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Introduction

1.1 Lattice models in theoretical physics

A major part of theoretical physics involves the construction and systematic analysis of mathematical models as a description of the physical world. For microscopic phenomena, in particular, the reference to models becomes quite explicit. The phenomena are often complex, and any theory that attempts to include every detail soon becomes intractable. It is more fruitful to develop models which ignore irrelevant details but, hopefully, capture the essential physics of the phenomena of interest. Thus we have the Heisenberg model of magnetic order, the Bardeen–Cooper– Schrieffer (BCS) model of superconductivity, and so on. It is important to note, at the outset, that the models we shall be discussing describe strongly interacting, and therefore highly correlated, systems of particles. These are difficult and interesting problems. Where interactions are absent, or weak, elementary treatments are possible and the resulting phenomena are generally unspectacular.

Why lattice models? In solid-state phenomena there is usually an underlying lattice structure, and the symmetry properties of this lattice play an important role in the analysis. Even the process of electrical conduction in metals or semiconductors can be equally well described in terms of localized quantum states or in terms of the more usual continuum picture. In quantum field theory, which is formulated in a space–time continuum, a lattice is often introduced for computational purposes. One can think of this in two ways: as an approximation to the continuum, which is then recovered as a limit at the end of the calculations, or as a necessary means of regulating the theory (i.e. controlling divergences) in calculating the Feynman path integral.

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To provide the reader with an overview of the subsequent material, which is often rather technical, we will introduce some of the models in a qualitative way,

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explain why they are interesting, and outline some of the important questions to be addressed.

1.2.1 The Ising model

As is well known, this model was proposed by Lenz to his student Ising in 1925 or so, as a simple model for ferromagnetism. It is defined in terms of a set of two-valued classical variables (usually termed 'spins') $\sigma_i = \pm 1$, at the N sites of a lattice, with an interaction energy

$$E(\{\sigma\}) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$
(1.1)

Here J (> 0) is an interaction constant, the sum is over nearest-neighbour pairs of sites $\langle ij \rangle$ on the lattice, and h is an external magnetic field. The interaction favours neighbouring spins being in the same state (either ++ or --) rather than in different states (+- or -+) because this minimizes the energy.

It is clear then that the most probable state(s), or the macroscopic thermodynamic state, will change with temperature. At high temperatures, provided that h is zero or small, the spins will be more-or-less randomly arranged due to thermal fluctuations, while at low temperatures they will tend to be aligned. Thus it is at least plausible that this simple model might reasonably describe the onset of magnetic order below the Curie temperature of a ferromagnet.

As is also well known, Ising solved the model exactly for a one-dimensional lattice and found no spontaneous magnetization and no phase transition. Thermal fluctuations in one dimension destroy the possibility of a non-zero magnetic moment at any non-zero temperature. In the two-dimensional case, however, Onsager's exact solution of the Ising model in zero field, which is regarded as one of the most important developments in the whole field, demonstrated the existence of a critical point with a divergent specific heat, and a spontaneous magnetization below the critical temperature. This showed, for the first time, that a careful statistical mechanical calculation could yield the kind of spectacular non-analytic behaviour characteristic of phase transitions in general.

Much of our current understanding of the physics of second-order phase transitions/critical points was first obtained from studies of the Ising model: the existence of critical exponents and of universality, the concept of a divergent correlation length at criticality, and the importance of thermal fluctuations at all length scales, leading to the ideas of renormalization (see e.g. Yeomans, 1992) Figure 1.1 shows typical configurations of Ising spins on a 64×64 square lattice at temperatures $T/T_c = 1.25$, 1.0, obtained from a Monte Carlo simulation. The existence of clusters of all sizes at the critical point is evident.

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Fig. 1.1. A typical configuration of Ising spins on a 64×64 square lattice at temperatures $T/T_c = 1.25$ (a) and $T/T_c = 1$ (b), obtained from a Monte Carlo simulation.



Fig. 1.2. (a) The temperature dependence of the specific heat of the Ising model in one (1D), two (SQ) and three-dimensions (SC). (b) The measured magnetization versus temperature of $DyPO_4$, compared with low-temperature series for the Ising model. From Rado (1970).

Although exact solutions exist for Ising models in two dimensions, there are no exact results for any three-dimensional lattice. Very precise and reliable results have been obtained, however, from two numerical methods: series expansions, the subject of this book, and Monte Carlo simulations. Figure 1.2(a) shows the temperature dependence of the specific heat of the Ising model in one, two and three dimensions. The one- and two-dimensional results are exact, while the threedimensional result is from series expansions (simple cubic lattice). Figure 1.2(b)

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shows the measured magnetization versus temperature of DyPO₄, compared with low-temperature series for the Ising model. The agreement is impressive.

As well as being a model for (uniaxial) magnets, the Ising model can be used to model many other kinds of system: binary alloys, lattice fluids and systems outside physics. We will describe the series expansion approach to the Ising model in Chapter 2.

1.2.2 The Ising model in a transverse field

In this model the Ising spins σ_i are replaced by Pauli operators σ_i^z , and an external field couples to the *x*-component, σ_i^x . The resulting Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$
(1.2)

This is now a fully quantum mechanical model, as the terms in H do not commute. We remind the reader of the usual matrix representation

$$\sigma^{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(1.3)

and the commutation rule

$$[\sigma_j^{\alpha}, \sigma_k^{\beta}] = 2i\delta_{jk}\epsilon_{\alpha\beta\gamma}\sigma_j^{\gamma} \tag{1.4}$$

where $\epsilon_{\alpha\beta\gamma}$ is the usual Levi–Civita symbol. We also note that many authors use the spin- $\frac{1}{2}$ operators $S_i^{\alpha} = \frac{1}{2}\hbar\sigma_i^{\alpha}$.

Historically this model appears to have been first used by de Gennes, to model the order–disorder transition in hydrogen bonded ferroelectrics, such as KH₂PO₄. Each H atom sits in a double-well potential and the two states can be regarded as the eigenstates of a 'pseudospin' operator σ^z . The transverse field term then describes tunnelling between the two states, and the parameter Γ is related to the tunnelling frequency. This is illustrated in Figure 1.3. The model has subsequently been used to describe a large variety of systems (see e.g. Chakrabarti *et al.*, 1996).

Apart from its role in describing real physical systems, this model is of interest for a number of fundamental theoretical reasons.

Unlike the classical Ising model discussed in the previous section, which has no intrinsic dynamics, the Ising model in a transverse field (for brevity the 'transverse field Ising model') is described by a proper Hamiltonian and does have intrinsic collective excitation modes ('spin waves') with an energy-momentum relation $\omega = \omega(\mathbf{k})$.

The transverse field Ising model can be solved exactly in one dimension at zero temperature (Pfeuty, 1970), and has a quantum phase transition at $\Gamma/J = 1$.



Fig. 1.3. (a) Structure of the ferroelectric material KH_2PO_4 (schematic). The tilted squares represent PO₄ tetrahedra, connected via hydrogen bonds (dashed lines). Each bond has a H atom in one of two equilibrium positions (filled and empty circles); (b) Double-well potential for a H atom. The lowest two eigenstates are shown as dashed lines, with tunnelling frequency $\Omega = 2\Gamma/\hbar$.

It is the simplest model to show such a transition, which results from strong quantum fluctuations rather than thermal fluctuations. The subject of quantum phase transitions is a very active one at present (Sachdev, 1999), and we shall investigate a number of quantum phase transitions in succeeding chapters. Here the transition is in fact a quantum critical point, with associated critical exponents which are found to be the same as the thermal critical exponents of the classical Ising model in two dimensions. This is an example of a rather general correspondence between ground state properties of a quantum model in d dimensions and thermodynamic properties of a corresponding classical model in (d + 1) dimensions (Appendix 8).

The transverse field Ising model cannot be solved exactly in dimensions d > 1. However series expansions can be used to locate the quantum critical point to high precision, and to study other properties. We will describe this approach in Chapter 4.

1.2.3 The Heisenberg model

Very soon after the development of quantum mechanics, Heisenberg and Dirac independently proposed that the phenomenon of magnetic order in solids might be understood on the basis of a model of exchange coupled quantum angular momenta ('spins'), with a Hamiltonian of the form

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1.5}$$

where the S_i are spin-S operators, the sum is over nearest-neighbour pairs, and the dot product is the usual

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$
(1.6)

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Fig. 1.4. (a) Structure of CuO_2 planes in cuprate high-T_c superconductors, and the antiferromagnetic state. The solid and empty circles represent Cu⁺⁺ and O⁻⁻ ions, respectively; (b) Measured spin-wave dispersion curve for a cubic manganite compound, compared with a model calculation. From Aeppli *et al.* (1997).

The model describes a ferromagnet (antiferromagnet) for J > 0 (< 0) respectively. Note that the Hamiltonian (1.5) is fully symmetric under rotations in spin space, with symmetry group O(3). This model has been intensively studied as the generic prototype for magnetic materials. The first systematic use of the model to describe real magnetic materials appears to be due to Van Vleck (1965). Figure 1.4 shows examples of two magnetic systems of current interest that are well described by the Heisenberg model.

The Heisenberg model (1.5) can be generalized to

$$H = -\sum_{\langle ij\rangle} \left[J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z \right]$$
(1.7)

when it is known as the XYZ model (or the XXZ model when $J_x = J_y \neq J_z$). The special case $J_z = 0$, $J_x = J_y$ is known as the XY model, and has been used as a lattice model of superfluid helium (for $S = \frac{1}{2}$). Obviously, with the freedom to vary the spin value, the degree of exchange anisotropy, the sign of the exchange constant, and the inclusion of further neighbour interactions we have a multi-dimensional space of possible Hamiltonians, with a resulting variety of properties and applications.

The isotropic Hamiltonian (1.5) has no long range order at finite temperatures in less than three dimensions. In three dimensions there is a critical point for both ferromagnetic (Curie point) and antiferromagnetic (Néel point) interactions. Unlike the case of the classical Ising model, the Curie and Néel temperatures differ slightly. The ground state of the ferromagnet is simple, with all spins aligned in an arbitrary direction, but for the anti-ferromagnet the situation is considerably more complex. In one dimension the famous solution of Bethe gives the wavefunction, and leads

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to an exact result for the ground state energy (see e.g. Takahashi, 1999). Very limited results are known, however, for general correlations or for thermodynamic properties. In two dimensions there are rigorous results for the existence of long-range order in the ground state for $S \ge 1$, and strong numerical evidence that this also the case for $S = \frac{1}{2}$.

The Heisenberg model also has interesting dynamical properties, including collective spin-wave excitations, which determine the low-temperature thermodynamics, higher energy bound states and time-dependent correlations which can be compared with neutron scattering studies of real materials.

Interesting recent developments, which have kept the Heisenberg model at the forefront of research, include the following.

- The discovery that, for the $S = \frac{1}{2}$ antiferromagnetic chain, the true elementary excitations are $S = \frac{1}{2}$ objects, termed 'spinons', rather than S = 1 magnons as previously supposed.
- The discovery that integer-spin antiferromagnetic chains differ in an essential way from half-integer spin chains, the former having an energy gap between the ground state and the lowest excitations ('Haldane gap') while the latter are gapless. This leads, *inter alia*, to fundamentally different low-temperature thermodynamics for the two cases, which is confirmed experimentally.
- The discovery of various compounds, usually low-dimensional, which have energy gaps, and attempts to understand these through Heisenberg models with competing interactions.

Series expansion methods have played an important role in understanding the Heisenberg model. This work will be described in Chapters 5, 6.

1.2.4 The Hubbard model

While models with localized spins do successfully describe an important class of real magnetic materials, it is nevertheless a restricted class since there are no charge degrees of freedom, i.e. no conduction electrons. A number of relatively recent discoveries, such as 'heavy fermion' behaviour in actinides, quantized Hall effects in high-mobility two-dimensional electronic systems, and the high-temperature cuprate superconductors, have pointed to the need for a better understanding of strongly correlated electron systems.

Perhaps the simplest generic model for strongly correlated electron systems is the Hubbard model, which arose from work of Hubbard and others in the 1960s on narrow-band metals. For a single band, the Hamiltonian is

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$
(1.8)

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Fig. 1.5. (a) The Hubbard model. The large circles represent orbitals at atomic sites, which may hold up to two electrons of opposite spin. Process A, in which a spin down electron hops from a doubly occupied site to an empty site decreases the energy by U; process B results in no energy change. (b) Electron density of states (schematic) showing the evolution of a 'Mott–Hubbard' gap for large U, and the origin of a metal-insulator transition.

where $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$ are creation and destruction operators, respectively, for electrons of spin σ on site *i*, and $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is the number of electrons of spin σ on site *i*. The first term represents non-interacting electrons of spin σ (\uparrow , \downarrow) 'hopping' between localized Wannier orbitals on nearest-neighbour sites of a lattice, the parameter *t* being determined by an overlap integral. This is just a one-electron theory, giving rise to a band of width $W \propto t$. The second term mimics the most important part of the Coulomb repulsion between electrons, giving a positive energy *U* for two electrons of opposite spin on the same site. Figure 1.5 shows the model pictorially and the development of a gap in the density of states arising from the Coulomb repulsion term. Many generalizations of this model have been proposed including multi-band models, the case of negative *U*, and the so-called 'extended Hubbard model', which includes a nearest-neighbour Coulomb repulsion. We shall not consider such cases here.

There is another important parameter in the model, the total electron density n = number of electrons per site. When n = 1, an average of one electron per site, the band is half-filled. For large U at half-filling the motion of the electrons is strongly suppressed and it can be shown that the lowest energy state has electrons of opposite spin at alternating sites, effectively a Heisenberg antiferromagnet, with exchange constant $J = 4t^2/U$. The removal of a fraction of the electrons from half-filling (generally referred to as 'doping' since this is precisely what happens in many real materials) allows the charge degrees of freedom to become active and leads to major changes in the physics of the model.

It is the presence of the U-term which introduces strong electron correlations, and makes the model much more difficult to analyse. Apart from some exact solutions

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in one dimension we have no really comprehensive knowledge of the physics of the model in the space of U/t, electron density n and temperature T. Much work has been done, using a variety of techniques including series expansions. Each method has its own strengths and weaknesses, and it is important to compare results from different approaches. We will describe the series approach to the Hubbard model and other models of strongly correlated electrons in Chapter 8.

1.2.5 Lattice gauge models

The lattice approach to gauge field theories was pioneered by Wilson (1974) as a non-perturbative approach to Quantum Chromodynamics (QCD), the standard theory of the strong interactions in particle physics. Subsequently, Monte Carlo simulations of lattice gauge models have become the preferred method for *a priori* calculations of the properties of QCD at low energies or large distances. Spin versions of these lattice gauge models were discussed even earlier, by Wegner (1971).

A lattice gauge model is primarily defined in terms of *link* variables or 'parallel transporters' U_{ij} , defined on the links between neighbouring sites *i* and *j* of the lattice. One may also introduce site variables or 'matter fields' ϕ_i residing on sites of the lattice. The link variables are taken to be elements of some gauge group *G*, and under gauge transformations the variables transform as

$$U_{ij} \to U'_{ij} = V_i U_{ij} V_i^{\dagger} \tag{1.9a}$$

$$\phi_i \to \phi_i' = V_i \phi_i \tag{1.9b}$$

where $U_{ji} = U_{ij}^{\dagger}$, and V_i is a unitary transformation belonging to the group *G*, which may vary according to the site *i*. This is an example of a 'local' or gauge transformation which may vary from one site to another, as opposed to a 'global' transformation which is the same at all sites.

We are interested in models where the terms in the lattice Hamiltonian (or action) are *invariant* under gauge transformations. Terms involving only link variables ('pure gauge' terms) will be invariant if they consist of ordered strings of link variables around a closed path on the lattice. The simplest example is a 'plaquette' interaction

$$P = \operatorname{Tr}\{U_{ij}U_{jk}U_{kl}U_{li}\}$$
(1.10)

where *i*, *j*, *k*, *l* form the corners of an elementary square of the lattice [Figure 1.6(a)]. The trace is taken because for a general group the U_{ij} will be matrix variables. It is easy to check that a term such as (1.10) is invariant under the transformation (1.9a). Invariant interactions can also be constructed from open strings of link variables

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Fig. 1.6. (a), (b): Interaction terms corresponding to different paths on the lattice. Link variables are denoted by directed arrows, and site variables by filled points. (c) The static quark potential for SU(3) Yang–Mills theory. From Stack (1984).

terminated by a matter field at each end, such as the nearest-neighbour interaction [Figure 1.6(b)]

$$\phi_i^{\dagger} U_{ij} \phi_j \tag{1.11}$$

The invariance of this term may also be verified by inspection.

The simplest example of a lattice gauge model is the Ising or Z_2 gauge model introduced by Wegner (1971)

$$H = \beta \sum_{\text{plaquettes}} \sigma_{ij} \sigma_{jk} \sigma_{kl} \sigma_{li}$$
(1.12)

where σ_{ij} is an Ising spin variable taking values ± 1 on each link (ij). This Hamiltonian is invariant under the Z_2 gauge group, where the transformation V_i either reverses the spin or leaves it unchanged on every link connected to site *i*.

A primary object of lattice gauge theory is to explain phenomena such as *con-finement* of quark and gluons in QCD. Figure 1.6(c) shows a Monte Carlo calculation of the potential between static quarks by Stack (1984). The linear rise of the potential at large radii provides convincing evidence that the quarks cannot escape from one another. We shall postpone further discussion of the physics of lattice gauge models, and their correspondence with continuum gauge field theories, until Chapter 9.

1.3 The important questions

In the previous section we introduced a number of generic models which will be the subjects of study in later chapters. In this section we will briefly discuss some of the