Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.56, 2016

Thermodynamics Property of Magnetic Materials in a Ferromagnetic System using the Ising Model

Akaninyene D. Antia Cyril C. Umoren
Department of Physics, University of Uyo, Nigeria

Abstract
There is hardly any branch of physics one can approach successfully without resorting to quantum statistical mechanics. It has been proven that the quantum mechanical description of a system gives accurate results. To use quantum statistical mechanics, the system are treated at their microscopic level. Most systems consist of many particles and in order o deal with such large numbers, one has to resort to statistical method related to the partition function of statistical mechanics. In this study, we haves used the partition function which is a statistical parameter to explore the thermodynamic properties such as Helmoltz free energy, Entropy, internal energy and heat capacity of a magnetic materials in a ferromagnetic system using the first and second dimensional Ising model. The results show that in one-dimensional model, phase transition does not occur at finite temperature but susceptibility of a system can be measured from the fluctuations in the magnetization in the second dimensional Ising model.

1. Introduction

The discovery of magnetic material predates the invention of writing. Humans were fascinated by the attractive or repulsive force between magnets and they assigned magical and esoteric values to these objects. Later the Chinese discovered the earth's field and use magnets as compass [1,2]. Electric and magnetic phenomenon was scientifically investigated, when placed in an external magnetic field of their own. It points either in the same direction (paramagnetism) or in the opposite direction (diamagnetism) [3,4]. Ferromagnetism is the ability of a paramagnetic material to retain spontaneous magnetization as the external magnetic field is removed [5,6]. The only ferromagnetic elements iron (Fe), Cobalt (Co), Nickel (Ni), Gadolinium (Gd) and Dysprosium (Dy) [7,8].

Ferromagnetic materials have a large, positive susceptibility in an external field, they exhibit strong attractive force to magnetic fields. They involve spin of electron of the outer layers because of their unpaired electrons so their atoms have a net magnetic moment. Even though electronic exchange forces in ferromagnetisms are very large, thermal energy eventually overcomes the exchange and produces a random effect. This occurs at a particular temperature called curie temperature (T_c) and above this temperature all ferromagnetic substances changes to paramagnetic substances. As $T \rightarrow T_c$ the magnetization goes to zero following a power law [9,10].

The Ising model [11] is a crude model for ferromagnetism, it was invented by Lenz who proposed it to his Ph.D student Ernest Ising. By 1925, Ising submitted his dissertation which was the first exactly solved one-dimensional case. This model receives great attention from both physicist and mathematicians in that; it is the simplest model of statistical mechanics where phase transitions can be vigorously established. The Ising model has a probabilities interpretation [12,13].

Heermann in 1990 discussed large-scale simulation of the two-dimensional kinetic Ising model. The dynamics of the system is specified by the transition probability of the Markova chain which will be realized by a Morite Carlo Algorithm [14]. He therefore calculated the dynamical critical exponent (z) for the Ising model defined by the Hamiltonian

$$H_{I\sin g} = -j \sum_{\langle i,\, j \rangle} S_i S_j \tag{1}$$

where $\langle i,\, j \rangle$ are nearest-neighbouring pair of lattice sites [15, 16].

Kosiorek et al in 2004 also studied the nanoscopic structures in the form of pyramids and can be fabricated on a bulk substrate. They considered the magnetic properties of a nanoscopic pyramid described by the model of localized and other spin ½ Hamiltonian using Ising model defined by [11, 12, 13].

$$H = -\frac{1}{2} I \sum S_{fl}\, S^{z}_{f'l'} \tag{2}$$

where I is the coupling parameter.

The aim of this paper is to determine the thermodynamic properties of magnetic materials in a ferromagnetic system using Ising model. In this work, we shall explore the use of the Ising model and apply it to thermodynamic properties of magnetic materials.

2.0 The Ising Model

In 1920, Wilhelm Lenz proposed a basic model of ferromagnetic substances to his Ph.D student Ernest Ising. By 1925, Ising was submitting his dissertation which was the first exactly solved one dimensional case, and as such was later called Lenz-Ising model [11, 12].

Let the exact states (microstate) in the system be S (S = 1, 2, 3,..... n), the energy of this microstate be E_s such that the partition function (z) which is a statistical parameter becomes

$$Z = \sum_s e^{-\beta E_s} \tag{3}$$

where β is the inverse temperature; $\beta = \frac{1}{K_B T}$ and K_B is the Boltzmann's constant.

The probability P_s that a system is in the state S is

$$P_s = \frac{1}{Z} e^{-\beta E_s} \tag{4}$$

Applying $\sum_s$ to both sides of Eq. (4) gives

$$\sum_s P_s = \frac{1}{Z} \sum_s e^{-\beta E_s} \tag{5}$$

Substituting Eq. (3) into Eq. (5)

$$\sum_s P_s = 1 \tag{6}$$

The average energy of the system is the total of the energies of the microstates weighted by their relative probabilities.

$$\langle E \rangle = \sum_s E_s P_s \tag{7}$$

Substituting Eq. (4) into Eq.)7) and taking note of Eq. (3) we obtain

$$\langle E \rangle = E_s \tag{8}$$

The Helmhpltz free energy function is given by

$$F = -KT \ln Z \tag{9}$$

$$\langle E \rangle = E_s = -KT \ln Z \tag{10}$$

Also $T = \frac{1}{\beta}$ which implies $K_B = 1$ so from Eq. (10)

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} \tag{11}$$

From fluctuation in energy in a canonical ensemble

$$\langle E \rangle = KT^2 C_v \tag{12}$$

where $C_v = \frac{\partial U}{\partial T}$ is the heat capacity and U is the internal energy of the system

But $U = \frac{1}{Z}$

$$C_v = \frac{\partial \left(\frac{1}{Z} \right)}{\partial T} = \frac{\ln Z}{\partial T} \tag{13}$$

Substituting Eq. (13) into Eq. (12) we have

$$\langle E \rangle = KT^2 \frac{\ln Z}{\partial T} \tag{14}$$

The entropy of the microstates can be defined from the statistical weights by using the function

$$S = K_B \ln \Omega(\vec{E}) \tag{15}$$

$\Omega(\vec{E})$ is the number of microstates with energy $\vec{E}$. From the first law of thermodynamics

$$\partial Q = \partial E + \partial W$$

where $Q =$ quantity of heat, $E =$ internal energy and $W =$ Work done on the system.

When the system is heated without any work $\partial W = 0$ then $\partial Q_{rev} = \partial E$

But $\partial Q_{rev} = Tds$ and hence

$$\partial E = Tds, \text{ thus } \frac{\partial S}{\partial E} = \frac{1}{T} \tag{16}$$

Equation (16) shows that the entropy will increase slowly as the temperature gets higher, but entropy will never decrease as the temperature increases. Equation (15) can also be defined directly in terms of the distribution function and the logarithm of the distribution function of a subsystem has the form.

$$\ln \Omega(\vec{E}) = \ln Z + \beta E \tag{17}$$

The mean value of Eq. (17) can be written as

$$\langle \ln \Omega(\vec{E}) \rangle = \ln Z + \beta E \tag{18}$$

The entropy of the system can then be written as

$$S = \ln \Delta E = -\ln \Omega(\vec{E}) \tag{19}$$

Substituting Eq. (17) into Eq. (19)

$$S = -(\ln Z + \beta E) \tag{20}$$

Substituting Eq. (20) into Eq. (15)

$$S = -K_B (\ln Z + \beta \langle E \rangle) \tag{21}$$

Equations (20) and (21) are equal since $K_B = 1$ and $\langle E \rangle = E_s$. Also from Eq. (16)

$$S = \frac{\partial E}{\partial T} \tag{22}$$

Substituting Eq. (10) into Eq. (22) we have

$$S = -\frac{\partial (KT \ln Z)}{\partial T} \tag{23}$$

Equation (23) shows that entropy will never decrease as the temperature increases.

3.0 Calculation of the Ising Model in one-dimension

In one-dimension Ising model, there is no external magnetic field. The energy is equal to the enthalpy as there will be no work done by the system. Each configuration is given by the Hamiltonian

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \tag{24}$$

The partition function thereby becomes

$$Z_N = \sum_{\sigma_1 = \pm 1} \dots \sum_{\sigma_N = \pm 1} \exp\left[\beta J \sum_{i+1}^{N-1} \sigma_i \sigma_{i+1} \right] \tag{25}$$

Using the hyperbolic function $e^x - e^{-x} = 2\cosh x$, Eq. (25) reduces to

$$\sum_{\sigma_N = \pm 1} \exp\{\beta J \sigma_{N-1} \sigma_N\} = 2\cosh \beta J \tag{26}$$

Substituting Eq. (26) into Eq. (3) we have

$$Z_N = [2\cosh \beta J] Z_{N-1}; \quad N = 0, 1, 2 \dots \tag{27}$$

$$Z_N = 2(\cosh \beta J)^{N-1} \tag{28}$$

The Gibb's free energy of the system is given as

$$G = -K_B T \ln Z_N \tag{29}$$

Substituting Eq. (28) into Eq. (29) and evaluating

$$G = -K_B T\left[\ln 2 + (N-1)\ln(\cosh \beta J)\right] \tag{30}$$

In the thermodynamics limit, that is, the limit of the free energy as N tends to infinity. Only the term proportional to N is important so Eq. (30) becomes

$$G = -NK_B T \ln(\cosh \beta J) \tag{31}$$

In the presence of magnetic field, the Hamiltonian becomes

$$H = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - h\sum_{i=1}^{N}\sigma_i \ , \tag{32}$$

where the spin labels run modulos N (i.e $N+i=i$) and $\sigma_i = \sigma_i + \sigma_{i+1}$.
The partition function for this new Hamiltonian can be written as

$$Z_N = \sum_{\sigma_i}\prod_{i=1}^{N}\exp\left\{\beta\left(J\sigma_i\sigma_{i+1} + \frac{h}{2}(\sigma_i\sigma_{i+1})\right)\right\} \tag{33}$$

Since the potential is very large, we introduce a 2 x 2 transfer matrix

$$P = \begin{bmatrix} P_{11} & P_{1-1} \\ P_{-11} & P_{-1-1} \end{bmatrix} \tag{34}$$

where $P_{11} = e^{\beta(J+h)}$ is the Hamiltonian

$P_{-1-1} = e^{\beta(J-h)}$ is the Lagrangian

$P_{1-1} = P_{-11} = e^{-\beta J}$ is the P. E when K. O-=0

We can now use the transfer matrix to describe our partition function in terms of a product of these transfer matrices.

$$Z_n = \sum_{\sigma_i} P_{\sigma_1\sigma_2}P_{\sigma_2\sigma_3}\ldots P_{\sigma_{N-1}\sigma_N} = TrP^N \tag{35}$$

Matrix P can be diagonalized and the eigenvalues λ_1 and λ_2 are the roots of the determinant in $\det(\rho - \lambda I = 0)$ and I is the 2 x 2 identity matrix.

$$P = \begin{bmatrix} e^{\beta(J-h)-\lambda} & e^{-\beta J} \\ e^{-\beta I} & e^{\beta(J-h)-\lambda} \end{bmatrix} = 0 \tag{36}$$

Evaluating the determinant and letting $\ell^{-2\beta I} \approx \infty$ as the potential energy function increases we have

$$\lambda^2 - 2\lambda e^{\beta J}\cosh \beta J - e^{-2\beta J} = 0 \tag{37}$$

Solving Eq. (37), we obtain

$$\lambda_{1,2} = e^{\beta J}\cosh \beta J \pm \sqrt{e^{2\beta J}\cosh^2 \beta J + e^{-2\beta J}} \tag{38}$$

But $\cosh^2 \beta J = \sinh^2 \beta J$ when the spin rotates at angle 45° for a one-dimensional Ising model. Similarly, the matrix P^N has eigenvalue λ_1^N and λ_2^N and TrP^N is the sum of the eigenvalues.

$$Z_n = \lambda_1^N + \lambda_2^N \tag{39}$$

Substituting Eq. (39) into Eq. (29)

$$G = -K_B T \ln\left(\lambda_1^N + \lambda_2^N\right) \tag{40a}$$

$$= -K_B T\left\{N\ln\lambda_1 + \ln\left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right]\right\} \tag{40b}$$

This approaches $-NK_B T\ln\lambda_1$ as N goes to infinity. Now taking this to the thermodynamics limit by substituting Eq. (38) into Eq. (40a)

$$G = -NK_B T\ln\left[e^{\beta J}\cosh \beta J + \sqrt{e^{2\beta J}\sinh^2 \beta J + e^{-2\beta J}}\right] \tag{41}$$

4.0 The Ising Model in two dimensions

The simplest two-dimensional lattice is a square lattice with $N = N_x \times N_y$

$$S_i = \pm 1,\ i = (i_x, i_y) \tag{42}$$
$$i_x = 0,\ 1,\ ..N_x - 1;\ i_y = 0, 1, \ldots N_y - 1$$

The simplest form of interaction is nearest-neighbour where S_i interacts with it's four neighbouring spin with the same coupling spin J

$$E = -J \sum_{\langle i,j \rangle} S_i, S_j - H \sum_i S_i \tag{43}$$

Here $\langle i, j \rangle$ represents a distant pair of nearest neighbour spins and H is a uniform external magnetic field. The most convenient type of boundary condition is separately periodic in each of the two dimensions:

$$S(i_x + N_x,\ i_y + N_y) = S(i_x, i_y) \tag{44}$$

With these boundary conditions, the total number of bonds is exactly 2N. There are 4 bond attached to each spin, but each bond is shared by two spins, thus the number of distinct bonds is 2N.

5.0 Thermodynamic Properties of Magnetic Materials using the Ising Model

We are now going to use the Ising model to determine the four thermodynamic properties such as Helmholtz free energy, the entropy, heat capacity and internal energy.

5.1 Helmholtz Free Energy

This property can be analyzed using Eq. (38). From the equation, it could be observed that when $J = 0$, the thermodynamic eigenvalue λ_1 is relevant, $\lambda_2 = 0$ and the Hlemholtz free energy per spin is obtained using Eq. (9) and Eq. (28) as

$$F = -NK_B T \ln(2\cosh \beta J) \tag{46}$$

where N is the number of particle per spin (i.e N = 0, 1, 2, ...).

5.2 Entropy

From the relation in Eq. (22) and carrying out the partial derivatives of in Eq. (46) we obtain the entropy for the ferromagnetic material as

$$S = NK_B \left\{ \ln\left[2\cosh\left(\frac{J}{K_B T}\right)\right] - \frac{J}{K_B T} \tanh\left(\frac{J}{K_B T}\right) \right\} \tag{47}$$

5.3 Internal Energy

The internal energy is the sum of Helmholtz free energy and the product of temperature and entropy $(E = F + ST)$ with the help of Eqs., we obtain the internal energy as

$$E = -NJ \tanh\left(\frac{J}{K_B T}\right) \tag{48}$$

5.4 Heat Capacity

The partial differential of the internal energy with temperature give heat capacity $\left(C_V = \frac{\partial E}{\partial T}\right)$ from Eq. (48)

$$C_V = \frac{\partial}{\partial T}\left[-JN \tanh\left(\frac{J}{K_B T}\right)\right] \tag{49}$$

$$C_V = \frac{NJ^2}{K_B T^2} \sec h^2 \left(\frac{J}{K_B T} \right) \quad (50)$$

6.0 Discussion

The thermodynamic properties of ferromagnetism have been explored using the transfer matrix form of the partition function using Ising model is presented in this paper and the variation of these properties with temperature are also discussed graphically. In Fig. 1, we have shown the behaviour of free energy of this system with change in temperature while the entropy and heat capacity as functions temperature are plotted in Fig. 2 and Fig. 3 respectively. Comparing thermodynamic properties of this system, it can be seen that for the internal energy, as temperature increases the internal energy increases negatively. But at low temperature $T \to 0; \langle E \rangle \to 0$ the entropy increases with temperature and this is in agreement with second law of thermodynamics $\Delta S \geq 0$ [17,18].

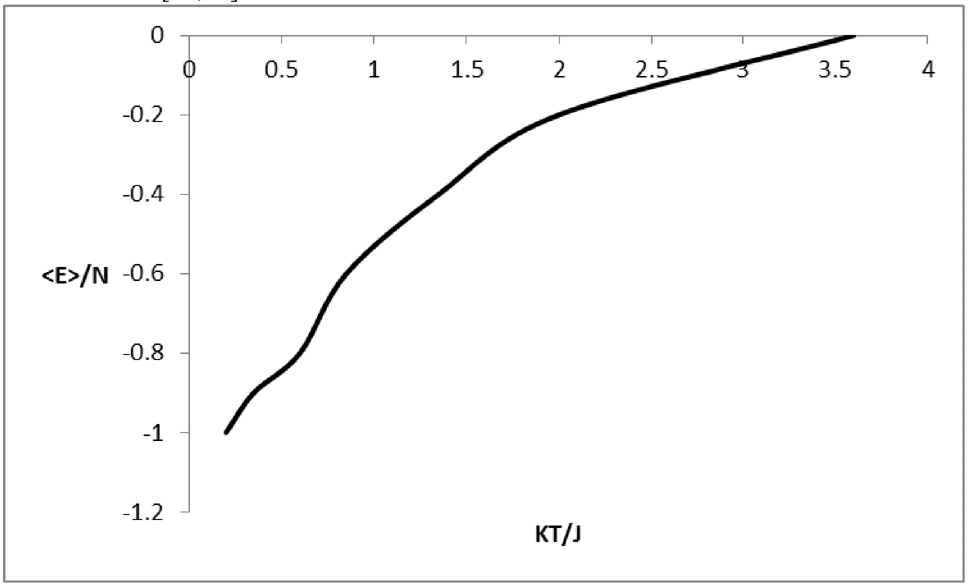

Figure 1: Free energy dependent on temperature

It is interesting to note that as $T \to \infty$, the entropies of the system approaches a constant value. The second law of thermodynamics is also still obeyed since $\Delta S = 0$ in the region for the heat capacity Cv, at the extreme[18]. Also as $T \to 0$, the heat capacity increases with increase in temperature and reach a maximum valued and then start decreases as $Cv \to K_B \left(\frac{J}{K_B T} \right)^2$ for the ferromagnetic system. Heat capacity increases with increase in temperature and has a maximum value and then decreases as $Cv \to K_B \left(\frac{J}{K_B T} \right)^2$ for ferromagnetic system.

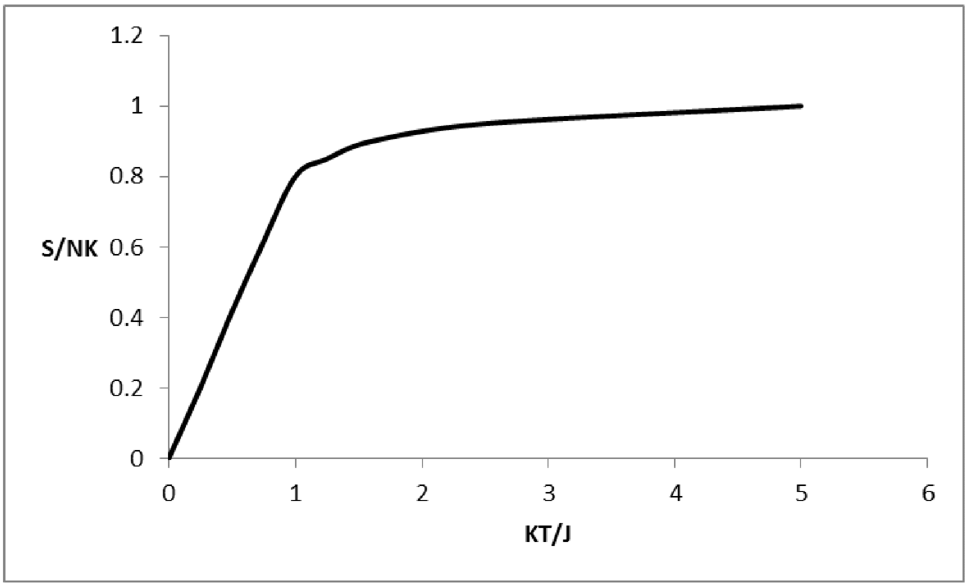

Figure 2: Entropy (S) as a function of temperature

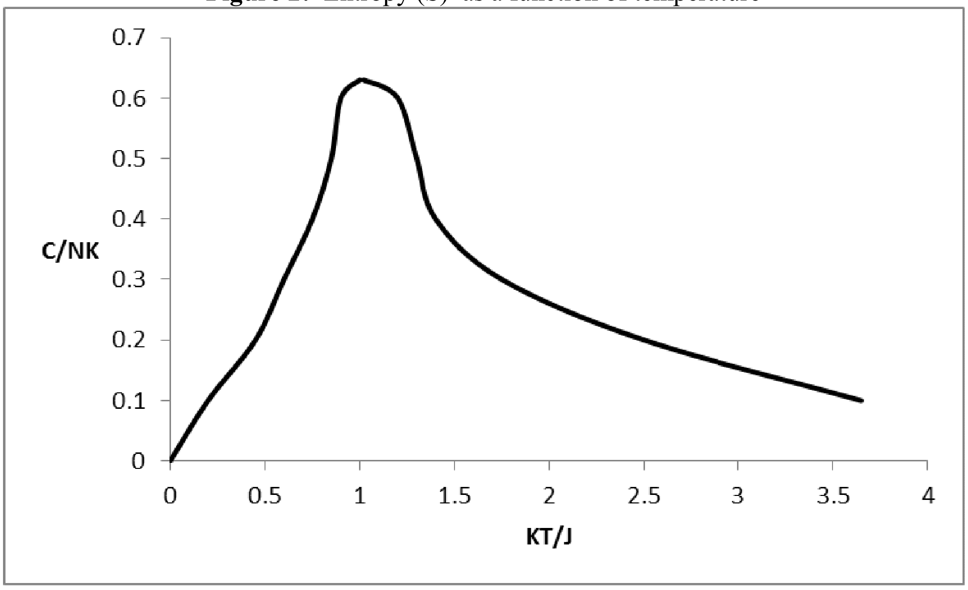

Figure 3: Heat capacity as a function of temperature.

Similarly, the free energy reduces at low temperature and increase (negatively) at high temperature. This is also in agreement with the theory of thermodynamics[19, 20].

7.0 Conclusion

We have been able to investigate the thermal properties of magnetic materials in a ferromagnetic system using first and second dimension Ising model. It is an interesting model as phase transition does not occur in the on-dimensional model at a finite temperature. But in the second-dimension, susceptibility of the system can be measured from the fluctuations in the magnetization. The susceptibility per spin can be determined by specific heat of the system and can also be measured using a fluctuation dissipation theorem. It is worthy to note here that each thermodynamic property of the ferromagnetic system considered has different behaviour. But each corresponding thermodynamic parameter for the system converges at extreme values of the temperature, that is, in the limits $T \rightarrow 0$ and $T \rightarrow \infty$. The behaviour of ferromagnetic system under change in temperature has been discussed as shown in Figures 1-3.

The work could be extended by looking more closely at the rotational variance that is observed in the sub-lattice prediction. Also as there is an oddity in the results at low temperatures, it could further be investigated to determine if it is affected by the lattice size as well as the current lattice configured.

References

1. Yoshioka, D. (2005). Statistical Physics. Department of Basic Science. University of Tokyo, Japan.

2. Vincent, M. (2011). Numerical Simulation of the Ising model on the union Jack Lattice. A thesis submitted for the degree of Doctor of Philosophy at the University of Queensland.
3. Fowler, R. & Guggenheim, E. (1940). Statistical thermodynamics of super-lattice. Proceedings of the Royal society of London series A, Mathematical and Physics Science 174(3): 189-206.
4. Ibach, H & Luth, H. (1992). Solid state physics. An introduction to theory and experiments. Narosa Publising House.
5. Heisenbye, A. (1928). Theoric Des Ferromagnetismus, Zeits-chirift Für Physik A. Hadrons and Nuclei 49: 619-636.
6. Kramers, A. & Wannier, H. (1941). Statistics of the two dimensional ferromagnet, part I. Physical Review 60: 252-262.
7. Strake, J. & Jaseur, M. (2003). Thermodynamics properties of exactly soluble transverse Ising on decorated plannar lattice. Journal of Physics 260: 415-425.
8. Kramers, A. & Wannier, H. (1941). Statistics of the two dimensional ferromagent. Part II. Physical review 60: 263-276.
9. Peirer, L. (1936). Ising model of ferromagnetism. Mathematical proceedings of the Cambridge philosophical society. Vol. 32: pp. 477-481.
10. Baxter, R. (1987). Triplet order parameter of the Triangular Ising model. Journal of Physics, A mathematical and General 8(11): 1795-1805.
11. Strauffer, D. (2007). Social Applications of Two-Dimensional Ising Model. Institution of Theoretical Physics Cologue University 0-50923 Koln, Germany.
12. Hohnisch, K. (2005). Social Applications of the two Dimensional Ising Model, Cologue University.
13. Schelling, T. (1971). Social Applications of Ising like model. 2005 Nobel Economist, New York.
14. Herrmann, W. (1995). Large-scale Simulation of the two-dimensional kinetic Ising Model: (19), D-69120. Heidelberg, Germany.
15. Jacyna-Qnyszkiewiez, Z. (2007). The Pyramid-like Ising Nanoscopic system Interaction with the substrate. Vol. 112.
16. Kosiorek, L., Borkowski, S. & Jacyna Qnyszkiewiez, Z. (2004). Pyramid-like Ising Nanoscopic system. Vol. 112.
17. Feynman, R. (1972). Lectures on statistical mechanics, Addison-Wesley. 59-72.
18. Free-Fermion, K. (1986). Checkerboard and Z-Invariant lattice models in statistical mechanics. Proceedings of Royal society of London, series A 404(1): 33-45.
19. Mariz, A., Herrmann, J. & De-Arcangelis, L. (1989). Comparative study of damage spreading in the Ising model using Heat-bath and Glauber Dynamics. Vol. 59: 3-4.
20. Quarie, D. (2000). Statistical mechanics. First Edition Sausalite, Califonia 94965. University Science Books. No. 55