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The Phase Transition of the 2D-Ising Model By Using Monte Carlo Method

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Abstract

In this project, the location of the phase transition in the two dimensional Ising model will be determined using Monte Carlo simulation with importance sampling. the magnetization per site $[\mu]$, energy per site $[J]$, magnetic susceptibility, specific heat of a Ferromagnetic materials are Calculated as a function of temperature T for 10×10, 20×20, 40×40, 50×50 spin lattice interaction by using Monte Carlo Simulation of the 2D Ising Model for some experimental values of ferromagnetic materials such as Gadolinium Chloride $(GdCl_3)$ at Curie temperature $T_c = 2.2\,J/k_B$, and ferromagnetic thin film from Nickel (N_i) growth on cooper (Cu) at Curie temperature $T_c = 2.772\,J/k_B$, in zero and nonzero magnetic field. It was noticed that above a certain temperature (T_c) the material will be in a paramagnetic state, this will lead to that the average magnetization will be decrease and the average energy increase, while below that temperature ,it will be in a ferromagnetic state, and the average magnetization will increase and the average energy decrease. Moreover, above a certain temperature spontaneous magnetization will be zero.

Keywords: Monte Carlo methods, the XYmodel.

الانتقال الطوري لنموذج ثنائي الأبعاد Ising باستخدام طريقة مونتي كارلو

الخلاصة

تم في هذا البحث تعيين موقع الانتقال الطوري ثنائي البعد لنموذج (Ising) باستعمال محاكاة المونتي كارلو لعينات من مواد فيرومغناطيسية مثل (كلوريد الكاديلينيوم $(GdCl_3)$, وغشاء رقيق فيرو من النيكل (N_i) على النحاس (Cu) , لحساب معدل المغناطيسيةالمكتسبة لكل موقع للذرات $[\mu]$, معدل الطاقةالمكتسبة لكل موقع $[J]$, القابلية المغناطيسية, السعة الحرارية , كدالة لدرجة الحرارة T لمصفوفة من تفاعلات شبيكة- برم ب 10×10, 20×20, 40×40, 50×50 ولبعض القيم العملية للعينات اعلاه عند درجات حرارة حرجة $T_c = 2.772\,J/k_B$, $T_c = 2.2\,J/k_B$ على التوالي . في مجال مغناطيسي $(H=0, H\neq0)$, حيث يلاحظ بان المواد بدرجة حرارة اعلى من (T_c) ستكون في حالة بارا مغناطيسية, مما يؤدي الى تناقص معدل المغناطيسية في هذه الحالة ويزداد بذلك معدل الطاقة, بينما يزداد معدل المغناطيسية عندما تكون (T_c) اقل حيث ستكون المواد في حالة فيرو مغناطيسية ويتناقص بذلك معدل الطاقة .

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Introduction

The Ising model itself can be formulated in two dimensions . The model is conveniently described in graph-theoretic terms, in which vertices represent atoms in a crystal and edges represent bonds between adjacent atoms. In the classic model, the graph is the standard “square” lattice in one, two, or three dimensions, so that each atom has two, four, or six nearest neighbors, respectively. There are two key sets of variables. First, each vertex i can be in one of two states, usually written as ± 1. Second, each edge has an assigned coupling constant, usually written as J_{ij}, where i and j are the two vertices. When neighboring vertices i and j are in states σ_i and σ_j, the interaction between them contributes an amount $-J_{ij}\sigma_i\sigma_j$ to the total energy H (the Hamiltonian) of the system, so that [1]

$$\mathrm{H}(\sigma) = -\sum_{(i,j)} J\sigma_i\sigma_j \quad \ldots(1)$$

where the sum is taken over all pairs of neighbors (i.e., edges of the graph). If J_{ij} is positive, then having neighbors in the same state $(\sigma_i = \sigma_j)$ decreases the total energy.

The goal of the Ising model is to understand how local interactions can give rise to long-range correlations. The computation of the partition function is essentially trivial in the one-dimensional case (see Figure 1a). It becomes a little more interesting with the addition of an “external field,” which can be viewed as an extra vertex with edges to all the other vertices (Figure 1b). [1]

The main state is to creates a lattice of randomly arranged spins at a given temperature. The spins then either flip or not by calculating the energy difference between the considered spin and its 4 nearest neighbors using the formula: [2]

$$\Delta U = 2J\cdot[i][j]\cdot(spin_{left}+spin_{right}+spin_{top}+spin_{bottom}) \quad \ldots\ldots.(2)$$

The spin then directly flips if $\Delta U \le 0$. If $\Delta U \ge 0$, it only flips if a randomly chosen number between 0 or 1 is smaller than the Boltzmann factor $\exp(-\Delta U / k_B T)$.The program starts at a certain given temperature and calculates whether the considered spin flips or not for a certain number of iterations. For each step we first performed l iterations to reach thermal equilibrium and then performed another $l/2$ iterations to determine the physical quantities

Energy per site, *Magnetization per site*, *Magnetic Susceptibility*, *Specific Heat*, [2,3,4].

2. Background

2.1 The phase transition of the 2D-Ising model

We can study the behavior of a magnet by using Monte Carlo method. ***A Monte Carlo algorithm*** is often a numerical Monte Carlo method used to find solutions to mathematical problems (which may have many variables) that cannot easily be solved, for example, by integral calculus, or other numerical methods. For many types of problems, its efficiency relative to other numerical methods increases as the dimension of the problem increases . Or it may be a method for solving other mathematical problems that rely on (pseudo-)random numbers [5].

We know that the expectation value of an observable A can be written as: [6]

$$\langle A \rangle = \frac{\sum_r A_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} \quad ....(3)$$

where A_r is the value of A for the state r. So given a system that has a discrete number of states, we could, (using a computer), calculate A for each state and weight these values by their Boltzman factors to find the average A. This might be feasible for a system with a small number of states, but, if we have for example a (20×20) and (40×40) etc., spin lattice interacting via the Ising model, there are 200^{400} states ,so we cannot possibly examine all of them .

2.2. Calculating Observables

We can obtain some qualitative information about our simulation by watching the spin array during a simulation. For high temperatures, the spins remain randomly aligned after long periods of equilibration, whereas for low temperatures, the spins end up pointing in mostly the same direction.

To get more quantitative results, we can measure the energy and the magnetization at each step of the routine. Before we start taking statistics, we should allow the system to equilibrate for a long time . We can then measure the magnetization by taking the sum of all the spins in the lattice, and we can calculate the energy by determining the energy for each spin and dividing by two for double counting.

The specific heat can also be written in terms of the variance of the energy: [6]

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

Where $\langle E \rangle = -\dfrac{\partial \ln Z}{\partial \beta}$

$$= -\frac{\beta}{T}\frac{\partial\langle E\rangle}{\partial\beta}$$

$$= \frac{\beta}{T}\frac{\partial^2 \ln Z}{\partial\beta^2}$$

$$Z = \sum e^{-E\beta}$$

Where Z= partition function

$$= \frac{\beta}{T}\frac{\partial}{\partial\beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial\beta}\right) =$$

$$\frac{\beta}{T}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial\beta}\right)^2\right]$$

$$= \frac{\beta}{T}\left[\langle E^2\rangle - \langle E\rangle^2\right] \quad ....(4)$$

Where $\beta = \frac{1}{k_B T}$

T = Temperature, k_B = Boltzman constant

Similarly, the magnetic susceptibility, χ, can be written in terms of the variance in the magnetization:

$$\chi = \frac{\partial\langle M\rangle}{\partial H} = \beta\langle M^2\rangle - \langle M\rangle^2 \, ..(5)$$

To determine the ***Energy per site*** we calculated the energy of the system after having reached thermal equilibrium Equation by summing up the over all energies of each spin as given by: [2]

$$E_{spin} = -J\cdot[i][j]\cdot(spin_{left} + spin_{right} + spin_{top} + spin_{bottom}) \quad .....(6)$$

In order to get $\langle E^2\rangle$ and $\langle M^2\rangle$, we squared the received energy in each iteration step and then proceeded in the same way as above. With these values, we can easily calculate the ***Magnetic Susceptibility*** in units (μ/k_B) and the ***Specific Heat*** in units $(J/k_B{}^2)$ using the following formula : [2]

$$\chi = \frac{1}{T}\left[\langle M^2\rangle - \langle M\rangle^2\right]$$

$$C_v = \frac{1}{T^2}\left[\langle E^2\rangle - \langle E\rangle^2\right] \quad ....(7)$$

To determine the location of the transition in the 2D-Ising model, we examined the mentioned quantities between a temperature of 2.2 (J/k_B) and 2.772 (J/k_B) with lattice size of 10×10, 20×20, 40×40, 50×50 spin lattice interactions.

4. Phase Transition in Physical Quantities

1. ***Magnetization for zero magnetic field***

The magnetization of a Ferromagnet as a function of temperature T in zero magnetic field $(H = 0)$ per site μ, where presented in figures (2,…,5), according to ***(ANNNI)*** model .

Figures (2, …, 5) indicate that all the points are based on the system that contains a small number of states, which have a 10×10, 20×20, 40×40 spin lattice interactions (i.e. number of rows and columns in lattice) via the Ising model by Monte Carlo Simulation of the 2D Ising Model for some experimental values of ferromagnetic materials such as Gadolinium Chloride $(GdCl_3)$ at Curie temperature $T_c = 2.2\, J/k_B$, and ferromagnetic thin film from Nickel (N_i) growth on cooper (Cu) at Curie temperature $T_c = 2.772\, J/k_B$.

one can to rely on Monte Carlo method that adopted is based on program as (Fortran Code 90). Therefore the parameters are using in this paper make us know the material ferromagnetic as{ $(GdCl_3)$, (N_i) growth on cooper (Cu) }before and at T_c according to the program .

We clearly see, that above a certain temperature (T_c) the material will be in a paramagnetic state, while below that temperature ,it will be in a ferromagnetic state. Moreover, above a certain temperature spontaneous magnetization will be zero. one can note from figures (2, 3) that values the average magnetization at site *(Axial Next Nearest Neighbor Ising)* case (1) first nearest neighbor will increase more (i.e. before the point T_c) due to the short period time for each step of 10×10, and 20×20 spin lattice interactions, with contrast with the average magnetization at the site *(Second Next Nearest Neighbor Ising)* case (2,3…..etc) second next nearest neighbor will little increase due to increase steps (long period time) for 40×40, 50×50 spin lattice interactions as in figures (4,5) (i.e. before the point T_c) . Therefore this average magnetization at high temperatures (i.e. after the point T_c) will be zero for all cases (1), (2,3,…) in sites *(ANNNI)* model

2. magnetization for nonzero magnetic field

One study the kink-like solutions by means of a MC simulation. In order to do that, One consider a classical *XY* model with two spin component in two dimensions (plane rotator model) under an external magnetic field, using as a initial configuration the kink solution given by eq(8) and calculating the total energy by eq (9). [7], as following

$$H = \sum_i \left(\sum_j \left(-\frac{J}{2} S_i S_j \right) - HS_i \right) \quad \text{…..(8)}$$

with J : coupling constant , H : external magnetic field . As the magnetic field increases/decreases more and more Spins align in the same direction as the field, Thus the average magnetization increases with the magnetic field until all spins are aligned parallel (i.e. before the point T_c) as in figures (6,8,10,12) but at a higher temperatures, and therefore more fluctuation of the spins (i.e. after the point T_c), because of this even (for example $H = 2$ and $H = -2, \ldots$) not all the spins are aligned parallel, for some experimental values of ferromagnetic materials such as Gadolinium Chloride $(GdCl_3)$ at curie temperature $T_c = 2.2\, J/k_B$, and the ferromagnetic thin film from Nickel (N_i) growth on cooper (Cu) at Curie temperature $T_c = 2.772\, J/k_B$.

We consider four different system sizes in two states, the first with short period time for each step of 10×10, 20×20 spin lattice interactions, at site *(ANNNI)* case (1) first nearest neighbor as in figures (6,8). The second increase steps (long period time) for 40×40, 50×50 spin lattice interactions at the site *(ANNNI)* case (2,3…..etc) second next nearest neighbor as in figures (10,12). For each system, in all simulations the external magnetic field consist of various values (H=0.5, 0.6, 1.2, 2) .

3. Magnetic Susceptibility

The magnetic susceptibility χ is a parameter that shows how much an extensive parameter changes when an intensive parameter increases. Thus, the magnetic susceptibility tells us how much the magnetization changes by increasing the temperature. From the figures in the magnetization one can see, at which transition, the magnetization rapidly decreases. Thus the magnetic susceptibility should show a fast increase to infinity. One can note also that at site *(ANNNI)* case (1) first nearest neighbor magnetic susceptibility will be order dropping (i.e. after the point T_c) , where $(\chi = 0)$, as in figures (14, 15) because short period time for each step of 10×10 and 20×20 spin lattice interactions, while at other site *(ANNNI)* case (2) second next nearest neighbor it will be disorder dropping with steps increase (long period time),where $(\chi = 0)$ for (50×50) spin lattice interactions as in Fig.16 .

It can be seen, that below and above T_c the magnetic susceptibility is about zero $(\chi = 0)$ and around T_c it goes to infinity. This shows that below and above the transition, the change in magnetization is almost zero, where at the transition, the change is infinite.

4. Spins and the Critical temperature:

One can obtain some qualitative information about our simulation by seeing the spin array (± 1) during a simulation, where

- At large T entropy wins : $M = 0$
- At small T energy wins : $M = \pm 1$

Figure (17) indicates that the average-magnetization (spin domains) per site $[\mu]$ at the spin positive sites $(+1)$, for 20×20 spin lattice interaction, will be (ferromagnetic) towards up at *(ANNNI)* case (1) first nearest neighbor in $(H = 0)$, while we note that the average magnetization for the spin negative sites (-1) will be (ferromagnetic) towards down at *(ANNNI)* case (2) second next nearest neighbor Ising model in magnetic field $(H = 0)$,where the Critical temperature for the ferromagnetic thin film from Nickel (N_i) growth on cooper (Cu) is $T_c = 2.772\, J/k_B$.

Therefore noticed that the highest temperature for which there can be nonzero magnetization at T_c for the two cases above (± 1). At this point, the system undergoes an order-to disorder transition, called a phase transition .

5 . Energy per site in nonzero magnetic field

The total energy of the system depends on the interactions of the particles with their nearest neighbor and with any external magnetic field.

The energy is given by $[8,9,10]$:

$$E = -B * \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} - J * \sum(neighborspins) * \begin{pmatrix} 1/2 \\ -1/2 \end{pmatrix} \quad \ldots\ldots(10)$$

One notes from figures (19, 21, 23, 25) that the average energy per site J for zero magnetic field that above a certain temperature (T_c) the material will be increased in the energy state, while below that temperature, it will be decreased in the energy state , with contrast with nonzero magnetic field (external magnetic field), which is average energy above a certain temperature (T_c) the material will be increase more, while below that temperature, it will be more from the energy state in zero magnetic field, because the magnetic field increases/decreases more and more Spins align in the same direction as the field, Thus the average energy increases with the magnetic field until all spins are aligned parallel, as in the figures (18,20,22,24).

6. Specific Heat

The specific heat tells us, how much the energy changes with increasing temperature. Thus we expect to see a divergence of the specific heat at the transition. The plot of the measured specific heat versus the temperature proofs the expectation well in zero magnetic field.

one can note from (fig.26) that values the (C_V) at site *(ANNNI)* case (1) first nearest neighbor will little due to the short period time for step of 10×10 spin lattice interactions, with contrast with the (C_V) at the site *(ANNNI)* (2,3…..etc) second next nearest neighbor will increase due to increase steps (long period time) for 20×20 spin lattice interactions as in (fig. 27) .we can calculate that up point in (C_V) at T_c represent final bound for energy changes with increasing temperature at $T_c < T$.

Conclusions

The solitonic-like solutions predicted by the continuum semi-classical two–dimensional *XY* -model are investigated using canonical Monte Carlo simulation. In particular, we verify the existence of kink states,
and study their degree of stability. These states, that were supposed to exist from approximate theories applied to the continuum limit of this model, are a new kind of solution of the XY model under external magnetic field. In the simulation several system sizes up to 10×10, 20×20, 40×40 spins were considered. The study of the static spin correlation between the initial and final configuration shows there exist a finite transition temperature *Tc*, which is independent of the system size. According to our simulation, at *T < Tc* the kink state is stable, and the degree of stability increases with system size.

Magnetization per site $[\mu]$, energy per site $[J]$, magnetic susceptibility, specific heat of a Ferromagnetic materials are Calculated as a function of temperature T for 10×10, 20×20, 40×40 , 50×50 spin lattice interaction of the 2D Ising Model for some experimental values of ferromagnetic materials such as Gadolinium Chloride $(GdCl_3)$ at Curie temperature $T_c = 2.2\,J/k_B$, and ferromagnetic thin film from Nickel (N_i) growth on cooper (Cu) at Curie temperature $T_c = 2.772\,J/k_B$, in zero and nonzero magnetic field.

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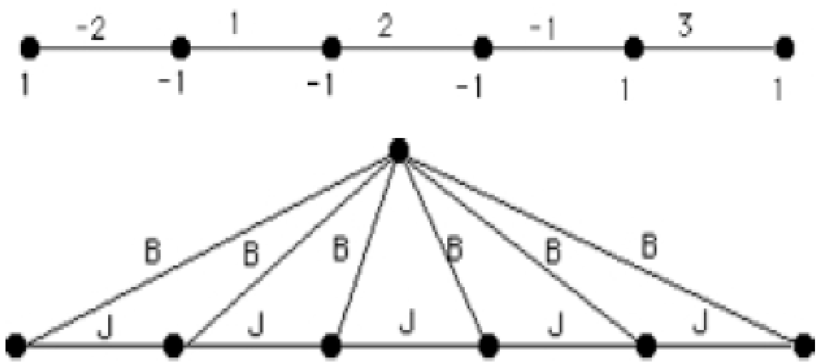


Figure (1): a) State and coupling constants for a one dimensional lattice .ground state is easy to find. b) One dimensional model with an external magnetic field.[1]

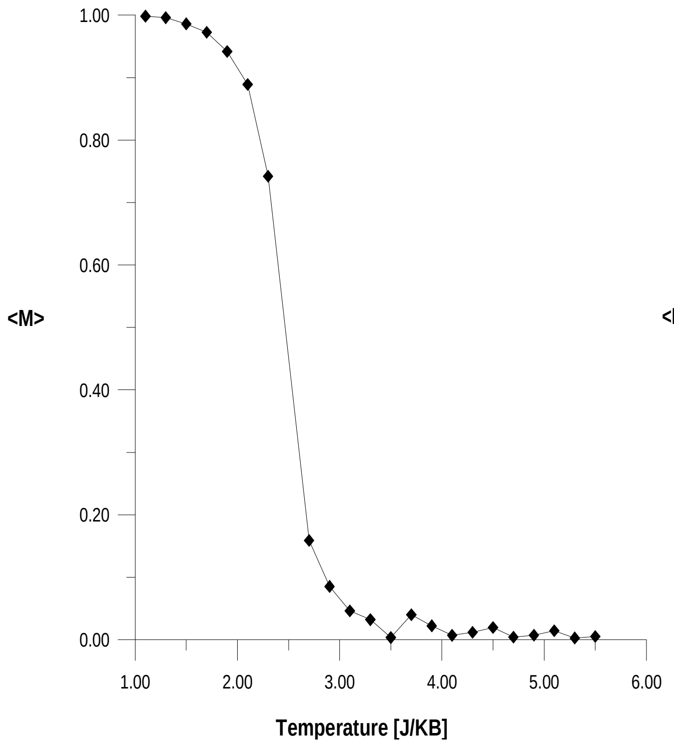


Figure (2):Average-magnetization per site [μ], of a ferroma as a function of temperature T, for 10*10 spin lattice interaction , at Tc=2.2 J/kB of Gadolinium Chloride($GdCl_3$

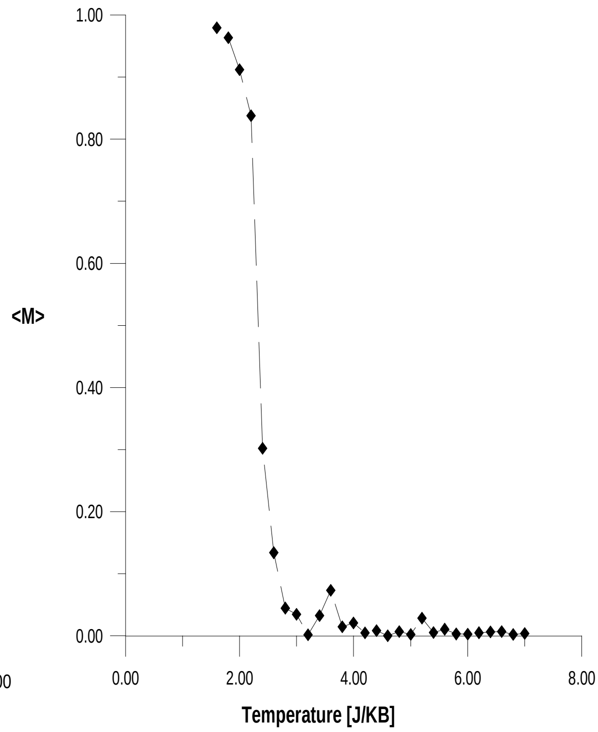


Figure (3):Average-magnetization per site[μ] of a ferromagnet asa function of temperature T, for 20*20spin lattice interaction ,at Tc=2.2 J/kB of Gadolinium Chloride($GdCl_3$).

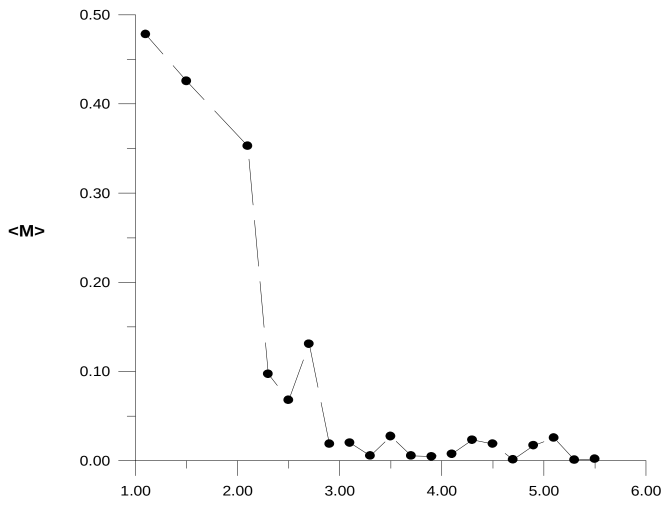


Figure (4): Average-magnetization per site [μ], of a ferromagnet as a function of temperature T, for 40*40 spin lattice interaction, at Tc=2.2 J/kB approximateof Gadolinium Chloride ($GdCl_3$).

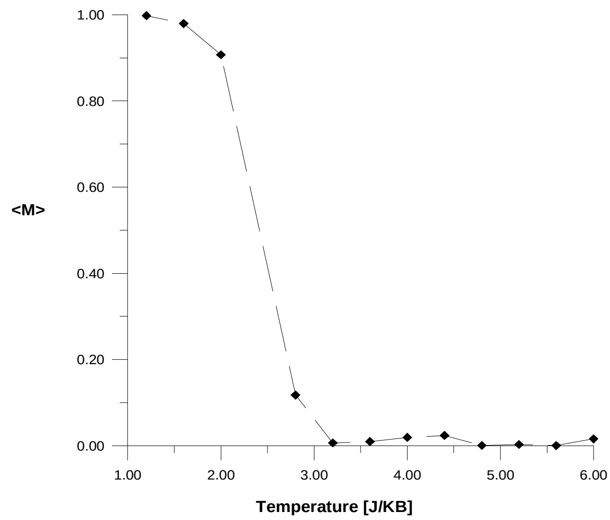


Figure (5): Average-magnetization per site [μ],of a ferromagnet as a function of temperature T,for 50*50 spin lattice interaction, at Tc=2.772 J/kB for thin film from Nickel (Ni) growthon cooper (Cu).

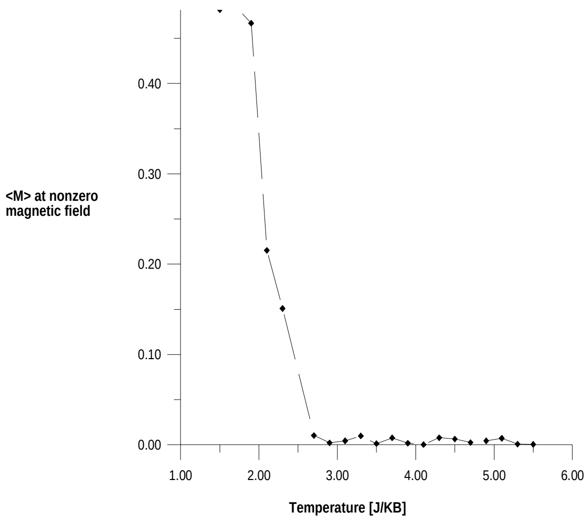


Figure (6):Average-Magnetization per site[μ] of a ferromagnet as a function of temperature T, for 20*20 spin lattice interaction in nonzero magnetic field (H=0.5) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

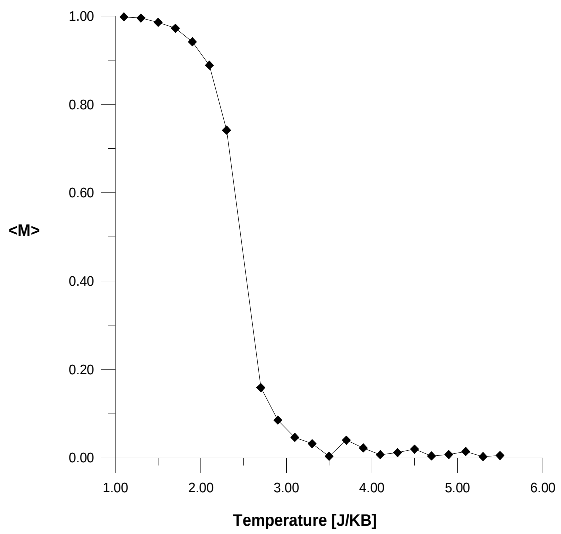


Figure (7):Average-magnetization per site [μ], of a ferromagnet as a function of temperature T, for 10*10 s lattice interaction in magnetic field (H=0) , at Tc=2.2 J approximate of Gadolinium Chloride($GdCl_3$).

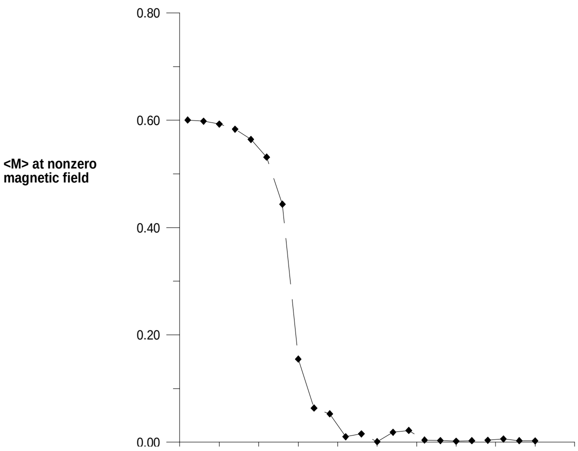


Figure (8):Average-magnetization per site [μ], of a ferromagnet as a function of temperature T, for 10*10 spin lattice interaction in nonzero magnetic field(H=0.6) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

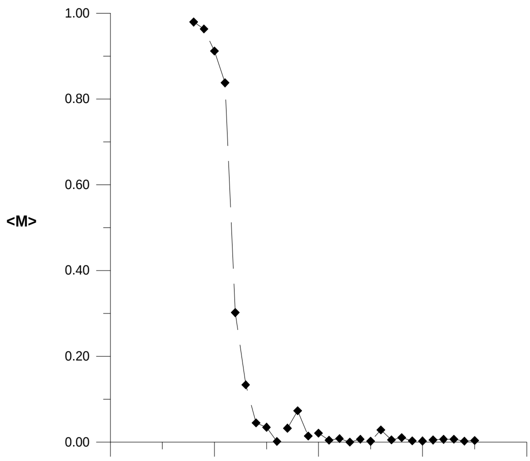


Figure (9):Average-Magnetization per site[μ] of a ferromagnet as a function of temperature T, for 20*20 spin lattice interaction in magnetic field (H=0),at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

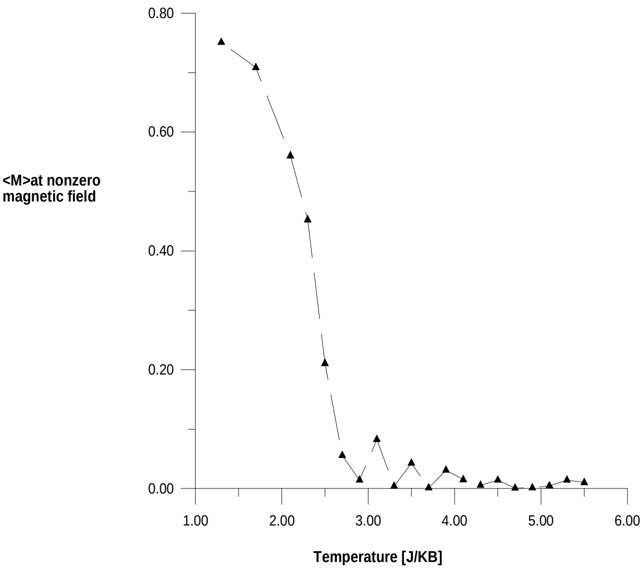


Figure (10):Average-magnetization per site[μ], of a ferromagnet as a function of temperature T, for 40*40 spin lattice interaction in nonzero magnetic field (H=1.2) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

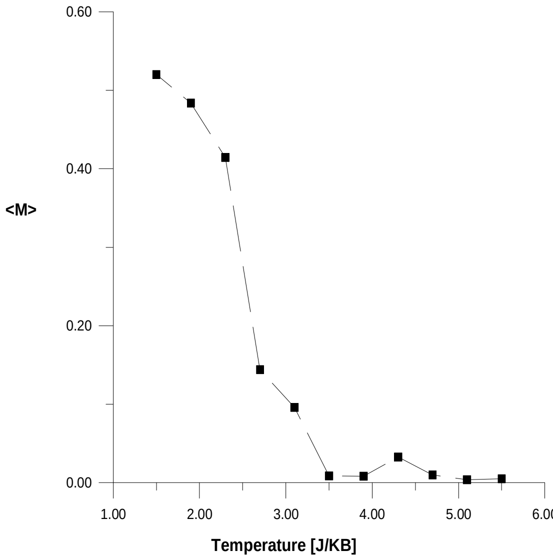


Figure (11): Average-magnetization per site [μ], of a ferromagnet as a function of temperature T, for 40*40 spin lattice interaction in magnetic field (H=0) , at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

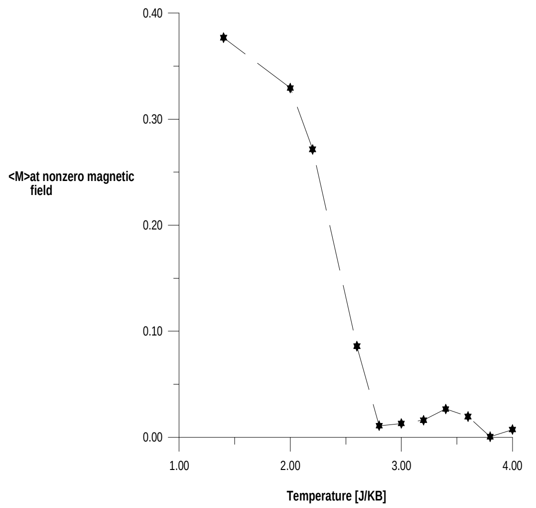


Figure (12):Average-magnetization per site [µ],of a ferromagn
a function of temperature T,for 50*50 spin lattice interaction
nonzero magnetic field (H=2) ,at Tc=2.772 J/kB for thin film fr
Nickel (Ni) growth on cooper (Cu).

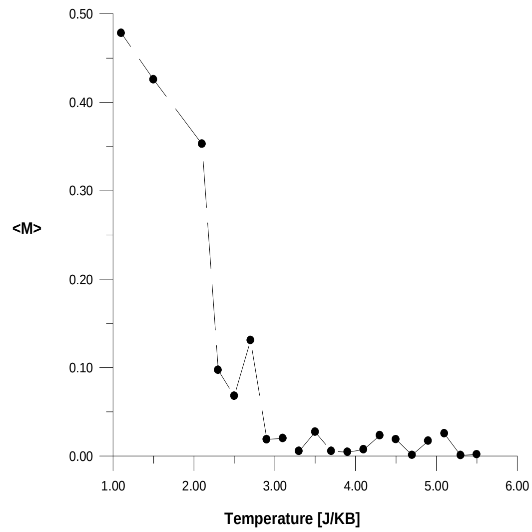


Figure (13):Average-magnetization per site[µ],of a ferromagnet as a function of temperature T,for 50*50 spin lattice interaction in magnetic field (H=0) ,at Tc=2.772 J/kB for thin film from Nickel (Ni) growth on cooper (Cu).

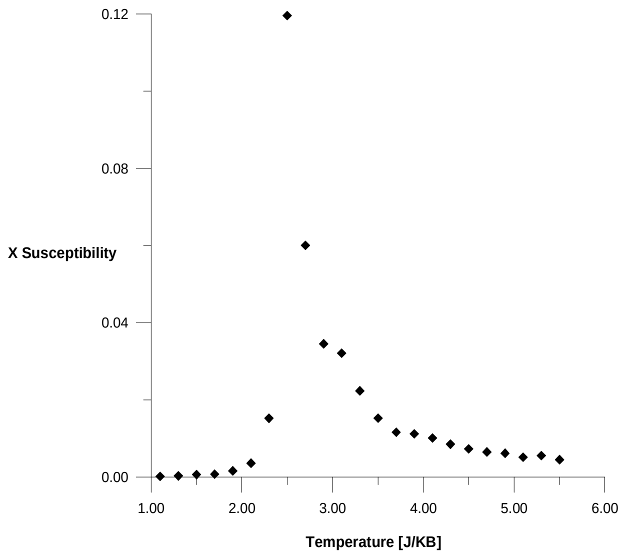


Figure (14):Magnetic susceptibility [µ /kB],of a ferromagnet as a function of temperature T, for 10*10 spin lattice interaction at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

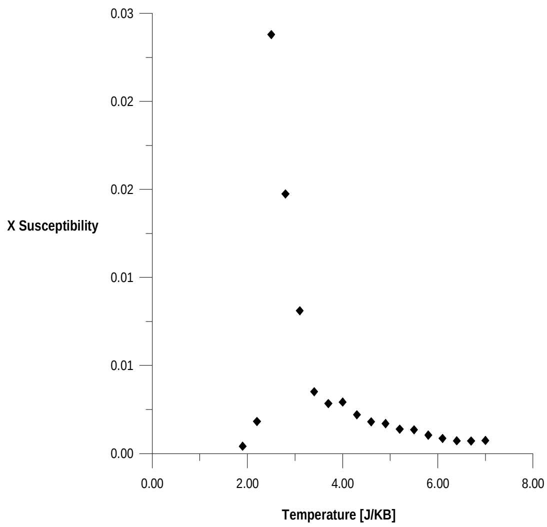


Figure (15): Magnetic susceptibility [µ/kB] of a ferromagnet as a function of temperature T, for 20*20 spin lattice interaction , at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

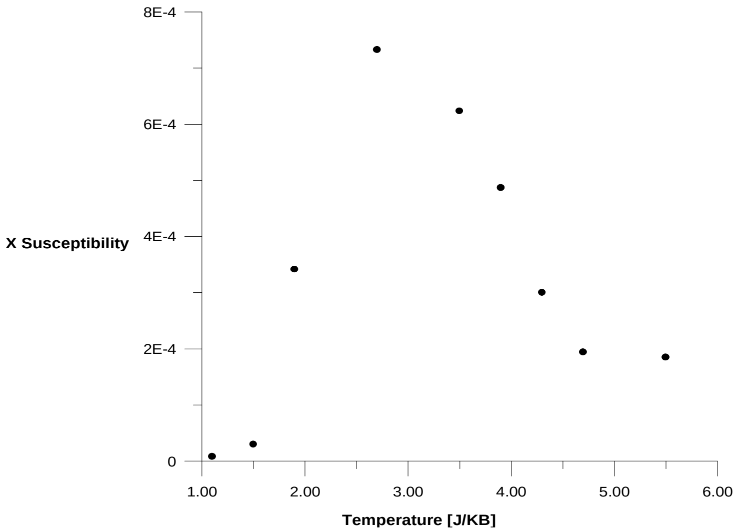


Figure (16):Magnetic susceptibility [μ /kB], of a ferromagnet as a function of temperature T,for 50*50 spin lattice interaction,at Tc=2.772 J/kB for thin film from Nickel (Ni) growth on cooper (Cu).

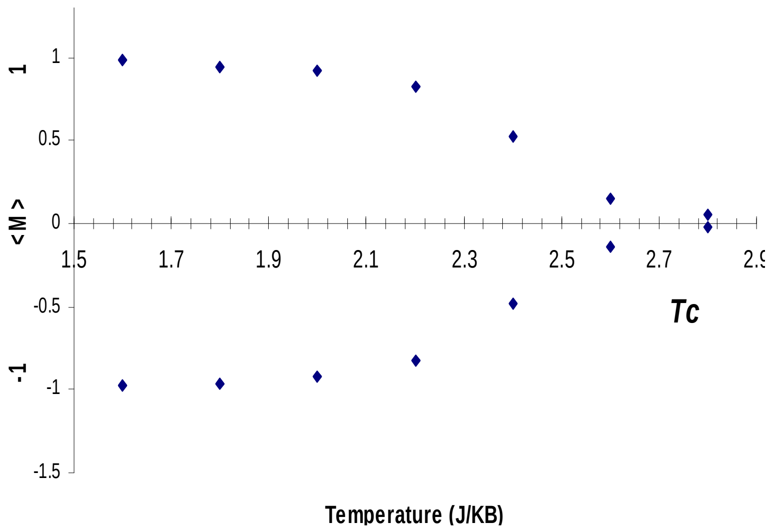


Figure (17) : Average-magnetization per site[μ],of a ferromagnet as a function of temperature T , for 20*20 spin lattice interaction for the spin array (+1,-1) at Tc=2.772 J/kB for thin film from Nickel (Ni) growth on cooper (Cu).

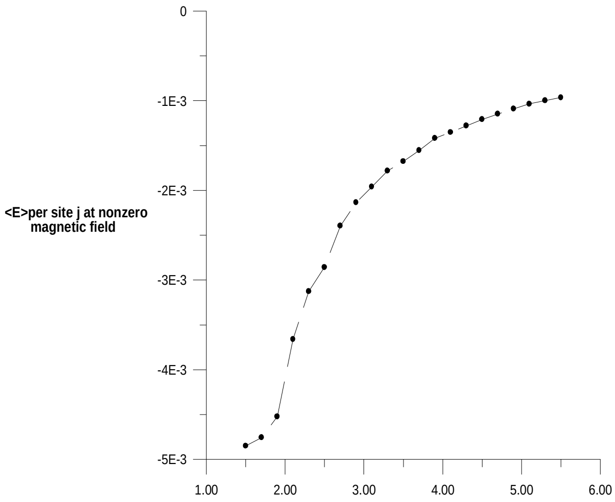


Figure (18):Average-energy per site[J], of a ferromagnet as a function of temperature T, for 20*20 spin lattice interaction in external magnetic field (H=0.5) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

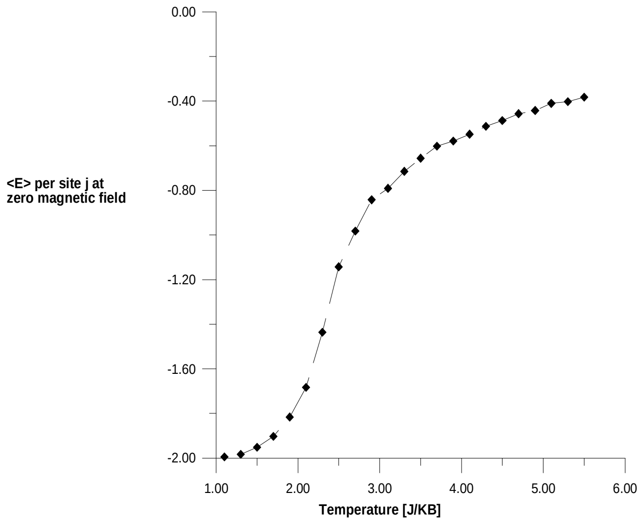


Figure (19): Average-energy per site [J], of a ferromagnet as a function of temperature T, for 10*10 spin lattice interaction in zero magnetic field (H=0) , at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$)

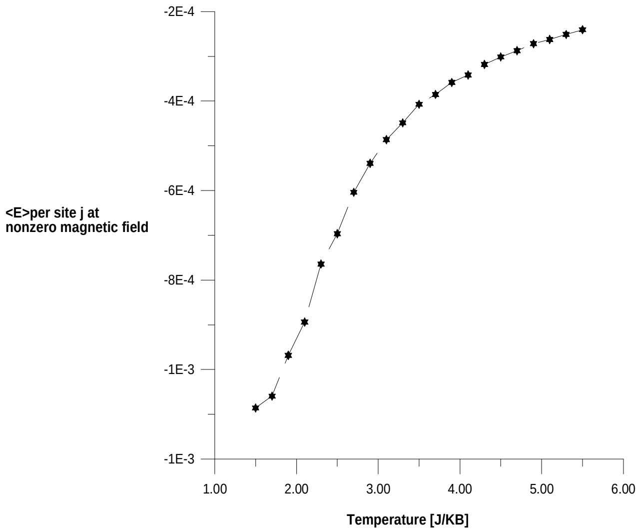


Figure (20): Average-energy per site [J], of a ferromagnet as a function of temperature T, for 10*10 spin lattice interaction in external magnetic field (H=0.6) , at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

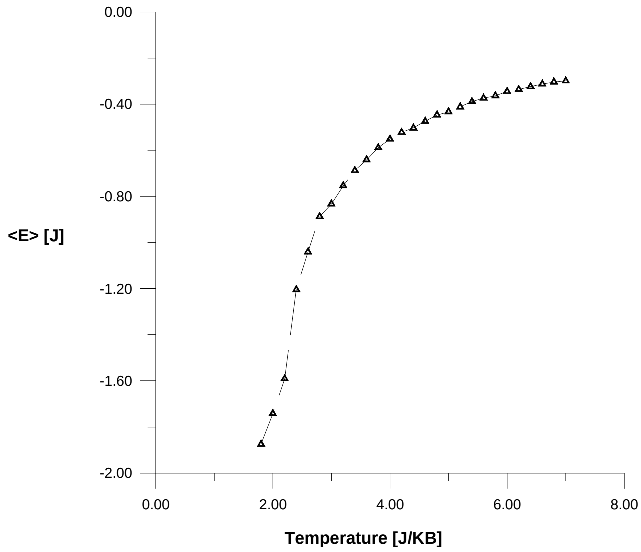


Figure (21):Average-energy per site[J], of a ferromagnet as a function of temperature T, for 20*20 spin lattice interaction in zero magnetic field (H=0) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).

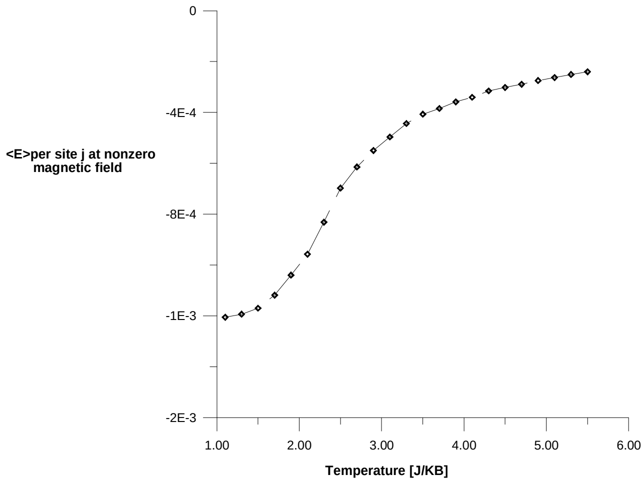


Figure (22): Average-energy per site [J], of a ferromagnet as a function of temperature T, for 40*40 spin lattice interaction in external magnetic field (H=1.2) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$)

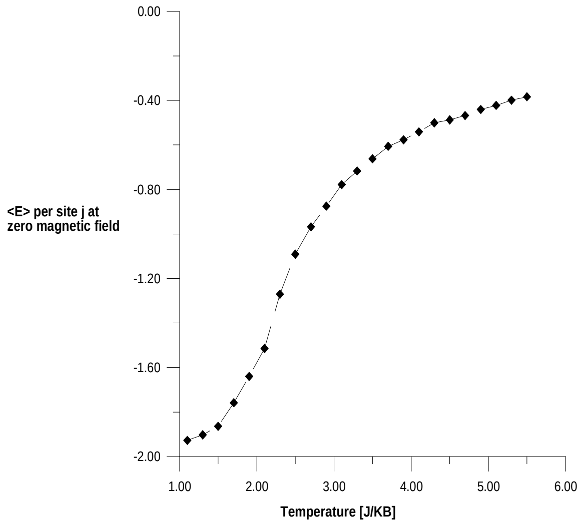
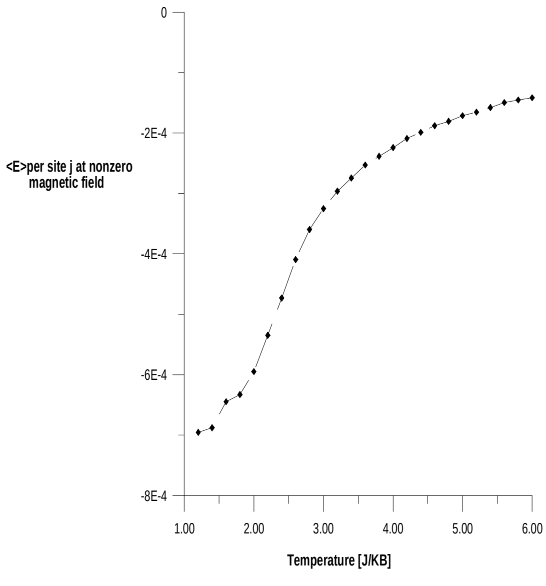
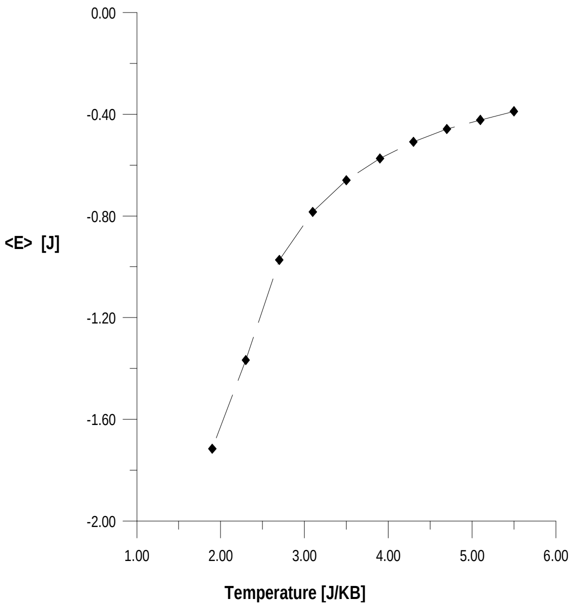


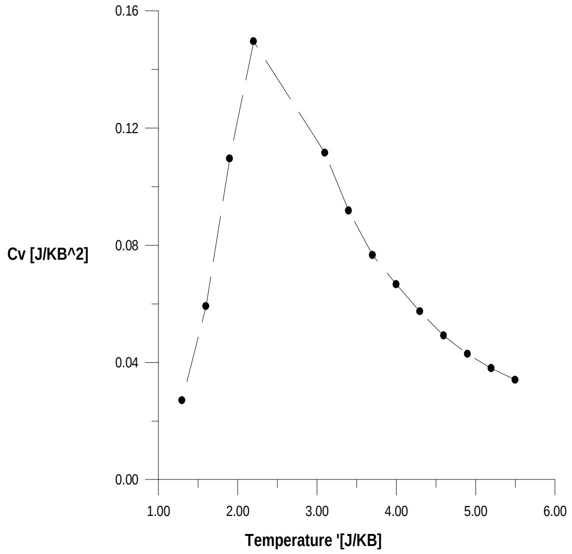
Figure (23): Average-energy per site [J], of a ferromagnet as a function of temperature T, for 40*40 spin lattice interaction in zero magnetic field (H=0) ,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).



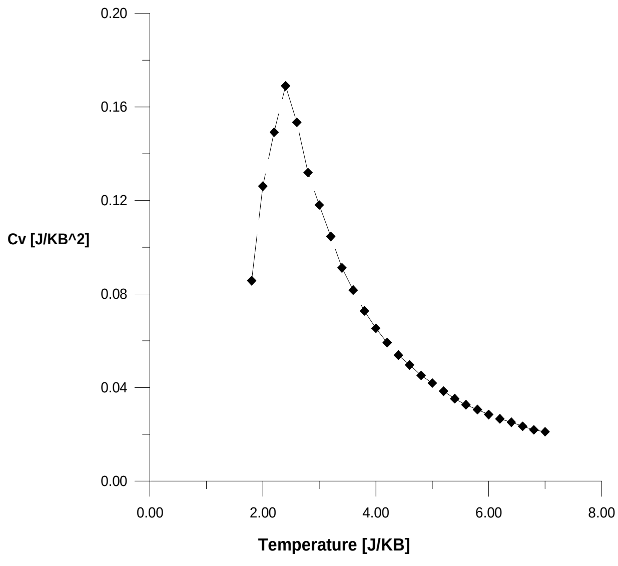
Figure(24): Average-energy per site [J], of a ferromagnet as a function of temperature T,for 50*50 spin lattice interaction in external magnetic field (H=2) ,at Tc=2.772 J/kB for thin film from Nickel (Ni) growth on cooper (Cu).



Figure(25): Average-energy per site [J], of a ferromagnet as a function of temperature T,for 50*50 spin lattice interaction in zero magnetic field (H=0) ,at Tc=2.772 J/kB for thin film from Nickel (Ni) growth on cooper (Cu).



Figure(26):Specific heat [J/kB ^2], of a ferromagnet as a function of temperature T, for 10*10 spin lattice interaction,at Tc=2.2 J/kB approximate of Gadolinium Chloride($GdCl_3$).



Figure(27):Specific heat [J/kB ^2] , of a ferromagnet as a functic temperature T, for 20*20 spin lattice interaction, at Tc=2.2 approximate of Gadolinium Chloride($GdCl_3$).