Chapter 1
Introduction

Abstract This chapter introduces the concept of atomic magnets and how they combine to form systems which have macroscopic magnetic properties. Since the magnetic moment of a single atom is closely associated with its angular momentum or spin, it is necessary to study spins in order to understand macroscopic magnetism. At the atomic level, the properties of atoms are described in terms of quantum mechanics and hence we need to study quantum spins and their interactions (quantum spin systems). The nature of the exchange interaction is discussed, and we distinguish between ferromagnetic and antiferromagnetic coupling. Finally we summarise the contents of subsequent chapters.

Quantum spin systems are normally first encountered when studying magnetism. A magnet displays its familiar properties, for example attraction of metallic objects, because it is made up of atoms some or all of which are themselves tiny magnets. They produce the observed effects when all or most of these atomic magnets align in the same direction so that the net effect is the sum of all the individual magnets and is thus of macroscopic scale. In order for these atomic magnets to align there must be a force between them. One possibility for this force is the normal magnetic dipole interaction which can produce a tendency for two magnetic dipoles to align either parallel or antiparallel or indeed at an arbitrary angle, dependent upon their relative positions. This is a long range interaction extending over many atomic spacings. However it turns out that the magnetic dipole interaction is too weak to explain the phenomenon of room-temperature magnetism. If this were the only possible interaction, magnetism on a macroscopic scale would only occur at very low temperatures, within a few degrees of absolute zero, where thermal fluctuations are very weak and not strong enough to disrupt the delicate ordering.

In fact all magnetic materials that are of practical consequence have their atomic magnets aligned by means of the exchange interaction. This is a direct consequence of the Pauli exclusion principle and is basically due to the electric forces between electrons in the atoms rather than magnetic forces. Since forces of electrical origin are much stronger than those of magnetic origin at an atomic scale this explains why the exchange interaction is powerful enough to permit macroscopic scale magnetism even at room temperature. The exchange interaction has a much simpler form than the magnetic dipole interaction. In addition it is very short range, being dependent

Parkinson, J.B., Farnell, D.J.J.: *Introduction*. Lect. Notes Phys. **816**, 1–5 (2010)
DOI 10.1007/978-3-642-13290-2_1

on overlap of atomic wave functions. These two facts make it rather easier to handle than a magnetic dipole interaction.

The magnetic moment of an atom is often due, at least partly, to the motion of the electrons around the nucleus. In a classical picture we can imagine the electrons “orbiting” the nucleus rather like a planet or asteroid orbiting the sun. Since the electron has an electric charge this effectively creates a minute current loop around the nucleus and by the well known laws of electromagnetism this current loop has an associated magnetic dipole. All atoms except hydrogen have more than one electron and often the magnetic dipoles of the electrons cancel out so that most atoms do not possess a net magnetic dipole. Again thinking classically, the electron orbiting the nucleus also has an angular momentum, so we expect and find that the magnetic dipole of an atom, where it exists, is associated with the angular momentum of the atom. In fact the study of microscopic behaviour of magnetic materials is often a study of how the angular momenta of the atoms interact rather than the magnetic moments and that will be the case in this book.

Detailed calculation of the exchange interaction is possible in many cases. In practice the form can often be expressed as

$$\mathcal{E} = \alpha \mathbf{S}_1 \,.\, \mathbf{S}_2 + \beta S_1^z S_2^z \tag{1.1}$$

where $\mathcal{E}$ is the energy of interaction between two atoms with angular momentum $\mathbf{S}_1$ and $\mathbf{S}_2$. Here we use the symbol $\mathbf{S}$ for the vector angular momentum for reasons that will become clear shortly.

The special case $\alpha = J$, $\beta = 0$ is called the isotropic Heisenberg interaction. The special case $\alpha = 0$, $\beta = J$ is called the Ising interaction. In either case if J is negative the lowest energy is obtained when the angular momentum vectors are parallel. For the Heisenberg case there is no favoured axis of alignment, but for the Ising case the favoured alignment is along the z-axis. If J is positive then the lowest energy is obtained when the vectors are antiparallel rather than parallel.

Both special cases and the more general case have been extensively studied. Since the Ising interaction is simpler mathematically than the Heisenberg, results in 1D (i.e. one dimension) are usually fairly simple, but in 2D extremely important and non-trivial results have been obtained, in particular the Onsager solution [1]. Because the mathematical formalism used for this is very different to that used in this book it is not given here.

We use the word model to mean a system containing many atoms interacting with each other, usually by means of nearest-neighbour interaction only. Virtually no exact results are known for the 3D Ising model although there are extensive numerical studies. In the Heisenberg case, many important and again non-trivial exact results are known in 1D, whereas in 2D and 3D the results are almost entirely numerical.

When the interaction favours parallel alignment of the magnetic atoms the result is a ferromagnet. Antiparallel alignment gives rise to antiferromagnets, which do not have a net macroscopic magnetic moment. Nevertheless, at the microscopic level these materials are probably more interesting than ferromagnets and their study has contributed greatly to our understanding of magnetism, especially the quantum mechanical properties. Some properties of antiferromagnets do manifest themselves on a macroscopic scale, for example the magnetic contribution to the thermal properties such as the specific heat.

If the interaction is not restricted to nearest-neighbours, or there is more than one type of magnetic atom present in the material, then other types of magnetism can occur. A ferrimagnet is one in which some atoms are aligned in one direction and others in the opposite direction, but there is a mismatch in the total magnetic moment in the two directions so that there is a net macroscopic moment. Spiral ordering can also occur in which the atoms do not align all along one axis, but the direction rotates as one moves through the material. Often, but not always, this results in a non-zero macroscopic magnetic moment. Ferrimagnets and spiral magnets will not be covered in this book.

In this book we shall consider spin systems. These are systems that consist of two or more particles each of which has an angular momentum and associated magnetic moment. As a result, study of these systems is effectively a study of certain types of magnetic materials. Usually the magnetic particles are atoms or ions of transition metals such as Mn, Ni or Fe or rare-earths such as Ce or Nd. The book by Mattis [2] has an excellent account of the history of magnetism.

Because this is such a vast topic we immediately restrict our attention to insulating materials, i.e. we shall not consider metallic magnets. We take the particles to be interacting by Heisenberg exchange which is electrical in origin and is normally much stronger than a magnetic interaction. The exchange interaction is in fact between the angular momenta of the particles but since their magnetic moment is proportional to the angular momentum it superficially appears as an interaction between the magnetic moments, albeit of a much simpler form than the magnetic dipole interaction.

We shall mainly consider the quantum case although there are many interesting classical results which we shall include in some places.

Heisenberg in 1925 [3] and Schrödinger in 1926 [4–6] established the basis of modern quantum mechanics. Their formalisms are somewhat different although equivalent. The Schrödinger formalism emphasises the explicit form of the wave function as obtained from the Schrödinger equation whereas the Heisenberg formalism expresses the wave function as a vector which represents a linear combination of basis states. The former is very successful in particular in atomic physics and in problems in which particles move in a potential well with or without the presence of electric and magnetic fields.

One area in which the Heisenberg formalism is especially useful is in the description of angular momentum. For the orbital angular momentum of single particles this can be done in the Schrödinger formalism, but for interacting particles, especially many-body systems, it is much more convenient to use the Heisenberg formalism. Indeed, for the intrinsic angular momentum of elementary particles, the spin, it is not possible to obtain a specific wave function. For baryons such as the neutron and proton this is because the internal structure in terms of quarks is rather complicated and in any case the quarks themselves have a spin, while the leptons such as the electron are believed to be point particles with no internal structure.

Most of the magnetism observed in practice is due to electrons. It may be associated with either the orbital angular momentum or the spin. For simplicity we shall refer to the angular momenta in all cases as spin even when it is wholly or partly due to orbital motion. The constant of proportionality between the magnetic moment and the angular momentum is different in the two cases and we write

$$\boldsymbol{\mu} = g\beta\mathbf{S}$$

where $\boldsymbol{\mu}$ is the magnetic moment, $\mathbf{S}$ is the spin measured in units of $\hbar$, $\beta = \dfrac{e\hbar}{2m}$ is the elementary unit of magnetic moment associated with unit spin, the Bohr magneton, and g is the gyromagnetic ratio which is 1 for orbital angular momentum, 2 for intrinsic spin and has an effective intermediate value when both are present.

We shall deal mainly with the ground state of the system and the elementary excitations from this. This implies $T = 0$ or $T \to 0$ and does not allow non-zero T for which much more detailed knowledge of the full eigenstates is needed. The exception to this is the 1D chain with $S = \frac{1}{2}$ where the extra information needed is available through the Bethe ansatz.

We shall consider all dimensionalities: 0D, 1D, 2D and 3D. 0D refers to finite-sized clusters or chains for which exact results can often be obtained. These are becoming of more interest in their own right but they can also shed light on the behaviour in higher dimensionalities. 1D (i.e. infinite chains) is the dimension in which dramatic exact quantum results for $S = \frac{1}{2}$ have been obtained.

Numerical results include the Density Matrix Renormalisation Group (DMRG) [7], which has been superbly successful in 1D where exact results are not available, e.g. for $S > \frac{1}{2}$. Many other numerical techniques exist, which are particularly important for 2D and 3D where it has proved difficult to use the DMRG. We shall describe one of these, the coupled cluster method, in detail in Chap. 10.

We shall mainly consider antiferromagnetic coupling with exchange interaction $J > 0$. For ferromagnetic coupling with negative J it is usually straightforward to write down the ground state in both quantum and classical cases. The elementary excitations are also usually simple to obtain, often in the form of spin waves or bound pairs of spin waves. The antiferromagnetic problem is much more difficult and also more interesting and shows much greater differences between the classical and quantum systems as is known from the analysis of the $S = \frac{1}{2}$ chain. We shall restrict our discussion mainly to systems with only nearest-neighbour exchange, although next-nearest-neighbour exchange is considered briefly in the final chapter. However, we shall allow the exchange to be anisotropic, and we shall also consider the effect of an applied magnetic field in some places.

Another interesting feature of antiferromagnetic systems is the possibility of frustration. This occurs when the system contains nearest-neighbour paths with odd numbers of atoms. The simplest example is a cluster of three atoms, each of which is nearest neighbour to both of the others. Since the antiferromagnetic exchange favours antiparallel alignment of nearest neighbours and this is not possible for all neighbours we use the term frustration. This can also happen in larger finite-sized clusters such as a five atom ring, a tetrahedron or an octahedron. It does not happen in 1D for nearest-neighbour-only exchange but it occurs in 2D, for example in triangular and Kagome lattices and in 3D, for example in the HCP lattice.

Again we emphasise that this is not intended to be a comprehensive account of spin systems which would be a formidable undertaking. Rather it is intended to fulfil two roles. Firstly we present an introduction to spin systems which should be of use to newcomers to the area, particularly graduate students. We then give a fairly detailed description of the $S = \frac{1}{2}$ chain which, because it has yielded so many exact results of a highly non-trivial and counter-intuitive nature, can reasonably be described as one of the crowning glories of many-body physics. Secondly we consider some of the most important approximate methods including an important modern technique, the coupled cluster method, and finally look at other work on these systems.

Lastly, we mention that there are, of course, numerous other books on magnetism and spin systems [2, 8–14]. As well as the the very comprehensive account given in Mattis [2], an excellent introductory text is the book by Caspers [8]. The present book differs from Caspers, partly in the choice of topics but also in the attempt to give complete details of the mathematics of some of the important results.

References

1. Onsager, L.: Phys. Rev. **65**(2), 117–149 (1944) 2, 7
2. Mattis, D.C.: The Theory of Magnetism I, Springer, Berlin (1981, 1988) 3, 5
3. Heisenberg, W.Z.: Physik **33**, 879 (1925) 3
4. Schrödinger, E.: Ann. Phys. **79**, 361, 489, 784 (1926) 3
5. Schrödinger, E.: Ann. Phys. **80**, 437 (1926) 3
6. Schrödinger, E.: Ann. Phys. **81**, 109 (1926) 3
7. White, S.R.: Phys. Rev. Lett. **69**, 2863 (1992) 4
8. Caspers, W.J.: Spin Systems. World Scientific, Singapore (1989) 5
9. Schollwöck, U., Richter, J., Farnell, D.J.J., Bishop, R.F. (eds.): Quantum Magnetism. Lecture Notes in Physics, vol. 645. Springer, Berlin (2004) 5
10. Diep, T.H.: Frustrated Spin Systems. World Scientific, Singapore (2004) 5
11. Auerbach A.: Interacting Electrons and Quantum Magnetism. Springer, New York, NY (1994) 5
12. Majlis, N.: The Quantum Theory of Magnetism. World Scientific, Singapore (2007) 5
13. Läuchli, A.M.: Quantum Magnetism and Strongly Correlated Electrons in Low Dimensions. Swiss Federal Institute of Technology, Zurich (2002) 5
14. White, R.M.: Quantum Theory of Magnetism. Springer, Berlin (1983) 5