Studies in Relaxation Dynamics of Complex Systems: Exact Solution of Hysteresis in One Dimensional Anti-ferromagnetic Random Field Ising Model at Zero Temperature

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I Ratnadeep Roy , hereby declare that the subject matter of this thesis is the record of work done by me, that the contents of this thesis did not form basis of the award of any previous degree to me or to the best of my knowledge to anybody else, and that the thesis has not been submitted by me for any research degree in any other University/Institute.

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Dedicated to
"Dadu"

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CHAPTER– I

I. Introduction

I.1 Importance of Exactly Solved Models

Statistical mechanics has made great strides in recent decades. The behaviour of systems in equilibrium is now understood quite well including phase transitions. Simple but exactly solved models have played an important role in the development of equilibrium statistical mechanics. Ising model [1] is one of the simplest and perhaps the most extensively studied model of cooperative behaviour in an extended system. The model is defined on a d-dimensional lattice, with lattice points denoted by $i=1, 2, 3, \ldots N$. We are interested in the thermodynamic limit $N \to \infty$. Each lattice point i is assigned a dynamical degree of freedom called an Ising spin S_i. An Ising spin is a binary variable. It can take the values 0 or 1, or any other set of two values depending on the context of the physical system. In modelling a magnetic system it is customary to assign the values +1 (up) or -1 (down) to S_i. The magnetization (per site) is simply the average orientation of the Ising spins, i.e.

$$m = \frac{1}{N}\sum_{i=1}^{N} S_i \qquad (I.1)$$

Nearest neighbour Ising spins are coupled to each other through an exchange interaction J. Thus an Ising model is characterized by the Hamiltonian

$$H = -J\sum_{nn} S_i S_j \qquad (I.2)$$

If $J > 0$ (ferromagnetic coupling), the interaction aligns nearest neighbour spins parallel to each other. This produces a long range ferromagnetic order in the system, and therefore a net magnetization. If the system is in thermal equilibrium with a heat bath at a temperature T, the thermal energy $k_B T$ acts to disrupt the long range order. We may expect long-range order to prevail at low temperatures, and disorder at high temperatures. There may be a phase transition from an ordered state to a disordered state at a critical temperature T_c given approximately by the equation $k_B T_c \approx zJ$, where z is the number of nearest neighbour of a site on a d-dimensional lattice, and k_B is the Boltzmann constant. The primary motivation in introducing the Ising model is to calculate T_c, and the singularities in the thermodynamic functions at the critical point.

The Ising model is easily solved in one dimension. It was solved by Ising in 1925 [2]. Surprisingly, the result showed that the critical temperature T_c in one dimension is equal to zero. The absence of long-range order at any finite temperatures is a special feature of one dimensional models with short-range interactions. It is now understood in a broader context as a result of theorems due to Landau, Mermin, and Wagner [3, 4]. This is an illustration of how exact solutions of very simple models can bring out a result of more general validity, and deepen our understanding.

Going beyond the one dimensional case, the simplicity of the Ising model turns out to be rather deceptive. The solution of the model in two dimensions is quite difficult. It was solved by Onsager in 1944 [5]. The Onsager solutions still remains a classic piece of work in equilibrium statistical mechanics and a required reading for a serious student of the subject. The solution was also extended to the case of a vanishingly small applied field in two dimensions [6]. The two dimensional Ising model in a finite applied field, and the three dimensional Ising model even in the absence of an applied field have not been solved exactly so far in spite of a great effort. However, extensive numerical studies of the three dimensional Ising model have been made, as also analytical studies based on perturbation theory (high temperature expansion) [7]. These studies have contributed greatly to the theoretical understanding of universality and scaling in critical phenomena [8-10].

I.2 Non – Equilibrium Phenomena

Following the success of equilibrium statistical mechanics, attention has turned increasingly to non-equilibrium phenomena. A basic difference between equilibrium and non-equilibrium phenomena is the role of relaxation dynamics in non-equilibrium phenomena. By relaxation, we mean a process by which a system lowers its free energy to attain thermal equilibrium with its surroundings. The equilibrium state is the state of lowest free energy of the system. The properties of a system in equilibrium are independent of the relaxation path taken by the system to reach equilibrium. This results in a great simplification in the formulation of equilibrium statistical mechanics. The relaxation dynamics of a system does not enter its equilibrium statistical mechanics. The success of equilibrium statistical mechanics arises from the fact that a great variety of physical systems relax very fast on the time scale of experimental observation. If the relaxation is slow or punctuated, we must take into account the relaxation dynamics of the system to understand its behaviour. This brings us to the subject of non-equilibrium statistical mechanics.

Non-equilibrium phenomena are generally as diverse as the systems exhibiting them. A first step towards their understanding would be to identify features that may have a weak universality going beyond the microscopic details of the system. Reasonable progress has been made in this direction. It has created several smaller fields of study which are better known by the key words such as coarsening , diffusion-limited-aggregation , viscous fingering [11-13], spinglasses [14-18], neural networks [19-25], persistence [26,27] etc. These keywords represent different aspects of weakly universal features seen in a wide variety of non-equilibrium phenomena. Simple models which provide an interesting caricature of these phenomena have been identified, studied numerically as well as analytically, and compared with experiments.

I.3 Hysteresis

Hysteresis is a common feature of non-equilibrium phenomena. Webster's New Collegiate dictionary tells us:

Hys-ter-e-sis: n [NL, fr. Gk *hysteresis* shortcoming, fr. *hysterein* to be late, fall short, fr. *hysteros* later] a retardation of the effect when the forces acting upon a body are changed (as if from viscosity or internal friction); esp.: a lagging in the values of resulting magnetization in a magnetic material (as iron) due to a changing magnetizing force. - **hys-ter-et-ic** adj.

It is clear that hysteresis represents history dependence of physical systems. The term is most commonly applied to magnetic systems: as the external field associated with the microphone is turned off, little magnetic domains created by the recorded voice in the tape do not return to their original configuration (by design, otherwise our record of the music would disappear !). Generally any system which is capable of several configurations of equilibria for given external conditions exhibits hysteresis. Hysteresis in a magnetic system is also the focus of this thesis. For the sake of completeness, we recall what is meant by hysteresis in a magnetic system. We take a magnet and drive it by a smoothly varying cyclic field of frequency ω. For simplicity we take the starting value of applied field to be very large and negative. Let us represent the applied field by the equation $h(t) = -h_o \cos \omega t$. Thus at the start of the hysteresis experiment, i.e. at time $t = 0$, the applied field is equal to $-h_o$. We assume that this initial value is large enough to saturate the magnetization in the downward direction, i.e. $m = -1$, at $t = 0$. As the applied field goes through a cycle the magnetization traces out a loop in the m-h plane. There are two values of magnetization for each applied field; the magnetization in increasing field being smaller than the magnetization in decreasing field. This indicates that we are observing a non-equilibrium effect where the response of the system lags behind the applied field. It may be expected that if the field is varied infinitely slowly, i.e. in the limit $\omega \to 0$, the system may be better able to keep pace with the applied field, and the hysteresis may disappear. This expectation is not always borne out by experiments and we shall say more on it later.

Suffice it to say here, that the existence of a loop even as $\omega \to 0$ is puzzling. In thermodynamic equilibrium, the system cannot exist in two distinct states except at a phase transition point. The hysteresis loop seems to indicate that the system has two thermodynamic states which are both stable at experimental time scales. This is a classic example of the conflicts between the predictions of classical equilibrium thermodynamics and empirical data that have existed since 19th century.

In experiments the hysteresis loops corresponding to subsequent cycles of the applied field often do not overlap each other perfectly. Rather, with each subsequent cycle of the applied field, the hysteresis loop shifts slightly and systematically. This is a complex phenomenon known as reptation [28]. We shall not go into it further in this thesis. We are concerned with simple hysteresis loops that connect the system between two states of oppositely saturated magnetization and which do not show reptation.

I.4 Analysis of Hysteresis Loops

Even the simple hysteresis loops mentioned above are difficult to obtain theoretically. Readers would appreciate that all hysteresis loops encountered by them are (most probably) of an experimental origin. Efforts to understand hysteresis theoretically were pioneered by Raleigh [29] and Preisach [30]. In the present work we attempt to obtain hysteresis loops theoretically from simple exactly solved models.

It is worthwhile to ask if there are any characteristics of hysteresis loops whose significance might go beyond the specifics of the physical system. For example, we expect the area of the hysteresis loop to vanish as $\omega \to 0$, irrespective of the system. It is interesting to investigate if the area vanishes as a (universal?) power of ω, or how it might depend on the parameters h_o, ω and T characterizing the field and the system. This question has been investigated by several authors [31-33]. It has been suggested that in the limit $h_{o,}\omega \to 0$, the area scales as $(h_o\omega)^{1/2}$ .The limit $\omega \to 0$ means that the time period of the applied field tends to infinity. In other words, the time over which the applied field changes significantly is much larger than any other time scales in the experiment. The time period of the applied field is one of the characteristic time scales for the system. The other time scale is determined by the thermal relaxation time of the system. In fact, in most systems, there is a whole spectrum of thermal relaxation times. In many practical cases the longest thermal relaxation time is larger than the time period of the applied field even if the field is cycled very slowly. In such cases the area of the hysteresis loop shows no indication of vanishing even if the applied field were to be cycled so slowly so as to take an entire life of an experimentalist to complete one cycle. The work presented in this thesis concerns these systems with infinitely slow thermal relaxation. We may conveniently set the temperature of the system equal to zero to model systems whose thermal relaxation is infinitely slow. The microscopic structure of magnetization loops in such systems can be broadly divided into two categories – (*i*) noisy, and (*ii*) smooth. The noisy structure is characteristic of ferromagnetic systems. Even though the applied field changes smoothly, the magnetization changes in sporadic jumps of irregular and unpredictable sizes. This is known as Barkhausen noise [34]. The Barkhausen noise shows an apparent power-law spectrum, and has been studied by several workers experimentally as well as theoretically [35-39]. It is a paradigm of non-equilibrium response of systems that respond to slow and smooth applied forces by avalanches. Other systems in this category are sandpiles [40,41], earthquakes, and avalanches of snow on mountains. The second category of systems respond relatively smoothly (i.e. without avalanches) but infinitely slowly to smoothly changing forces. These systems are characteristic of anti-ferromagnetic interactions. The anti-ferromagnetic interactions ensure that an Ising spin that has flipped in response to a changing external field generally acts to stop its immediate neighbours from flipping. As we shall see below, there are exceptions to this rule. Occasionally a nearest neighbour may flip but the process does not continue beyond the nearest neighbour. There are no avalanches in this category of relaxation. Examples of physical systems showing this behaviour are amorphous anti-ferromagnets, glasses and spinglasses which continue in a metastable state for a long time and then transit to another by small localized events sans avalanches [42-44].

1.5 Complexity

Complexity is a topic of current research activity in a number of fields including statistical mechanics, computer science, mathematics and biology. Within such diverse groups it is not surprising that the term complexity is used with several shades of meaning. We shall not go into the various definitions of complexity, rather we will briefly mention what we understand by complexity in an intuitive way in the context of recent research, and then state more specifically in the context of this thesis. Generally we can describe an extended system at two levels: microscopic level and macroscopic level. Complexity refers to the richness of the description at the macroscopic level. Consider two examples: water (as a chemical) and an animal (a biological system). At the macroscopic level water is adequately described by stating the phase in which it exists e.g. is it liquid, vapour or ice? The phase in turn is specified uniquely by the temperature and pressure. There are critical points for water where two phases may coexist but generally it has a unique macrostate. On the contrary if our system is a biological system, its macroscopic description may be rich (an animal may run, sleep, eat, jump ...).

The variety of the macroscopic description is taken as an indication of complexity.

From this point of view, clearly all traditional physical systems are simple and apparently complexity is not relevant in the world of physics. However, in the last years the situation has changed: it has been found that there are many disordered physical systems for which the macroscopic description is quite rich. An example that is easy to visualize is a heteropolymer, i.e. a polymer composed of a sequence of many different functional units. Typical biological heteropolymers are proteins, DNA and RNA. Sometimes it happens that the same heteropolymer at low temperature folds in a unique way, but in other cases more than one folding is possible. If the heteropolymer may fold in many different ways, we can consider each folding as a different phase and such a system is a complex system [45, 46]. Other physical systems like spinglasses have similar properties; they have been carefully investigated and structure of different phases of the systems has been studied in details. It is striking that these systems have a rather interesting chaotic behaviour: a small change in the form of the system may completely upset the macroscopic behaviour. This effect becomes more and more pronounced by increasing the size of the system. In the case of large systems the macroscopic behaviour is extremely difficult to predict because it is sensitive to a huge number of microscopic details.

This kind of difficulty is not without precedent in physics. Indeed the observation that for a given system the actual trajectory is extremely sensitive to the initial conditions (as billiard balls), destroyed the hope of computing the trajectory of a large system in a precise way (apart a few exceptions). However the birth of statistical mechanics is related to this difficulty; the unpredictability of the trajectory in a deterministic sense makes possible to obtain probabilistic predictions for the behaviour of the system for generic initial conditions. The main proposal of Boltzmann was to give up the possibility of predicting the evolution of the system for given initial conditions and to concentrate the attention on the study of the most likely evolution starting from generic initial conditions. In the same way we can give up the possibility of computing which are all the macroscopic descriptions of a particular complex system. Doing so we gain the possibility of obtaining statistical predictions on its behaviour. The statistical predictions however are different from the ones of usual statistical mechanics. In usual statistical mechanics the system is nearly always in one given macrostate and we compute the probability distribution of several different microscopic realizations of the same macrostate. Here we predict the probability of having a given number of simultaneously available macrostates and the relations among the different macrostates. Other interesting quantities that can be computed are, for example the average time spent by a system in a given macrostate before jumping into another macrostate.

For a large class of systems, a generic choice of the system implies the existence of many macroscopic states. In other words if the system is chosen in a random way, the macroscopic behaviour is automatically very rich. We do not need to tune the parameters that control our system in order to have many different macroscopic states because this feature is present in the generic case. We can summarize the situation by saying that microscopic randomness generates complexity.

I.6 Quenched Disorder and Separation of Time Scales

Disorder is really unavoidable in any thermodynamic system. The reason is that any system must have a finite entropy at a non zero temperature. However, there may be instances of small disorder e.g. a tiny fraction of point defects in an otherwise perfect crystal, or a large disorder that is characteristic of liquids. This separation of disorder between small disorder and large disorder does not have a sharp dividing line, but the meaning is intuitively clear. Similarly, there is another classification of disorder into two categories: annealed and quenched. This classification is based on the relaxation dynamics of the system. Thermodynamic systems have several modes of relaxation. The number of modes maybe infinitely large, and each mode has a different rate of relaxation. If the disorder is able to relax well over experimental time scales, we call it annealed disorder. Annealed disorder is the kind of disorder seen in very slowly cooled liquids and metals. If the disorder is not able to relax itself over the time periods of experimental observation i.e. if it remains frozen for all practical purposes, we call it quenched disorder. Examples of quenched disorder are glasses, spinglasses, and other amorphous solids. It is quenched disorder that gives rise to a large number of macrostates of the system and hence to complex behaviour.

Again, the dividing line between what can relax and what remains frozen is not very sharp. It depends on the period over which the system is observed. Suppose the time of observation is τ_0, and the time of relaxation (inverse of relaxation rate) is τ_r. Quenched disorder corresponds to the case, $\tau_r >> \tau_0$. Even in this case, there is small probability that the slowest relaxation modes may affect the system during observation. However, for theoretical convenience, we shall impose a strict separation of time scales in the analysis of the system. Relaxation processes which occur extremely slowly will be assumed not to occur at all. Consider for example a glass. There is natural separation of time scales in this example. The mean positions of atoms change extremely slowly, while the vibrations around the mean positions (phonons) are fast. Quenched disorder assumes that the mean positions do not change at all.

In quenched systems, a fraction of the degrees of freedom is assumed to remain strictly frozen during the life time of the system, and the remaining degrees of freedom evolve in this frozen background. Due to the randomly frozen background in which the system has to evolve, its evolution depends strongly on the initial state i.e. the history of the system. If the time period of observation were truly infinite and all relaxation processes were allowed the evolution of the system will be punctuated by long-lived metastable states. Over practical time periods, the system explores only a limited phase space corresponding to the domain of a metastable state. Going back to our example of phonons in a glass, the glassy solid can only explore those phonon modes which are possible in the frozen configuration of the mean positions of atoms. It is not possible for the system to explore phonon modes belonging to a different realization of the distributions of mean positions of atoms.

Systems with quenched disorder have a large number of metastable states. As we discussed in the preceding section, the existence of several metastable states or macrostates give rise to complex behaviour. We shall take an extended system to be a complex system, if its free energy has a thermodynamically large number of local minima in the phase space of the system, and the local minima are separated from each other by thermodynamically large energy barriers. Spinglasses are our paradigm of complex systems, and spinglass behaviour that of complexity. The local minima are the metastable states of the system. Large barriers mean that the metastable states have a very long lifetime. A system may stay in the same metastable state during the period of experimental observation. Thus the observed properties of the system should be obtained by averaging the system over the thermodynamic domain of a single metastable state, and then taking a second average over the distributions of local minima of free energy. The barriers separating various local minima are assumed to be random and mainly larger than thermal energy of the system. Experience with spinglasses and other random systems has shown that Ising models with quenched random interactions or quenched field on sites, produce a free energy landscape of the kind indicated above. However, models with quenched interactions have not been solved exactly even in the mean field approximation [17]. Random field Ising models (RFIM) are more amenable to exact solution. In the following, we describe the nature of the work done on the RFIM so far before taking it up for further analysis in this thesis.

I.7 Random Field Ising Model

The random field Ising model (RFIM) has played an important role in understanding disordered systems. It first came into prominence around 1975, when Imry and Ma [47] argued that Ising magnets with quenched random field were capable of sustaining a long range order in two dimensions. It was an appealing argument, and a kind of clear statement which was lacking in the context of other prominent models of quenched disorder, e.g. the Sherrington-Kirkpatric (random bond) model of a spinglass. Thus several people were attracted to the study of the equilibrium statistical mechanics of the random field Ising model. Soon a controversy was generated. Dimensional reduction arguments based on field theoretic methods [48] showed that the lower critical dimensionality of RFIM was three rather than two as predicted by Imry and Ma. It took some years to resolve that the application of the dimensional reduction method in this context was unjustified because it necessarily assumed the existence of a unique solution of the field equations. It was shown that the field equations for systems with quenched disorder have a large number of solutions (metastable states). Due to the presence of numerous metastable states in the system, the numerical simulations proved rather difficult and inconclusive, and the initial enthusiasm for the model faded in due course.

Some years later, interest in RFIM revived for the same reason it had faded earlier. Its richness in metastable states was a deterrent in the study of its equilibrium properties, but made a good model for the study of non-equilibrium phenomena in glassy and complex systems. These systems are characterised by extremely slow relaxation, and history dependent effects which arise from the presence of several metastable states in the system. Recently Sethna et al [49] used the RFIM to study hysteresis and other related phenomena such as the return point memory effect, and Barkhausen noise. Hysteresis is a kinetic phenomena, and therefore one needs to put in a dynamics in the model. Sethna et al employed the zero-temperature Glauber dynamics of Ising spins. It showed remarkable success in reproducing the observed features of hysteresis and other phenomena mentioned above. The success of the Sethna model is not unreasonable. It forms a minimal model which takes into account the most important aspects of hysteresis. For complex systems of the kind indicated above, the zero-temperature dynamics is a reasonable approximation to the finite temperature dynamics on laboratory time scales. The thermal energies are anyway much smaller than barrier heights, therefore it is a reasonable approximation to assume that the thermal energy is zero. Although the dynamics is deterministic, there is a stochastic aspect to it coming from the randomness of the quenched field. The metastable states of the RFIM become fixed points (stable states) under the zero-temperature dynamics. This simplifies their numerical as well as analytic characterization. However, the model retains the key features of the original problem. There is a broad distribution of energy barriers between nearby stable states. When the system is driven by a smoothly increasing applied field, it jumps from a stable state to a nearby stable state of lower energy when the applied field crosses the barrier between the two states. As the barriers are random variables, the trajectory of the system is not smooth. On a microscopic scale, it consists of irregular jumps in the magnetization (Barkhausen noise).

For ferromagnetic systems, experiments show that there is a broad distribution of the size of the magnetization jumps. Averaged over the entire hysteresis loop, jump distribution shows power laws over several decades (usually three). This has led to suggestions that there is a self-organized criticality in the system. The Sethna model provides a framework for examining this question. Although it does not appear to support self-organized criticality in the system, but there is a "plain old critical point" on each half of the hysteresis loop. At this point, the magnetization jumps show true power laws. The critical region appears to be rather broad. Thus approximate power laws are expected over a wide sector of the hysteresis loop. The extensive study of the Sethna model is based on numerical simulations of the model, and its analysis in the mean field approximation. For ferromagnetic interactions, the zero temperature hysteresis loops, the distribution of sizes of the Barkhausen jumps, and minor hysteresis loops have been determined exactly in one dimension as well as on a Bethe Lattice [50-56].

1.8 Our Work

This thesis is a first step towards an exact determination of the non-equilibrium response of an anti-ferromagnet with quenched disorder. As indicated in the previous section, much of the effort in solving Ising models with quenched disorder has been focused on ferromagnetic models. To the best of our knowledge, exact solution of hysteresis in an anti-ferromagnetic Ising model with quenched disorder has not been attempted so far, although the problem was posed and solved approximately a few years ago [57,58]. In view of this situation we decided to determine the hysteretic response of the anti-ferromagnetic random field Ising model (AFRFIM). We were forced to make further simplifications by necessity. We limited our effort to one dimensional AFRFIM, zero-temperature Glauber dynamics, and the case when the applied field is ramped up and down infinitely slowly. In spite of these simplifications, it proved difficult to find the solution of the model for a general, unbounded, continuous distribution of the random field at par with the solution of the ferromagnetic RFIM [50-56]. The reason lies in the qualitative difference between the zero-temperature dynamics with ferromagnetic interactions and that with anti-ferromagnetic interactions. The ferromagnetic case is abelian [52], i.e. if we start with any stable configuration of Ising spins, and then increase the external field and allow the system to relax, the final stable configuration reached is same and independent of the order in which the unstable spins are flipped. Also, in the relaxation process no spin flips more than once. In the anti-ferromagnetic case, the order in which the unstable spins are relaxed is important, and a spin which has flipped up in increasing field may flip down again at a higher field.

In the first instance [59, 60], we considered a bounded, rectangular distribution of the random field of width 2Δ, with $\Delta \leq |J|$, where $|J|$ is the magnitude of the nearest neighbour anti-ferromagnetic interaction. In this case, the numerical simulation of the model shows that the magnetization on the lower hysteresis loop takes the form of three ramps separated by two plateaus. The model and its numerical simulations are described in Chapter II. The analysis of the three ramps is presented in Chapters III, IV, and V. We could not immediately generalize our solution for small disorder $(\Delta \leq |J|)$ to the case of large disorder $(\Delta \geq |J|)$, and to unbounded distributions of the random field. Some progress has been made in this direction, but only recently. This is presented in Chapter VI. Finally Chapter VII contains a summary of our results and concluding remarks.