Revisiting 2D Lattice Based Spin Flip-Flop Ising Model: Magnetic Properties of a Thin Film and Its Temperature Dependence

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Abstract
This paper presents a brief review of Ising's work done in 1925 for one dimensional spin chain with periodic boundary condition. Ising observed that no phase transition occurred at finite temperature in one dimension. He erroneously generalized his views in higher dimensions but that was not true. In 1941 Kramer and Wannier obtained quantitative result for two-dimensional Ising model and successfully deduced the critical temperature of the system. In 1944 Onsager explicitly obtained free energy in zero fields. Though only 1dimensional formula has been derived in this review paper but Monte Carlo simulations results verify the established part of experiment and theory and explore the temperature dependence of magnetic property of thin film in 2D case. The paramagnetic case with spin coupling coefficient J=0 and anti-ferromagnetic cases with J=0.50, 0.75 & 1.0 are studied at temperatures kT=0.20, 0.30, 0.40, 0.50, 0.60, 1.0, 1.5 & 2.0. The change in behavior from anti-ferro to para is also observed and explained at high T values. I have demonstrated data writing for application purpose by writing number 10 on a thin anti-ferromagnetic tape (i.e. 2D film).
Key word: Spin wetting, Monte Carlo Simulation, Ferromagnetism, Paramagnetism

Introduction

Magnetism is a subject that is taught at various levels of courses in India and parts of the world. The 10th standard students are introduced with the magnetic properties of ferromagnetic, paramagnetic and diamagnetic materials. Experimentation with magnetic materials including experiments as drawing the line of magnetic lines of earth magnetic field lines with a compass needle starts as a part of school curriculum. At latter stages of learning as Bachelor of Science the students are taught basic theory of magnetism, which further deepens at Master level. Of course at research level it involves all the teaching-learning process in definite ways when one wants to explore the fascinating world of magnetism with questions in mind-"What is magnetism? How it is produced? What are the possible applications of these magnetic materials?"

We know magnetic properties of certain materials from many centuries. Chinese noted that magnetite or lodestone found in open pits was attracted by earth's magnetic field. The ferromagnetic properties of elements like iron, nickel, cobalt etc are very well understood and there is a fully developed experimental and theoretical branch of physics dedicated to magnetic properties of materials and its applications. The magnetic materials are broadly classified into paramagnetic, diamagnetic, ferromagnetic, anti-ferromagnetic and ferrimagnetic etc. which are widely used for day-to-day applications. The inventions and manufacturing of new devices and appliances have become a need of the hour because of the huge demand of the growing population of the world in order to provide to a solution to various problems of mankind and also for making it better and safer. This century is going to be century of technology especially that of nanotechnology when the miniaturization process has

reduced the dimension(s) of the functional materials to few hundred nanometers- Poole & Owenes (2009).

In paramagnetic materials atoms have one unpaired electron in their outermost subshell. So, each atom can contribute either spin angular momentum +1/2 or -1/2 i.e. S=±1/2. So, there exist a net magnetic moment because of electron spin with each atom even though the electron may be said to posses no orbital angular momentum. The quantity Bohr magneton μ_B has a magnitude $\mu_B = 9.27 \times 10^{-24}$ A-m^2. The orbital magnetic moment contribution is given by $m_l \mu_B$ where m_l is the magnetic quantum number. In real practice the electrons do posses some orbital angular momentum and contribute to magnetic moment. Because of this fact orbital motion is taken into account in general. If the electron possesses non-zero orbital angular momentum and significantly interplays with the spin motion of the electron, then the total angular momentum J is taken into account to carry out the energy calculations.

$$J = L + S \tag{1}$$
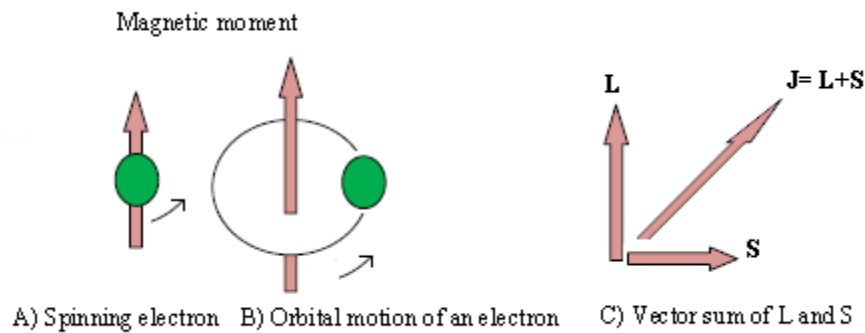$$J^2 = J(J+1)h^2 \tag{2}$$

Figure:1 Pictorially represents the origin of spin and orbital angular moments [Beiser .,1995) an electron in an atom.
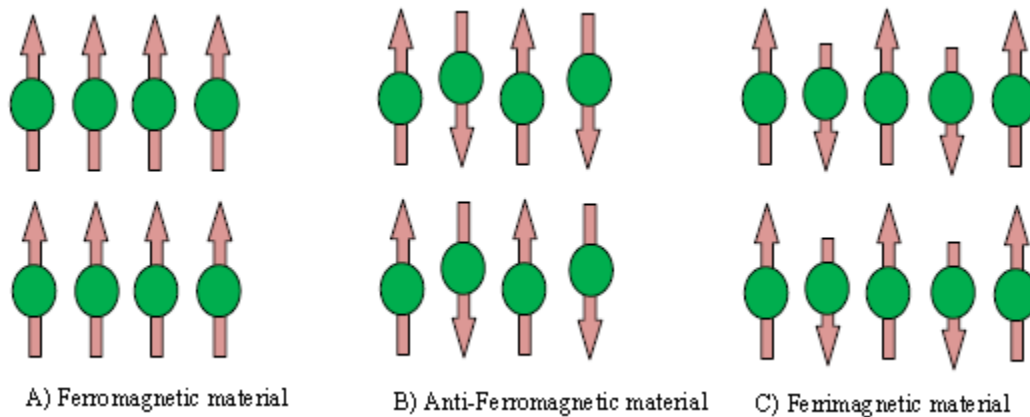

Figure:2 Pictorial representation of spin arrangements in different tyes of magnetic materials

Expectation value of the z-component of the angular momentum is given by-

$$J_z = m_J h \tag{3}$$
$$m_J = -J, -J+1, -J+2, \ldots\ldots to \ldots\ldots -J-1, J \tag{4}$$

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The magnetic moment is given by-

$$\mu_z = -\mu_B g_J m_J \qquad (5)$$

$$g_J = 1 + \frac{\left[\left(J(J+1) + S(S+1) - L(L+1)\right)\right]}{\left[2J(J+1)\right]} \qquad (6)$$

The energy of the system $U = -|\mu||B|Cos\theta$ (7)

The energy levels are split in (2J+1) sub levels if there is coupling between orbital angular momentum and the spin angular momentum of an electron. Thus an anomalous behavior is observed by these paramagnetic cases-Tanner (1995). If the electron spin dominates and orbital magnetic moment is left then the electrons can either move to spin up or down states depending on which one is energetically favored by the external magnetic field. In metals when electrons are in conduction band of course, the orbital contributions to magnetic moments are readily zero. In paramagnetic metals the magnetic moment contributions can be calculated by Pauli's formula [3]-

$$\mu = -g_S \mu_B S; \quad g_s = 2 \qquad (8)$$

Stern-Gerlach experiments have proven the there exist two spin angular moment states for electrons as $S = \pm\dfrac{h}{2}$. The weak effect of paramagnetism in metals because of free electrons is known as Pauli paramagnetism.

In presence of external magnetic field, paramagnetic materials are weakly attracted by the field where as the diamagnetic materials are weakly expelled from the field. In Gouy balance, a paramagnetic sample appears to weigh more and a diamagnetic sample appears to weigh less when the magnetic field is turned on- Atkins & Paula (2002). For paramagnetic material magnetic susceptibility χ is positive where as χ has very small but negative value for diamagnetic materials of the order of 10^{-5} [see Table-1]. In diamagnetic materials atoms have paired electrons in their outermost shell so that the magnetic moment vector of the two electrons points opposite and cancel each other. According to the Langevin theory of diamagnetism, in presence of external magnetic field the orbital motion of one of the electron is energetically favored by the presence of the external magnetic field and it's the frequency of this electron is increased. Thus the magnitude of the magnetic moment is also increased. Vice-versa another electron suffers because of unfavorable energy conditions produced by the presence of the external magnetic field and the magnitude the magnetic moment is shortened. This process yields a net magnetic moment inside the material $\Delta M = \pm er^2\Delta\omega/2 = \pm e^2 Br^2/4m$ -Resnick & Halliday (1991).

$$\text{Magnetic field density } B = \mu_0 \left(M + H\right)$$
$$= \mu_0 \left(1 + \chi\right)H \qquad (9)$$

Here M=Magnetization ≡χH; H=Applied Field Strength; χ=Magnetic Susceptibility

Ferromagnetic materials show strong magnetization in presence of external magnetic field. These have pre-existing small spin domains in which all the spins are aligned in same direction but again the various domains may point in different directions in absence of external magnetic field. In presence of

external magnetic fields these substances show strong magnetization because of the growth of the spin domains, which is energetically favored ones. The orientation of the net spin of the domain also takes place in the direction so that the contribution because of the magnetic field lowers the energy of the system. The spin wetting of domain leads to increase in size of domains, which have been speculated around the decade of ninety with the advent of high-resolution microscope. Thus surface induced effects can play a vital role in properties like ferromagnetism. I have recently reported surface dominated wetting and dewetting phenomena and precipitation in conserved binary mixture using 2D and 3D lattice based Glauber spin exchange kinetics with anti-ferromagnetic case- Singh (2011) and Singh (2012). Though these 2D and 3D problems focus on mixing and dewetting in absence of magnetic field and only surface fields are present in form of chemical potentials in the models but these problems are different with this current problem under discussion in the sense that those discuss disordered binary mixture whereas the problem under discussion deals with complete ordering. The author would suggest going through the references Singh (2011) and Singh (2012) and would leave any further details. Ferromagnetism is shown by transition metals as iron, cobalt, nickel and some of the rare earth metals such as gadolinium (Gd). Magnetic susceptibility is as high as 10^6 for ferromagnetic materials. So that H<< M, we can write-

$$B \cong \mu_0 M \qquad\qquad (10)$$

Manganese Oxide (MnO) is a ceramic material, which shows anti-ferromagnetic behavior. Mn^{2+} ions possess predominantly net spin magnetic moment. Orbital contribution to moment is not significant. O^{2-} ions do not posses any magnetic moment. The neutron scattering experiment suggests from the Brag's law that the two Mn^{2+} spins are oppositely oriented yielding a net contribution of the magnetic cell zero- Tanner (1995). In neutron scattering the scattering process takes place as per Brags's law: $2d_{hkl} \sin\theta = n\lambda$, because of the interactions of magnetic moments of the incident neutron beam and the magnetic moments of possessed by the atoms at different lattice points. NiO and $KNiF_3$ also show anti-ferromagnetism.

There are some ceramics of chemical composition MFe_2O_4, which exhibit permanent magnetization. Here M stands for metallic elements. In this type of material there exists net magnetic moment after the coupling between anti-parallel spins of Fe^{2+} and Fe^{3+} i.e. two states of Fe. This is ferrimagnetism. It has similarities with ferromagnetism but differs in spin orientation.

Paramagnetic materials		*Diamagnetic materials*	
Material	*Susceptibility χ_m (SI units)*	*Material*	*Susceptibility χ_m (SI units)*
Manganese Sulfate	3.70×10^{-3}	Gold	-3.44×10^{-5}
Aluminum	2.07×10^{-5}	Mercury	-2.85×10^{-5}
Chromium chloride	1.51×10^{-3}	Silver	-2.38×10^{-5}
Chromium	3.13×10^{-4}	Aluminum oxide	-1.81×10^{-5}
Titanium	1.81×10^{-4}	Copper	-0.96×10^{-5}
Sodium	8.48×10^{-6}	Silicon	-0.41×10^{-5}

Table-1 Magnetic susceptibility of some paramagnetic and diamagnetic materials

Brief Theory of Para and Ferromagnetism: Simulation Results and Explanation

In 1925, Ising gave an exact solution to the problem of one-dimensional periodic chain as follows. If there are N spin sites such that each spin can flip up or down, the magnetization depends on the nearest neighbor spin coupling, the magnitude of the external magnetic field and the temperature of the system. We can obtain an expression for the average magnetization of 1D thin film starting from the Hamiltonian of the system as follows- Pathria & Beale (2011) and Huang (1987):

$$H_N\{S_i\} = -J\sum_{n.n} S_i S_j - \mu B \sum_{i=1}^{N} S_i \tag{11}$$

We can write equation (11) in symmetrical form as:

$$H_N\{S_i\} = -J\sum_{\substack{i=1 \\ <i,j>}}^{N} S_i S_{i+1} - \frac{1}{2}\mu B \sum_{i=1}^{N}\left(S_i + S_{i+1}\right) \tag{12}$$

The partition function of the system is obtained through all possible configurations of the system and is defined by:

$$Q_N(B,T) = \sum_{S_1=\pm1}\cdots\sum_{S_N=\pm1} Exp\left[\beta\sum_{i=1}^{N}\left\{JS_iS_{i+1} + \frac{1}{2}\mu B\left(S_i + S_{i+1}\right)\right\}\right] \tag{13}$$

Using a Matrix Operator P as follows:

$$\langle S_i|P|S_{i+1}\rangle = Exp\left[\beta\left\{JS_iS_{i+1} + \frac{1}{2}\mu B\left(S_i + S_{i+1}\right)\right\}\right] \tag{14}$$
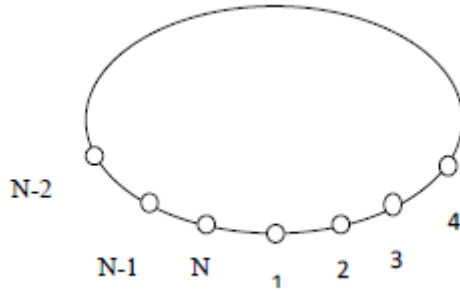

Figure: 3 *Shows a string of one dimensional string of N atoms. Because of periodic boundary conditions even though the system size is finite but the (N+1) site represents 1ˢᵗ site, N+2 represents 2ⁿᵈ site and so on. Thus the system behaves as an ensemble of infinite system in real after a reasonable run time or MC Cycles (i.e. Monte Carlo Cycle- One MC Cycle is completed when all spins get one chance to flip-flop in 2D lattice) so that most of the spin sites gets a permutation chance to flip-flop in to complete the configuration space.*

We can write Equation (3) as-

$$Q_N(B,T) = \sum_{S_i=\pm1}\cdots\sum_{S_N=\pm1}\langle S_1|P|S_2\rangle\langle S_2|P|S_3\rangle\cdots\langle S_{N-1}|P|S_N\rangle\langle S_N|P|S_1\rangle \tag{15}$$

Since each spin S_i can take spin up and spin down two values $S_i = \pm 1$ so the expression

$$\sum_{S_{i}=\pm 1}\sum_{S_{i+1}=\pm 1} Exp\left[\beta J S_i S_{i+1} + \frac{1}{2}\mu\beta\left(S_i + S_{i+1}\right)\right] \qquad (16)$$

yields four terms which will produce same matrices for the all (i, i+1) pairs of neighboring spins, so one can write the transfer matrix P as follows:

$$P = \begin{pmatrix} e^{\beta(J+\mu B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu B)} \end{pmatrix} \qquad (17)$$

For apposite spins $\frac{1}{2}\mu\beta(S_i + S_{i+1}) = 0$ only βJ will contribute to the operator. Since this is repeated N times in our problem, the problem is simplified. So, we can obtain the partition function as –

$$Q_N(B,T) = \sum_{S=\pm 1}\langle S | P^N | S\rangle = Trace\left(P^N\right) = \lambda_1^N + \lambda_2^N \qquad (18)$$

Here λ_1 and λ_2 are the Eigen values of the matrix P. The Eigen values can be obtained by the determinant –

$$\begin{pmatrix} e^{\beta(J+\mu B)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu B)} - \lambda \end{pmatrix} = 0 \qquad (19)$$

$$\lambda^2 - 2\lambda e^{\beta J} Cosh\left(\beta\mu B\right) + 2Sinh\left(2\beta J\right) = 0 \qquad (20)$$

We get-

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = e^{\beta J} Cosh\left(\beta\mu B\right) + 2Sinh\left(2\beta J\right) = 0 \qquad (21)$$

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = e^{\beta J} Cosh\left(\beta\mu B\right) \pm \left\{e^{-2\beta J} + e^{2\beta J} Sinh^2\left(\beta\mu B\right)\right\}^{\frac{1}{2}} \qquad (22)$$

In general we have $\lambda_2 < \lambda_1$ so that $\left(\dfrac{\lambda_2}{\lambda_1}\right)^N \to 0$

The condition of thermodynamic limit $N \to \infty$ (i.e. system with infinitely large number of particles) is achieved by periodic boundary conditions in molecular simulation of various problems. Now we get

$$\ln Q_N(B,T) \cong N\ln\lambda_1 \qquad (23)$$

$$\frac{1}{N}\ln Q_N(B,T) = \ln\left[e^{\beta J} Cosh\left(\beta\mu B\right) + \left\{e^{-2\beta J} + e^{2\beta J} Sinh^2\left(\beta\mu B\right)\right\}^{\frac{1}{2}}\right] \qquad (24)$$

Now, the Helmholtz free energy can be written as:

$$A(B,T) = -NJ - NkT \ln\left[Cosh(\beta\mu B) + \left\{e^{-4\beta J} + Sinh^2(\beta\mu B)\right\}^{\frac{1}{2}}\right] \quad (25)$$

The internal energy of the system can be written as:

$$U(B,T) \equiv -T^2 \frac{\partial}{\partial T}\left(\frac{A}{T}\right) \quad (26)$$

$$U(B,T) = -NJ - \frac{N\mu B Sinh(\beta\mu B)}{\left\{e^{-4\beta J} + Sinh^2(\beta\mu B)\right\}^{\frac{1}{2}}} + \frac{2NJe^{-4\beta J}}{\left[Cosh(\beta\mu B) + \left\{e^{-4\beta J} + Sinh^2(\beta\mu B)\right\}^{\frac{1}{2}}\right]\left\{e^{-4\beta J} + Sinh^2(\beta\mu B)\right\}^{\frac{1}{2}}}$$

$$<M(B,T)> \equiv -\left(\frac{\partial A}{\partial B}\right)_T = \frac{N\mu Sinh(\beta\mu B)}{\left[e^{-4\beta J} + Sinh^2(\beta\mu B)\right]^{\frac{1}{2}}} \quad (27)$$

Ising carried out this one-dimensional analysis and observed that no phase transition occurred at finite temperature in one dimension. He erroneously generalized his views in higher dimensions but that was not true. In 1941 Kramer and Wannier obtained quantitative result for two-dimensional Ising model and successfully deduced the critical temperature of the system. In 1944 Onsager explicitly obtained free energy in zero fields- Pathria & Beale (2011) and Huang (1987).

$$\chi_0(T) = \frac{N\mu^2}{kT}e^{2J/kT}$$

$$(28)$$

Simulation Results and Explanation

In this paper, I have studied a problem of two dimensional spin lattice of 100×100 size. The spins are assigned initial values of ±1/2 in a random fashion so that ½ of the sites are populated with spin up and ½ of the sites are populated with spin down. Initial net spin of the thin film is taken to be zero. Now each spin is visited one by one and a trail attempt to flip its spin is made. The energy change in flipping the spin is calculated. If a random number (p) chosen between 0-1 is lesser than the Boltzmann factor (i.e. $p < Exp[-\Delta E/k\, T]$) the spin flip move is accepted else the original spin is restored- Binder & Heermann (1992) and Singh (2008). Only nearest neighbor interactions are taken into account. The coupling constant J is also varied as J=0.0, 50, 0.75 & 1.0. The temperature observations are done for T=0.20, 0.30, 0.40, 0.50, 0.60, 1.0, 1.5 & 2.0. The External field variations are done in in steps of 0.20 units of B from -6.0 to +6.0. The average magnetization vs external magnetic field results are plotted for different temperatures and coupling coefficients. J=0 corresponds to perfect paramagnetic behavior which follows a $<M> = N \mu \tanh(\beta\mu B)$ curve. A positive J enhances magnetization and develops a spin correlation enhancing magnetization. This indicates for ferromagnetic behavior. For $\beta J \to \infty$, the magnetization curve becomes a step function indicating a singularity at T=0. The susceptibility of the system is given by equation [28]. As T becomes higher and higher the coupling effect become weaker and after certain high temperature as T=2.0 in this paper one can see that the thin film behavior matches with that of the case of the J=0 i.e. paramagnetic. Remarkable thing is to note that at enough high temperatures the spin agitations become more pronounced and disordered. So, system loses its spin correlations. These results correspond to Neel temperature. The lower temperatures have spin ordering effects in system. Higher magnetic field does the same job. [See Figure- 4, 5 & 6]

Fig. 4 shows average magnetization per unit volume vs applied external magnetic field at different temperatures kT=0.20, 0.30, 0.40 & 0.50. For lower temperatures one can observe that the saturation values of magnetization are achieved even for the low magnetic field values of B=±2.5. The Boltzmann constant k is taken to 1.0 unit is all runs. All data points are obtained after running the equilibrating the system for 4000 Monte Carlo Cycles. Fig. 5 Shows average magnetization per unit volume vs applied external magnetic field at different temperatures kT=0.60, 1.0, 1.50 & 2.0 relatively in higher range. For higher temperatures one can observe that the saturation values of magnetization is not achieved even for the high magnetic field values of B=±6.0. At higher temperatures as T=2.0, the trend curve matches with that the case of J=0 i.e. paramagnetic case in Fig. 6. After certain critical temperature the anti-ferromagnetic behavior transit to paramagnetic behavior. All data points are obtained after running the equilibrating the system for 4000 Monte Carlo Cycles. Fig. 6 Shows average magnetization per unit volume Vs applied external magnetic field for different spin coupling coefficient J=0.0, 0.50, 0.75 & 1.0 at temperature kT=0.50.For higher J values one can observe that the saturation values of magnetization is achieved at slower rate even for the higher magnetic field values of B. It is something new in the sense that one would classically think of faster alignment of spins with high values of spin coupling but an intuitive argument is that the long range spin correlations slows down the magnetization process and thus requires more time and strength of external magnetic field to achieve the saturation value of magnetization in case of 2D thin films at low temperatures as T=0.50 in this case. At higher temperatures as T=2.0, the trend curve matches with that the case of J=0 i.e. paramagnetic case in this figure. Above certain critical temperature called Neel temperature the anti-ferromagnetic behavior transit to paramagnetic behavior.

In Figure 7, I have demonstrated data writing 2D thin films. Fig. 7 shows writing number 10 on 2D thin film which has random spins 50 % of each ±1/2.The shaded reason has opposite magnetic field to that of rest of the film. In this case external magnetic field applied is |B|=6.0 SI units (It requires appropriate scaling here). Ten has been chosen for demonstration of data writing on magnetic film for the reasons that it is an indication of perfection in many part of the world. For lower values of B, data writing would create more noise. Also important thing is to note that in B-H curve field reversal causes hysteresis loss in case of ferromagnetic tapes, selection field choice becomes also important to manufacturers though the discussion on the subject is omitted in this paper.
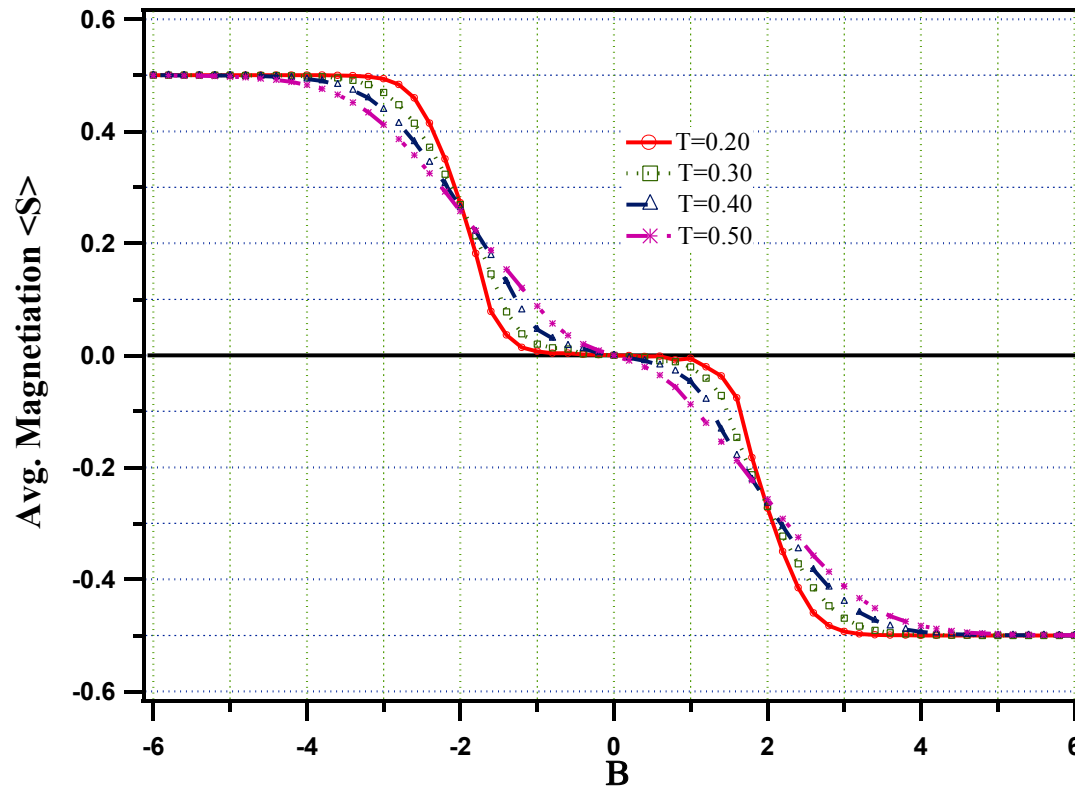
Figure 4 *Shows average magnetization per unit volume Vs applied external magnetic field at different temperatures kT=0.20, 0.30, 0.40 & 0.50. For lower temperatures one can observe that the saturation values of magnetization are achieved even for the low magnetic field values of B=±2.5*
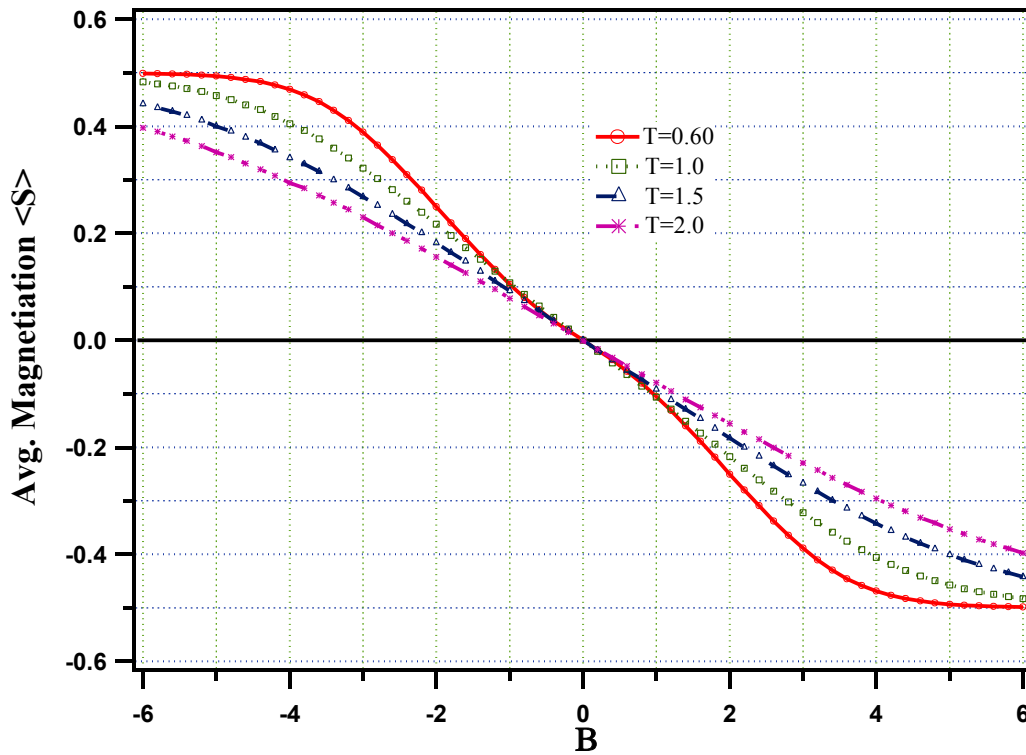
***Figure 5** Shows average magnetization per unit volume Vs applied external magnetic field at different temperatures kT=0.60, 1.0, 1.50 & 2.0 relatively in higher range.*
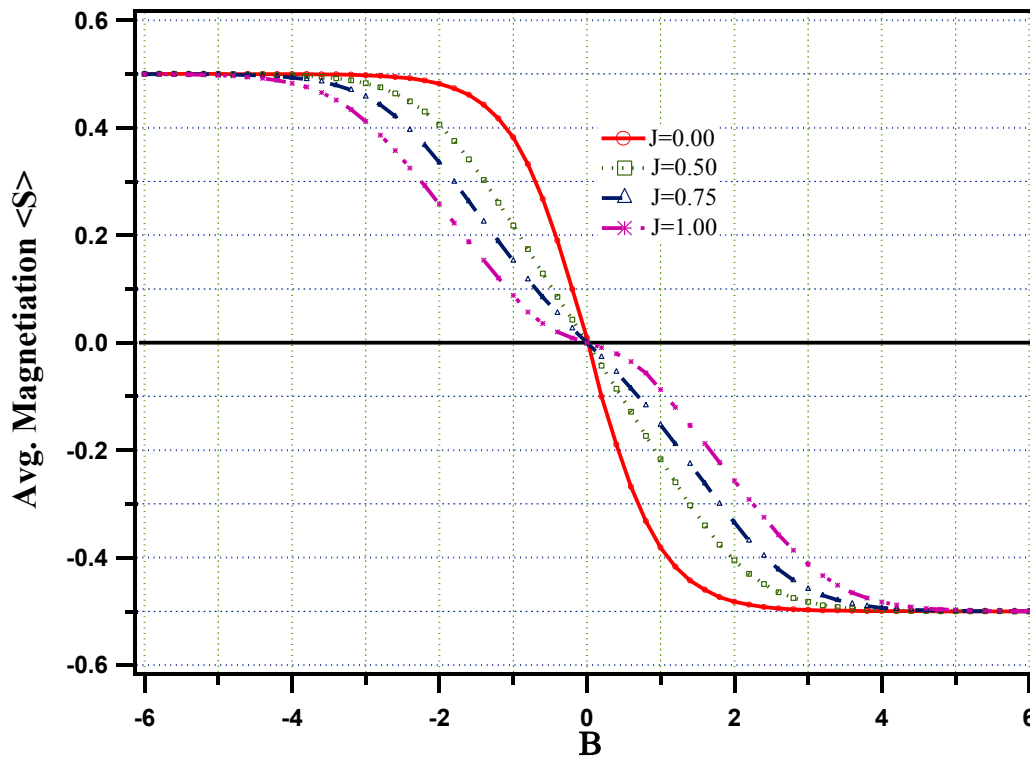

***Figure 6** Shows average magnetization per unit volume Vs applied external magnetic field for different spin coupling coefficient J=0.0, 0.50, 0.75 & 1.0 at temperature kT=0.50.*
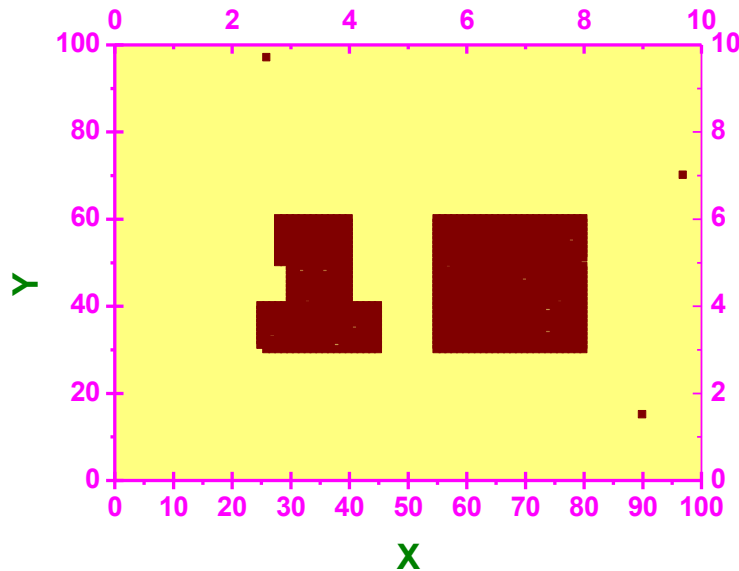
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Conclusion

The author hopes that this paper explores this old but computationally advance topic of magnetism to educators and students giving insight into the subject with a newer approach which has emerged as a new branch of science bridging the gap between experimentation and theory. The temperature dependence of magnetization of 2D thin film with cases of J=0 and J>0 has been discussed to throw light on paramagnetism and anti-ferromagnetism which indeed have been experimentally verified and now have become parts of many advance text and research books. The case of J<0 i.e. ferromagnetism has been omitted in this paper for the sake making coherence on the subject. This subject is of vital importance as for as its technological application is concerned. As for example low-carbon steels are used as lowest garde core materials. Iron-Silicon alloys are used to reduce transformer noise. Cold Rolled Grain Oriented (CRGO) steel carries better magnetic properties and has low hysteresis losses. Alnico alloys are mechanically hard and breakable. Their magnetic properties are highly stable against temperature variation, shock etc. Rare earth magnetic alloys like Sm-Co alloys are used in medical devices such as thin motors in implantable pumps and valves. Fe-Cr-Co alloys are used in making permanent magnets for telephone receivers. Nd-Fe-B alloys are used in making light and compact electric motors. Soft Mg-Mn ferrites, Mn-Cu ferrite etc. are used as memory or logic operation devices in computers as switching devices and in information storage. Hard ferrites as Barium ferrites are used for making permanent magnets.

Acknowledgement

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