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Investigation Of Ground State Of Spins In Ising Model For A Specific Value Of Interaction Strength J(I,J)=J And Establishment Of Numerical Relationship Between Hamiltonian And Magnetic Moments Of Spins

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Abstract: *Interaction between spins in Ising model depends on the nature of the interaction strength (J(I,j)) acting between spins. Different nature of interaction strength produces a variety of ground states, such as for ferromagnetic type interaction ground state is with all spins either up or down, on the other hand for anti ferromagnetic spins ground state consists of anti parallel spins. Here I have treated interaction strength to depend on the relative spacing (r(i,j)) of interacting spins and have found ground state with a specific r(i,j) dependence of J(I,j).*
Keywords- *Interaction strength, Ising model, Ising Hamiltonian, Magnetic moment, Spins & temperature*

I. Introduction

From Ising model we know that in absence of external field the Hamiltonian [1] of a spin- system can be written as:

$$H = \sum_{\substack{i,j \\ i \neq j}}^{N} J_{ij}\ \sigma_i \sigma_j$$

Here J_{ij} represents the interaction strength acting between spins σ_i and σ_j, where N is total no. of spins.

Depending on the nature of interaction between spins a spin –system can have different ground states. At absolute zero (T=0), the ground state of a ferromagnetic system (J_{ij}<0) is the one with all spins being at either up (+1) or down (-1) state. The magnitude of J_{ij} is a measure of interaction strength acting between i'th and j'th spin. J_{ij} can vary from spin to spin.

For our present discussion I assume that for any two spins σ_i and σ_j, if their separation $|\boldsymbol{r_i} - \boldsymbol{r_j}|$ is maintained constant then the interaction strength acting between them also remain constant. So, actually what I have assumed is that the interaction strength acting between spins for a particular substance is a function of their separation only, i.e.

$$J_{ij} = J(|\boldsymbol{r_i} - \boldsymbol{r_j}|) = J(\boldsymbol{r_{ij}})$$

For simplicity I assume $J_{ij}\ \alpha\ r_{ij}^{-n}$ --------------------------- (1.1)
Where 'n' is some non negative integer.

I shall check for some n=0 case in the following sections.

II. Theoretical calculations and analysis

Putting n=0 in equation (1.1) we obtain ,

$$J_{ij}\ \alpha\ r_{ij}^{-0}$$

$$J_{ij} = J\, r_{ij}^{-0} \quad \{\text{ J= proportionality constant}\}$$

$$J_{ij} = J \quad \text{------------------------- (2.1)}$$

For simplicity I choose J= ±1. So J_{ij} = ±1 ---------------------------------- (2.2)

From equation (2.2) we can clearly see that J_{ij} depends neither on the location of spins nor on their spacing. This means any two spin on the lattice will experience same interaction strength acting between them. The choice of n=0 does not become fruitful to large lattices but it is effective for small domains which responds to external excitation as a single spin as if they spins in such domains are strongly attached to each other.
The Hamiltonian of i'th spin σ_i interacting with all other spins σ_j's in a spin –system can be written as,

$$H = \sigma_i \sum_{\substack{j \\ i\neq j}}^{N} J_{ij}\ \sigma_j \text{-------------------- (2.3)}$$

Now using (2.2) on (2.3) we obtain,

$$H = \pm\sigma_i \sum_{j,\, i\neq j}^{N} \sigma_j \text{ ------------------------------ (2.4)}$$

In equation (2.4) '+' sign in r.h.s. stands for anti ferromagnetic interaction and '-' sign stands for ferromagnetic interaction. Further discussion on each of the cases has been done in the following subsections.

2.1 Ferromagnetic case

For ferromagnetic interaction equation (2.4) becomes,

$$H_i = -\sigma_i \sum_{j,\, i\neq j}^{N} \sigma_j$$

$$= -\sigma_i \left(\sum_{j=1}^{N} \sigma_j - \sigma_i\right)$$

$$= -\sigma_i (m - \sigma_i) \qquad \{\text{where } m = \textstyle\sum_{j=1}^{N} \sigma_j \text{ ; N = total no. of spins}\}$$

$$= -\sigma_i m + \sigma_i^2$$

$$= -\sigma_i m + 1 \qquad \{\text{As } \sigma_i^2 = 1\}$$

Therefore, $H_i = -\sigma_i m + 1$ -------------------- (2.5)

From equation (2.5) we see that minimum energy state for i'th spin is the one for which all spin is in the same state i.e. either all up(1) or all down(-1). This can be proved as follows,

If for 'N' no. of spins all spins are up then, $m=\sum_{j=1}^{N} \sigma_j = \sum_{j=1}^{N} 1 = N$ and $\sigma_i=1$; hence from equation (2.5) we get,

$$H_i = -N + 1 \text{ ----------------------- (2.6)}$$

Again if all the spins were down then m= -N and σ_i= -1; hence from equation (2.5) we get,

$$H_i = -(-1)(-N) + 1 = -N + 1 \text{ ---------(2.7)}$$

Equation (2.6) & (2.7) proves our previous inference. Since minimum energy state for any individual spin requires all other spins in the same state we can make one more inference that the ground state at absolute zero is the one for which all spins are in the same state.

The total Hamiltonian in this case can be calculated from equation (2.5) as follows,

$$H = \sum_{i=1}^{N} H_i = -m \sum_{i=1}^{N} \sigma_i + \sum_{i=1}^{N} 1 = -m^2 + N \text{ ------------------- (2.8)}$$

Now, in the ground state m= ±N at absolute zero; So from equation (2.8) we get,

$$H = -N^2 + N \text{ --- (2.9)}$$

As soon as the temperature rises from absolute zero spin starts flipping and therefore the first term in the r.h.s. of equation (2.8) reduces. Therefore we may write the ground state Hamiltonian for a spin –system in equilibrium at temperature T as follows,

$$H(T) = -m^2(T) + N \text{ ---------------------- (2.10)}$$

2.2 Anti ferromagnetic case

Equation (2.4), for anti ferromagnetic interaction takes the following form,

$$H_i = \sigma_i \sum_{j,\, i\neq j}^{N} \sigma_j \text{ --------------------- (2.11)}$$

In this case we have to treat even no. of spins and odd no. of spins distinctly. Because for even no. of spins with ground state being nearby spins in anti parallel formation net magnetic moment is zero while for odd no. of spins the same is one non vanishing spin which may be either up or down. Both cases are treated separately in the following subsections.

2.2.1 Even no. of spins

In this case we get from equation (2.11) that,

$$H_i = \sigma_i \sum_{j,\, i\neq j}^{N} \sigma_j$$

$$= \sigma_i \left(\sum_{j=1}^{N} \sigma_j - \sigma_i\right) \text{ ------------------------- (2.12)}$$

$$= \sigma_i (0 - \sigma_i) \ \{\text{Since N= even ; pairs of spins cancel each other}\}$$

Therefore,

$$H_i = -\sigma_i^2 = -1 \text{ ----------------------------- (2.13)}$$

Total Hamiltonian of the system in this case is,

$$H = \sum_{i=1}^{N} H_i = \sum_{i=1}^{N} (-1) = -N \text{ -------------------(2.14)}$$

Above equation is valid at absolute zero only. Above absolute zero the term $\sum_{j=1}^{N} \sigma_j$, in equation (2.12) does not become zero as anti ferromagnetic alignment is gradually lost as temperature is increased from absolute zero. Say at temperature T, $\sum_{j=1}^{N} \sigma_j = x(T)$. Hence from 2.12 we get,

$$H_i = \sigma_i(x(T) - \sigma_i)$$
$$= \sigma_i x(T) - \sigma_i^2$$
$$= \sigma_i x(T) - 1$$

So, at T, total Hamiltonian becomes

$$H = \sum_{i=1}^{N} H_i = x(T) \sum_{i=1}^{N} \sigma_i - \sum_{i=1}^{N} 1$$

$$H = \sum_{i=1}^{N} H_i = x^2(T) - N \quad \text{------------------------ (2.15)}$$

2.2.2 Odd no. of spins

In this case we get from equation (2.11) that,

$$H_i = \sigma_i \sum_{j, i \neq j}^{N} \sigma_j$$
$$= \sigma_i \left(\sum_{j=1}^{N} \sigma_j - \sigma_i\right)$$
$$= \sigma_i(y - \sigma_i) \quad \{ y=\pm 1; \text{ y is the non vanishing spin at ground state at absolute zero}\}$$
$$= \sigma_i y - \sigma_i^2$$

Therefore,

$$H_i = \sigma_i y - 1 \quad \text{------------------------ (2.16)}$$

Total Hamiltonian is,

$$H = \sum_{i=1}^{N} H_i = y \sum_{i=1}^{N} \sigma_i - \sum_{i=1}^{N} 1$$

$$H = y^2 - N = 1 - N \quad \text{----------- (2.17)} \qquad \{\text{as } y=\pm 1 \text{ so } y^2=1\}$$

Above equation is satisfied at absolute zero only. As temperature rises above the value $y=\pm 1$ does not hold because flipping of spins occur generating more non vanishing spins. So at temperature T, equation (2.17) can be redefined as follows,

$$H(T) = y^2(T) - N \quad \text{-------------- (2.18)}$$

Here y(T) is the no. of non vanishing spins upon summation over spin –system at temperature T.

III. Validity check of theoretical analysis via computer simulation

To check the validity of equations depicting the relationship between total Hamiltonian and magnetic moment for different cases as discussed in section II, I performed a number of Monte Carlo simulations[2] using Metropolis algorithm[2] with two dimensional square lattices of different sizes and found the fore said equations to be correct. For the sake of completeness, here I am giving some of the results in tabular form for each case and discussing the results.

Table 1

Lattice size	Interaction type	Temperature(T)	Simulated value of H(T)	M(T)	N	Calculated value of H(T) from theory using simulated value of M(T) { $H(T) = -m^2(T) + N$ }
20x20	Ferromagnetic	0	-159600	± 400	400	-159600
20x20	Ferromagnetic	100	-159600	± 400	400	-159600
20x20	Ferromagnetic	200	-148596	± 386	400	-148596
20x20	Ferromagnetic	300	-107184	± 328	400	-107184
20x20	Ferromagnetic	350	-81396	± 286	400	-81396
20x20	Ferromagnetic	420	-10004	± 102	400	-10004

In Table 1, equality of column 4 and column 7 establishes the agreement of theory and simulations for ferromagnetic interactions.

Table 2

Lattice size	Interaction type	Temperature(T)	Simulated value of H(T)	x(T)	N	Calculated value of H(T) from theory using simulated value of x(T) { $H(T) = x^2(T) - N$ }
20x20	Anti ferromagnetic	0	-400	±0	400	-400
20x20	Anti ferromagnetic	100	-336	±8	400	-336
20x20	Anti ferromagnetic	200	-384	±4	400	-384
20x20	Anti ferromagnetic	300	-384	±4	400	-384
20x20	Anti ferromagnetic	3000	276	±26	400	276

In Table 2, equality of column 4 and column 7 establishes the agreement of theory and simulations for anti ferromagnetic interactions with even no. of spins.

Table 3

Lattice size	Interaction type	Temperature(T)	Simulated value of H(T)	y(T)	N	Calculated value of H(T) from theory using simulated value of y(T) { $H(T) = y^2(T) - N$ }
21x21	Anti ferromagnetic	0	-440	±1	441	-440
21x21	Anti ferromagnetic	100	-432	±3	441	-432
21x21	Anti ferromagnetic	1000	-320	±11	441	-320

In Table 2, equality of column 4 and column 7 establishes the agreement of theory and simulations for anti ferromagnetic interactions with odd no. of spins.

3.1 Nature of H vs N curves for different cases

In this subsection I have presented nature of Hamiltonian vs system size curve graphically by simulating two dimensional lattices of different sizes for different cases as discussed in above sections.

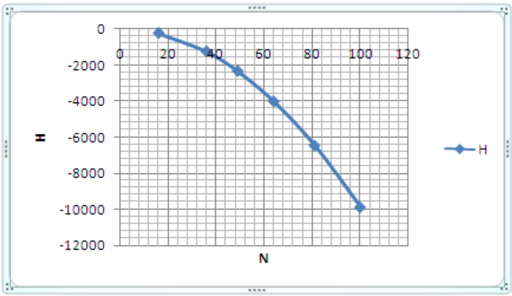

Figure 1: For ferromagnetic interaction at T=0

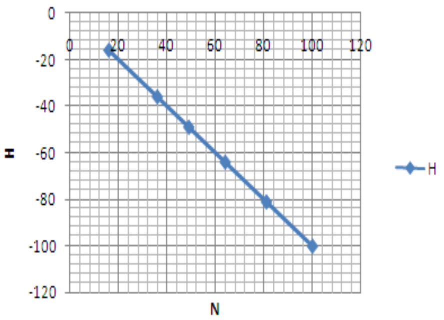

Figure 2: For anti ferromagnetic interaction at T=0 for even no. of spins

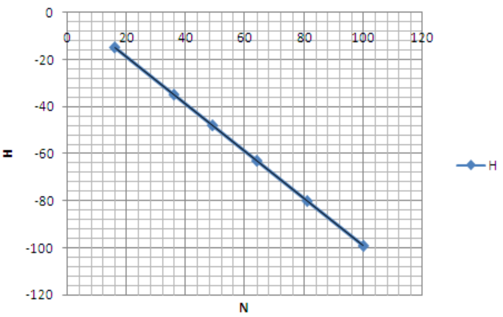

Figure 3: For anti ferromagnetic interaction at T=0 for odd no. of spins

Fig. 1 shows some nonlinear and somewhat parabolic type of variation of H with N which is in accordance with equation (2.9). Fig. 2 &3 shows linear relationship between H and N as expected from equations (2.14) & (2.17) respectively.

IV. Conclusions

In the present work a relationship between Hamiltonian and magnetic moment of spin systems have been established for a special case where it is supposed that any spin can interact with any other spin of the system with identical interaction strength. Such assumption simplifies the complexity of finite size effect because all spins are interacting with each other as if there is no boundary. If we interchange a boundary spin to any other position total Hamiltonian remains unchanged. Since total Hamiltonian is blind of spins positions, it may be possible that spins are continuously changing their states keeping their macro state defined by total Hamiltonian unchanged. Further enlightenment is necessary to come to such conclusion. This situation of interaction strength not being dependent of separation of spins, might happen for highly diluted magnetic systems, where small sized domains are developed.

References

[1] Michael P. Marder, Classical Theories of Magnetism and Ordering(John Wiley & Sons,2010)

[2] Gould H. & Tobochnik J. Introduction to Computer Simulation Methods (Addison – Wesley Publishing Company,1988)