N+/N = ½(1 + m)$$

$$N-/N = ½(1 - m)$$

$$M/N = (N+ - N-)/ N = m$$

$$mN = N+ - - \qquad (4)$$

Then

$$E_I = -\epsilon\gamma N/2[1/4(1+m)^2 + 1/4(1-m)^2 - ½(1+m)(1-m)] - HmN$$

$$= -\epsilon\gamma N/2(m^2) - HmN \qquad (5)$$

In above equation m is wide range parameter which shows magnetization in ferromagnetic system, at very high temperature, where one expects m=0, where, as at less temperature m is not equals to zero. Bragg-Williams method has shown this in very decent manner as it is in the following section.

The number of microstates of arrangement of spin over the N lattice sites by the number of ways we can pick up N+ out of N,

$$\Omega = N! / N+! (N - N+)! = N! / N+! \ -! \quad (6)$$

Since entropy is defined as the logarithm of number of microstates, we have

$$S = k \ln \Omega \quad (7)$$

$$S = k \ln (N! / N+! \ -!)$$

After simplification, entropy can be re-expressed as

$$S = -Nk [½(1 + m)\ln (1 + m) + ½(1 - m)\ln (1 - m) - \ln 2] \quad (8)$$

Then construct Bragg-Williams function

$$A(T,m) = EI - TS \quad (9)$$

Using (5) and (8) one gets,

$A(T,m) = -\epsilon \gamma N/2 (m2) - HmN + NkT [½(1 + m)\ln (1 + m) + ½(1 - m)\ln (1 - m) - \ln 2]$ (10)

The equilibrium value of m is calculated by ƏA(T,m)/ Əm = 0 so that

$$\ln[(1 + m)/ (1 - m)] = (\epsilon \gamma m + H) / kT = 2x \text{ (say)} \quad (11)$$

After simplification

$$m= \tanh x \quad (12)$$

which is result of weiss theory. For H=0, the spontaneous magnetic moment is

$$Ms = N \tanh (\epsilon \gamma Ms/NkT) \quad (13)$$

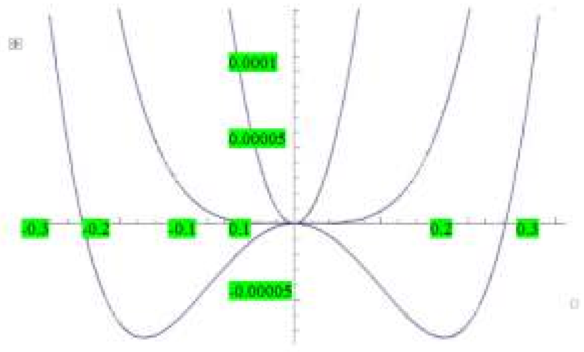

Diagram:- The plot drawn for A(m,T) , where x axis denote the values of m and y axis denote the values of T. In this plot the top value of T=Jz is 1:05 and middle value is 1 and bottom value is 0:99.

In the above diagram behavior of A(m,T) is shown. A(m,T) has a minimum at m=0 if T>Jz. For finite non zero values of m and T<Jz A(m,T) is minima. Ising Hamiltonian spin symmetry liable for symmetric plot. At T =Tc=Jz shifting of minima will start from zero to non-zero values. Where Tc represent the critical temperature. Around the critical temperature Tc the phase change continuously into second order phase transition. The Gibbs free energy and its first order derivative also continuous function in second order phase transition.

5. CONCLUSION

To conclude, we have seen that BW theory helps to understand phase transitions appearing in completely different areas in physics. Ising model of ferromagnetic to non-feromagnetic transition. This is a second order phase transition. This theory helps us to understand how to transform a matter from one phase to other around the critical temperature. In the second order phase transition the properties of the matter change around the critical temperature but states remains same.

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