Chapter

The Ising Model: Brief Introduction and Its Application

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Abstract

Though the idea to use numerical techniques, in order to solve complex three-dimensional problems, has become quite old, computational techniques have gained immense importance in past few decades because of the advent of new generation fast and efficient computers and development of algorithms as parallel computing. Many mathematical problems have no exact solutions. Depending on the complexity of the equations, one needs to use approximate methods. But there are problems, which are beyond our limits, and need support of computers. Ernst Ising published his PhD dissertation in the form of a scientific report in 1925. He used a string of magnetic moments; spin up (+1/2) and spin down (−1/2), and applied periodic boundary conditions to prove that magnetic phase transition does not exist in one dimensions. Lars Onsager, latter, exactly solved the phase transition problem in two dimensions in 1944. It is going to be a century-old problem now. A variety of potential applications of Ising model are possible now a days; classified as Ising universality class models. It has now become possible to solve phase transition problems in complex three-dimensional geometries. Though the area of spinotronics still needs more engagements of computational techniques, its limited use have provided good insights at molecular scale in recent past. This chapter gives a brief introduction to Ising model and its applications, highlighting the developments in the field of magnetism relevant to the area of solid state physics.

Keywords: surface-directed phase separation, wetting-dewetting, Monte Carlo simulation

1. Introduction

Ernst Ising (**Figure 1**) was born on May 10, 1900, in Loe Koln. He started schooling in 1907 and obtained his diploma at the gymnasium there in the year 1918. After brief military training, he studied mathematics and physics at Gottingen University in the year 1919. After a short gap, he continued his studies and learnt astronomy apart of other subjects. He got focused to theoretical physics at the suggestion of Professor W. Lenz. He started investigating ferromagnetism under supervision of W. Lenz by the end of the year 1922. Ising published short paper in 1925 as a summary of his doctoral thesis [1, 2]. He exactly calculated partition function for one-dimensional lattice system of spins. Ising had first proven that no phase transition to a ferromagnetic ordered state occurs in one dimension at any temperature.

His argument in the favor of his mathematical note was very simple. Suppose, if one of the spins get flipped at a random position because of thermal agitation, there

is no force available, which can stop the neighboring spins to flip in the same direction. And this process will go on and on, and completely ordered state will not remain stable at a finite temperature. Thus no phase transition will occur at a finite temperature. Ideally speaking, any ordered state will always remain like a metastable state at finite temperature and nothing more. Molecular motion seizes at absolute zero temperature. So, one may expect that no spin fluctuations may occur at absolute zero temperature. Henceforth, the stable ordered state is a natural outcome at absolute zero temperature. But, it cannot be said to be a critical temperature in true sense. The existence of phase transition at this temperature has no physical meaning, because there is no temperature below it. After going through some approximate calculations, Ising purportedly showed that his model could not exhibit a phase transition in two and three dimensions, either. Latter, his conclusion was proven to be erroneous [1, 2] (**Figure 2**).

Barry Simon has quoted it very well "This model was suggested to Ising by his thesis advisor, Lenz. Ising solved the one-dimensional model, and on the basis of the fact that the one-dimensional model had no phase transition; he asserted that there was no phase transition in any dimension. As we shall see, this is false. It is ironic that on the basis of an elementary calculation and erroneous conclusion, Ising's name has become among the most commonly mentioned in the theoretical physics literature. But history has had its revenge. Ising's name, which is correctly pronounced "E-zing", is almost universally mispronounced "I-zing"."

Ising's paper credited Wilhelm Lenz for his original idea, who had first proposed it in the year 1920. W. Lenz was Ising's research supervisor. It has been often rendered as Lenz-Ising model in many citations. Lenz suggested that dipolar atoms in crystals are free to rotate in quantized manner. He proposed quantum treatment of dipole orientations, though in its classical version, Ising considered only two spin states, i.e., $S = \pm ½$. Ising discussed his results with Professor Lenz and Dr. Wolfgang Pauli, who was teaching at Hamburg at that time. Ising's work was first cited by famous contemporary scientist Heisenberg. Heisenberg was first one to realize the failure of Lenz-Ising model. In order to explain ferromagnetism, he developed his own theory, using complicated interactions of spins. There

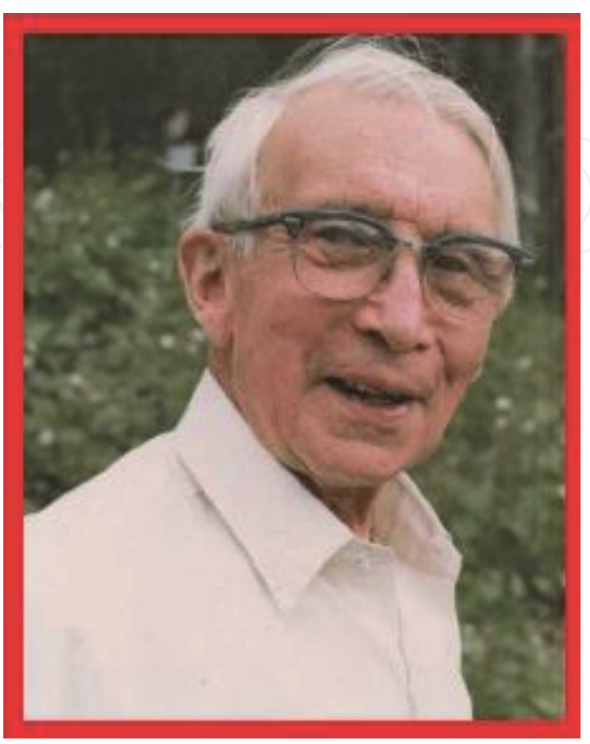

Figure 1.
Ernst (Ernest) Ising (May 10, 1900–May 11, 1998).

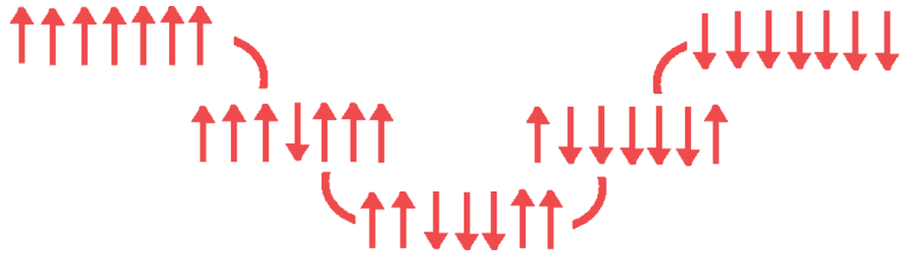

Figure 2.
Random spin flipping in one-dimensional system.

are more scientists in the list, whose contribution to Lenz-Ising model or simply say Ising model must be cited here, because of their historical relevance. They have greatly enriched and contributed to this new model. This list includes scientists like Gorskly (1928), R. H. Fowler (1930), Bragg and Williams (1934), R. Peierls (1936), J. G. Krikwood (1938), Hens Bethe (1939), Kramers and Wannier (1941), and Onsager (1942). They further extended Ising model to a new class of problems.

2. Application of Ising model

Ising model has been extensively used for solving a variety of problems [3–18]. Some of the problems are discussed, here, with appropriate examples.

2.1 Phase separation and wetting/dewetting

Ising model was first exploited for investigating spontaneous magnetization in ferromagnetic film (i.e. magnetization in the absence of external magnetic field). An example case of Ising model using metropolis algorithm is shown in **Figure 3**. Transition temperature depends on the strength of the inter-spin exchange coupling; the dominating term governs the kinetics, when long-range interactions are introduced in the calculations. Latter, it was used to study phase separation in binary alloys and liquid-gas phase transitions (i.e., condensation of molecule in one region of space of the box). Binary alloys constitute of two different atoms. At temperature T = 0, Zn-Cu alloy; known as brass, gets completely ordered. This state is said to be β-brass. In β-brass state, each Zn atom is surrounded by eight copper

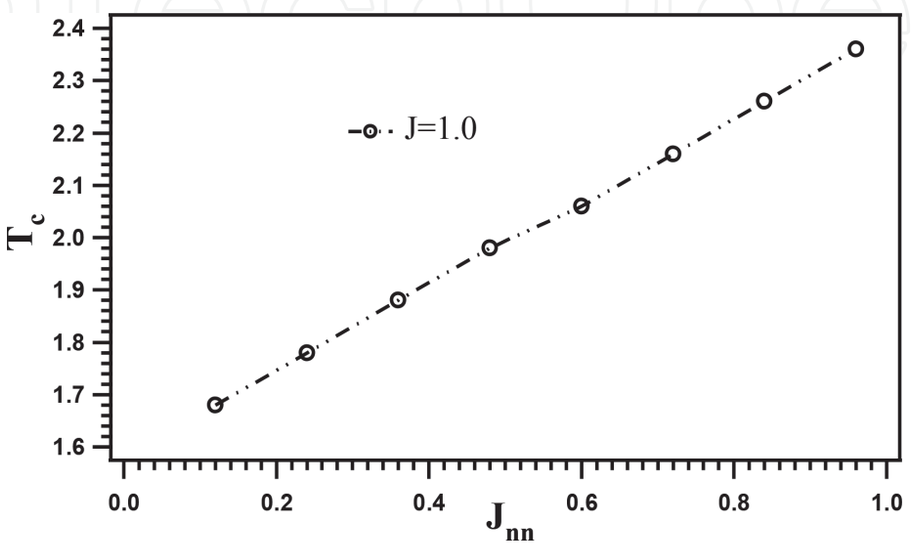

Figure 3.
Variation in critical temperature vs. next nearest exchange coupling for a bcc lattice (reproduced with permission from Singh [3]).

atoms, placed at the corners of the unit cell of the body-centered cubic structure and vice versa. The occupation of each site can be represented by:

$$n_i = \begin{cases} 1 & \text{if site i is occupied by atom A} \\ 0 & \text{if site i is occupied by atom B} \end{cases} \quad (1)$$

The interaction energy between A-A, B-B, and A-B type of atoms are represented by ε_{AA}, ε_{BB}, and ε_{AB}, respectively. Phase separation has been studied vastly, using Ising model [4–6]. A phase is simply a part of a system, separated from the other part by the formation of an interface; that essentially means that two components aggregate and form rich regions of A and B type of molecules with an interface in between them. The evolution of two distinct phases, when an initial random but homogeneous mixture is annealed below a definite temperature, is known as phase separation. Phase separation leads to discontinuity and inhomogeneity in the systems. This happens because the phase-separated regions are energetically more stable. Phase separation has been an old problem and has been extended to study diverse phenomena ranging from magnetic liquid-liquid phase separation to protein-protein phase separation in biological systems. This process has also been studied in the presence of external surfaces having affinity to one type of atom or molecule (**Figure 4a**). Both theoretical and experimental methods have been exploited and have been found in close agreement. Formation of long ridges and circular drops has been reported numerous occasions using lattice-based Ising model. For example, one may look into John W. Cahn research paper published in *The Journal of Chemical Physics* in the year 1965. The TEM image taken for Vycor, in which one phase had been leached out and the voids were filled with lead (**Figure 4b**).

2.2 Lattice-based liquid-gas model

Yang and Lee first coined the term lattice gas in the year 1952. A lattice should have larger volume (V) than the number of lattice molecules (N), so that some of the nodes or lattice vertices are left empty (i.e., N < V). No lattice vertex can be occupied by more than one particle. The interaction potential between two atoms at lattice sites i and j is given by Eq. (2):

$$U(rij) = \begin{cases} -\in & if\ \mathrm{S_i} = \mathrm{S_j} = 1.0 \text{ and rij} = 1.0 \\ \infty & \text{if rij} = 0.0 \\ 0 & \text{else} \end{cases} \quad (2)$$

For surface affinity of lower surface to i^{th} liquid molecule, we chose:

$$V(ri) = \begin{cases} -\dfrac{J_0}{r(i)} & if\ \mathrm{S_i} = 1.0 \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

The occupation number (n_i) of a lattice site i is given by:

$$n_i = \begin{cases} 1 & \text{if site i is occupied} \\ 0 & \text{if site i is un} - \text{occupied} \end{cases} \quad (4)$$

One example case is shown in **Figure 5**. Here, we chose lattice size of $128 \times 128 \times 48$. The fluid-fluid molecule and wall-liquid molecule interactions are defined, respectively, in Eqs. (2) and (3). In canonical ensemble, the three-dimensional lattice is swept one by one; by choosing sites regularly with one of its

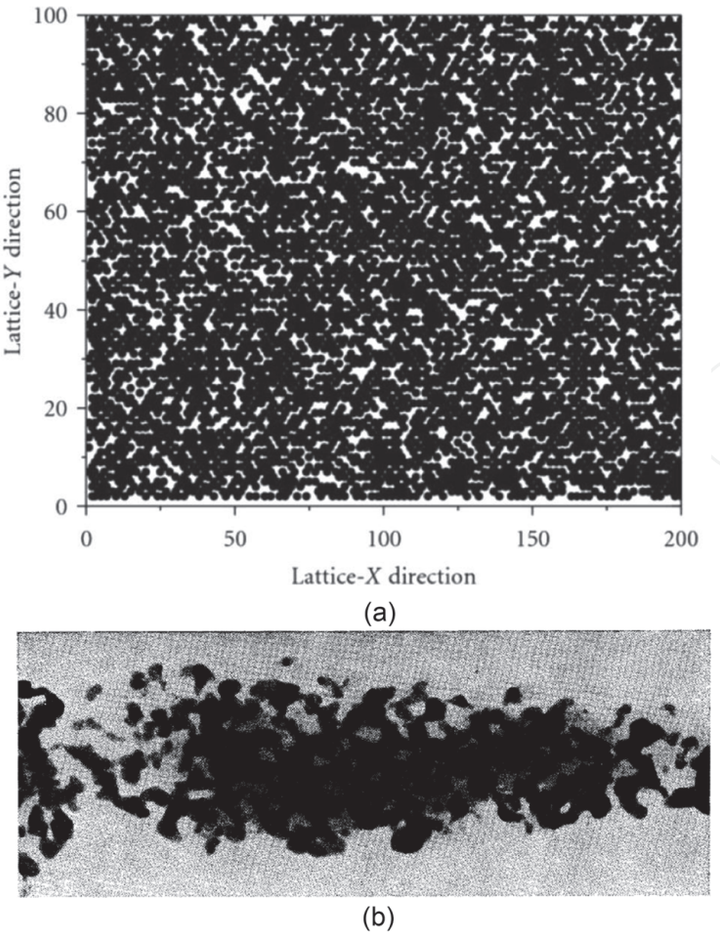

Figure 4.
(a) Surface-directed phase separation and dewetting in conserved binary mixture using two-dimensional lattices of size 200 × 100 nodes. The conserved components are taken in ratio 70:30 at T = 0.70. Majority component is attracted by upper and lower substrates, whereas the minority component has repulsive interaction with the two interfaces. Periodic boundary conditions are applied along X-direction. The micrograph is taken after completion of 30,000 Monte Carlo cycles using Kawasaki exchange method (the figure is reproduced with permission from Singh [5]). (b) Shows Transmission Electron Microscope (TEM) image of unsintered Vycor with one phase replaced by lead (X 200000). Reproduced with permission from W. G. Schmidt and R. J. Charles, Journal of Applied Physics 35, 2552 (1964); doi: 10.1063/1.1702905.

nearest neighbor (i.e., i = n and i + 1 = n + 1). Change in energy is calculated during exchanging of these two sites; the exchange move is accepted, if Exp $[-\Delta E/k_BT]$ is found to be greater than or equal to a random number generated between [0, 1]. For all cases of studies here, $\varepsilon = 1$ and $J_0 = 12.0$, and only the lower surface is functional, while the upper surface has only hard-sphere interaction with the fluid molecules. Average number density for liquid-like molecules is taken as 0.25 [16].

Figure 6 shows micrograph of self-aligned liquid columns. The system evolves from an initial homogeneous mixture of liquid- and gas-like molecules obtained by annealing the system at high temperature for few thousand MC cycles. Dynamic Monte Carlo simulation has been used with continuous but random trial movements of the molecules. The lattice-based Ising model using Eqs. (2) and (3) is also supposed to give same results, at least qualitatively.

2.3 Spin glasses

Crystalline solids possess short- and long-range order along its crystal axes and maintain its periodicity in three dimensions. Liquids possess only short-range order, and its molecules have no long-range correlation. Liquid molecules retain only short-range order. Gases possess neither of the two. These are the three phases, in which any matter may exist. What are the glasses then? Glasses are solids,

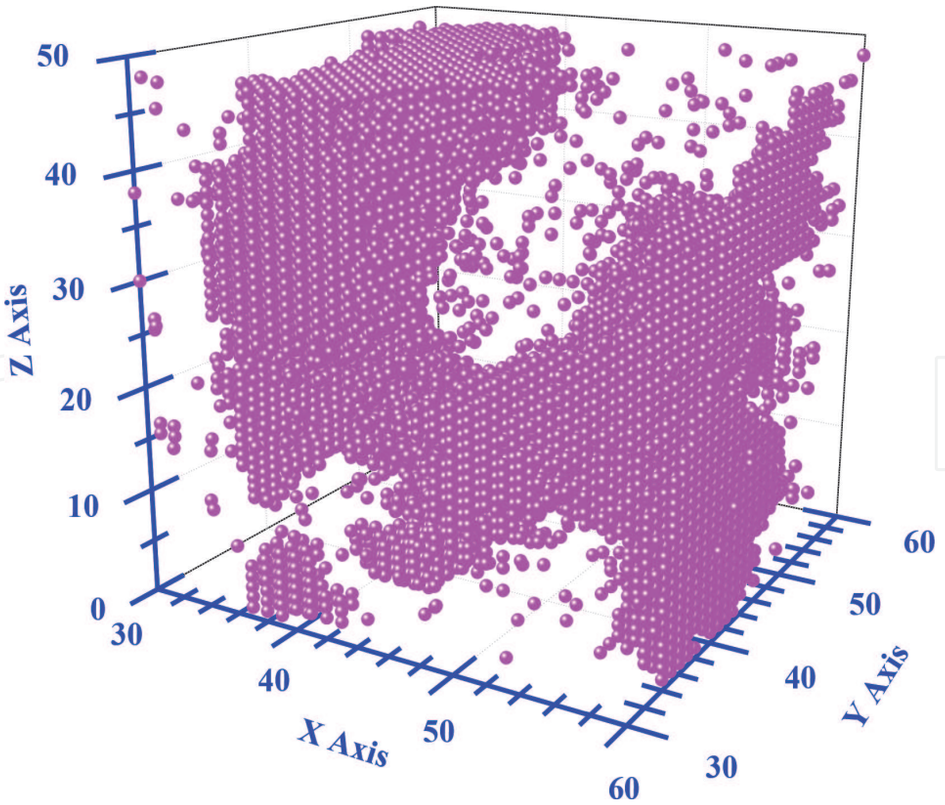

Figure 5.
Micrograph for box thickness H_z = 48 after completion of 20 K M C cycles (figure is reproduced with permission from proceedings, Singh [16]).

possessing no long-range order. Molecules may only locally arrange themselves to minimize its free energy. If the molecular arrangement is completely random, then a term "random media" is assigned to that. Glasses are understood as supercooled liquids. If a liquid is frozen abruptly, so that the molecules do not get sufficient time to organize themselves, some local order can be retained inside the frozen liquid. Glasses have one peculiar property. These retain relatively higher entropy even at quite low temperatures. One example is Mn doped in metals as impurity. Mn atoms interact with other Mn so (i.e. impurity atom) via RKKY interaction $J_{ij}(r) \sim \frac{\cos(2k_F r)}{(k_F r)^3}$. Because of the oscillations in it, the interactions remain random. Such spin systems are classified as spin glasses. There is great deal of frustrations in spin orientations; so on many occasions, these are also referred as "frustrated spin glasses."

Lenz-Ising model did not remain limited to above problems only, but it was extensively used to study liquid mixtures, ternary and quaternary alloys, polymer and their mixtures, random walk problem, and many others. The important aspect of Ising model is that a variety of problems (including some problems mentioned above) can be investigated by the similar kind of modeling and approach all together. It is no longer necessary to develop a different kind of theory for each type of cooperative phenomenon. Despite of all the above, it has been ironical that the inventor of the model, Ernst Ising, gave up the idea on working it, any further presuming that his model has no physical significance. He realized after two decades that he had become famous for his model because of the results obtained by other scientist based on his model, rather by his own work. It has been a queer sensation that the results of Ising model matched with any experimental data or the model was bit artificial. As for as the exponents were concerned, they were of universal nature, and a wide variety of systems have the same Ising exponents. The experimental evidence in favor of it remained a challenge, for many decades. In the

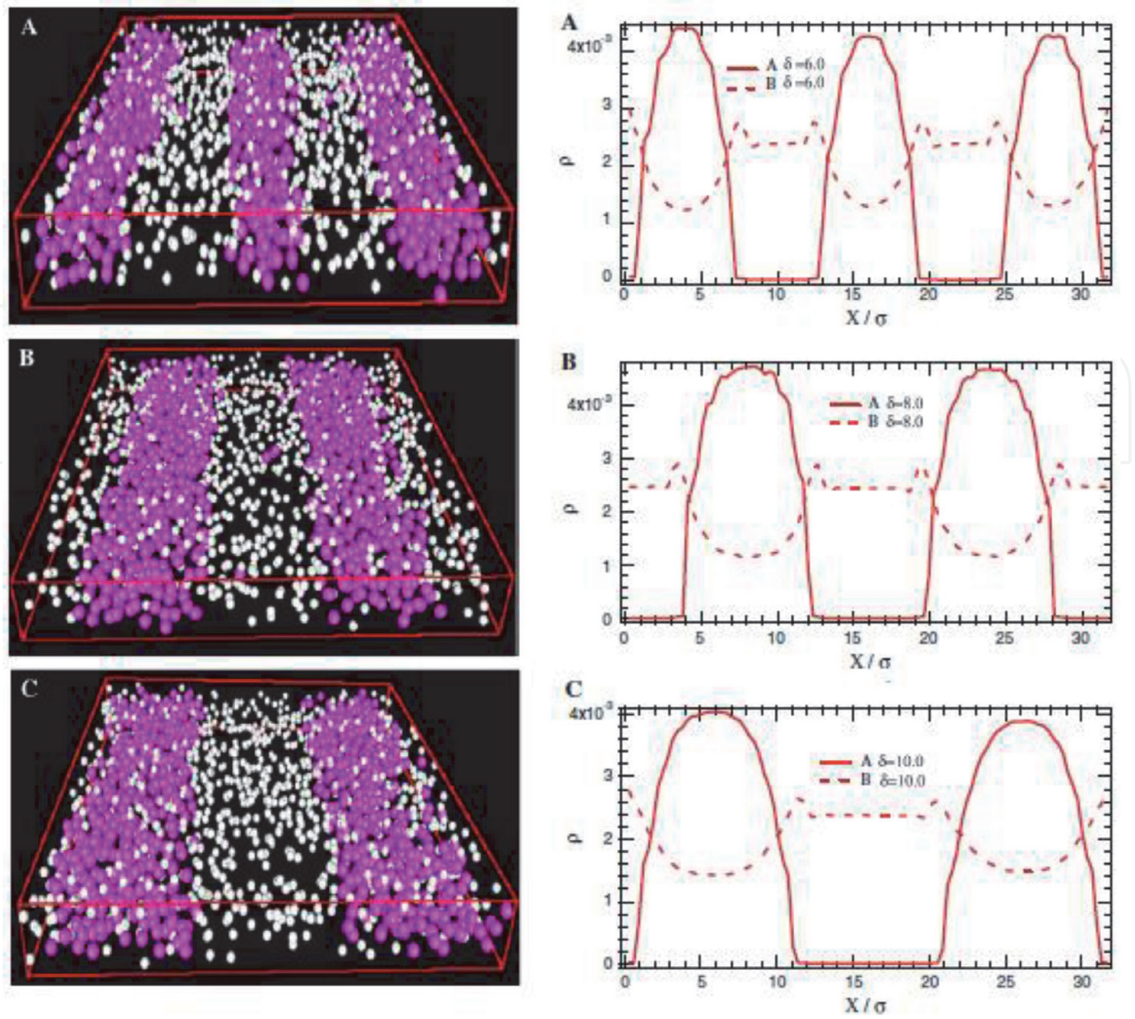

Figure 6.
Self-assembled channels formed in confined geometry; the system starts with a random mixture of square-well fluid (A-type) and hard-sphere (B type) particles. The chemically patterned surface has affinity to (A-type) with interaction range $\lambda_{A\text{-}A}$ = 1.5, $\lambda_{A\text{-}B}$ = 1.5, $\lambda_{Wall\text{-}A}$ = 2.0; interaction strengths were taken as ε_{AA} = 1.0, ε_{AB} = 0.5, and $\varepsilon_{Wall\text{-}A}$ = 3.0. Average number density of the system has been taken as ρ = 0.40. Pore width H = 4.0 and composition ratio A:B = 50:50 were taken for all cases of studies. The micrograph and density data were taken after completion of 40 × 10^5 Monte Carlo cycles (the figure is reproduced with permission from Singh et al. [14]).

year 1974, an alloy was found, which first showed that its magnetic behavior exactly matched with the Onsager result.

3. Mathematical formulation in one dimension

Various textbooks are available nowadays, which discuss Ising model and its applications in greater details [19–22]. Here, brief theory of one-dimensional Ising model is presented. H, Q, and A stands for Hamiltonian, partition function, and free energy of the system, respectively:

$$H_N\{S_i\} = -J\sum_{n,n} S_i S_j - \mu\, B \sum_{i=1}^{N} S_i \tag{5}$$

$$H_N\{S_i\} = -J \sum_{\substack{i=1 \\ <i,j>}}^{N} S_i S_{i+1} - \frac{1}{2}\mu B \sum_{i=1}^{N} (S_i + S_{i+1}) \tag{6}$$

$$Q_N(B,T) = -\sum_{S_1=\pm 1} \ldots\ldots\ldots\ldots \sum_{S_{N=\pm 1}} e^{\beta\sum_i^N \left\{JS_iS_{i+1}+\frac{1}{2}\mu B(S_i+S_{i+1})\right\}} \tag{7}$$

$$\langle S_i|P|S_{i+1}\rangle = e^{\beta\left\{JS_iS_{i+1}+\frac{1}{2}\mu B(S_i+S_{i+1})\right\}} \tag{8}$$

$$Q_N(B,T) = \sum_{S_i=\pm 1} \ldots\ldots\ldots\ldots \sum_{S_{N=\pm 1}} \langle S_1|P|S_2\rangle\langle S_2|P|S_3\rangle \ldots\ldots\ldots\ldots \langle S_{N-1}|P|S_N\rangle\langle S_N|P|S_1\rangle \tag{9}$$

$$Q_N(B,T) = \sum_{S_i=\pm 1} \sum_{S_{i+1}=\pm 1} e^{\beta JS_iS_{i+1}+\frac{1}{2}\mu\beta(S_i+S_{i+1})} \tag{10}$$

$$P = \begin{pmatrix} e^{\beta(J+\mu B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu B)} \end{pmatrix} \tag{11}$$

$$Q_N(B,T) = \sum_{S=\pm 1} \left\langle S\middle|P^N\middle|S\right\rangle = Trace\left(P^N\right) = \gamma_1^N + \gamma_2^N \tag{12}$$

$$\begin{pmatrix} e^{\beta(J+\mu B)} - \gamma & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu B)} - \gamma \end{pmatrix} = 0 \tag{13}$$

$$\gamma^2 - 2\gamma e^{\beta J}\cosh(\beta\mu B) + 2\sinh(2\beta J) = 0 \tag{14}$$

$$\begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = e^{\beta J}\cosh(\beta\mu B) + 2\sinh(2\,\beta J) = 0 \tag{15}$$

$$\begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = e^{\beta J}\cosh(\beta\mu B) \pm \left\{e^{-2\beta J} + e^{2\beta J}\,sinh^{\,2}(\beta\mu B)\right\}^{1/2} \tag{16}$$

$$\gamma_2 < \gamma_1;\ \left(\frac{\gamma_2}{\gamma_1}\right)^N \to 0 \tag{17}$$

$$ln\,Q_N(B,T) \cong N ln\,\gamma_1 \tag{18}$$

$$\frac{1}{N}\,ln\,Q_N(B,T) \cong \ln\left[e^{\beta J}\cosh(\beta\mu B) + \left\{e^{-2\beta J} + e^{2\beta J}\,sinh^{\,2}(\beta\mu B)\right\}^{1/2}\right] \tag{19}$$

$$A(B,T) = NJ - Nk_BT\ ln\left[\cosh(\beta\mu B) + \left\{e^{-4\beta J} + sinh^{\,2}(\beta\mu B)\right\}^{1/2}\right] \tag{20}$$

$$U(B,T) \equiv -k_BT^2\frac{\partial}{\partial T}\left(\frac{A}{k_BT}\right) \tag{21}$$

$$U(B,T) \equiv -NJ - \frac{N\mu B sinh(\beta\mu B)}{\left\{e^{-4\beta J} + sinh^{\,2}(\beta\mu B)\right\}^{1/2}} + \frac{2NJe^{-4\beta J}}{\left[\cosh(\beta\mu B) + \left\{e^{-4\beta J} + sinh^{\,2}(\beta\mu B)\right\}^{1/2}\right]\left\{e^{-4\beta J} + sinh^{\,2}(\beta\mu B)\right\}^{1/2}} \tag{22}$$

Some thermodynamic functions are defined as follows:

$$\overline{M}(B,T) \equiv -\left(\frac{\partial A}{\partial B}\right)_T = \frac{N\mu\ \sinh(\beta\mu B)}{\left[e^{-4\beta J} + sinh^{\,2}(\beta\mu B)\right]^{1/2}} \tag{23}$$

$$\chi \equiv \frac{\partial M}{\partial B} \rightarrow \chi_0(T) = \frac{N\mu^2}{k_B T} e^{2J/k_B T} \tag{24}$$

3.1 Case A: free boundary with zero field

Partition function is given by:

$$Q\ (0,T) = \sum_{S_1} \ldots\ \ldots \ldots \sum_{S_{N-1}} e^{K\sum_{i=1}^{N-1} S_i S_{i+1}} \tag{25}$$

Here, K = β J.
We now define a new variable:

$$\sigma_i = S_i S_{i+1}; Here\ i = 1, 2, \ \ldots\ \ldots \ldots N-1 \tag{26}$$

Then we can assign σ to two values, i.e., ±1:

$$\sigma_i = \begin{cases} +1 & if\ \ S_i = S_{i+1} \\ -1 & if\ \ S_i = -S_{i+1} \end{cases} \tag{27}$$

In order to consider contributions from all possible configurations $\{S_1, S_2, S_3 \ldots \ldots \ldots S_N\}$, we need to provide the set of numbers $\{\sigma_1, \sigma_2, \sigma_3 \ldots \ldots \ldots \sigma_{N-1}\}$; here each S_i can take two values as ±1. Configuration in a lattice description means a particular set of values of all spins; if there are N numbers of vertices, there will be 2^N different configurations as a result of permutation and combination of spins. The space, thus formed with these configurations, is called configuration space. Here, summing over σ_i will give only half value of Q, henceforth, we can write:

$$Q\ (0,T) = 2\sum_{\sigma_1} \ldots\ \ldots \ldots \sum_{\sigma_{N-1}} e^{K(\sigma_1+\sigma_2+\sigma_3 \ldots \ldots \ldots \ldots \ldots +\sigma_{N-1})} \tag{28}$$

$$Q\ (0,T) = 2\sum_{\sigma_1} \ldots\ \ldots \ldots \sum_{\sigma_{N-1}} e^{K(\sigma_1+\sigma_2+\sigma_3 \ldots \ldots \ldots \ldots \ldots +\sigma_{N-1})} \tag{29}$$

$$Q\ (0,T) = 2(2coshK)^{N-1} \tag{30}$$

3.2 Case B: periodic boundary with zero field

Now, the partition function is given by:

$$Q\ (0,T) = \sum_{S_1} \ldots\ \ldots \ldots \sum_{S_{N-1}} e^{K\sum_{i=1}^{N-1} S_i S_{i+1} + K S_N S_1} \tag{31}$$

Here, $S_{N+1} = S_1$

$$Q\ (0,T) = \sum_{S_1} \ldots\ \ldots \ldots \sum_{S_{N-1}} e^{K(\sigma_1+\sigma_2+\ldots\ \ldots\ \ldots \sigma_{N-1}) + K\sigma_1\sigma_2 \ldots\ \ldots\ \ldots \sigma_{N-1}} \tag{32}$$

Since $(S_i)^2 = 1$, we can write $S_1S_N = S_1.\ S_2.\ S_2.\ S_3.\ S_3 \ldots\ \ldots\ \ldots\ \ldots\ S_{N-1}.\ S_{N-1}.\ S_N$

$$Q\ (0,T) = 2\sum_{\sigma_1} \ldots\ \ldots \ldots \sum_{\sigma_{N-1}} e^{K(\sigma_1+\sigma_2+\ldots\ \ldots\ \ldots \sigma_{N-1})} \sum_{n=0}^{\infty} \left(\frac{K\sigma_1\sigma_2\sigma_3 \ldots \sigma_{N-1}}{n!}\right)^n \tag{33}$$

Here, second part in exponential has been converted into a summation series:

$$Q\left(0,T\right)=2\sum_{n=0}^{\infty}\frac{K^n}{n!}\left[\sum_{\sigma}\sigma^n e^{K\sigma}\right]^{N-1} \tag{34}$$

$$Q\left(0,T\right)=2\sum_{n=0}^{\infty}\frac{K^n}{n!}\left[e^{K}+(-1)^n e^{-K}\right]^{N-1} \tag{35}$$

$$Q\left(0,T\right)=(2\cosh \mathrm{K})^N+(2\sinh \mathrm{K})^N \tag{36}$$

It can be shown that in thermodynamic limit, (i.e. $N\rightarrow\infty$), the free energy of the system converge to a finite value. Readers are left with the exercise. So, periodic boundary condition, as shown in **Figure 7** (invented by Ising), really helps one to get rid of constructing infinitely large systems. Using appropriate boundary conditions, one may obtain realistic results using large but finite number of spins.

4. Critical phenomena

A lot of research work has been dedicated to observe system behavior near critical points [23–27]. The relevant thermodynamic variables exhibit power-law dependences on the parameter $(T-T_c)$ specifying the distance away from the critical point. The critical points are marked by the fact that different physical quantities pertaining to the system pose singularities at the critical point. These singularities are expressed in terms of power laws of $(T-T_c)$ characterized by critical exponents. As, for example, magnetization <M> identified as an order parameter in magnetism, shows dependence on critical temperature (T_c), with exponent β as follows other exponents are also listed below.

Reduced temperature $t\equiv(T-T_c)/T_c$.
α: specific heat c $(t)\sim t^{-\alpha}$; $B\equiv h=0$.
β: spontaneous magnetization M (t) $\sim(-t)^{\beta}, T\leq T_c$, $B\equiv h=0$.
γ: magnetic susceptibility $\chi=\partial M/\partial h, T\sim|t|^{-\gamma}$, $B\equiv h=0$.
δ: critical Isotherm M (h) $\sim|h|^{1/\delta}$ sgn (h), $t=0$.
ν: correlation length, $\xi\sim|t|^{-\nu}$, $B\equiv h=0$.
η: correlation function G $(r)\sim r^{(-d+2-\eta)}$, $t=0$, $B\equiv h=0$.

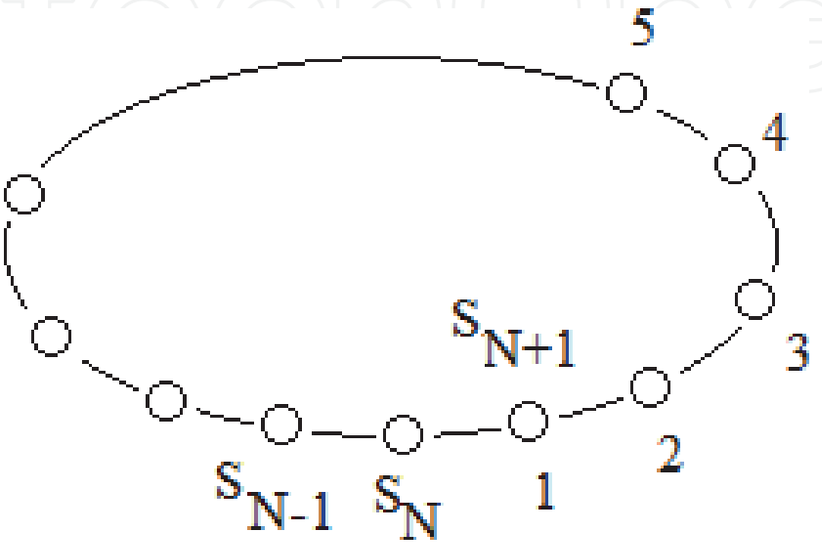

Figure 7.
Representation of periodic boundary conditions in a one-dimensional Ising chain.

4.1 Scaling hypothesis and renormalization group theory

Kadanoff first suggested that, when a system is near critical temperature, individual spins may be grouped into blocks of spins [23]. It is possible because of the fact that the spin-spin correlation length becomes exceedingly large near T_c and details of individual spins no longer remain important. In transformed system, each block plays the role of a single spin. Now, the spin variable associated with a single block is denoted by symbol σ_i. σ_i can take values ± 1. The new system is composed of N′ spins (**Figure 8**).

$$N' = l^{-d}N \tag{37}$$

Lattice constant:

$$a' = la \tag{38}$$

In order to preserve the spatial density of the degrees of freedom of spins in the system, the spatial distances are rescaled by the factor l.

$$r' = l^{-1}r \tag{39}$$

Now, the partition function can be updated as follows:

$$Q = \sum_{\{\sigma_i\}} e^{[-\beta H_N\{\sigma_i\}]} \tag{40}$$

This idea was first propounded by Kadanoff, and was later developed by Wilson. This process is also referred as decimation process. A new exchange coupling constant is assigned for interaction between σ_i. This new construction of lattice does not alter the free energy of the system, and it remains the same as obtained by the original method. The rescaling process helps to find relations between various exponents. More detailed discussion on this topic can be found in standard textbooks of *Statistical Mechanics* by Patharia, Huang, etc. Since this process involves

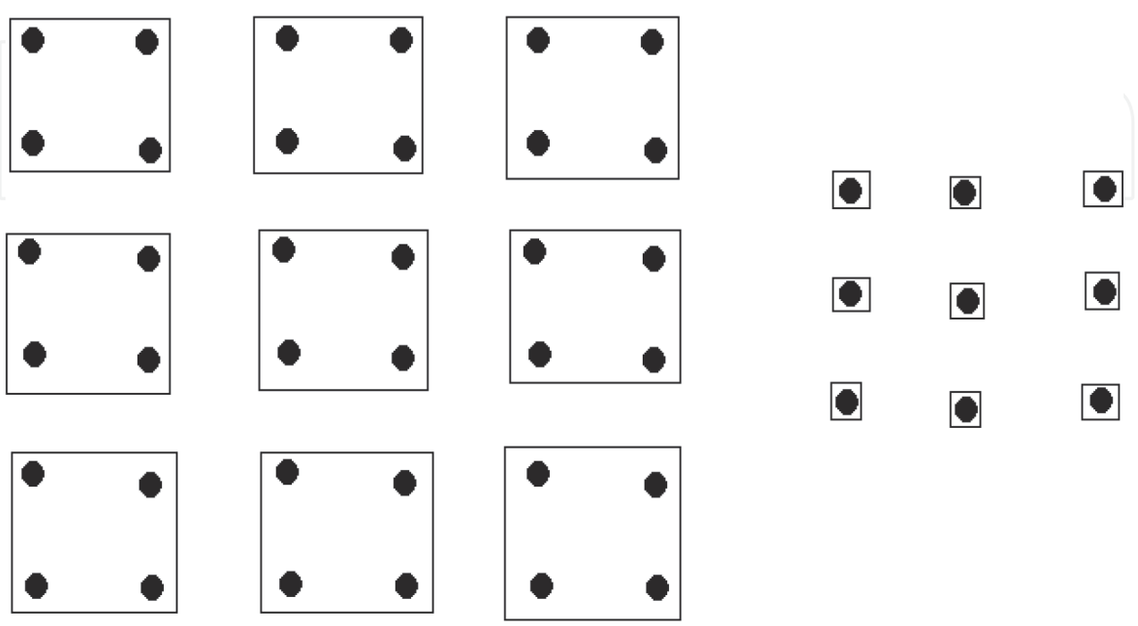

Figure 8.
Spin decimation process in a two-dimensional square lattice. A small cluster of 36 spins gets transformed into 9 nodal points.

length transformation or a change of scale, Wilson introduced the concept of renormalization group theory after removing certain deficiencies in Kadanoff's scaling hypothesis. A greater detail of this is omitted here, because that is beyond the scope of the chapter.

5. Physical realization: simulation results based on Ising model

We now discuss some of the simulation results obtained using Ising model. **Figure 9** shows spontaneous magnetization for a simple cubic crystal (i.e., scc lattice). As the strength of exchange coupling between spin-up and spin-down (J_{AB}) decreases, the critical temperature lowers down. Lower values of J_{AB} weaken the spin flip-flop mechanism; henceforth the system requires further cooling, so that the spin-spin correlation overcomes the fluctuations. Spontaneous magnetization occurs in the absence of external magnetic field [28]. The confirmation of spontaneous process is further confirmed in **Figure 10**. **Figure 10** is plotted for spin

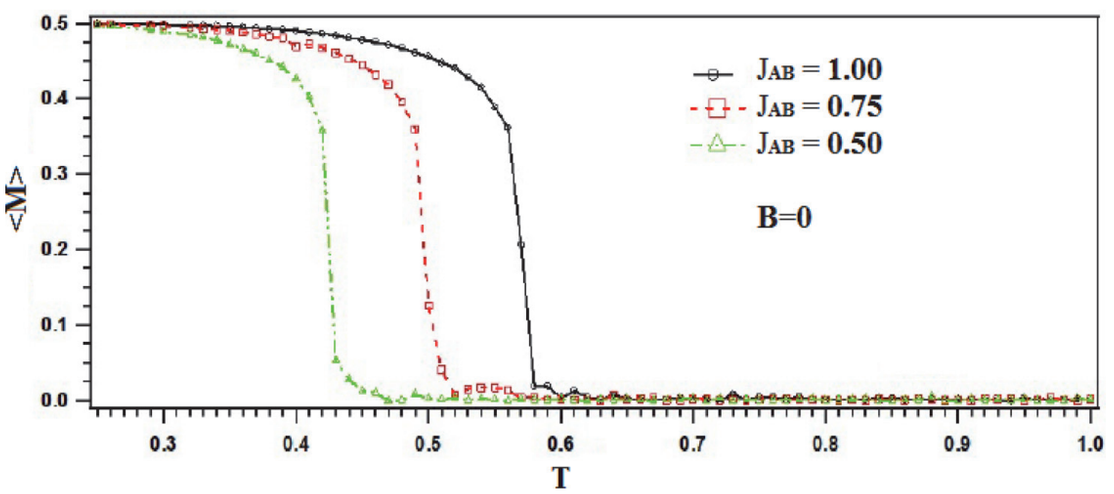

Figure 9.
Spontaneous magnetization in two-dimensional thin film (this figure is reproduced with permission from Singh [28]).

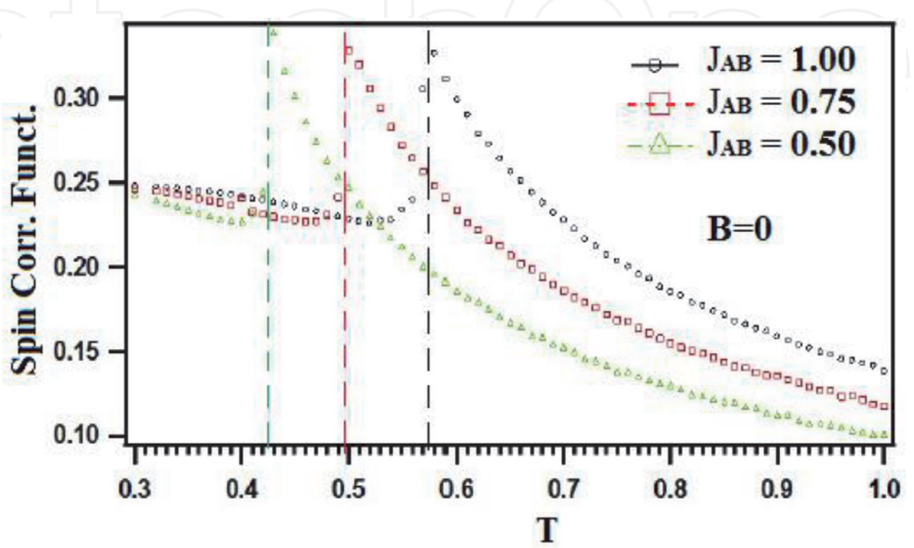

Figure 10.
Correlation function vs. temperature for a two-dimensional thin film. Spontaneous magnetization is marked by discontinuity in it (this figure is reproduced with permission from Singh [28]).

correlation function vs. temperature of the system [28]. The critical temperature is marked by the presence of discontinuity in it. Above critical temperature, the magnetization abruptly falls to zero, which is an indication of paramagnetic state. The critical temperature in ferromagnetic thin film is known as Curie temperature. We observe similar kind of behavior with antiferromagnetic films, though below critical point (also known as Neel temperature), the net average magnetization becomes zero, because opposite spins are energetically favored in this case. The schematic diagram is shown in **Figure 11** [28]. Magnetization vs. external magnetic field curves are plotted in **Figure 12(a)–(d)** for different sets of parameters [28].

Simulation results obtained for a magnetically striped system as schematically shown in **Figure 13** are reported in **Figures 14–17** [29]. One or two alternate rectangular regions are created, using external field. **Figure 14** shows the gradual transition at the interface, where a definite value of external field suddenly gets zero. The spin polarizations in two regions show sharp boundary. The magnetized film, in presence of magnetic field, induces the magnetic zones in proximity where its close external field is zero. Micrograph also indicates for spin-spin phase separation. The corresponding average magnetization vs. temperature and spin correlation function vs. temperature are also plotted in **Figures 15** and **16**, respectively, but these studies are done using Monte Carlo simulation with semi-infinite free boundary conditions. It has been observed that these systems have relatively high critical transition temperatures. **Figure 17** shows the magnetization process with two alternate magnetized zones [29].

Low-dimensional magnetic heterostructures play vital role in spinotronics. Ferromagnets can induce magnetic ordering through a 40-nm-thick amorphous paramagnetic layer, when placed in its close proximity. One has to reconcile with long-range magnetic interaction to correctly measure the extent of induced magnetization. Readers may go through the *Nature Communications* article of F. Magnus et al. published in the year 2016 [17]. The magnetic properties of ferromagnetic materials with reduced dimensions get altered; when the thickness of a film is

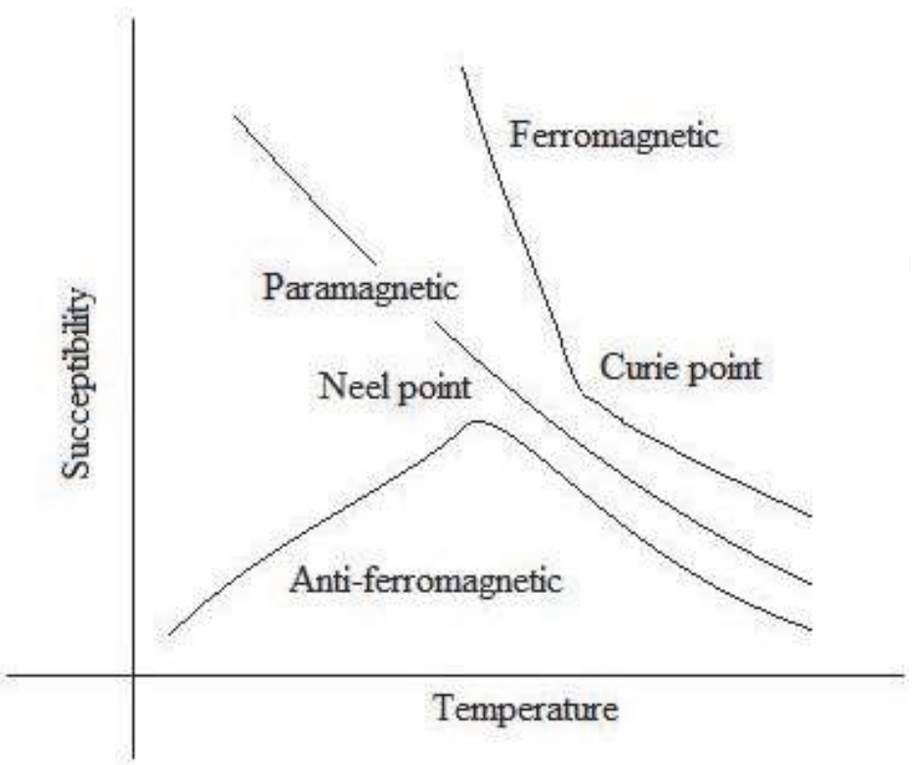

Figure 11.
Schematic representation of ferromagnetic to paramagnetic and antiferromagnetic to paramagnetic transitions.

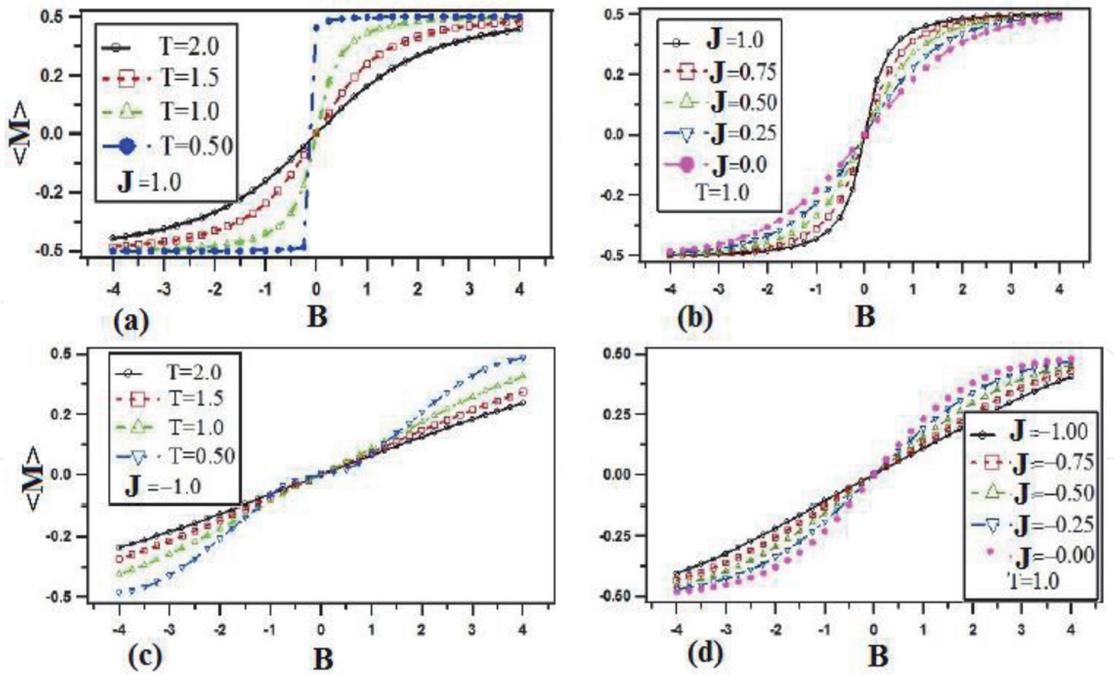

Figure 12.
(a) Magnetization vs. external fields at different temperature T = 0.50, 1.0, 1.5, and 2.0. (b) Magnetization vs. external fields for different exchange couplings J = 0.0, 0.25, 0.50, 0.75, and 1.0. These cases are for ferromagnetic thin films. (c) Magnetization vs. external fields at different temperature T = 0.50, 1.0, 1.5, and 2.0. (d) Magnetization vs. external fields for different exchange couplings J = 0.0, 0.25, 0.50, 0.75, and 1.0. These cases are for antiferromagnetic thin films (this figure is reproduced with permission from Singh [28]).

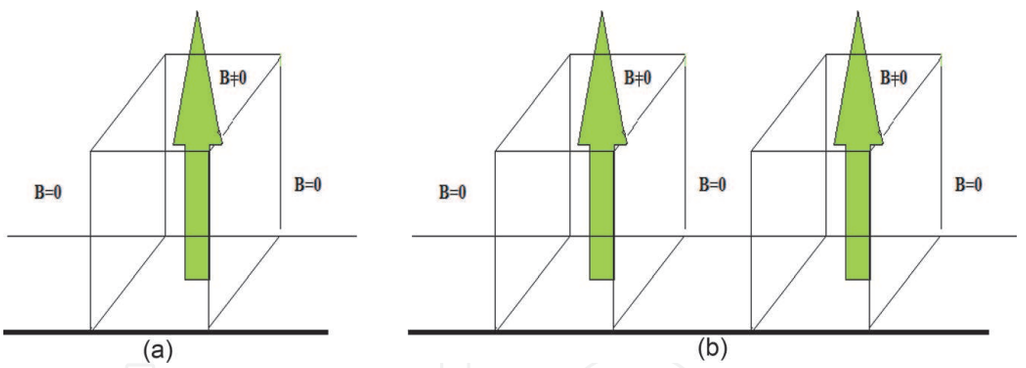

Figure 13.
(a) The system with one slab of size $n_x \times n_y \times n_z = 50 \times 100 \times 100$ exposed to an external magnetic field. (b) The system with two alternate slabs of size $n_x \times n_y \times n_z = 50 \times 100 \times 100$ exposed to an external magnetic field.

reduced below a critical value, the ferromagnetic to paramagnetic transition disappears [18]. Finite-size effects may also weaken or enhance magnetic interactions at the boundaries, as well as restrict the evolution of spin-spin correlation length. Extension of these ideas to model magnetic heterostructures, comprising of multiple magnetic and/or nonmagnetic layers, gives insight into interfacial phenomena. Many current and emerging technologies are based on this central problem. This may be very useful in understanding and exploring problems as metal-insulator transition, which is at the core of many state-of-the-art technologies. Henceforth, computational techniques, especially Ising model, can now be extended to develop and enrich science, for making new technologies. Though, its use can be said at the nascent stage, but with the advancement in computer hardware and efficient algorithms, it's applications in areas related to spinotronics appears to be bright.

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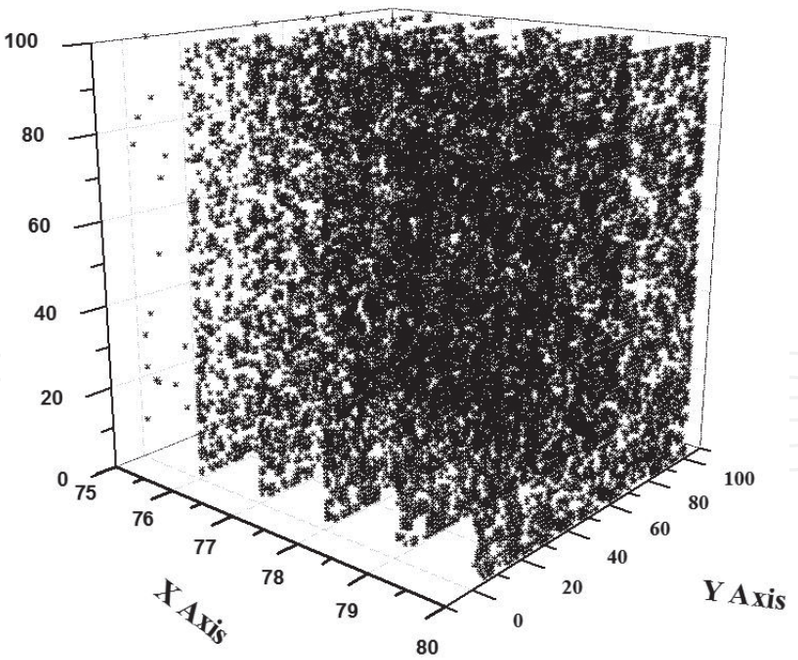

Figure 14.
The micrograph of the coexisting phases in the regions of close proximity of the magnetic barrier indicating for the presence of depletion layer near the barrier.

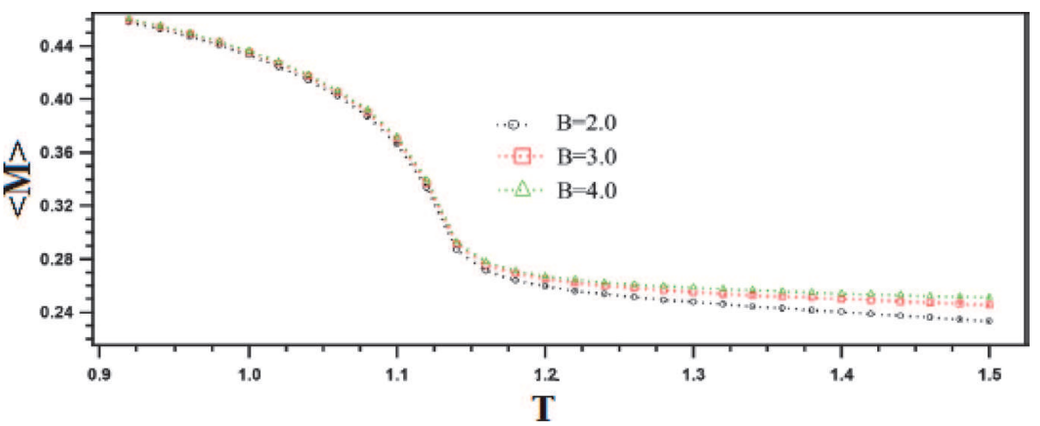

Figure 15.
Magnetization vs. temperature for magnetically striped system. Only one region experiences the presence of external magnetic field as illustrated in ***Figure 12(a)****. This simulation is done for simple cubic lattice with semi-infinite free boundary conditions (the figure is reproduced with permission from Singh [29]).*

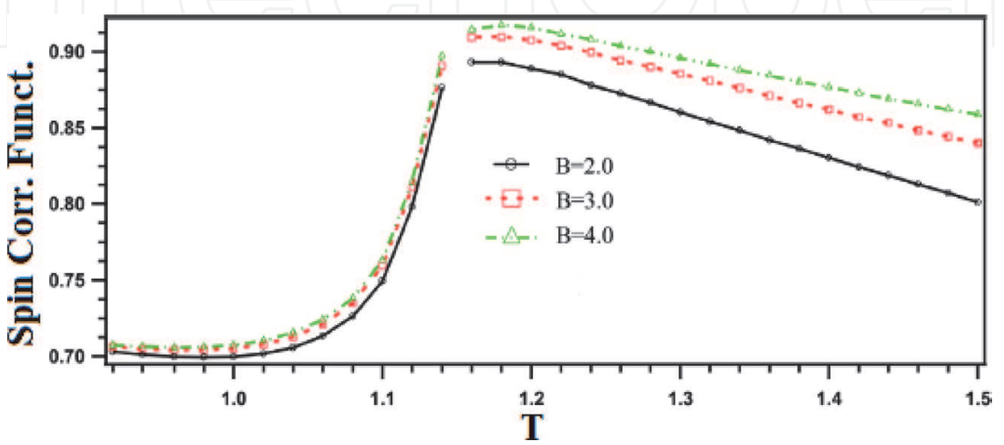

Figure 16.
Spin correlation function vs. temperature for magnetically striped system. Only one region experiences the presence of external magnetic field as illustrated in ***Figure 13(a)****. This simulation is done for simple cubic lattice with semi-infinite free boundary conditions (the figure is reproduced with permission from Singh [29]).*

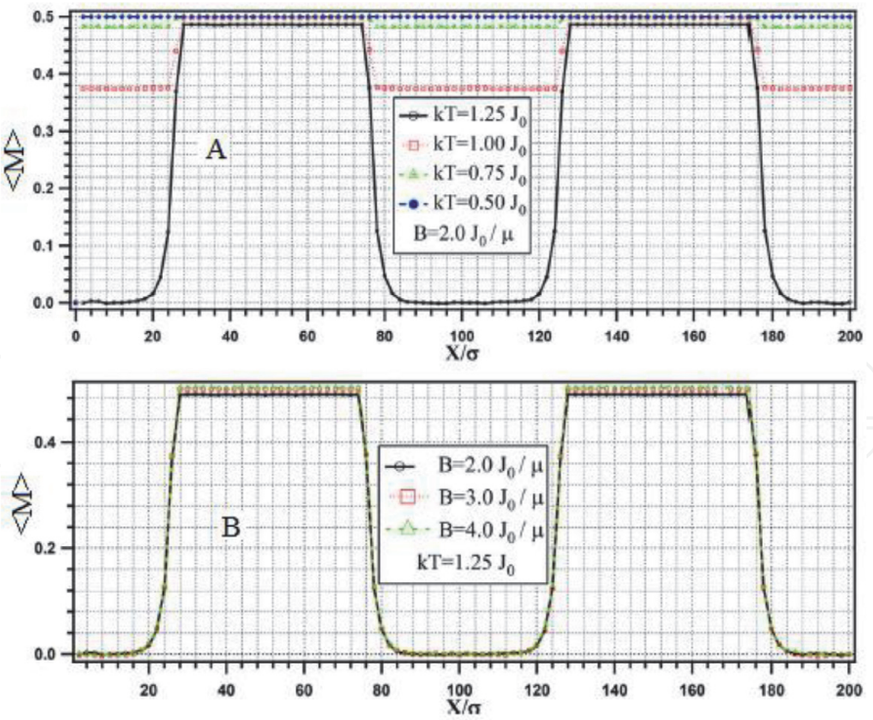

Figure 17.
Magnetization vs. temperature for magnetically striped system. Two alternate regions experience the presence of external magnetic field as illustrated in ***Figure 12(b)****. This simulation is done for simple cubic lattice with semi-infinite free boundary conditions (the figure is reproduced with permission from Singh [29]).*

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References

[1] Brush SG. History of the Lenz-Ising model. Reviews of Modern Physics. 1967;**39**(4):883-893. DOI: 10.1103/RevModPhys.39.883

[2] Niss M. History of the Lenz–Ising model 1950–1965: From irrelevance to relevance. Archive for History of Exact Sciences. 2009;**63**:243-287. DOI: 10.1007/s00407-008-0039-5

[3] Singh SP. Curie temperature of Ising ferromagnetic film and its dependence on nn exchange coupling. AIP Conference Proceedings. 2018;**1953**: 140015. DOI: 10.1063/1.5033190

[4] Singh SP, Singh K, Roychoudhury M. Monte Carlo simulation for diffusion limited surface directed phase separation. Proceedings of the National Academy of Sciences, India—Section A. 2008;**78**:79-83

[5] Singh SP. Spinodal theory: A common rupturing mechanism in spinodal dewetting and surface directed phase separation (some technological aspects and the significance of dipole-quadrupole interaction in spinodal dewetting). Advances in Condensed Matter Physics. 2011;**2011**:526397. DOI: 10.1155/2011/526397

[6] Singh SP. Spatial correlation in 2D and 3 D thin films of conserved binary mixtures in presence of wetting of substrates by preferred majority component: Interpretation in real scenario. Applied Nanoscience. 2012;**2**: 365-369. DOI: 10.1007/s13204-012-0094-8

[7] Pan AC, Chandler D. Dynamics of nucleation in the Ising model. The Journal of Physical Chemistry. B. 2004; **108**:19681-19686. DOI: 10.1021/jp0471249

[8] Sonsin AF et al. Computational analysis of 3D Ising model using Metropolis algorithms. Journal of Physics: Conference Series. 2015;**630**:012057. DOI: 10.1088/1742-6596/630/1/012057

[9] Katsoulakis MA, Plechac P, Bellet LR. Numerical and statistical methods for the coarse-graining of many-particle stochastic systems. Journal of Scientific Computing. 2008;**37**:43-71. DOI: 10.1007/s10915-008-9216-6

[10] Lundow PH, Markstrom K, Rosengren A. The Ising model for the bcc, fcc and diamond lattices: A comparison. Philosophical Magazine. 2009;**89**(22-24):2009-2042. DOI: 10.1080/14786430802680512

[11] Montroll EW, Potts RB, Ward JC. Correlations and spontaneous magnetization of the two dimensional Ising model. Journal of Mathematical Physics. 1963;**4**:308-322. DOI: 10.1063/1.1703955

[12] Huang R, Gujrati PD. Phase transitions of antiferromagnetic Ising spins on the zigzag surface of an asymmetrical Husimi lattice. Royal Society Open Science. 2019;**6**:181500. DOI: 10.1098/rsos.181500

[13] Singh SP. Revisiting 2D lattice based spin flip-flop Ising model: Magnetic properties of a thin film and its temperature dependence. European Journal of Physics Education. 2014;**5**(3): 8-19

[14] Singh SP, Singh JK, Sharma A. Adsorption of gas like molecules on self-aligned square well fluid channels under confinement of chemically patterned substrates. Applied Nanoscience. 2013;**3**: 179-187. DOI: 10.1007/s13204-012-0118-4

[15] Singh SP. Monte Carlo simulation of microscopic viscosity and rupturing thin polymer film near melt: A molecular

perspective. Physics Letters A. 2017;**381**: 1321-1327. DOI: 10.1016/j.physleta.2017.02.011

[16] SP Singh, A Kumari Singh, Formation of liquid structures and investigation of its interfacial properties using lattice based liquid-gas model, Proceedings of International Conference on Nanoscience and Nanotechnology, 29th Nov.-01st Dec. 2019, VIT, Vellore, Tamil Nadu, India

[17] Magnus F et al. Long-range magnetic interactions and proximity effects in an amorphous exchange-spring magnet. Nature Communications. 2016;**7**:11931. DOI: 10.1038/ncomms119311

[18] Singh SP. Specific heat capacity: Thickness critical spontaneous magnetization in striped ferromagnetic thin films. AIP Conference Proceedings. 2018;**1953**:040020. DOI: 10.1063/1.5032640

[19] Patharia RK, Beale PD. Statistical Mechanics. 3rd ed. Academic Press; 2011

[20] Huang K. Statistical Mechanics, 2nd Ed. Wiley; 2008

[21] Chandler D. Introduction to Modern Statistical Mechanics. USA: Oxford University Press; 1987

[22] Binder K, Heermann D. Monte Carlo Simulation in Statistical Physics, 1868-4513. Berlin Heidelberg: Springer-Verlag;

[23] Kadanoff LP. Scaling Laws for Ising models near Tc*. Physics. 1966;**2**(6): 263-272. DOI: 10.1103/PhysicsPhysiqueFizika.2.263

[24] Holovatch Y. Introduction to renormalization. Condensed Matter Physics. 2006;**9**(2(46)):237-262. DOI: 10.5488/CMP.9.2.237

[25] Kaya T. A new approach to real space renormalization group treatment of Ising model for square and simple cubic lattice. International Journal of Modern Physics B. 2018;**32**(23):1850252. DOI: 10.1142/S0217979218502521

[26] Nauenberg M. Renormalization group solution of the one−dimensional Ising model. Journal of Mathematical Physics. 1975;**16**:703-705

[27] Carneiro CEI, Henriques VB, Salinas SR. Renormalisation group calculations for a spin-1 Ising model with bilinear and biquadratic exchange interactions. Journal of Physics A: Mathematical and General. 1987;**20**: 189-197. DOI: 10.1088/0305-4470/20/1/027

[28] Singh SP. First observations of entropy vs free energy in lattice based modeling for spin coarsening in conserved and non-conserved binary mixtures: The phenomenological study of phase transitions in 2D thin films. Nanosystems: Physics, Chemistry, Mathematics. 2015;**6**(6):882-895. DOI: 10.17586/2220-8054-2015-6-6-882-895

[29] Singh SP. Temperature induced spin polarization in magnetically striped ferromagnetic film: The coexisting phases and the two regime behavior. Macromolecular Symposia. 2017;**376**(1): 1600193. DOI: 10.1002/masy.201600193