Theoretical Tools for Spin Models in Magnetic Systems

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To Rosangela, Henrique and Guilherme

Contents

Preface

Magnetism is an exciting area of research in condensed matter presenting a variety of exotic phases and critical phenomena and several technological applications. We can study simple models, which are theoretically tractable and yet display quantitative correspondence with real systems.

This book is addressed to people with an interest in magnetism, mainly spin systems. There are excellent advanced textbooks and review papers on the subject. Still, it was my experience that a book was needed, dedicated to the basic concepts with a more elementary treatment for researchers starting in the area. Very little in the text is my original contribution. Most of the material was collected from the literature. However, it would take a long time for the interested student to gather all the topics in the literature. I have tried to make the material mostly self-contained, and references to more advanced treatment are indicated. It is supposed that the reader has some familiarity with the subject at a level as the one presented in the book by Blundel [1]. To keep the text short, I have left out some themes such as one-dimensional models, path-integral formalism and the treatment of continuous systems, and in this context, the nonlinear sigma model.

In chapter 1, I introduce the Heisenberg model and discuss the ground state of the ferromagnet and the antiferromagnet. A short introduction to the Hubbard model is given. In chapter 2, the spin-wave formalism is presented for the ferromagnet and the antiferromagnet. The XY model is studied using a self-consistent harmonic approximation. I finish the chapter with a brief introduction to the Jordan–Wigner transformation and Majorana fermions. In chapter 3, I look at the antiferromagnetic triangular lattice and the antiferromagnetic square lattice in the presence of an external magnetic field. I introduce the Dzyaloshinskii–Moriya interaction, treat the nonlinear spin-wave theory in a mean-field approach, and finally present a modified spin-wave method.

In chapter 4, I describe lattices with three different sites: the honeycomb, the checkerboard, and the Union Jack lattices. To treat the antiferromagnetic lattices, I introduce a generalized Bogoliubov transformation. Chapter 5 is dedicated to the study of formalisms that are more general than the spin-wave theory and can be used to study magnetically disordered phases. I develop the Schwinger boson technique and use it to study valence bond solids and frustrated systems. The use of fermion operators is also mentioned. In chapter 6, I present bond operators adequate to treat dimerized phases and the Schwinger SU(3) bosons. I survey quantum phase transitions, nematic phases, and the Heisenberg model with biquadratic interaction. Chapter 7 is dedicated to the study of dynamics. I introduce the linear response theory, correlation functions, spin transport, the Kubo formulas, the Green function technique, and the memory function formalism. In chapter 8, I develop perturbation theory to calculate the retarded Green function, also called the Feynman propagator, for a many-body system. There are excellent books leading with the subject and discussing in full detail Green functions in the context of perturbation theory. In this chapter, I go straight to the point to teach the reader how to calculate

Feynman diagrams. Magnon topological insulators have been the cause of substantial interest in recent years, and in chapter 9 I explore briefly topological effects in ferromagnets and antiferromagnets. In chapter 10 I present a brief introduction to topological spin liquids. This chapter complements chapter 5, but it is more specific and can be skipped if the reader is not interested in the subject. An overview of numerical methods used in spin models is presented in chapter 11. In appendix A, a short account of group theory is presented to introduce some concepts used in the book. Finally, in appendix B, I finish with a Green function theory specific to spin Hamiltonians. The exercises vary in difficulty and complement the text with specific examples. References are given for the most difficult exercises.

The book by Eriksson *et al* [2] covers some material lacking in the present book, and in that sense both books complement each other.

References

[1] Blundell S 2003 *Magnetism in Condensed Matter* (Oxford: Oxford University Press)

[2] Eriksson O, Bergman A, Bergqvist L and Hellsvik J 2016 *Atomistic Spin Dynamics: Foundations and Applications* (Oxford: Oxford University Press)

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Chapter 1

The Heisenberg model

We start with a lattice, in one, two, or three dimensions. There are several kinds of lattices, and sometimes we even consider a continuum model. Now, in each lattice site i, we put a spin $\vec{S}_i$, with $\vec{S}_i^{\,2} = S(S+1)$ where S is an integer or a half odd integer. In most cases, one is interested in $S = ½$ and sometimes in $S = 1$. The classical limit where $S \to \infty$ is also of interest. The most straightforward interaction between two spins is given by $\vec{S}_i \cdot \vec{S}_j$. Using quantum mechanics, we can arrive at this term (see, for instance, Auerbach [1] and Maplis [2]). Still, I am not going to do that here and assume that the reader is familiar with the procedure. The basic Hamiltonian in magnetism is the so-called Heisenberg model. This model describes the interaction between spins in a lattice with N sites where generally, $N \to \infty$. This is a many-body problem that usually cannot be exactly solved, and many numerical techniques solve the equations for a finite number of sites. When we do analytical calculations, most of the time, we treat free particles (called quasiparticles) described by a quadratic Hamiltonian. The interaction between particles is then handled via perturbation theory or using a mean-field approach where a quadratic Hamiltonian replaces the true Hamiltonian of the system with renormalized temperature-dependent parameters. Let us start our journey.

The following Hamiltonian represents the Heisenberg model

$$H = \frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i \cdot \vec{S}_j, \tag{1.1}$$

wherein the sum i and j run over all sites on a lattice, $J_{ij} = J_{ji}$ is symmetric, and the factor ½ corrects the double-counting of the bonds. Spin components on the same site obey the commutation relations

$$\left[S_j^{\alpha},\, S_j^{\beta}\right] = i\sum_{\gamma}\varepsilon_{\alpha\beta\gamma}S_j^{\gamma} \qquad (\alpha, \beta, \gamma = x, y, z). \tag{1.2}$$

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Spins on different sites commute with each other. The coefficients J_{ij} are called exchange constants, and for most of the text, we assume $J_{ij} = J$, and nearest-neighbor interactions. If $J < 0$, the energy is minimized when the spins are parallel to each other, and we have a ferromagnetic model. For $J > 0$, antiparallel orientation is instead favored, and we have an antiferromagnet. Defining

$$S_j^+ = S_j^x + iS_j^y, \quad S_j^- = S_j^x - iS_j^y, \tag{1.3}$$

we can write (1.1) as

$$H = \frac{1}{2}\sum_{ij} J_{ij}\left(\frac{S_i^+ S_j^- + S_i^- S_j^+}{2} + S_i^z S_j^z\right). \tag{1.4}$$

At high temperatures, the spins are disordered due to the strong thermal fluctuations, and the expectation value of each spin vanishes: $\langle \vec{S}_i \rangle = 0$. For an operator A, we define

$$\langle A \rangle = tr(\rho A), \tag{1.5}$$

where ρ is the density matrix. For mixed states ρ is given by

$$\rho = \sum_n p_n |n\rangle\langle n|, \tag{1.6}$$

where p_n is the probability of occupation of the eigenstate $|n\rangle$. For a pure state $|\psi\rangle$, the density matrix is given by $\rho = |\psi\rangle\langle\psi|$. In the canonical ensemble, as will be the case treated here, we have

$$\langle A \rangle = \frac{1}{Z}\sum_n e^{-\beta E_n} \langle n|A|n\rangle, \tag{1.7}$$

where $Z = tr(e^{-\beta H})$. It may happen that below some critical temperature, T_c, the spins order magnetically, and on average, they point along some definite direction: $\langle \vec{S}_i \rangle \neq 0$. The existence of T_c depends on the dimensionality, the type of lattice, and the range of the interactions. I will discuss the details later. If there is a T_c below this temperature $\langle \vec{S}_i \rangle$ will increase when we decrease T and will reach a maximum value at zero temperature. The critical temperature is called the Curie temperature in ferromagnets and the Néel temperature T_N in antiferromagnets.

1.1 Ground state for the ferromagnet

For a spin S we have the basis $|S, m\rangle$ with

$$\vec{S}^2|S, m\rangle = S(S+1)|S, m\rangle, \quad S^z|S, m\rangle = m|S, m\rangle. \tag{1.8}$$

Since we are considering lattices where all spins have the same eigenvalue S we write $|m\rangle$. For a lattice, the basis is spanned by the product states $|m_1\rangle, |m_2\rangle, \ldots, |m_N\rangle$.

On this basis, the last term in (1.4) is diagonal, but the other two terms are not. Defining the total spin $\vec{S} \equiv \sum_i \vec{S}_i$ it is easy to show that

$$[S^x, H] = [S^y, H] = [S^z, H] = 0. \tag{1.9}$$

Then we can find simultaneous eigenstates of H, $\vec{S}^2$ and S^z. We will start with states where m_i has the maximum value S. This means that all spins are aligned in the z-direction. We write

$$|\psi\rangle = |S\rangle_1 |S\rangle_2 \ldots |S\rangle_N, \tag{1.10}$$

where $|S\rangle_i$ means $|m = S\rangle$ for the spin at the site i. Here we take $J_{ij} > 0$, and for the ferromagnet, we write equation (1.4) with a minus sign. Acting with H on (1.10) we get

$$H|\psi\rangle = -\frac{1}{2}\sum_{ij} J_{ij}\left(\frac{1}{2}S_i^+ S_j^-|\psi\rangle + \frac{1}{2}S_i^- S_j^+|\psi\rangle + S_i^z S_j^z|\psi\rangle\right), \tag{1.11}$$

but $S_i^+ S_j^-|\psi\rangle = S_i^- S_j^+|\psi\rangle = 0$, and so we can write

$$H|\psi\rangle = -\frac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z|\psi\rangle = -\frac{S^2}{2}\sum_{ij} J_{ij}|\psi\rangle. \tag{1.12}$$

Thus $|\psi\rangle$ is an eigenstate of H. There are $2S_{tot} + 1$ of such states since H is invariant under rotations in the spin space. However, a state $|\phi\rangle = |m_1\rangle\ |m_2\rangle\ \ldots\ |m_N\rangle$ is generally not an eigenstate of H. We have

$$\begin{aligned}\langle\phi|H|\phi\rangle &= -\frac{1}{2}\sum_{ij}\left(\frac{1}{2}\langle\phi|S_i^+ S_j^-|\phi\rangle + \frac{1}{2}\langle\phi|S_i^- S_j^+|\phi\rangle + \langle\phi|S_i^z S_j^z|\phi\rangle\right)\\ &= -\frac{1}{2}\sum_{i,j} J_{ij} m_i m_j.\end{aligned} \tag{1.13}$$

If $J_{ij} \geqslant 0$ for all i and j, then $J_{ij} m_i m_j \leqslant J_{ij} S^2$ and we conclude

$$\langle\phi|\ H\ |\phi\rangle \geqslant -\frac{S^2}{2}\sum_{ij} J_{ij}. \tag{1.14}$$

Therefore, all eigenenergies, in particular the ground state energy, are larger than or equal to $-(S^2/N)\sum_{ij} J_{ij}$. However, $|\psi\rangle$ is an eigenstate to this energy and therefore it must be a ground state if $J_{ij} \geqslant 0$ for all i, j. We have found then that the fully polarized state is the ground state.

1.2 Spontaneous broken symmetries

Spontaneous symmetry breaking happens when the Hamiltonian has a symmetry and hence a conserved quantity, but the ground state of the system does not have that symmetry. The Hamiltonian of the Heisenberg model given by equation (1.1) is rotationally symmetric. If we rotate all spins by the same angle, the Hamiltonian does not change. The total spin of the system, as we have seen, commutes with the Hamiltonian and hence is conserved. However, the symmetry is broken spontaneously

in the ferromagnet's ground state where a single unique direction has been chosen along which all the spins have lined up, and the ground state is not invariant under rotation. When the symmetry that is broken spontaneously is continuous, such as the rotation of spins discussed above, there are infinitely many ground states. (Note that there are a finite number of ground states when the broken symmetry is discrete, such as a spin inversion in the Ising model, to be discussed later.) In the case of spontaneously broken continuous symmetry, the low-lying excitation with energy $E(\vec{k})$ does not have a gap. That is, $E(\vec{k}) \to 0$ as $\vec{k} \to 0$. This result is known as the Goldstone theorem. More details of the theorem can be found in Auerbach [1].

1.3 Ground state for the antiferromagnet

In most cases, the antiferromagnetic ground state is more complicated than the ferromagnetic ground state, and few rigorous results are known about the ground state of the general Heisenberg model. One case where a rigorous result exists is where one has an antiferromagnet on a bipartite lattice. In such a lattice, all sites are divided into two disjoint subsystems A and B so that $J_{ij} = 0$ if $i,j \in A$ or if $i,j \in B$. Hence, one has interactions only between sites from different lattices. As an example, we have the square lattice shown in figure 1.1.

For a bipartite lattice with $J_{ij} \geqslant 0$ in Hamiltonian (1.4), we might naively assume that the ground state is fully polarized but with the spins in opposite directions for the two sublattices. This state is called the Néel state. It is the true ground state for the classical model, but it is not for the quantum case. For instance, the ground state of a four-site spin ½ antiferromagnetic chain is given by

$$|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle - 2|\uparrow\downarrow\uparrow\downarrow\rangle - 2|\downarrow\uparrow\downarrow\uparrow\rangle.$$

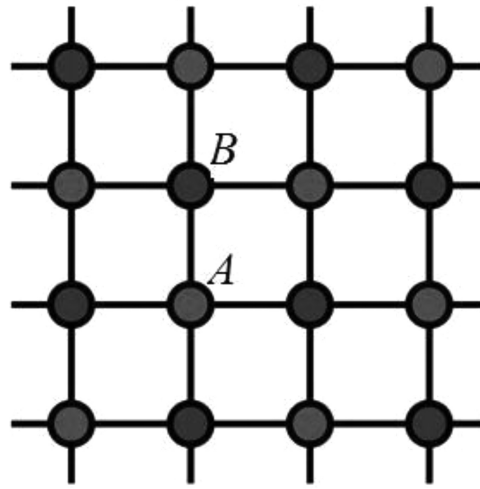

Figure 1.1. The bipartite square lattice with sublattices A and B.

The Néel state can be written as

$$|\psi\rangle = \prod_{i\in A} |S\rangle_i \prod_{j\in B} |-S\rangle_j. \tag{1.15}$$

The states $|\pm S\rangle$ are eigenstates of S^z for the given lattice site with eigenvalues $\pm S$.

We have

$$H|\psi\rangle = \sum_{i\in A}\sum_{j\in B} J_{ij}\left(\frac{1}{2}S_i^+ S_j^- |\psi\rangle + \frac{1}{2}S_i^- S_j^+ |\psi\rangle + S_i^z S_j^z |\psi\rangle\right). \tag{1.16}$$

Note that

$$S_i^+ S_j^- |\psi\rangle = 0, \tag{1.17}$$

and

$$H|\psi\rangle = \sum_{i\in A}\sum_{j\in B} J_{ij} \times \left(\frac{1}{2}[S(S+1) - S(S-1)] \ldots |S-1\rangle_i \ldots |-S+1\rangle_j - S^2\right)|\psi\rangle. \tag{1.18}$$

So, $|\psi\rangle$ is not even an eigenstate of H. We present an important theorem without demonstration. The proof is given in chapter 5 of Auerbach [1].

Marshall's theorem: *The absolute ground state $|\psi_0\rangle$ for equal size sublattices A and B is a singlet of the total spin*

$$S_{tot}|\psi_0\rangle = 0. \tag{1.19}$$

Marshall's theorem does not uniquely determine the ground state, and many other total-spin singlets are not the ground state.

As we saw, due to the spin rotational invariance of the coupling, the antiferromagnetic interaction drives neighboring spins isotropically antiparallel. The ground state can be achieved by forming an overall singlet with $S_{tot} = 0$ (as follows from Marshall's theorem). The difficulty is that this condition does not fix the state uniquely. The number of singlets grows exponentially as a function of the lattice size (Fazekas [3]), and most of the singlets have a complicated structure. For spin ½ the basic singlet is given by

$$[i,j] = \frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle). \tag{1.20}$$

Singlet states of more than two spins are obtained by letting all the spins participate in pair bonds. Let us consider as an example a four-site spins ½ Heisenberg model on a square (a single plaquette). The singlet basis can be chosen to consist of the two states shown in figure 1.2.

Other states can be written as a combination of the above basis, as shown in figure 1.3.

The ground state of this four-site Heisenberg model is given by [3]

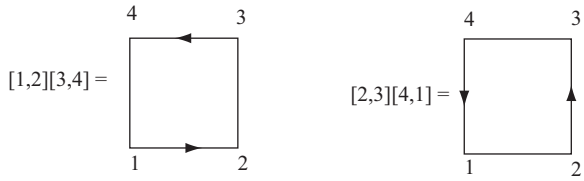

Figure 1.2. Singlet basis.

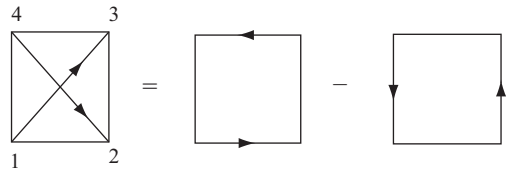

Figure 1.3. [1, 3][4, 2] = [1, 2][3, 4] − [2, 3][4, 1]. This state is a combination of the basis in figure 1.2.

$$\psi_0 = \frac{1}{\sqrt{2}}([1, 2][3, 4] + [2, 3][4, 1]), \tag{1.21}$$

with energy $E_0 = -2J$ (which is quite different from the Néel state). ψ_0 is a superposition of two states with parallel bond configurations on the square. Each state given by the parallel bonds is not an eigenstate of the Hamiltonian, and thus not the ground state. The Hamiltonian flips the bonds on the square between horizontal and vertical configurations of the parallel bonds. The ground state is hence given by the superposition (1.21). The situation remains the same if we go to larger configurations. Only in the thermodynamic limit (when $N \to \infty$), the Néel ground state (for the isotropic square lattice) becomes asymptotically degenerate with the exact singlet ground state. However, there are models for which the ground state is not the Néel state even when the number of sites goes to infinity.

1.4 Excited states for the ferromagnet

In this section, I will consider the excited states of a ferromagnet. I take $S = 1/2$, but it can be easily generalized for other values of spins. For simplicity, let us study a one-dimensional chain. Each spin has two neighbors, and so we can write

$$H = -J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}. \tag{1.22}$$

As we have seen, the ground state of the system $|\psi_0\rangle$ consists of all the spins lying along the z-direction, and we have

$$H|\psi_0\rangle = -\frac{NS^2}{2}|\psi_0\rangle. \tag{1.23}$$

To create an excitation, we flip a spin at site j and consider the state $|\psi_j\rangle = S_j^- |\psi_0\rangle$. This state is the ground state with the spin at site j flipped:

$$|\psi_0\rangle = \ldots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots$$
$$|\psi_j\rangle = \ldots \uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow \ldots$$

Thus, we have changed the total spin of the system by ½ - (- ½) = 1. This excitation has, therefore, an integer spin and is a boson. Acting with H on $|\psi_j\rangle$ we obtain

$$H|\psi_j\rangle = J[(-NS^2 + 2S)\,|\psi_j\rangle - S|\psi_{j+1}\rangle - S|\psi_{j-1}\rangle], \tag{1.24}$$

and we see that $|\psi_j\rangle$ is not an eigenstate of the Hamiltonian. We get an eigenstate by summing over all configurations with a spin flipped at each site j and writing

$$|\psi_q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqr_j} |\psi_j\rangle \tag{1.25}$$

where e^{iqr_j} is a phase factor, which describes a plane wave of wave number q. Such waves are known as 'spin waves'. The state $|\psi_q\rangle$ is essentially a flipped spin delocalized. A single spin deviation does not appear on a particular site but is instead distributed over all of the sites in the lattice. It is easy to see that

$$H|\psi_q\rangle = E(q)|\psi_q\rangle, \tag{1.26}$$

where

$$E(q) = -NS^2J + 2JS(1 - \cos qa), \tag{1.27}$$

and a is the lattice spacing. This result can easily be extended to higher dimensions. A ferromagnet is perfectly ordered at $T = 0$, but at non-zero temperature, the order is disrupted by spin waves. The energy of a spin-wave is quantized, and the quantum of energy of a spin-wave is called a *magnon*.

1.5 Translational symmetry

I will consider the same problem taking a linear chain in a ring (that is, with periodic boundary condition). The system is invariant if we displace all spins by one (or more) site. Let T be the translation operator, which takes a spin at the site l into the site $l + 1$. We have

$$TS_l^\gamma T^\dagger = S_{l+1}^\gamma \quad (\gamma = x, y, z), \tag{1.28}$$

and

$$T\,|\alpha\rangle = \alpha\,|\alpha\rangle, \tag{1.29}$$

where $|\alpha\rangle$ and α are eigenvectors and eigenvalues of T. If we have N sites, applying T N times we return to the first site. Thus, $\alpha^N = 1$. The solutions are then

$$\alpha = e^{-iK} \quad \text{with} \quad K = (2\pi/N)n, \quad n = 0, 1, \ldots, N - 1.$$

We can write the eigenstates of H as

$$|S^T, S_z^T, K\rangle, \tag{1.30}$$

where

$$\begin{aligned} \vec{S}^2 |S^T, S_Z^T, K\rangle &= S^T(S^T+1)|S^T, S_Z^T, K\rangle, \\ S_Z^T |S^T, S_Z^T, K\rangle &= S_Z^T |S^T, S_Z^T, K\rangle, \\ T |S^T, S_Z^T, K\rangle &= e^{-iK} |S^T, S_Z^T, K\rangle, \end{aligned} \tag{1.31}$$

with $0 \leqslant S^T \leqslant NS$, $S_z^T = NS, NS-1, \ldots, -NS$.

We know from quantum mechanics that translational invariance is associated with the conservation of linear momentum. In the following, I consider the state with one spin flipped. We can write an eigenstate of T as

$$|\phi\rangle = c_1 |- + + + \ldots\rangle + c_2 |+ - + + \ldots\rangle + \ldots \tag{1.32}$$

$$T |\phi\rangle = c_1 |+ - + + + \ldots\rangle + c_2 |+ + - + + \ldots\rangle + \ldots \tag{1.33}$$

But $T|\phi\rangle = e^{-iK}|\phi\rangle$, which leads to

$$e^{-iK}c_2 = c_1, \ldots, \rightarrow e^{-iK}c_n = c_{n+1}, \ldots, \tag{1.34}$$

so, $c_n = e^{-iKn}$ and thus

$$|\phi\rangle = e^{iK} |- + + + \ldots\rangle + e^{2iK} |+ - + + \ldots\rangle + e^{3iK} |+ + - + +\rangle + \ldots \tag{1.35}$$

We have N eigenvalues of T. We also have one energy for each value of K. For instance, for $N = 4$ we have

$$|\phi\rangle = e^{iK}|- + + +\rangle + e^{2iK}|+ - + +\rangle + e^{3iK}|+ + - +\rangle + e^{4iK}|+ + + -\rangle, \tag{1.36}$$

with $K = 0, \pi/2, \pi, 3\pi/2$.

1.6 Two spin waves

The state with two flipped spins is given by

$$|\psi_{ij}\rangle = S_i^- S_j^- |\psi_0\rangle. \tag{1.37}$$

For the ferromagnet, this is a state with two magnons. Note that for $S = ½$ there is no state $|\psi_{ii}\rangle$. We can put the first spin flipped at N sites. The second spin flipped at $N-1$ sites. Since a permutation does not change the state, we have $N(N-1)/2$ states. For $S > ½$, we can have two flipping at the same site, and therefore N additional states, leading to a total of $N(N+1)/2$ states. I am not going to present the calculation of two spin-wave states here. For this calculation, see Feynman [4]. It is important to mention that now we have bound states, and we can look upon the problem as a scattering of two quasiparticles. In the same way, we can treat three or more spin deviations.

1.7 Long-range order

Suppose that we have a rotationally invariant Hamiltonian H_0. We add an ordering field h, which breaks the rotational symmetry, and write

$$H = H_0 - hS_q^z, \tag{1.38}$$

where

$$S_q^z = \sum_i e^{i\vec{q}\cdot\vec{r}_i} S_i^z. \tag{1.39}$$

The magnetization per site is given by

$$m_q(h) = \frac{1}{NZ} tr\left(e^{-\beta H} S_q^z\right). \tag{1.40}$$

We consider here lattices that are symmetric under reflection about the origin. For $h > 0$ we have $m_q(h) > 0$ since the applied field induces the magnetization. We say that the system has a spontaneously broken symmetry if the magnetization is finite in the thermodynamic limit, as we take the field h to zero from above. That is

$$\lim_{h\to 0^+} \lim_{N\to\infty} m_q(h) \neq 0. \tag{1.41}$$

Note that the order of limits matter. We define the correlation functions as

$$S^{\alpha\alpha}(\vec{q}) = \lim_{h\to 0^+} \frac{1}{ZN} tr\left(e^{-\beta H} S_q^\alpha S_{-q}^\alpha\right). \quad \alpha = x, y, z. \tag{1.42}$$

If $h = 0$, the correlations are independent of the direction α.

1.8 Mermin and Wagner's theorem

The theorem says that for the quantum Heisenberg model

$$H = \frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i \cdot \vec{S}_j, \tag{1.43}$$

with short-range interactions that obey

$$\frac{1}{2N}\sum_{i,j} |J_{ij}||\vec{r}_i - \vec{r}_j| < \infty, \tag{1.44}$$

there can be no true long-range order at finite temperatures in one and two dimensions. The theorem does not apply at $T = 0$. If there is a unique ground state and a gap in the excitation spectrum, the ground state of the Heisenberg model must be disordered. The proof of the above statement is presented in Auerbach [1]. Note that gapless excitations do not imply long-range order. For example, the spin half Heisenberg antiferromagnet in one dimension has gapless excitation but no long-range order at zero temperature.

1.9 The Ising model

In this book, I will study several spin Hamiltonians. Here I will mention only one specific case: the Ising model described by the Hamiltonian

$$H = -\frac{J}{2}\sum_{ij} S_i^z S_j^z. \tag{1.45}$$

It is the simplest model in magnetism since $|m\rangle_1\,|m\rangle_2 \ldots |m\rangle_N$ is an eigenstate of the Hamiltonian. The model has an ordered phase below the critical temperature in three and two dimensions. It is perhaps one of the most studied models, mainly in statistical physics, and it can be applied to several different systems where we have a variable that can take only two values. Its importance is that it is one of few solvable models in one and two dimensions where we can compute thermodynamic quantities exactly. As concerning magnetic systems, for a material to be Ising-like, the ground state of the ion model must be a doublet well separated from the excited states.

1.10 Brillouin zone

Suppose we have a lattice with lattice vectors [5]

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3, \tag{1.46}$$

where n_i are integers and $\vec{a}_i$ are the primitive vectors. The reciprocal lattice is generated by basis vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ given by

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)}, \quad \vec{b}_3 = \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}. \tag{1.47}$$

The vectors of the reciprocal lattice are then

$$\vec{K}_n = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3 \quad (n_i\text{: integer}). \tag{1.48}$$

If we express the vector $\vec{q}$ as

$$\vec{q} = q_1\vec{b}_1 + q_2\vec{b}_2 + q_3\vec{b}_3, \tag{1.49}$$

then the component q_i has the values

$$q_i = \frac{n_i}{N_i}, \tag{1.50}$$

where N_i is the number of unit cells in the $\vec{a}_i$ direction, and the total number of lattice points is equal to $N = N_1N_2N_3$. We have N independent $\vec{q}$ vectors. The first Brillouin zone is the region surrounded by planes bisecting the vectors connecting the origin and neighboring reciprocal lattice points.

In general, we have to integrate a function in the Brillouin zone. To show how this is done, we start with the simple case of one dimension, where we have the well-known result

$$\int_{-b}^{b} f(x)dx = \sum_{i=1}^{N} f(x_i)\Delta x, \tag{1.51}$$

where $\Delta x = 2b/N$. We can write (1.51) as

$$\frac{1}{N}\sum_{i=1}^{N} f(x_i) = \frac{1}{2b}\int_{-b}^{b} f(x)dx. \tag{1.52}$$

If we have a lattice in one dimension of length a, the reciprocal lattice is given by $-\pi/a \leqslant k \leqslant \pi/a$. With $b = \pi/a$, we have

$$\frac{1}{N}\sum_{i=1}^{N} f(k_i) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} f(k)dk. \tag{1.53}$$

This result can easily be generalized to an integral in the Brillouin zone in d-dimensions

$$\frac{1}{N}\sum_{i} f(\vec{k}_i) = \frac{V}{(2\pi)^d}\int_{BZ} d^d\vec{k}, \tag{1.54}$$

where V is the volume of the unitary cell. For the square or cubic lattice, the calculation is straightforward. If the unitary cell is a rectangle with sides a and b, the Brillouin zone is given by: $-\pi/a \leqslant k_x \leqslant \pi/a, -\pi/b \leqslant k_y \leqslant \pi/b$. However, the integral is more elaborated in other kinds of lattices. Note that it is usual to take the lattice parameter a as unity.

1.11 Mean-field approximation for the classical ferromagnetic Heisenberg model

The magnetization is $\vec{m}_i = \mu_B g\vec{S}_i$, and the total magnetization $\vec{M} = \sum_i \vec{m}_i$. In the case of interaction with only an external field $\vec{B}$, the energy of the system is

$$E = \sum_i E_i = -\mu_0\vec{B}\cdot\sum_i \vec{m}_i = -\mu_0\mu_B g\vec{B}\cdot\sum_i \vec{S}_i = -\mu_0\mu_B gSB\sum_i \cos\theta_i, \tag{1.55}$$

where θ_i is the angle between the magnetic field and the orientation of the spin. The partition function is given by

$$Z_1 = \int \sin\theta\, d\theta d\phi\, \exp(\beta\mu_0\mu_B gSB\cos\theta) = 4\pi\left[\frac{\sinh r}{r}\right], \tag{1.56}$$

where $r = \beta\mu_0\mu_B gSB$.

From the free energy $F = -k_B T \ln Z_1$, we get the magnetization (in the field direction)

$$M = -\frac{1}{\mu_0}\left(\frac{\partial F}{\partial B}\right) = \mu_B g S N\left[\coth(r) - \frac{1}{r}\right] = \mu_B g S N L(r), \tag{1.57}$$

where $L(r) = \coth(r) - 1/r$ is the Langevin function.

Now we consider the classical ferromagnetic Heisenberg model in the presence of an external field. We have for the energy

$$E = -J\sum_{\langle i,j\rangle}\vec{S}_i \cdot \vec{S}_j - \mu_0\mu_B g\vec{B} \cdot \sum_i \vec{S}_i. \tag{1.58}$$

In the mean-field approximation, we replace the interaction between spins by an interaction with a field generated by the mean orientation of the spins (that is, we replace one of the $\vec{S}_i$ by its average $\langle\vec{S}_i\rangle$). We write then

$$E = -Jz\langle\vec{S}\rangle \cdot \sum_i \vec{S}_i - \mu_0\mu_B g\vec{B} \cdot \sum_i \vec{S}_i = -(Jz\langle\vec{S}\rangle + \mu_0\mu_B g\vec{B}) \cdot \sum_i \vec{S}_i, \tag{1.59}$$

where z is the number of nearest neighbors. We assume that the direction of the z-axis is in the direction of the magnetic field. The direction of $\langle\vec{S}\rangle$ is also in the z-axis direction and its modulus is $\langle S\rangle$. Using equation (1.56) we have for the magnetization

$$M = \mu_B g N S L(f), \qquad f = \beta S(Jz\langle S\rangle + \mu_0\mu_B g B). \tag{1.60}$$

However, $M = N\mu_B g\langle S\rangle$, and so we can write

$$\langle S\rangle = SL[\beta S(Jz\langle S\rangle + \mu_0\mu_B g B)]. \tag{1.61}$$

We have to solve (1.61) numerically. For $B = 0$ we find a finite solution for $T < T_c$, where T_c is given by

$$T_c = \frac{JzS^2}{3k_B}. \tag{1.62}$$

We can use the mean-field theory described above only to study ordered phases because we assume $\langle\vec{S}_i\rangle \neq 0$. The antiferromagnet can be treated on the same line, noting that now we have two sublattices.

The reader can easily perform the above calculation for the quantum case. Instead of the integral (1.56), one has a discrete sum over the quantum states that can be calculated using the formula

$$a + ax + ax^2 + \ldots + ax^{L-1} = \sum_{j=1}^{L} ax^{j-1} = \frac{a(1 - x^L)}{1 - x}, \tag{1.63}$$

where L is the number of terms in the series, which in this case is $L = 2J + 1$.

1.12 Landau theory for phase transitions

The Landau theory of phase transitions is based on the view that phase transitions have universal properties, in that they depend only on the nature of the order

parameter and not on the finer details of the system. In general, the order parameter vanishes in the disordered phase and takes a non-zero value in the ordered phase. However, correlations and fluctuations are ignored in the theory. The central hypothesis is that we may expand the free energy in a power series in the order parameter in the vicinity of the critical point that we take as the magnetization m. Here we consider a ferromagnet [6]. The equilibrium value of m is then the value that minimizes the free energy. For cases where $F(m, T) = F(-m, T)$, the most general expansion for F is

$$F(m, T) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6 + \ldots \tag{1.64}$$

where we use fractional coefficients just for convenience. We have

$$\frac{\partial F}{\partial m} = 0 = b(t)m + c(T)m^3 + d(T)m^5 + \ldots \tag{1.65}$$

First, we consider the case where $c, d, e, \ldots > 0$. To obtain a magnetically ordered state, one must suppose that the coefficient of the term m^2 passes through zero at some temperature T_c. We write then

$$b(T) = \gamma(T - T_c), \tag{1.66}$$

near $T = T_c$. If c is positive, nothing new is added by the term d, and this term may then be neglected. The magnetization (for zero applied field) is found from

$$\gamma(T - T_c)m_s + c(T_c)m_s^3 = 0. \tag{1.67}$$

So that either $m_s = 0$ or

$$m_s^2 = (\gamma/(c(T_c))(T_c - T). \tag{1.68}$$

For $T \geqslant T_c$ the only real root of (1.68) is at $m_s = 0$ because γ and c are positive. Thus, T_c is the Curie temperature. For $T < T_c$ the minimum is at

$$m_s = (\gamma/c(T_c))^{1/2}(T_c - T)^{1/2}. \tag{1.69}$$

This phase transition is a second-order phase transition because the magnetization goes continuously to zero at the transition temperature.

The transition is first order (the magnetization drops discontinuously to zero at the transition temperature) if c is negative. We must then retain d and take it as positive to restrain it from going to minus infinite. The equilibrium condition is

$$\gamma(T - T_c)m_s - |c(T_c)|m_s^3 + d(T_c)m_s^5 = 0. \tag{1.70}$$

So that either $m_s = 0$ or

$$\gamma(T - T_c) - |c(T_c)|m_s^2 + d(T_c)m_s^4 = 0. \tag{1.71}$$

The Landau theory, although very useful, is a mean-field theory and cannot correctly describe critical points, where it should be complemented by scaling laws

and renormalization group theory. At a critical point, a thermodynamic function generally contains a term regular in t, where $t = T/T_c - 1$, plus a singular part that behaves like a power of t [7]. The power is the critical *exponent*. When the external magnetic field is zero, we define the following exponents as $t \to 0$:

$$\begin{aligned} M &\sim |t|^{\beta} \qquad \text{(Order parameter)}, \\ \chi &\sim |t|^{-\gamma} \qquad \text{(Susceptibility)}, \\ C &\sim |t|^{-\alpha} \qquad \text{(Heat capacity)}, \end{aligned}$$

where ~ means 'singular part is proportional to' (note that β here is not $1/k_B T$). Critical exponents are universal in that they do not depend on the details of the physical system and are the same for several classes of systems. For instance, for the ferromagnet, they depend on the dimensionality of the lattice, the range of interaction, and the dimensionality of the order parameter (actually the symmetry of the order parameter). The mean-field theory gives $\beta = ½$ (independent of the space dimension). The critical exponents calculated using the mean-field theory differ from the true ones in dimensions 1, 2 and 3. The theory is only correct when the system's space dimension is higher than a certain dimension called the *upper critical dimension*.

1.13 The Hubbard model

The simplest model of a solid is to consider atoms as a collection of sites, each with a single level (orbital). The Pauli principle constrains the sites to four configurations: empty, a single electron with spin-up, a single electron with spin-down, and finally occupation by a pair of electrons with opposite spins. In the so-called tight-binding model, electrons can hop between lattice sites without interacting with each other. In its simplest form, electron hopping can only occur between nearest-neighbor sites, and all hopping processes have the same kinetic energy$-t$. The kinetic energy term in the Hamiltonian is a term that destroys an electron of spin σ on site i and creates it on a neighbor site j (or vice-versa). In the Hubbard model [8], we have an additional term that considers the electrons' interaction via a screened Coulomb repulsion. In the Hamiltonian, we have a term which is zero if the site is empty or has only a single electron, but has the value U if electrons doubly occupy the site with opposite spins since the most significant interaction will be for two electrons on the same site. The Hamiltonian is then written as:

$$H = -t \sum_{\langle i,j\rangle\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{j\downarrow} - \mu \sum_{i} (n_{i\uparrow} + n_{i\downarrow}), \tag{1.72}$$

where

$$n_{\sigma i} = c_{\sigma i}^{\dagger} c_{\sigma i}, \tag{1.73}$$

and $c_{\sigma i}$ are fermion operators. The symbol $\langle i, j\rangle$ means that hopping occurs only between two adjacent sites. The last term is a chemical potential that controls the filling. We refer to the situation where there is one electron per site as 'half-filling'. Depending on the value of U, the model describes a metallic or an insulating state.

If the Coulomb repulsion is large, the electrons are less likely to hop to a neighboring site, and they self-localize on a given lattice site. The electrons can virtually hop to another site and back. However, the material is an insulator and will not conduct. Such a material with an odd number of electrons per unit cell that does not conduct because of Coulomb repulsion is called a Mott insulator, as opposed to band insulators, resulting from filled energy bands. If t/U is large, electrons are essentially free. However, if $U/t \gg 1$, the electrons are localized. The kinetic energy term favors two neighboring site-localized electrons to have antialigned spins, as a hop to a neighboring site is not allowed due to the Pauli exclusion principle. Hence, at half-filling and in the large repulsion limit, the most elementary model that captures the dominant interaction in Mott-insulators is the spin ½ antiferromagnetic Heisenberg model with $J \sim t^2/U$,

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1.74}$$

with the spin given by

$$\vec{S}_i = \frac{\hbar}{2} c^{\dagger}_{\sigma i} \tau_{\sigma\sigma'} c_{\sigma' i}, \quad \text{(no sum in } i\text{)} \tag{1.75}$$

where $\vec{\tau}$ are the three Pauli matrices. For the derivation of this result, see Fradkin [9]. Note, however, that equation (1.74) is only the leading term of the effective Hamiltonian. If we go to higher orders, we obtain also ring-exchange processes, second-neighbor interactions, etc. For instance, up to the third order in the strong coupling expansion, we get the following three spin ring-exchange term [10]

$$H_3 = J_3 \sin\phi \sum_{\Delta ijk} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k), \tag{1.76}$$

where J_3 is the three spin ring-exchange couplings constant around an elementary triangle $\Delta_{i,j,k}$ on the square lattice formed by the sites *i, j, k* in a counterclockwise way and ϕ is the magnetic flux enclosed through $\Delta_{i,j,k}$. The scalar spin chirality in $\Delta_{i,j,k}$ is defined by

$$\chi_{ijk} = \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k). \tag{1.77}$$

This term acts as a fictitious magnetic flux for the Hubble model's conduction electrons and gives rise to a nontrivial topology.

I am not going to study the Hubbard model in this book. The above introduction was only to show that the antiferromagnetic Heisenberg model can be used to study strongly correlated systems.

1.14 Exercises

1.1. Consider the one-dimensional ferromagnetic Ising model with Hamiltonian

$$H = -2J \sum_{i=1}^{N-1} S_i^z S_{i+1}^z - 2J S_N^z S_1^z,$$

where the last term was added so that we have periodic boundary conditions.

a) Show that the operator $\eta_i = 4S_i^z S_{i+1}^z$ has eigenvalues $+1$ or -1.

b) Using η_i show that the partition function is $Z = [2\cosh(J/2k_BT)]^N$.

1.2. Calculate the partition function and the transition temperature for the quantum ferromagnetic Heisenberg model in three dimensions, using the mean-field approximation.

1.3. Consider the two-site Hubbard model with 2 electrons and $U = 0$. Calculate the ground state eigenstates and eigenenergies.

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