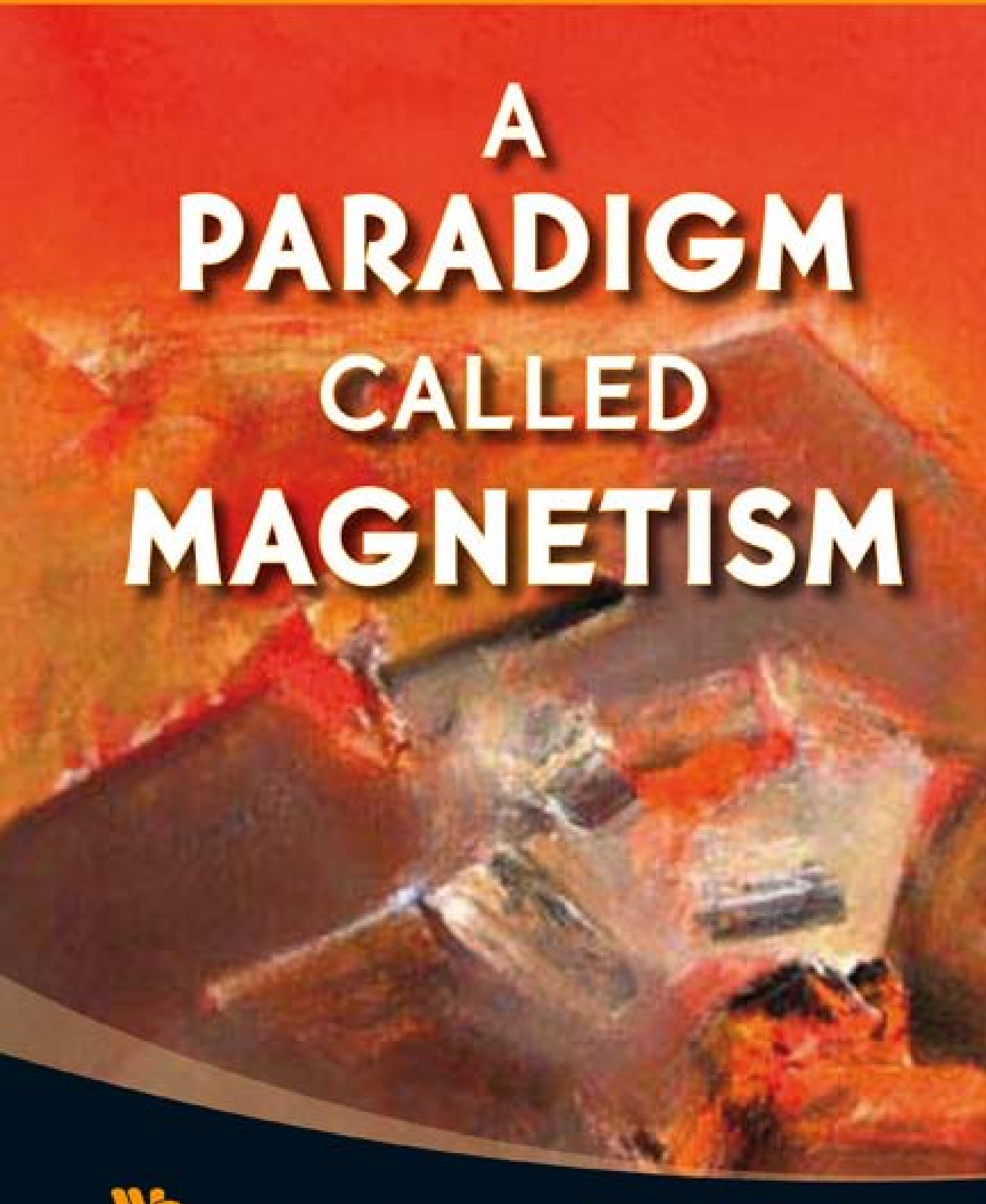
Sushanta Dattagupta

A PARADIGM CALLED MAGNETISM



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Preface

Magnetism is truly a very old subject. The first reference to a magnetic material, magnetite or the famed loadstone, can be found in Greek literature in astonishingly early times like 800 B.C. Yet the subject remains modern. It appeals to extremely basic issues of physics– magnetism as a material property is a direct result of one of the fundamental forces of nature governed by electromagnetic interactions. At the same time, this property forms the core of technology, influencing power-generation, biomedical applications through, for instance, magnetic resonance imaging, computer industry with the aid of memory devices and chips, just to name a few. Our objective in this volume is not to dwell on the myriad applications of Magnetism but to highlight the rich structure of its theory. It is remarkable to recount how many extraordinary ideas of physics ensue while teaching a course in Magnetism. To mention some: the first instance of velocity-dependent potentials in Mechanics is encountered in treating the Lorentz force on a charged particle in a magnetic field, the first example of the violation of time reversal is stumbled upon when we consider the Zeeman interaction of a spin in an external magnetic field, and so on.

Given this background to the wide applicability of the concepts of Magnetism, the purpose of these Lecture Notes is to further amplify how the subject has influenced developments in other diverse areas of Physics and how models used in Magnetism can help to clarify a variety of apparently unrelated phenomena. Magnetism is essentially a quantum mechanical subject. Yet its classical limits such as those described by Heisenberg or Ising-like models have far reaching applications to a plethora of topics in phase transitions. Thus, while the ideas of symmetry-breaking and scaling first appeared in Magnetism, they soon pervaded other topics of not just condensed matter physics, but even distant terrains of field theory and high energy physics. Similarly, the concepts of disorder and frustration, embedded in magnetic spin glass systems, are also common to structural glasses. In the domain of non-equilibrium effects too, examples derived from Magnetism help to elucidate the underlying issues of relaxation and dissipation.

With the preceding preamble, the Lecture notes are chapter-wise divided as follows. Chapter 1, consisting of three sections, deals with the by-now well-known phenomena which first appeared in the context of Magnetism but have had important bearing in many other subjects. In section 1.1, we discuss the Mermin-Wagner-Berezinskii theorem on symmetry-breaking in the context of the Heisenberg magnet and its implications in ϕ^4 field theory. The latter forms the backbone of section 1.2 that is devoted to universality and consequent scaling relations which are the underlying concepts in critical point phenomena. In section 1.3 we discuss the issue of multicriticality and point out how the models originally introduced to describe this phenomenon in what are called metamagnets, found their application to tricritical points in 3_{He} - 4_{He} mixtures and even to bicriticality and tetracriticality in an open, nonequilibrium system such as a two-mode ring laser. From chapter 2 onwards, we turn to more recent topics. In chapter 2, we introduce the contemporarily relevant topic of the quantum critical point, again in the context of the Ising model but now in a transverse magnetic field, which finds its realization in rare-earth magnetism. The model helps illustrate the occurrence of quantum phase transitions in a variety of phenomena. The same model allows us to deal with the inter-connected concept of disorder and frustration, which is the subject of chapter 3. Again, the important ideas were first observed in dilute magnets alloyed with metals, called spin glasses. In chapter 4, we move from equilibrium to nonequilibrium statistical mechanics and show how the well-established ideas of spin-lattice and spin-spin relaxations, which are at the heart of magnetic resonance systems, can be further developed to obtain coarse-grained models of phase ordering and pattern formation, seen in many systems as competition between nonlinear interactions and nonequilibrium effects. In chapter 5, we discuss important nonequilibrium phenomena seen in an assembly of single-domain nanomagnetic particles. The concomitant relaxation and memory effects are found to be a consequence of the interplay between polydispersity and inter-particle interactions. Similar memory or aging effects are observed in very different systems of relaxor ferroelectrics, shape-memory ferroelectric materials and structural glasses. The concepts discussed in chapter 4 in the context of magnetic response and relaxation behaviour find their counterparts in the recently-developed subject of dissipative quantum systems, discussed in detail in chapter 6. Therein we analyze the significance of coherence to decoherence transitions using a magnetic paradigm of Diamagnetism, which is intrinsically a quantum phenomenon, for which the boundary of the container plays a critical role. Thus dissipative diamagnetism is prototypical of decoherence in mesoscopic structures. Our final example is from a large spin quantum system that finds its realization in molecular magnets, and in which mesoscopic quantum tunneling can be seen. The influence of environment-induced dissipation makes this system yet another example of observing coherence to decoherence in quantum to classical crossover phenomena.

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Contents

Chapter 1

An Assortment of Well-Established Concepts

1.1. Symmetry-Breaking

The dynamics of a many body system are determined in terms of a Hamiltonian. The Hamiltonian is characterized by its invariance properties under all transformations that belong to a group, reflecting the underlying symmetries of the system. An extremely rich example of such a system is the one governed by interacting magnetic spins S and described by what is called the Heinsenberg Hamiltonian:

$$\mathcal{H} = -J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \,. \tag{1.1}$$

The summation is over sites i and j, and is restricted to nearest neighbours, as indicated by the angular brackets $<\ >$. The term J is usually referred to as the exchange interaction [1-5].

We may now enlist all the invariance properties of $\mathcal{H}$. The most basic of all these, as is indeed the fundamental attribute of all mechanical systems, is the invariance under time translation. The implication of this invariance is that the total energy is constant, as it must be for a conservative mechanical system. The second invariance property, again shared by most mechanical systems, is the one exhibited under time reversal. As the time t is reversed to $-t$, each spin operator such as S_i has its sign flipped, because S transforms like the orbital angular momentum operator. There is however no overall change in sign for the pair i and j. Time reversal symmetry is fundamental to electromagnetic forces and is broken only due to dissipation, or the presence of an external magnetic field. The third property, which is what we would like to focus onto, relates to the invariance of $\mathcal{H}$ under the simultaneous rotations of all spins through an arbitrary angle about an arbitrary axis. The group of transformations that leaves the Hamiltonian invariant is the symmetry group, denoted by G.

If the Heisenberg Hamiltonian does not make a distinction between different orientations, as discussed above, how does it then describe ferromagnetism which is associated with a unique directionality of the magnetization? Recall that the thermodynamic state of a system is governed by the minimum of the Helmholtz free energy $F = U - TS$, U being the internal energy, S the entropy and T the temperature. For instance, for the magnetic system at hand, the system would choose those spin configurations for which F is minimized. Thus, at high temperatures, the entropy dominates and the maximally disordered state has the highest entropy. This implies that the high temperature equilibrium state is paramagnetic with no average alignment of spin, i.e. the magnetization is zero. Therefore, the paramagnetic phase is invariant under the same group G as its Hamiltonian. On the other hand, at low temperatures, U dominates over TS and the ground state of $\mathcal{H}$ is the one in which all the spins are aligned along the same direction. (Note the negative sign in the right hand side of Eq. (1).) This low temperature equilibrium phase is a ferromagnetic one with nonzero average spin $<S> = <S_i>$, independent of the site index i, or equivalently a magnetization, $m = \mu V_o^{-1} <S>$, V_o being the volume of a unit cell and μ the magnetic moment per spin. At a critical temperature T_c called the Curie temperature the system undergoes a phase transition from the entropy dominated paramagnetic state to the energy dominated ferromagnetic state. Thus the magnetization m, which is zero in the paramagnetic phase and becomes non-zero in the ferromagnetic phase, is appropriately called the order parameter of the low temperature phase. It is invariant under rotations about an axis parallel to itself but changes under rotations about all axes that are oblique to itself. Therefore, the ordered phase has a lower symmetry than the full symmetry of the group G — it is a broken symmetry phase, as it breaks the symmetry of the Hamiltonian [6, 7].

The important concept of symmetry-breaking transitions, as enumerated above, transcends the subject of Magnetism to many other areas of Condensed Matter Physics and even to Quantum Field Theory and Particle Physics [8]. Indeed many of the ideas of symmetry and symmetry-breaking transitions in Magnetism, as encapsulated in the Heisenberg or Heisenberg-like models, can be carried over to different fields. We may recall that the most common form of phase transitions in condensed matter physics is encountered in the case of fluids (gases or liquids). A fluid is the highest symmetry phase of matter which is invariant under the Euclidean group of all translations, rotations and reflections. As the external field such as pressure and temperature are varied one sees a series of phase transitions. The most common low temperature phase is a crystalline solid for which the symmetry is lowered from that of the fluid phase. As it turns out the gas-liquid phase transition can be discussed in complete analogy with the magnetic phase transition. While this will be dealt with in Sec. 2 below we want to mention here that in Quantum Field Theory, the idea of symmetry-breaking in a Heisenberg magnet finds its echo in the Lagrangian of n-coupled scalar fields in what is called a ϕ^4 theory. Although the Lagrangian and hence the equations of motion are invariant under a continuous group of transformations, the ground state, called now the vacuum, is not invariant — the symmetry appears spontaneously broken. This phenomenon is completely akin to a Heisenberg magnet which exhibits spontaneous (i.e. in the absence of an applied magnetic field) magnetization below the Curie temperature. Further, just as in the case of Heisenberg magnets wherein low temperature excitations are described by spin waves (whose quanta are magnons), the consequence of continuous symmetry-breaking in field theory is the appearance of massless excitations called the Goldstone Bosons. Indeed, it is this similarity between Magnetism and Particle Physics which has helped establish the deep relationship between Field Theory and Statistical Mechanics [9-11].

To further underscore this similarity, mentioned in the paragraph above, we may recall the famous Mermin-Wagner-Berezinskii (MWB) theorem [12-14]. It states that a system with a continuous symmetry (such as the Heisenberg model under continuous rotations) cannot have a spontaneously broken symmetry in dimensions less than or equal to two. The theorem is most conveniently proved in a simpler version of the

Heisenberg model called the *XY*-model. In the *XY*-model the longitudinal components (along the z-axis about which the symmetry of the Heisenberg model is expected to be broken) are assumed suppressed. Thus Eq. (1.1) yields

$$\mathcal{H}_{xy} = -J \sum_{<ij>} (S_{ix} S_{jx} + S_{iy} S_{jy}). \tag{1.2}$$

The Hamiltonian in Eq. (2), like the one in Eq. (1.1), is invariant under continuous and arbitrary rotations about the z-axis. In the classical limit Eq. (1.2) may be written as

$$\mathcal{H}_{xy} = -J \sum_{<ij>} \cos(\theta_i - \theta_j). \tag{1.3}$$

Further, in order to obtain the continuous limit of Eq. (1.3) in which the lattice spacing a is arbitrarily small, we can expand the cosine term to yield

$$\mathcal{H} = \frac{J}{4} \sum_{ij} \gamma_{ij} (\theta_i - \theta_j)^2 - \xi JN + \text{higher order terms}. \tag{1.4}$$

In Eq. (1.4), ξ is the number of nearest neighbours (the 'coordination number' of the lattice). The restriction on the summations over *i* and *j* being over nearest neighbours (indicated by angular brackets in Eq. (1.3)) is removed but is reimposed through the introduction of a matrix γ_{ij} which is defined as

$$\begin{aligned} \gamma_{ij} &= 1, \text{ if } i \text{ and } j \text{ are nearest neighbors}, \\ &= O, \text{ otherwise}. \end{aligned} \tag{1.5}$$

Neglecting the constant and the higher order terms in Eq. (1.4) the continuum version is

$$\mathcal{H}_{xy} = \frac{1}{2} \int d^d x p [\nabla \theta(\vec{x})]^2, \tag{1.6}$$

where *d* is the spatial dimensionality and

$$p = \frac{\xi J}{2d} a^{2-d} . \tag{1.7}$$

In the *XY* model the spin vector can point in any direction in the *XY*-plane, but if the symmetry is broken, one direction is preferred. Assuming that direction to be the *X*-axis the order parameter is

$$< \cos\theta >= R\left[\frac{1}{Z}\int D[\theta(\vec{x})]e^{-i\theta(\vec{x})}e^{-\beta\mathcal{H}_{xy}}\right]. \tag{1.8}$$

where Z is the partition function and $\beta = (k_B T)^{-1}$, k_B being the Boltzmann constant and T the temperature. Using the 'Gaussian' property of H_{xy} due to which all cumulants of the fluctuations in $\theta(x)$ beyond the second order vanish, we find

$$< \cos\theta(\vec{x}) > = e^{-\frac{1}{2}<\theta^2(\vec{x})>} . \tag{1.9}$$

Furthermore

$$< \theta^2(\vec{x}) > = -\sum_q \frac{\partial}{\partial\left(\frac{1}{2}\beta\rho q^2\right)} \ln Z_q , \tag{1.10}$$

where $\vec{q}$ is the wave vector that is Fourier-conjugate to $\vec{x}$, and

$$Zq = \left(\frac{2\pi}{\beta\rho q^2}\right)^{\frac{1}{2}} \tag{1.11}$$

Thus

$$< \theta^2(\vec{x}) > = \sum_q \left(\frac{1}{\beta\rho q^2}\right). \tag{1.12}$$

which, in the continuum limit yields

$$< \theta^2(\vec{x}) > = \frac{1}{2\beta\rho} \frac{d^d q}{(2\pi)^d} \frac{1}{q^2} = \frac{1}{4\pi^2 \rho\beta} \frac{\Lambda^{d-2}}{(d-2)} , \tag{1.13}$$

where Λ is the wave number cut off. Equation (1.13) measures the degree to which the order parameter value is diminished from its zero temperature (saturation) value due to classical thermal fluctuations. Evidently as the dimension d approaches the value 2 the fluctuations grow inordinately thereby destroying the order (cf. Eq. (1.9)). This result then proves the celebrated MWB theorem by establishing that fluctuations destroy long range order for a system with continuous symmetry in dimensions less than or equal to two. Physically speaking, the long-wavelength (low q) modes make 'weighty' contributions in low dimensions, thermal excitation of which averages out the orientation of the average spin angular momentum.

The MWB theorem, first derived in the context of magnetism, has been restated by Coleman in Field Theory. As mentioned earlier, spontaneous symmetry-breaking yields a zero mass Goldstone boson. However, in a two-dimensional space-time it is not possible to construct a massless scalar field operator due to severe infrared (or large wavelength) divergences, as indicated above [15].

While the XY-model discussed above is one kind of anisotropy-limit of the Heisenberg model, a different kind of anisotropy ensues when the transverse components of the spin are suppressed and only the longitudinal components are led to interact. This yields the much studied Ising model the Hamiltonian of which can be written as [16, 17]

$$\mathcal{H}_{IS} = -J \sum_{<ij>} S_{iz} S_{jz} \,. \tag{1.14}$$

Unlike the Heisenberg or the XY-model, the Ising model is evidently endowed with discrete symmetry. This symmetry is classified under a group called Z_2 that comprises just two elements: the identity and an element whose square is the identity. This Ising or Z_2 symmetry is broken in those phase transitions which have just two ordered states with order parameters simply differing in sign. Naturally there is no MWB theorem in the Ising case, which does exhibit a phase transition in two dimensions. The discrete symmetry has a further consequence that there is no mass-less Goldstone bosons — the spin wave spectrum (depicting the magnon frequency versus the wave number) has a gap at large wavelengths [18].

The Ising model has a special place in history as it provides a vindication of the subject of statistical mechanics through the path breaking work of Onsager who obtained an exact solution for the partition function of the model in two dimensions. Thus the existence of phase transition, a phenomenon that occupies the centre stage in the subject of thermodynamics, could be demonstrated in terms of a microscopic theory namely that of statistical physics [19].

It is interesting to note that although the Ising model was first introduced as a model of a Heisenberg-like magnet in the limit of extreme anisotropy, such as due to crystal field effects, the majority of its applications is in different fields such as gas-liquid transitions or ordering in alloys. Thus, in the context of gas-liquid transitions, it is a common practice to think of a lattice-gas model wherein a lattice is imagined to consist of cells. Each cell can be occupied by a liquid-like particle, or be empty, to depict a gas-like particle. Hence, the basic statistical variable is a binary one, like in the Ising magnet, but now is a 'pseudo spin' whose upward projection indicates an occupied cell whereas a downward projection implies a vacant cell. If we define the order parameter as the deviation of the density from its average (of the liquid and gas densities of the corresponding coexisting phases) value, the ordered states of liquid and gas are again characterized by equal and opposite (in sign) order parameters, exactly as in the case of the Ising magnet. Indeed this identification of the order parameter allows us to describe the phenomena near the critical point of a gas-liquid phase transition in complete analogy with a paramagnet-to-ferromagnet transition [17]. This is further linked with the concept of 'universality', a subject of Sec. 1.2.

As mentioned above, the discrete binary symmetry of the Ising model finds yet another application to materials science. Consider then a solid alloy of just two elements. Each lattice site is imagined to be occupied by either an A or a B-type of atom. Thus the occupation variable is once again an Ising pseudo-spin, but now one encounters two distinct phenomena depending on whether the exchange parameter J in Eq. (1.14) is positive or negative. If $J > 0$, corresponding to ferromagnetic ordering of the spins in the low-temperature phase, one would see clustering of A-rich (i.e. domains of up spins) and B-rich