Chapter 9
Other Approximate Methods

Abstract Exact diagonalisations of the type presented in the previous chapter are typically limited to relatively small numbers of lattice sites. In this chapter approximate methods that may be applied to larger systems are discussed. The variational method is discussed as one method of simulating the properties of quantum spin systems, although an exact enumeration of the basis states in a given sector becomes prohibitive in terms of computational cost for larger lattices. Monte Carlo simulation allows us to treat larger lattices using the variational method. This discussion leads on to a more general description of the quantum Monte Carlo simulation of quantum spin systems. Finally, the topics of perturbation theory and of series expansions are explored. Series expansions obey the linked cluster theorem and so yield results valid in the infinite-lattice limit from the outset. The spin-half Heisenberg model on the linear chain is used as a test-case for all of these methods. We show that even simple applications of these methods give improved results for the ground-state energy compared to the classical result.

9.1 Introduction

The finite-size calculations, described in the previous chapter, are only one way of obtaining results numerically. The coupled-cluster method, described in detail in the next chapter is also a numerical method which deals directly with the infinite lattice. In this chapter we mention the variational method and its stochastic version, the Variational Monte Carlo method, the Green Function Monte Carlo method and also perturbation theory/series expansions. Some of these, e.g., series expansions, deal directly with the infinite lattice, although others such as Monte Carlo are generally applied to a finite lattice and the results then extrapolated in the infinite-lattice limit.

9.2 Variational Method

The variational method, widely used in theoretical physics, can also be applied to 2D and 3D quantum spin systems in a simple and straightforward manner. An important point to note about the variational method is that the approximate bra

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and ket states are Hermitian conjugates of each other (unlike in the coupled cluster method described later) so that the calculated ground-state energy is a strict upper bound on the true value. If the result depends upon some parameter in the wave function then minimising with respect to this parameter, i.e. varying it to find the minimum, can lead to a good approximation to the true value. The ground state wave function is less reliably obtained as some important features may have been neglected in the initial trial wave function.

For example, in an antiferromagnetic spin system we usually know that the ground state is a state with total spin equal to 0. The true ground state must consist of a linear combination of states in the set $\{I\}$ which is the set of all Ising states for which $S_T^z \equiv \sum_i S_i^z = 0$. Thus the ground state wave function is

$$|\Psi\rangle \;=\; \sum_I c_I |I\rangle. \tag{9.1}$$

The ground-state energy is given by the Schrödinger equation as normal

$$H|\Psi\rangle \;=\; E_g|\Psi\rangle$$

and applying $\langle\Psi|$ on the left gives

$$E_g = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

or

$$E_g = \frac{\sum_{I_1,I_2} c_{I_1}^* c_{I_2} \langle I_1|H|I_2\rangle}{\sum_I |c_I|^2}. \tag{9.2}$$

Now we make an approximation to the coefficients in such a way that there is one or more parameters in the coefficients which can be varied.

An example is the choice for a spin-half system given by

$$c_I = u_{ij}(p_i^{\uparrow} p_j^{\downarrow} + p_i^{\downarrow} p_j^{\uparrow}), \tag{9.3}$$

where the indices i and j run over all lattice sites. $p^{\uparrow}$ and $p^{\downarrow}$ are projection operators for the 'up' and 'down' states of the spins, where

$$\begin{aligned} p^{\uparrow}|\uparrow\rangle &= 1|\uparrow\rangle \quad p^{\uparrow}|\downarrow\rangle = 0|\downarrow\rangle \\ p^{\downarrow}|\uparrow\rangle &= 0|\uparrow\rangle \quad p^{\downarrow}|\downarrow\rangle = 1|\downarrow\rangle. \end{aligned}$$

In terms of the normal spin operators

$$p^{\uparrow} \equiv \frac{1}{2} + S^z : \qquad p^{\downarrow} \equiv \frac{1}{2} - S^z,$$

and the $\{u_{ij}\}$ are parameters.

Note that it is slightly easier to deal with the equivalent spin system after a unitary rotation of the local axes of the spin by 180° on one sublattice. This changes the Hamiltonian slightly, but crucially means that the c_I coefficients must be positive from the Marshall-Peierls sign rule. An example is the choice for a spin-half system (after rotation of the local spin axes) given by

$$c_I = u_{ij}(p_i^{\uparrow} p_j^{\uparrow} + p_i^{\downarrow} p_j^{\downarrow}), \tag{9.4}$$

where the indices i and j run over all lattice sites.

A possible choice of these parameters is the 'two-site' approximation known as the Jastrow Ansatz, in which the u_{ij} are all zero if i and j are not nearest neighbours. A simple version of this is to set u_{ij} equal to some number α when i and j are nearest-neighbours and to zero in all other cases. There is now a single parameter, α, to be adjusted in the final result.

For small enough lattices, we enumerate all of the states in the Ising basis either by hand (or for larger lattices computationally), and so we are able to calculate all of the contributions to the ground-state energy of Eq. (9.2). We obtain a value for the ground-state energy in terms of α and then minimise with respect to it. Hence, we obtain a 'variational' value for the ground-state energy. Because the ground-state energy thus found is an upper bound of the 'true' value, this is very useful both as an estimate of the ground-state energy in itself and also as a test for other approximate methods. If another approximate method produces a ground-state energy higher than the simple variational estimate then it is unsatisfactory.

Finally, we may find estimates of other ground-state expectation values easily as we have direct access to the (approximate) wave function written in terms of expansion coefficients with respect to the Ising basis.

9.3 Variational Monte Carlo Method

However, we may not be able to enumerate all Ising states in the basis even using very intensive computational approaches (and in the relevant ground-state subspace) for very large lattices, i.e., those of very many spins. This is particularly true for 2D and 3D lattices and for higher spin quantum number. In this case we use a method called Monte Carlo simulation in order to carry out the enumeration of states approximately. Clearly, not all states are equal in their contribution to the ground-state energy and this method allows us to choose those states that are 'most important.' Furthermore, the error of the estimate of ground-state expectation values decreases in a statistically well-understood manner with the length of the simulation.

We begin the Monte Carlo treatment of the variational problem by rewriting the ground-state energy of Eq. (9.2) in the following form:

$$\begin{aligned} E_g &= \frac{\sum_{I_1,I_2} c^*_{I_1} c_{I_2} \langle I_1|H|I_2\rangle}{\sum_I |c_I|^2} \\ &= \frac{\sum_{I_1} |c_{I_1}|^2 \sum_{I_2} \frac{c_{I_2}}{c_{I_1}} \langle I_1|H|I_2\rangle}{\sum_I |c_I|^2} \\ \Rightarrow \quad E_g &= \sum_I P(I) E_L(I). \end{aligned} \tag{9.5}$$

$P(I)$ is interpreted as a probability for the state I and is given by

$$P(I) = |c_I|^2 / \sum_J |c_J|^2.$$

(The index J represents a sum over all Ising basis states, though it will disappear as we shall see shortly). The local energy with respect to the state I is given by

$$E_L(I) = \sum_{I_2} \frac{c_{I_2}}{c_I} \langle I|H|I_2\rangle.$$

We start from a given state in the relevant ground-state Ising basis and we define an acceptance probability $A(I \to I')$ from state I to state I' given by

$$A(I \to I') = \min\left[1, \frac{P(I')K(I)}{P(I)K(I')}\right], \tag{9.6}$$

where $K(I)$ indicates the number of states accessible from state I via the 'off-diagonal' terms in the Hamiltonian. (The denominator $\sum_J |c_J|^2$ in both $P(I)$ and and $P(I')$ is identical and so cancels in Eq. (9.6).) We choose a state I' to be one of these $K(I')$ states and now use the Metropolis algorithm in order to decide if we should accept this new state I' or if we should stay with the old one, I. We generate a random number η from a uniform distribution in the range 0 to 1 and we test if our acceptance probability $A(I \to I')$ is greater than η. If it is then we accept the new state and otherwise we retain the original state. It is this element of randomness or chance that leads to the name of the method (i.e., Monte Carlo) for obvious reasons.

We now repeat the process for the new state I' in order to form yet another state I'', and so on. As is common in Monte Carlo simulations we repeat this process many times and we form an average of the local energies (and 'local' estimates of all other ground-state expectation values similarly) as we go along. Again, we note

that the ground-state energy again forms an upper bound on the 'true' ground-state energy, but within the limits of the error bars due to the Monte Carlo simulation in this case. The estimate of the ground-state energy may be minimized computationally for the variational Monte Carlo estimate presented here. This is simple to achieve in practice and a robust estimate of the ground-state energy may be formed in a straightforward manner for the nearest-neighbour two-spin approximation. This process becomes more difficult as we include longer-range correlations and higher-order terms in the approximation for the c_I coefficients. However, we would expect the accuracy of the results to increase also as we add in more such terms and, again, we would obtain an upper bound on the ground-state energy.

It is interesting to apply the variational Monte Carlo (VMC) method to the spin-half one-dimensional antiferromagnetic ($J>0$) Heisenberg model on a chain of finite length, which can be solved by the exact diagonalisation method as described above. For example, we obtain an estimate of the ground state energy of $E_G/N = -0.423729(3)J$ ($\alpha = 1.773$) for the Heisenberg model on a chain of $N = 20$ sites with periodic boundary conditions. Note that α is the strength of the nearest-neighbour correlations in u_{ij} in Eq. (9.4) and that $M = 10^{10}$ Monte Carlo iterations were used in this simulation. This result lies above and is reasonably close to the exact diagonalisation result of $E_G/N = -0.445219J$ for the $N = 20$ chain with periodic boundary conditions, which is itself not too far from the exact Bethe ansatz result of $E_G/N = 1/4 - \ln 2$ ($= -0.443147$) in the infinite-lattice limit. Indeed, we see that 89% of the correlation energy of the $N = 20$ Heisenberg chain has been captured by using this simple two-body nearest-neighbour Ansatz. Furthermore, this result also illustrates the fact mentioned earlier that variational methods provide an upper bound on the ground-state energy of a system because the ket and bra states are always Hermitian conjugates of each other. We may also apply VMC to much larger lattices than exact diagonalisations because the computational cost needed to carry out VMC is much lower. However, caution should be used when interpreting the results of variational studies because they might actually provide quite a poor approximation to the 'true' ground-state wave function while still yielding deceptively good results for the ground-state energy.

Despite this, however, it is true to say that variational methods have an important role to play in understanding quantum spin systems, especially in providing upper bounds on the ground-state energy which can then be compared with results of other approximate methods. In the next chapter we shall describe a method called the coupled cluster method (CCM) that allows us to systematically refine the approximation level to include higher order terms in the wave function. The CCM is strictly speaking a bi-variational method, and since the bra and ket states are not explicitly constrained to be Hermitian conjugates of each other, it does not yield an upper bound to the energy. However, this negative aspect is offset by many positive aspects, not-the-least that one may obtain results for the infinite lattice ($N \to \infty$) from the outset.

9.4 The Green Function Monte Carlo Method

There are many forms of Monte Carlo in science [1–6] and its use is ubiquitous. Thus, even in the fairly restricted area of quantum spin systems, the variational Monte Carlo method is only one of a number of approaches that use Monte Carlo techniques. Another example, used for calculating zero temperature properties, is the Green function Monte Carlo method. This provides an estimate of the true ground-state energy and other properties directly and so there is no need to minimise the ground-state energy with respect to any parameters of the wave function.

It uses 'power iteration' of the Hamiltonian in which one repeatedly operates with the Hamiltonian on an initial starting state $|I_0\rangle$ (in the relevant ground-state subspace). For a large number M of operations $H^M|I_0\rangle \stackrel{M\to\infty}{\longrightarrow} K|\Psi\rangle$, where K is a constant and $|\Psi\rangle$ is the eigenstate of H which has the eigenvalue with the largest magnitude, normally the ground-state. This method is frequently used in exact diagonalizations of finite-sized systems in order to isolate the ground-state wave function and its energy. Often the Lanczos technique can also be used to drastically reduce the number of iterations compared to the direct 'power" iteration method.

However, for the Green function Monte Carlo, this property of power or direct iteration turns out to be quite useful. This is because each time we apply the Hamiltonian new Ising states in the approximate wave function are created. The Green function method represents these states by a set of 'walkers' where each walker has transition probabilities $A(I \to I')$ to go from state I to state I' and associated local energies. The estimate of the ground-state energy is given by the average of the local energies over all walkers for a given number of iterations M. Again, each move is accepted or rejected randomly and so we obtain a 'random walk' for each of the individual walkers through the set of basis states.

For Green function Monte Carlo, however, we also need to know the signs of the expansion coefficients c_I beforehand in order to ensure that the transition probabilities are always positive; if we utilize signs that are wrong then we will sample the underlying probability distributions incorrectly and so our estimates will also be incorrect. Fortunately, there exist a number of such rules for the signs of the expansion coefficients, the most famous of which is the Marshall-Peierls sign rule [7] for the Heisenberg model for bipartite lattices. Bipartite lattices are those lattices such as that linear chain, square and cubic latices that can be decomposed into two neighbouring sublattices. The estimates of the ground-state properties of lattice quantum spin systems thus obtained using Green function Monte Carlo present the most important of the approximate methods for 2D (and to lesser extent 3D) unfrustrated systems. However, the application of Monte Carlo is severely limited by the presence of the 'sign problem' for frustrated spin systems. Frustration is an effect in which different terms in the Hamiltonian compete. Classically, this means that the ground-state energy per bond is lower than that of a comparative unfrustrated system. By contrast, perhaps the best evidence of frustration occurs in the analogous quantum system is that no such sign rule can be created. Examples of frustrated systems are the triangular lattice antiferromagnet and the J_1–J_2 model

with antiferromagnetic nearest- and next-nearest-neighbour terms of bond strengths J_1 and J_2, respectively. Some of these systems will be considered in more depth later on. However, we note that variational Monte Carlo may still be applied for those cases in which no sign rule exists. Furthermore, a more sophisticated Monte Carlo approach called fixed-node Monte Carlo may be employed in these cases also. However, a description of this method lies beyond the scope of this text.

9.5 Perturbation Theory

There are many other approximate methods which have been applied to quantum spin systems. We finish by briefly mentioning one of these, the perturbation method.

The basic idea here is to divide $\mathcal{H}$ into two parts and treat one part as a perturbation, even if it is not very small. For example, a system with anisotropic exchange, called the 'XXZ-Model', in any number of dimensions has Hamiltonian

$$\mathcal{H} = \frac{J}{2} \sum_i \sum_\rho \left[S_i^z S_{i+\rho}^z + \gamma \left(S_i^x S_{i+\rho}^x + S_i^y S_{i+\rho}^y \right) \right]$$

where ρ runs over all nearest neighbours on the opposite sublattice and γ is the anisotropy parameter. Writing this as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

where

$$\mathcal{H}_0 = \frac{J}{2} \sum_i \sum_\rho S_i^z S_{i+\rho}^z$$

and

$$\mathcal{H}_1 = \frac{J}{2} \gamma \sum_i \sum_\rho (S_i^x S_{i+\rho}^x + S_i^y S_{i+\rho}^y)$$

$\mathcal{H}_0$ is a simple Ising model and its exact ground state is the antiferromagnetic Néel state. Clearly for small values of γ, $\mathcal{H}_1$ is small and can be treated as a perturbation. Hence, using perturbation theory, one can calculate corrections to the ground state energy. One can also calculate correlations. The method has the advantage that it works for all S and all dimensions including 3D.

As an illustration, we calculate the first few orders of the (Rayleigh-Schrödinger) perturbation series for the energy $E_G = E_0 + \gamma E_1 + \gamma^2 E_2 + \cdots$ for the $S = \frac{1}{2}$ case explicitly. It is useful to rotate the the axes by 180° on one sublattice so that notionally the classical Néel (unperturbed) state $|0\rangle$ has all spins pointing upwards, and this

has the effect that $H_0 = -\frac{J}{2}\sum_i \sum_\rho S_i^z S_{i+\rho}^z$ and $H_1 = -\frac{J}{4}\gamma \sum_i \sum_\rho (S_i^+ S_{i+\rho}^+ + S_i^- S_{i+\rho}^-)$. The zeroth-order term in the series for the energy is now simply:

$$E_0 = \langle 0|H_0|0\rangle = \frac{-NnJ}{8},$$

where n is the number of nearest neighbours (1D: $n = 2$; 2D: $n = 4$; and, 3D: $n = 6$).

The first-order correction is given by $E_1 = \langle 0|H_1|0\rangle$. H_1 acting on $|0\rangle$ produces pairs of nearest-neighbour down spins for each lattice site i. Denoting one such state as $|i, i+\rho\rangle$ and noting that

$$\langle 0|i, i+\rho\rangle = 0$$

we see immediately that

$$E_1 = 0. \tag{9.7}$$

The second-order term in the series for the energy is given by

$$E_2 = \frac{1}{2}\sum_i \sum_\rho \frac{|\langle i, i+\rho|H_1|0\rangle|^2}{(E_0 - E_0^{(i,i+\rho)})}, \tag{9.8}$$

where the factor of $\frac{1}{2}$ is to avoid over-counting, and where

$$\begin{aligned} E_0^{(i,i+\rho)} = \langle i, i+\rho|H_0|i, i+\rho\rangle &= (E_0 + J) \quad \text{in 1D} \\ &= (E_0 + 3J) \quad \text{in 2D} \\ &= (E_0 + 5J) \quad \text{in 3D.} \end{aligned}$$

Furthermore, $\langle i, i+\rho|H_1|0\rangle = J\gamma/2$, so

$$\begin{aligned} E_2 = \frac{Nn}{2} \times \frac{(J/2)^2}{(E_0 - E_0 - J)} &= -\frac{NJ}{4} \quad \text{in 1D} \\ = \frac{Nn}{2} \times \frac{(J/2)^2}{(E_0 - E_0 - 3J)} &= -\frac{NJ}{6} \quad \text{in 2D} \\ = \frac{Nn}{2} \times \frac{(J/2)^2}{(E_0 - E_0 - 5J)} &= -\frac{3NJ}{20} \quad \text{in 3D.} \end{aligned}$$

Thus, to second-order for the 1D chain we obtain $E_G/N = -\frac{J}{4}(1+\gamma^2)$. Although perturbation theory assumes small γ, the result for $\gamma = 1$, $E_G/N = -\frac{J}{2}$, is nearer to the exact result of $-0.443147J$ (to 6 decimal places) than the zeroth-order value of $E_0/N = -\frac{J}{4}$, although it is still some distance away from the exact result.

Clearly, better accuracy can be obtained by including additional terms in the series, although this process becomes increasingly difficult to do analytically. Numerical computational techniques can, however, determine the series to high orders in γ.

Some of the earliest results were obtained by Bullock (1965) [8] and later ones by Singh (1989) [9]. For the antiferromagnetic ground state energy in 2D with $S = \frac{1}{2}$, Singh obtained the result

$$\frac{4E_G}{J} = -2 - \tfrac{2}{3}\gamma^2 + 0.00370370\gamma^4 - 0.00632628\gamma^6 - 0.00330085\gamma^8 - 0.00124740\gamma^{10} + \ldots \quad .$$

As noted above, even though the basic premise of perturbation theory is that $\mathcal{H}_1$ (and thus γ) is small, this series can give a reasonable estimate of the ground state energy even for the Heisenberg model with isotropic exchange, i.e. $\gamma = 1$.

Even with the use of powerful computers only a finite number of terms in the series can be calculated. A method of improving the results is to approximate the missing higher order terms using Padé approximants. This works well for many cases, although sometimes it is necessary to apply a transformation to avoid unphysical singularities. Using this approach (often also referred to as "series expansions" [10]), excellent results for the Heisenberg antiferromagnet have been achieved. Results of series expansions are discussed in the final chapter of this book.

Every numerical method has its own particular strengths and weaknesses. For example, for small systems, exact diagonalisations provide 'exact' results as the name suggests, and so are in some sense incontrovertible, which is a strong advantage of the method. However, the method is restricted to lattices with relatively small numbers of sites, $N \sim 40$ especially in 2D and 3D, even with the aid of high-performance computing. The DMRG method [11–14] provides essentially exact results for quasi-1D lattices, but has had only limited success in 2D.

As described above, another important method is the quantum Monte Carlo method (see, e.g., Refs. [4, 5]). In principle, this method gives results in which the accuracy is limited only by the amount of computational power available because the accuracy of the results increases in a statistically well-understood manner with the length of the Monte Carlo simulation. However, the method suffers from the 'sign-problem' and cannot be easily applied to 'frustrated' quantum spin systems.

Clearly there is a wide range of approximate techniques, each with advantages and disadvantages. In the following chapter we shall give a detailed account of a technique called the coupled cluster method (CCM) which has been applied to quantum spin systems only fairly recently. This is a technique related to that of cumulant series expansions and has important 'linked-cluster' properties. This method also gives results in the infinite-lattice limit ($N \to \infty$) from the outset, although it does not automatically provide an upper bound on the energy of the ground state or any other state.

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