

Chapter 8

Numerical Finite-Size Calculations

Abstract Numerical methods have been used extensively for studies of quantum spin systems. In subsequent chapters we shall describe some of these methods, which make use of sophisticated approximation techniques developed in many areas of quantum many-body theory. However, in this chapter we first look a very simple numerical method that does not involve any theory other than the assumption that the properties of small systems change smoothly as the size of the system increases to the limit of infinite numbers of atoms. The technique is to take a small finite-sized system with N atoms, where N can be any number from 2 upwards. For these small systems, every basis state can be written down explicitly and all the matrix elements of the Hamiltonian in the basis can be calculated. The matrix is then diagonalised numerically and hence the eigenstates and eigenvalues calculated. Usually the largest N is of the order of 20 for full diagonalisation and 40 for partial diagonalisation. Clearly the ground state energy and the energies of the elementary excitations are obtained directly. Also the partition function can be constructed directly for full diagonalisation because all the eigenvalues are known. This opens the way to study of the non-zero temperature properties of these systems.

8.1 Introduction

In previous chapters we considered two exact 1D methods:

1. The Bethe Ansatz applied to the $S = \frac{1}{2}$ Heisenberg chain.
2. The method of Jordan and Wigner applied to the $S = \frac{1}{2}$ XY chain.

These exactly solvable systems are known as *integrable* systems. They comprise only a few very specialised systems, which are nevertheless extremely important because much more detailed information is available for them than for other systems.

We have also considered one approximate method, namely spin-wave theory, especially for antiferromagnets which is valid in all dimensions. Spin-wave theory is useful in practice but is not easy to improve in a systematic way.

In this section we describe another approximate method which applies very generally and which is systematic. This method is useful for estimating the ground

state properties, i.e. for systems with $T = 0$. It also works well for medium and high T , but is least accurate for low T ($\neq 0$). Again we shall mainly consider antiferromagnets.

We shall describe the essential features of the method. However, because it has been very widely used it is only possible here to give one or two examples of its application which we hope will give an indication of its power.

Suppose we wish to find the ground state energy for a system of N atoms where $N \rightarrow \infty$. As noted above, most systems are not integrable, examples being

- a. Systems with $S \geq 1$.
- b. Systems with interactions which are not nearest-neighbour.
- c. Systems with other types of interaction between spins such as biquadratic $(\mathbf{S}_i \cdot \mathbf{S}_j)^2$.
- d. Systems with dimension higher than 1.

For many of these cases a powerful method is to calculate results numerically for small systems, typically $N \lesssim 40$, for several different values of N and then try to extrapolate $N \rightarrow \infty$.

The pioneering work was done by Bonner and Fisher (1964) [1] who considered the 1D (chains and rings) XXZ model with $S = \frac{1}{2}$ and a magnetic field.

$$\mathcal{H} = -2J \sum_j \Delta \left[S_j^z S_{j+1}^z + (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) \right] - B \sum_j S_j^z. \quad (8.1)$$

(Note the factor of 2 compared to earlier chapters.) This is a system which can be dealt with by Bethe Ansatz (BA) and so the accuracy of some of the numerical results, such as the ground state energy, can be checked directly with the exact result. Other properties of the ground state, such as correlations between different spins, which cannot be easily obtained by the BA can now be estimated numerically. Also results for non-zero T can be found. Mostly it has been used for 1D systems as it is more difficult to treat 2D systems that are large enough to make extrapolations meaningful. However, for some systems accurate results in 2D for the ground state have been found and some of these are discussed in the final chapter. For the same reason there are virtually no results in 3D.

8.2 A Simple Example

The method involves direct diagonalisation of the full Hamiltonian for a short chain (open ends) or ring (periodic boundary conditions). We illustrate the method for the Heisenberg Hamiltonian, i.e. (8.1) with $\Delta = 1$ and $B = 0$, for a ring of $N = 4$, $S = \frac{1}{2}$ atoms. We also put $J = 1$ for simplicity. Hence

$$\mathcal{H} = 2 \sum_j S_j \cdot S_{j+1} = 2 \sum_j \left[S_j^z S_{j+1}^z + \frac{1}{2} (S_j^- S_{j+1}^+ + S_j^+ S_j^-) \right] \quad (8.2)$$

where blank regions contain only 0s. Note the block-diagonalisation due to S_T^z being a good quantum number.

Clearly this matrix can now be easily diagonalised numerically to find all the eigenvalues, the lowest of which is the ground state energy.

The system also has translational symmetry because of the periodic boundary conditions. This means that we can Fourier transform in terms of wavevectors k . For this small system these can be written directly as a new basis, which for the $S_T^z = 0$ subspace has the form

$$\begin{aligned}\phi_1 &= \frac{1}{\sqrt{2}}(|+-+ - > +|-+-+ >) & k = 0 \\ \phi_2 &= \frac{1}{\sqrt{2}}(|+-+ - > -|-+-+ >) & k = \pi \\ \phi_3 &= \frac{1}{2}(|++- - > +|-++- > +|--++ > +|+-- + >) & k = 0 \\ \phi_4 &= \frac{1}{2}(|++- - > +i|-++- > -|--++ > -i|+-- + >) & k = \frac{\pi}{2} \\ \phi_5 &= \frac{1}{2}(|++- - > -|-++- > +|--++ > -|+-- + >) & k = \pi \\ \phi_6 &= \frac{1}{2}(|++- - > -i|-++- > -|--++ > +i|+-- + >) & k = \frac{3\pi}{2}\end{aligned}$$

with similar states for the $S_T^z = \pm 1$ subspace. (The $S_T^z = \pm 2$ subspaces only have one state in so this is automatically a $k = 0$ state.)

Note that these states are of the form

$$\phi = \frac{1}{\sqrt{N_T}} \sum_j e^{ikj} (T)^j \psi$$

where ψ is one of original basis states, T translates by 1 unit and N_T is the number of distinct states which are related to ψ by translation. This greatly reduces the size of the matrix to be diagonalised. One can also make use of the reflection symmetry to create a basis whose states have only real coefficients, e.g. $(\phi_4 + \phi_6)$ and $i(\phi_4 - \phi_6)$ instead of ϕ_4 and ϕ_6 , which enables the Hamiltonian matrix have purely real entries and thus be easier to handle numerically. The ground state wave function is given by “ $\phi = (\sqrt{2}\phi_1 - \phi_3)/\sqrt{3}$, which gives an overall ground-state energy eigenvalue of -4 .”

8.3 Results in 1D

In Table 8.1 and Fig. 8.1 we show the results that Bonner and Fisher obtained for the ground state energy per atom of the Heisenberg antiferromagnetic chain using this method. (Note the factor of 2 in Eq. (8.1).) As can be seen the results extrapolate very accurately as straight lines when plotted as a function of $\frac{1}{N^2}$ rather than $\frac{1}{N}$. Also note the separate lines for chains with odd and even numbers of atoms, both of which converge to the exact value of $\frac{1}{2} - 2 \ln 2$ as $N \rightarrow \infty$.

Clearly the results in this case where the exact result is known are very good, and for other 1D systems which are not exactly soluble the results are generally excellent.

Table 8.1 Finite-size results for the ground-state energy of spin-half Heisenberg chains of (odd/even) length N with periodic boundary conditions (note the factor of 2 compared to earlier results of Bethe Ansatz)

N	Even	N	Odd
4	-1.00000	3	-0.50000
6	-0.93425	5	-0.74721
8	-0.91277	7	-0.81577
10	-0.90309	9	-0.84384
12	-0.8979	11	-0.85799
∞	-0.88629	∞	-0.88629

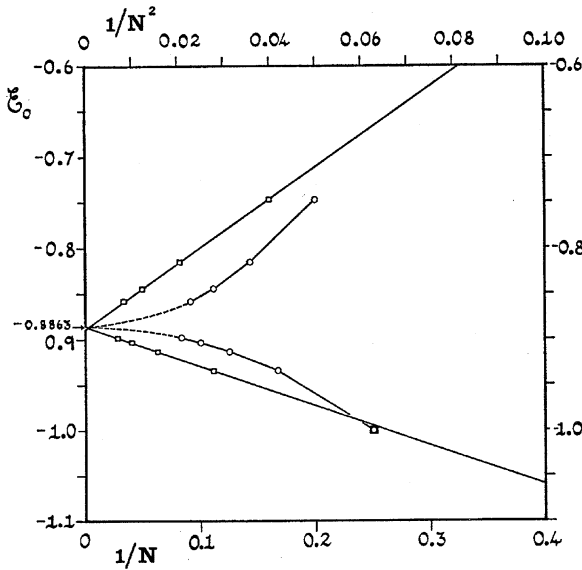


Fig. 8.1 Bonner and Fisher’s [1] original figure for the ground state energy of the linear Heisenberg antiferromagnetic chain. (Antiferromagnetic ground-state energies versus $1/N$ (circles) and versus $(1/N)^2$ (squares) for pure Heisenberg rings ($\gamma = 1$).) (Reprinted with permission from Bonner and Fisher [1]. Copyright 1964 by the American Physical Society)

Because all the eigenvalues can be calculated for small systems of size N it is quite straightforward to calculate the partition function:

$$Z_N = \sum_i e^{-\beta E_i},$$

and from this we can calculate any other thermodynamic quantity such as specific heat. Bonner and Fisher’s result is shown in Fig. 8.2. As can be seen the convergence is good for $T \gtrsim 1$.

At the time of Bonner and Fisher’s paper there were very few $T \neq 0$ results available, even for $S = \frac{1}{2}$. Later work by Yang and Yang (1966) [2-4] and Takahashi (1971) [5] enabled some of these quantities to be calculated exactly using the Bethe Ansatz for the $S = \frac{1}{2}$ chains. The numerical method is much more general, however,

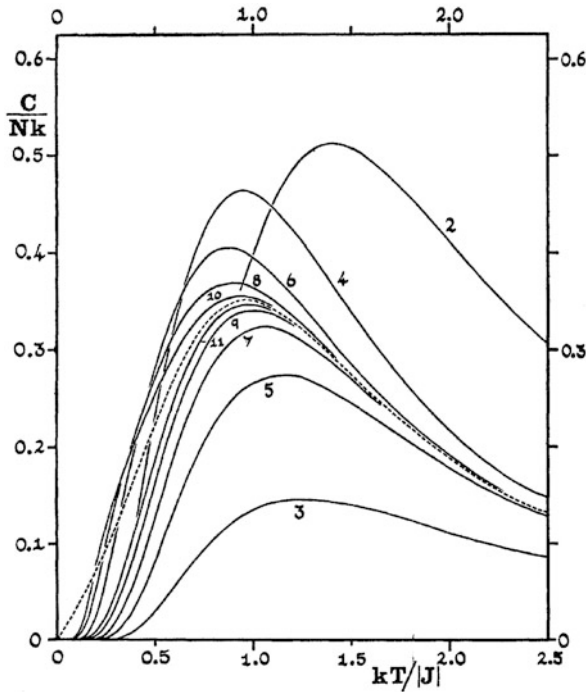


Fig. 8.2 Bonner and Fisher's [1] original figure for the specific heat of the linear Heisenberg anti-ferromagnetic chain. (Variation of specific heat with temperature for anti-ferromagnetic Heisenberg chains: finite N , *solid lines*; estimated limit $N \rightarrow \infty$, *dashed line*.) (Reprinted with permission from Bonner and Fisher [1]. Copyright 1964 by the American Physical Society)

and works well for many of the systems mentioned at the beginning of this chapter, e.g. $S \geq 1$, for which the Bethe Ansatz method is not applicable.

Another important result which was confirmed by this method is the existence of an energy gap between the ground state and the first excited state of linear chains with an isotropic Heisenberg interaction. This gap is known to be zero, i.e. there is no gap, in the limit $N \rightarrow \infty$ for $S = \frac{1}{2}$. However, in 1982 Haldane [6, 7] predicted that for $S = 1$ (and any other integer value of S) the gap would be non-zero. Haldane's method involved a transformation of the chain of separate atoms into a continuum limit and then using field theoretical methods. He was not able to prove the result exactly and initially people were surprised and somewhat sceptical.

However numerical results by Botet and Jullien (1983) [8], using the above techniques rapidly produced evidence that the result was correct. Figure 8.3 is from Parkinson and Bonner (1985) [9] and gives results for longer chains. If the gap for $S = 1$ were zero then the points would have to lie on a curve similar to the one shown with dots and dashes, which seems unlikely.

Much later, in 1993, the value of the gap in energy was obtained to very great accuracy by the density matrix renormalisation group method (DMRG) by White

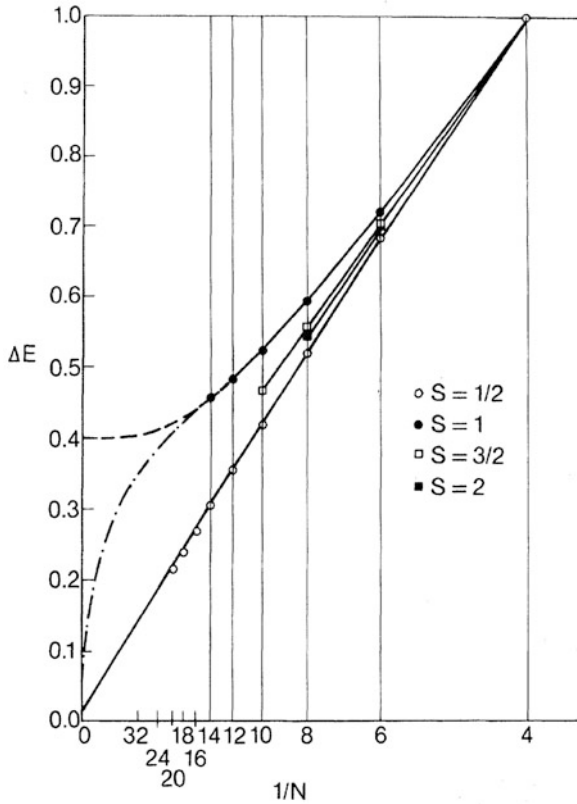


Fig. 8.3 Plot of the energy gap of the linear Heisenberg antiferromagnetic chain for different S

and Huse [10] and the value is 0.4105(1) in units of the exchange J . The DMRG is another quite different numerical technique which works extremely well in 1D but is not easy to extend to 2D.

This non-zero gap for integer spin S is evidence of a completely different type of ground state which is disordered and has correlations which decay exponentially. The systems with $S = \text{integer} + \frac{1}{2}$ including the Bethe Ansatz soluble case $S = \frac{1}{2}$ are believed to have ordered ground states in which correlations decay algebraically.

8.4 Results in 2D

As mentioned earlier, the method can be used in 2D. For a square lattice one can choose small square sections containing N atoms and with periodic boundary conditions. If the square section has sides parallel to the axes of the square then the number of suitable square sections is five, namely 2×2 , 3×3 , 4×4 , 5×5 and 6×6 . 6×6 would have $N = 36$, and which is almost at the limit of what can be

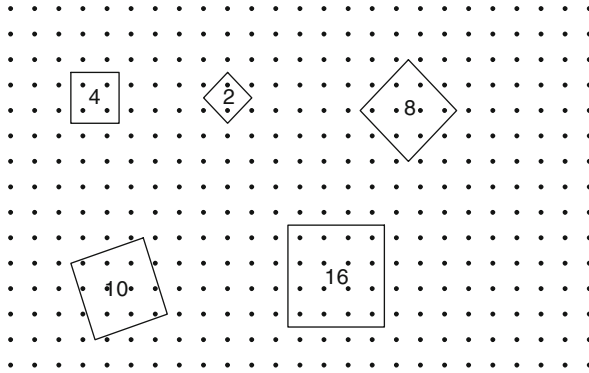


Fig. 8.4 Square sections of an infinite square lattice with $N = 2, 4, 8, 10, 16$ which would tile the entire lattice if repeated indefinitely

handled numerically for the ground state, e.g., via the Lanczos method. However, an ingenious way around this, introduced by Oitmaa and Betts (1977) [11], is to use square sections with periodic boundary conditions where the edges of the square are not parallel to the axes. This is shown in Fig. 8.4 for sections with $N = 2, 4, 8, 10$ and 16. Similar constructions are also available for $N = 18, 20$, etc. Using these one can plot the ground state energy and other quantities as a function of $1/N$ or $1/N^2$ just as for 1D systems.

The limiting factor in all of these calculations is the very rapid growth in the size of the basis as N increases. For $S = \frac{1}{2}$ systems the number of basis states is 2^N so for $N = 20$, $2^{20} = 1048576$. For $S = 1$ number of states is 3^N etc. The matrices are somewhat smaller than this because of translational symmetry and reflection symmetry in 1D and also rotational symmetry in 2D. Nevertheless, the largest values of N that can be fully diagonalised in 1D are approximately of order 20 for $S = \frac{1}{2}$, 14 for $S = 1$ and 10 for $S = \frac{3}{2}$. In 2D the maximum N are slightly greater because there is more symmetry but, of course, it is \sqrt{N} which determines the size of the section in 2D and this is much smaller. Larger systems may be considered for partial diagonalisation, e.g., for the ground state and low-lying excited states. Indeed, results of numerical finite-size calculations for the ground states of 2D antiferromagnets (referred to also as “exact diagonalisations”) are presented in the final chapter of this book. It is clear that in 3D lattices one cannot use large enough sections for the method to be useful at the moment.

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