COMPUTATIONAL QUANTUM MAGNETISM

Boulder 2003 Summer School

Introduction- The Style and Goal of These Lectures

The goal of these lectures is to describe three computational approaches to quantum magnetism. At the same time, by illustrating these techniques with applications to the Heisenberg and Hubbard Hamiltonians, we will learn some of the underlying physics of two of the most fundamental models in the field. We will begin with exact diagonalization. Next we will examine world line Quantum Monte Carlo (QMC), and, finally, determinant QMC.

This is a lot of ground to cover. My intent is to provide the implementation of the methods, with, in the case of the QMC methods, a minimum of emphasis on proving why they work. We will limit ourselves to establishing plausibility, and leave the very important issue of rigorous justification to those who are interested in this deeper level of understanding.

Because we do not have extensive computational facilities here, I am not providing codes for you to examine and play around with. However, I will provide a fairly complete description of the key elements ('subroutines') involved in the construction of such codes. And, of course, I welcome any questions you have about implementing the algorithms.

No description of a technique for solving problems is complete without an assessment of its limitations. Thus, a final goal is for you to have an appreciation of the *weaknesses* of computational approaches to complex many body quantum problems, as well as their strengths.

Lecture I- Exact Diagonalization

A. Some Review

In this first lecture I will introduce the two most commonly used lattice models of quantum magnetism, the Heisenberg and Hubbard Hamiltonians, and the most straightforward of all methods for solving such many body problems: exact diagonalization. In doing this, we will learn a bit of their basic physics and the relation between them. This lecture will also then serve as an essential introduction to Lectures II and III which deal with Quantum Monte Carlo (QMC) approaches.

The Heisenberg and Hubbard models have finite dimensional Hilbert spaces when considered on finite lattices. The basic idea of the exact diagonalization method is extremely simple: We choose a basis, enumerate all the states, figure out the associated matrix of H and then call some (canned) routine to diagonalize it. With the eigenstates in hand we can compute all the properties of the system exactly, with no error bars. We can also easily get the properties as a function of temperature (thermodynamics) and even as a function of time (dynamics). Sound too good to be true? We'll see what the drawback is shortly.

Let's start by establishing/reviewing some notation. We learn in our early quantum mechanics courses that the commutation relations of the angular momentum operators constrain the values of the square of the total angular momentum $S^2 = S_x^2 + S_y^2 + S_z^2$ and its components. The eigenvalues of S^2 are restricted to $j(j+1)$ with $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ (Here, and throughout these notes, I will set $\hbar = 1$.) For a given j, the eigenvalues of S_x, S_y, S_z are $m = -j, -j+1, ... + j$. Because the different components do not commute, we can only specify the eigenvalue of one of them. It is usual to select S_z as the preferred component, and to denote by $|j, m\rangle$ the associated eigenstates:

$$\begin{aligned} S^2 \ |j,m\rangle &= j(j+1) \ |j,m\rangle \\ S_z \ |j,m\rangle &= m \ |j,m\rangle. \end{aligned} \tag{1}$$

Rather than working with S_x and S_y directly, it is useful to introduce linear combinations, the raising and lowering operators,

$$\begin{aligned} S_+ &= S_x + iS_y \\ S_- &= S_x - iS_y, \end{aligned} \tag{2}$$

whose action on the states is

$$\begin{aligned} S_+ \ |j,m\rangle &= \sqrt{j(j+1) - m(m+1)} \ |j, m+1\rangle \\ S_- \ |j,m\rangle &= \sqrt{j(j+1) - m(m-1)} \ |j, m-1\rangle. \end{aligned} \tag{3}$$

Because the operators do not change j, it is conventional to drop reference to it and denote $|j, m\rangle$ more simply by $|m\rangle$. We will also specialize to the case of spin-$\frac{1}{2}$ where the

messy square roots reduce to unity, and simplify further the notation for the two choices $|m\rangle$ from $|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ to $|+\rangle$ and $|-\rangle$. In this compact notation we have, $S_+|-\rangle = |+\rangle$, $S_-|+\rangle = |-\rangle$. Of course, $S_+|+\rangle = 0$ and $S_-|-\rangle = 0$ as well.

Let's first consider a single quantum spin interacting with an external field $\vec{B}$. We may choose our z axis to be along the field direction so that $\vec{B} = B\hat{z}$, so the Hamiltonian is,

$$H = -\vec{B} \cdot \vec{S} = -BS_z. \tag{4}$$

The two states $|+\rangle$ and $|-\rangle$ are eigenstates of H with eigenvalues $E_\lambda = \pm B/2$:

$$H|\pm\rangle = \pm B/2|\pm\rangle. \tag{5}$$

The partition function is

$$Z = \sum_\lambda e^{-\beta E_\lambda} = 2\cosh(\beta B/2). \tag{6}$$

The magnetization is

$$\langle S_z\rangle = Z^{-1}\sum_\lambda \langle\lambda|S_z|\lambda\rangle e^{-\beta E_\lambda} = \frac{1}{2}\tanh(\beta B/2), \tag{7}$$

and the magnetic susceptibility

$$\chi = \frac{d\langle S_z\rangle}{dB} = \frac{1}{4}\beta\ [\cosh(\beta B/2)]^{-2}. \tag{8}$$

Notice that $\chi \propto 1/T$ as $T \to 0$, the familiar 'Curie law' which describes the magnetic susceptibility of an isolated magnetic atom.

B. Exact Diagonalization of the Heisenberg Model

The Heisenberg model describes a set of quantum mechanical spins localized on a set of sites i, and interacting on neighboring sites $\langle ij\rangle$ through inter-atomic exchange,

$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j. \tag{9}$$

Other lecturers will discuss the physical origin of this interaction, as well as typical values of J for different materials.

Let's consider the two site Heisenberg model,

$$H = J\,\vec{S}_1 \cdot \vec{S}_2 = J\,[S_{1,x}S_{2,x} + S_{1,y}S_{2,y} + S_{1,z}S_{2,z}] = J\,[\frac{1}{2}(S_{1,+}S_{2,-} + S_{1,-}S_{2,+}) + S_{1,z}S_{2,z}] \tag{10}$$

There are four states in the Hilbert space, since each z component can take on one of two values. We will denote these by $|S_{1,z}S_{2,z}\rangle = |++\rangle$, $|--\rangle$, $|+-\rangle$, $|-+\rangle$.

Before solving the two site Heisenberg model by constructing the matrix for H and diagonalizing, we'll get the answer with a trick. We write,

$$H = J\,\vec{S}_1 \cdot\ \vec{S}_2 = \frac{1}{2}J\,[(S_1 + S_2)^2 - S_1^2 - S_2^2]. \tag{11}$$

We can replace S_1^2 and S_2^2 with a *constant* $j(j+1) = \frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$, since these operators give the same value on all states in the Hilbert space. Now we know that $S_1 + S_2$ can take the two possible values $S_1 + S_2 = 0, 1$ when we add two spin-$\frac{1}{2}$ angular momenta. The choice $S_1 + S_2 = 1$ is three-fold degenerate, corresponding to $S_{1z} + S_{2z} = -1, 0, 1$. We conclude that the eigenvalues of H are $\frac{1}{2}J[1(1+1) - \frac{3}{4} - \frac{3}{4}] = +\frac{1}{4}J$ (three-fold degenerate) and $\frac{1}{2}J[0(0+1) - \frac{3}{4} - \frac{3}{4}] = -\frac{3}{4}J$ (nondegenerate).

Constructing the matrix of H and diagonalizing yields the same result.

$$\begin{aligned} H|++\rangle &= +\frac{1}{4}J\,|++\rangle \\ H|--\rangle &= +\frac{1}{4}J\,|--\rangle \\ H|+-\rangle &= -\frac{1}{4}J\,|+-\rangle + \frac{1}{2}J\,|-+\rangle \\ H|-+\rangle &= -\frac{1}{4}J\,|-+\rangle + \frac{1}{2}J\,|+-\rangle. \end{aligned} \tag{12}$$

Thus the matrix for H (with the basis vectors in the order listed above) is

$$H = \frac{1}{4}J \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 2 \\ 0 & 0 & 2 & -1 \end{pmatrix}. \tag{13}$$

Two of our basis vectors, $|++\rangle$ and $|--\rangle$ are already eigenstates of H with eigenvalue $\frac{1}{4}J$. These are the states with $S_1 + S_2 = 1$ and $S_1^z + S_2^z = 1, -1$. We need to form symmetric and antisymmetric linear combinations of the other two to get the remaining eigenvectors: $\frac{1}{\sqrt{2}}\,(\,|+-\rangle + |-+\rangle\,)$ and $\frac{1}{\sqrt{2}}\,(\,|+-\rangle - |-+\rangle\,)$. These have eigenvalues $\frac{1}{4}J$ and $-\frac{3}{4}J$ respectively. Confirming our earlier analysis with the method using the square of the total spin, we find three eigenvectors of eigenvalue $\frac{1}{4}J$, and a single eigenvector of eigenvalue $-\frac{3}{4}J$. The 'singlet' is the ground state for $J > 0$ (antiferromagnetic coupling).

An external field $\vec{B} = B\hat{z}$ shifts the eigenvalues without changing the eigenvectors. This is obvious since $B\hat{z}$ couples to $S_{z,\mathrm{tot}} = S_{z,1} + S_{z,2}$ which commutes with H. The degeneracy of the triplet is lifted, with the eigenvalues becoming $\frac{1}{4}J \to \frac{1}{4}J - B, \frac{1}{4}J, \frac{1}{4}J + B$, while the singlet eigenvalue is unaltered. The magnetic susceptibility χ now depends very differently depending on whether the ground state is the singlet ($J > 0$, antiferromagnetic) or the triplet ($J < 0$, ferromagnetic). In the latter case we still have the Curie law as T is lowered, while in the former case χ vanishes as $T \to 0$. Singlet formation and the suppression of the magnetic susceptibility is a commonly occuring feature of Hamiltonians like the Heisenberg, Hubbard, and Periodic Anderson Models, with fascinating links to the Mott metal-insulator transition and other phenomena.

It is amusing that the four site Heisenberg model is also amenable to an analysis through examining the squares of the angular momentum. We note,

$$H = J\,[\vec{S}_1\cdot\vec{S}_2 + \vec{S}_2\cdot\vec{S}_3 + \vec{S}_3\cdot\vec{S}_4 + \vec{S}_4\cdot\vec{S}_1] = \frac{1}{2}J\,[\,(\vec{S}_1+\vec{S}_2+\vec{S}_3+\vec{S}_4)^2 - (\vec{S}_1+\vec{S}_3)^2 - (\vec{S}_2+\vec{S}_4)^2\,] \tag{14}$$

The possible values of $S_1 + S_3$ are $0, 1$ and likewise for $S_2 + S_4$. When $S_1 + S_3 = 0$ and $S_2 + S_4 = 0$ are combined we get a single total spin $S_1 + S_3 + S_2 + S_4 = 0$ state. Putting together $S_1 + S_3 = 1$ and $S_2 + S_4 = 0$ yields three $S_1 + S_3 + S_2 + S_4 = 1$ states, as does combining $S_1 + S_3 = 0$ and $S_2 + S_4 = 1$. Adding $S_1 + S_3 = 1$ and $S_2 + S_4 = 1$ yields one $S_1 + S_3 + S_2 + S_4 = 0$ state, three $S_1 + S_3 + S_2 + S_4 = 1$ states, and five $S_1 + S_3 + S_2 + S_4 = 2$ states.

In the sector formed by putting together $S_1 + S_3 = 0$ and $S_2 + S_4 = 0$, the eigenvalue is $\frac{1}{2}J[0(0+1) - 0(0+1) - 0(0+1)] = 0$. In the sector formed by putting together $S_1 + S_3 = 1$ and $S_2 + S_4 = 0$, the (three) eigenvalues are $\frac{1}{2}J[1(1+1) - 1(1+1) - 0(0+1)] = 0$. The same holds for the sector formed by putting together $S_1 + S_3 = 0$ and $S_2 + S_4 = 1$. In the sector formed by putting together $S_1 + S_3 = 1$ and $S_2 + S_4 = 1$, the eigenvalues are $\frac{1}{2}J[2(2+1) - 1(1+1) - 1(1+1)] = J$ for the five total spin 2 states, $\frac{1}{2}J[1(1+1) - 1(1+1) - 1(1+1)] = -J$ for the three total spin 1 states, and $\frac{1}{2}J[0(0+1) - 1(1+1) - 1(1+1)] = -2J$ for the spin 0 state.

The biggest cluster for which this specialized approach works is the four site case we just considered. In general one must resort to explicitly constructing and diagonalizing H. For four sites, the dimension of H is $2^4 = 16$. Enumerating the basis vectors $|S_{z,1}S_{z,2}S_{z,3}S_{z,4}\rangle$ in the order

$$|++++\rangle, |+++-\rangle, |++-+\rangle, |+-++\rangle, |-+++\rangle, |++--\rangle, |+-+-\rangle, |-++-\rangle,$$
$$|+--+\rangle, |-+-+\rangle, |--++\rangle, |---+\rangle, |--+-\rangle, |-+--\rangle, |+---\rangle, |----\rangle$$

yields

$$H = \frac{1}{4}J \begin{pmatrix}
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2 & -4 & 2 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 2 & -4 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4
\end{pmatrix} \tag{15}$$

The block structure of H is a consequence of the fact that H commutes with $S_{z,\mathrm{tot}}$, the blocks above corresponding to $S_z^{\mathrm{tot}} = 2, 1, 0, -1, -2$. The maximum block dimension is six, and occurs for $S_z^{\mathrm{tot}} = 0$. Taking advantage of the block structure of the matrix for H in calling the diagonalization routine speeds up the computation of the eigenvalues

and eigenvectors significantly. Other symmetries like the commutation of H with $S^2_{\rm tot}$, and momentum (translation invariance) can further reduce the size of the blocks, but also significantly increase the complexity of the construction of H.

It becomes awkward to compute the matrix elements by hand as the number of sites grows. Writing a program to get the matrix elements is, however, very simple. The basic ingredients are (i) a convention for numbering the states, that is, a function which computes the state number n given the z components of spin on all sites, $\{S^i_z\}$; and (ii) a function which reverses the process and gets $\{S^i_z\}$ given the state number n. One possible choice is:

$$n = 1 + \sum_i 2^{i-1}\ (S_{z,i} + \frac{1}{2}). \tag{16}$$

with the inversion formulae,

$$\begin{aligned} S_{z,1} &= -\tfrac{1}{2} + \mathrm{mod}[n-1, 2] \\ S_{z,2} &= -\tfrac{1}{2} + \mathrm{mod}[\tfrac{1}{2}(n-1-(S^1_z+\tfrac{1}{2})), 2] \\ S_{z,3} &= -\tfrac{1}{2} + \mathrm{mod}[\tfrac{1}{4}(n-1-(S^1_z+\tfrac{1}{2})) - 2(S^2_z+\tfrac{1}{2})), 2] \end{aligned} \tag{17}$$

etc.

The construction of the matrix for the Hamiltonian then proceeds by looping through the states n, computing the associated spin configuration, and looking at all pairs $\langle i,j\rangle$ of neighboring sites to see if spins are antiparallel. If they are, the spins are exchanged and the new state number n' is computed. The entries $H(n,n')$ and $H(n',n)$ are then set to $\frac{1}{2}J$. From the spin configuration the diagonal entry is also obtained by computing the sum of $S_{z,i}S_{z,j}$ for all pairs $\langle ij\rangle$. Once H is constructed, a standard matrix diagonalization routine can be called.

The procedure outlined above does not put the matrix in block diagonal form. That is, the states with the same $S_{z,\rm tot}$ are not adjacent. However, pulling out the different blocks, or constructing the sub-blocks of H with similar procedures is straightforward.

It should be clear that many interesting variations of the Heisenberg model are easily studied once a Heisenberg code has been written. For example, implementing the XXZ Hamiltonian, in which the coupling J_z between the z components of spin and the coupling J_{xy} between the x and y components of spin are allowed to be different, is simply a matter of multiplying the off diagonal elements of H by the ratio J_{xy}/J_z. Adding a next nearest neighbor interaction J_2 involves using the same construction, but looking at different pairs of sites to exchange up and down spins. Likewise, to include an external magnetic field in the z direction involves adding an additional term to the diagonal elements of H.

C. The Heisenberg Model- Measuring Correlation Functions

The eigenstates and eigenvalues determine all physical observables. The average energy is especially trivial since it only involves the eigenvalues,

$$\begin{aligned} \langle E \rangle &= Z^{-1} \sum_\lambda E_\lambda e^{-\beta E_\lambda} \\ Z &= \sum_\lambda e^{-\beta E_\lambda}. \end{aligned} \tag{18}$$

Quantities which are diagonal in the S_z basis are also straightforward. Let us denote by c_λ^n the coefficients of the expansion of eigenvector $|\lambda\rangle$ in the basis state $|n\rangle$. (These are commonly returned by canned routines as the columns of the matrix which diagonalizes H.) Then for example,

$$\langle\, S_{z,i} S_{z,j} \,\rangle = Z^{-1} \sum_\lambda \langle\lambda|\, S_{z,i} S_{z,j} \,|\lambda\rangle\; e^{-\beta E_\lambda} = Z^{-1} \sum_\lambda \sum_n |c_\lambda^n|^2 \,\langle n|\, S_{z,i} S_{z,j} \,|n\rangle\; e^{-\beta E_\lambda}. \tag{19}$$

The matrix elements $\langle n|\, S_{z,i} S_{z,j} \,|n\rangle$ are obtained using the same function identifying the spin components $\{S_{z,i}\}$ of a state $|n\rangle$ which was used to construct H.

Expectation values of non-diagonal operators are slightly more complex. For example

$$\langle\, S_{+,i} S_{-,j} \,\rangle = Z^{-1} \sum_\lambda \langle\lambda|\, S_{+,i} S_{-,j} \,|\lambda\rangle\; e^{-\beta E_\lambda} = Z^{-1} \sum_\lambda \sum_n \sum_m c_\lambda^m c_\lambda^n \langle n|\, S_{+,i} S_{-,j} \,|m\rangle\; e^{-\beta E_\lambda} \tag{20}$$

The matrix elements $\langle n|\, S_{+,i} S_{-,j} \,|m\rangle$ can be obtained using both the function identifying the spin components $\{S_{z,i}\}$ and also the function which computes the new state $|m\rangle$ obtained by the action of $S_{+,i} S_{-,j}$ on $|n\rangle$.

In constructing an exact diagonalization code it is advisable to check a few quantities which should be equal by symmetry, for example on a 2-d square lattice $\langle S_{z,i} S_{z,i+\hat{x}} \rangle$ and $\langle S_{z,i} S_{z,i+\hat{y}} \rangle$. My experience is that a vast majority of coding errors are caught by this simple check. It is also often useful to compute the expectation value of the energy using the expectation value of all the operators in H and combining them, and comparing to the simple expression Eq. (18) obtained from the eigenvalues alone.

The obvious drawback of the exact diagonalization approach is the system size it is able to handle. Even using symmetries of the Hamiltonian, the matrix to be diagonalized grows exponentially with the number of sites. Typically, diagonalization methods are limited to a few tens of lattice sites, where the exact number is determined by the number of possible values of the degrees of freedom at each site (and the effort the programmer is willing to make!). On such small lattices, most of the lattice sites are on the surface of the cluster, and so it is important to use periodic (or anti-periodic) boundary conditions to reduce the finite size effects.

To explore the systematic effects of the restriction to finite size it is useful to be able to compare results on lattices of different extent. One trick to facilitate this is to consider non-standard tilings. For example, rather than considering only 2x2, 3x3, 4x4, ... lattices, one can tile the 2-d square lattice with other configurations such as groups of eight sites,

$$\begin{array}{ccccc} & & A & B & \\ C & D & E & F & \\ & G & H & & \end{array} \tag{21}$$

as follows:

$$\begin{array}{ccccccccc} & & & & A & B & & & \\ & & & C & D & E & F & & \\ & & A & B & G & H & A & B & \\ C & D & E & F & C & D & E & F & \\ & G & H & A & B & G & H & & \\ & & C & D & E & F & & & \\ & & & G & H & & & & \end{array} \tag{22}$$

This construction corresponds to dividing the 2-d lattice into $\sqrt{8}$ by $\sqrt{8}$ squares whose axes are rotated with respect to the grid lines defining the array of sites. Notice that the natural connections which implement periodic boundary conditions can be seen from the picture. For example, site B has neighbors C (above), A (left), G (right) and E (below).

A further reason for looking at these oddly shaped lattices in two dimensions has to do with special symmetries of the 4x4 lattice which is frequently studied in 2-d exact diagonalization. It is easy to verify that the 4x4 lattice has the same connectivity as the 2x2x2x2 lattice in four dimensions. That the 4x4 lattice has unusual properties can be illustrated by the observation that correlation functions between observables separated by $\hat{x} + \hat{y}$ are identical to those separated by $2\hat{x}$ or $2\hat{y}$!

D. The Heisenberg Model- A Few Results

These lectures are mostly about the methodology for studying quantum magnetism numerically. However, a few results are useful for illustration.

Figure 1 shows the specific heat of the 1-d Heisenberg model as determined by exact diagonalization. In order to get a feeling for various finite size effects, we compare results for $N = 4$, $N = 8$, and $N = 12$ sites. The differences between $N = 8$ and $N = 12$ are relatively minor. In one dimension, $\langle E \rangle$ and C can be computed exactly in the thermodynamic limit using the Bethe Ansatz. If one compares to this method, one finds that the $N = 12$ values are very close to $N = \infty$, as the match between $N = 8$ and $N = 12$ already suggests might be the case. Careful inspection of Fig. 1 reveals that much of the dependence of C on N occurs at low temperatures. This is a consequence of the fact that on a finite lattice there is a discrete energy spectrum and hence a finite gap between the ground and excited states. This gap results in exponential dependence of observables on temperature, in contrast with the power law behavior which might result, for example, from the existence of ungapped spin wave excitations.

It is a general feature of finite cluster calculations that measurements which involve local correlations are usually quite accurately obtained even on small lattices. Unfortunately, one

is often interested in long range order, and hence in the asymptotic behavior of operators separated by large distances. Exact diagonalization has little to say about these issues.

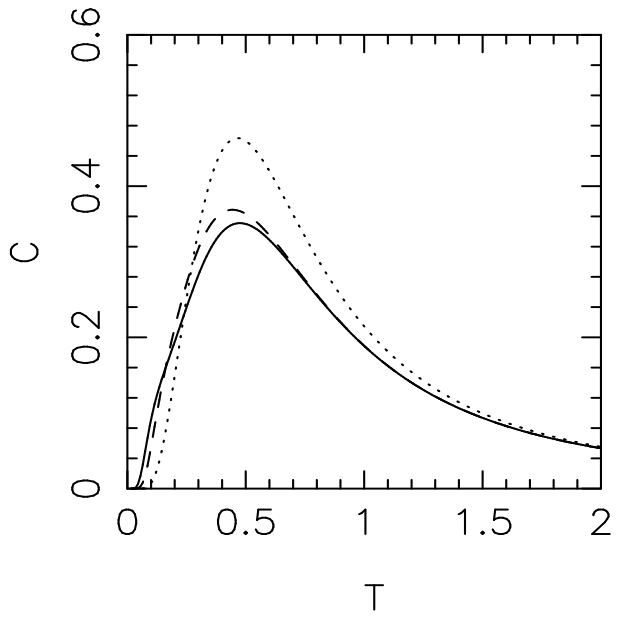

FIG. 1: The specific heat per site of the 1-d Heisenberg model for $N = 4$ (dotted line), $N = 8$ (dashed line), and $N = 12$ (full line). Here $J = 1$.

E. Exact Diagonalization of the Hubbard Model

The Heisenberg Hamiltonian describes a set of localized magnetic moments interacting via an exchange coupling. The Hubbard Hamiltonian, on the other hand, models *itinerant* electrons,

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{23}$$

Here the operators $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ create or destroy, respectively, an electron of spin σ at site i. The operators $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ count the number of electrons of spin σ at site i.

We will provide a lot less detail for the exact diagonalization procedure of the Hubbard model, since much of the commentary above for the Heisenberg model can be carried over.

We begin by considering the two site Hubbard model, whose Hilbert space has dimension sixteen. Consider the largest subspace, the sector with one spin up and one spin down electron. We denote by $|\uparrow\downarrow \quad 0\rangle, |0 \quad \uparrow\downarrow\rangle, |\uparrow \quad \downarrow\rangle$, and $|\uparrow \quad \downarrow\rangle$, the state with a spin up electron and a spin down electron on site 1, and site 2 empty; the state with a spin up electron and a spin down electron on site 2, and site 1 empty; the state with a spin up on site 1 and a spin down electron on site 2; and the state with a spin up on site 2 and a spin down electron on site 1, respectively.

It is easy to see that the associated matrix for the Hamiltonian is

$$H = \begin{pmatrix} U & 0 & -t & -t \\ 0 & U & -t & -t \\ -t & -t & 0 & 0 \\ -t & -t & 0 & 0 \end{pmatrix} \tag{24}$$

It is immediately obvious that two of the eigenvalues of H are 0 and U. Two others are $\frac{1}{2}(U \pm \sqrt{U^2 + 16t^2})$. If we expand the last two eigenvalues in t/U we get $-4t^2/U$ and $U + 4t^2/U$, and see the emergence of the energy scale $J = 4t^2/U$. The significance of J will be discussed further below.

The action of the kinetic energy term in the Hubbard model is very similar to that of the exchange term $S_{+,i}S_{-,j} + S_{+,j}S_{-,i}$ of the Heisenberg model. So the same ideas that worked for the Heisenberg case for labeling the states and for getting occupations from the state number and *vice-versa* can be used here to constuct functions which compute the matrix elements automatically. One very important difference, though, is the existence of minus signs which arise from the anticommutation of the fermion operators on different sites. In one dimension, these minus signs can be eliminated for near-neighbor hopping with a choice of appropriate boundary conditions. Indeed, this is one way of understanding the existence of exact maps between fermions and quantum spins, like the Jordan-Wigner transformation, in 1-d. In 2-d, it is no longer possible to eliminate the minus signs.

We briefly discussed boundary conditions for the Heisenberg model. In one dimension, for the Hubbard model, it is sometimes useful to alternate periodic and antiperiodic boundary conditions for lattices of size $4n$ and $4n+2$. With that alternation, measured quantities monotonically approach the large spatial size limit rather than oscillating above and below the asymptotic value.

F. Relation to The Heisenberg Model

The Heisenberg model emerges as a limit of the Hubbard model when t/U is small. To see this, note that the sector of the two site Hubbard model with one up and one down spin, considered above, can be expandied to include all sectors with two electrons, by adding the states $|\uparrow\ \uparrow\rangle$, and $|\downarrow\ \downarrow\rangle$. These states are eigenstates of H with eigenvalue 0. All together, the two electron space of the two site Hubbard model has four 'small' eigenvalues $0, 0, 0$, and $\frac{1}{2}(U - \sqrt{U^2 + 16t^2}) \approx -4t^2/U$ and two 'large' ones U and $\frac{1}{2}(U + \sqrt{U^2 + 16t^2})$. The large eigenvalues are associated with eigenvectors whose components have significant mixtures of the states with doubly occupied sites. The existence of the two groups of states whose eigenvalues are separated by U is a reflection of the 'upper and lower Hubbard bands'. The 'Mott-Hubbard' gap in the spectrum gives rise to a metal-insulator transition. In the two site Heisenberg model we had three eigenvalues $J/4$ and one $-3J/4$. Apart from a trivial shift in energies, this is the same spectrum as that of the small eigenvalue sector of the Hubbard model, with the identification $J = 4t^2/U$.

G. The Hubbard Model- A Few Results

Let's think about the commonly studied half-filled case of the Hubbard model when we have a density of electrons equal to the number of sites of the lattice. One of the central features of the Hubbard model is the existence of two energy scales: U controls the 'charge fluctuations' that is, the extent to which sites on the lattice can deviate from having precisely one electron each, while J controls the preference for neighboring sites to have antialigned as opposed to parallel spins.

The fluctuation in charge is often analyzed by looking at 'moment formation'. One defines the square of the z component magnetic moment on a site i by $\langle m_{z,i}^2 \rangle = \langle (n_{i,\uparrow} - n_{i,\downarrow})^2 \rangle = 1 - \langle n_{i,\uparrow} n_{i,\downarrow} \rangle$, where we have used the fact that the lattice is half-filled. The local moment is one for singly occupied sites and zero for doubly occupied or empty sites. The effect of U can be viewed either as a suppression of doubly occupied (and empty) sites, $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle \to 0$ or, equivalently, as the development of well defined moments $\langle m_{z,i}^2 \rangle \to 1$.

In Figure 2 we show $\langle m_{z,i}^2 \rangle$ as a function of temperature T for a four site Hubbard cluster with $t = 1$ and $U = 8$. We see that at a temperature scale set by U the local moment crosses over from its high temperature value $\langle m_{z,i}^2 \rangle = \frac{1}{2}$ to its low temperature value $\langle m_{z,i}^2 \rangle \approx 1$. The deviation of $\langle m_{z,i}^2 \rangle$ from unity at $T = 0$ is an effect of the 'quantum fluctuations' associated with finite U.

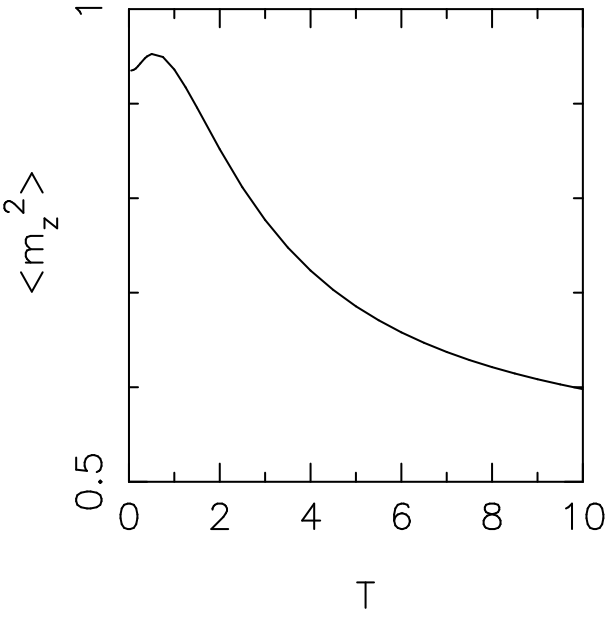

FIG. 2: Local moment of the Hubbard model for $N = 4$ sites. Here $t = 1, U = 8$ and the lattice is half-filled. The local moment develops at a temperature scale T set by U.

In Figure 3 we show the near neighbor spin correlations $\langle S_{z,1} S_{z,2} \rangle$ and next near neighbor spin correlations $\langle S_{z,1} S_{z,3} \rangle$ as a function of temperature T. Again we choose $t = 1$ and $U = 8$ on a half-filled lattice. We see that antiferromagnetic correlations set in on the smaller temperature scale T set by J. The tendency towards antiferromagnetism for the

half-filled Hubbard model is evident in the negative value of the near-neighbor and positive value of the next-near-neighbor spin correlations.

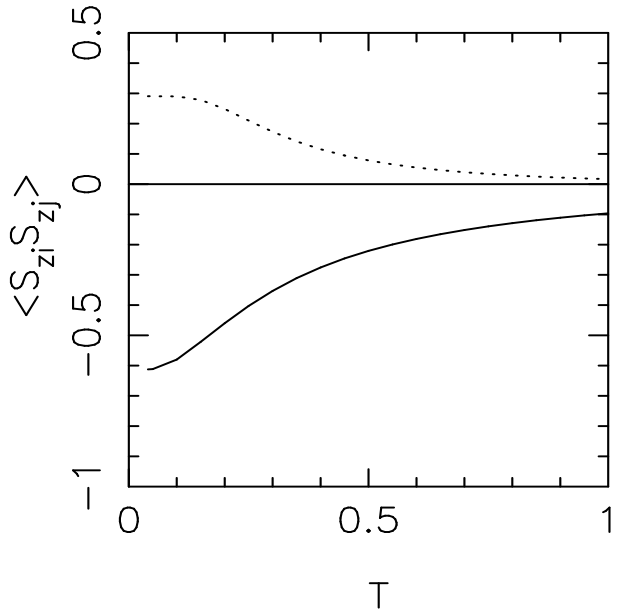

FIG. 3: Near-neighbor (full line) and next-near-neighbor (dotted line) spin correlations of the Hubbard model for $N = 4$ sites. Here $t = 1, U = 8$ and the lattice is half-filled. The correlations develop at a temperature scale T set by $J = 4t^2/U = 0.5$.

The question of whether the spin correlations are truly long ranged at $T = 0$ is highly nontrivial, and was settled partly through very careful Quantum Monte Carlo simulations. The analogous question of whether the doped Hubbard model, where the average density of electrons is not half-filled, has long range d-wave superconducting order is much less convincingly answered.

In lecture 3 we will see the specific heat of the half-filled Hubbard model and how it reflects both moment formation at $T \approx U$ and moment ordering at $T \approx J$.

H. Variations of Exact Diagonalization

A variant of the exact diagonalization method is the Lanczos algorithm, which allows you to work on somewhat larger lattices at the expense of yielding only the ground state eigenvector. Implementing the Lanczos algorithm involves acting with the matrix H on vectors, and therefore the procedure described above for constructing H also serves as the kernel for a Lanczos code. Variants of the Lanczos approach are available to look at some excited state properties.

The 'density matrix renormalization group' (DMRG) method is another very powerful method for ground state properties of many body systems. DMRG involves explicit diagonalization of finite dimensional Hilbert spaces, with the added inspiration of a systematic truncating of the Hilbert space as the system is 'grown' spatially.

I. Closing Thoughts

It is interesting how much of our insight into many body model Hamiltonians has been obtained by this most prosaic of all methods – exact diagonalization. Besides 'bread-and-butter' physics like antiferromagnetic correlations and the Mott-Hubbard gap, even rather subtle issues can be explored. Very early exact diagonalization studies of the two dimensional Hubbard model, for example, hinted at the possibility of phase separation of holes doped into the half-filled antiferromagnetic state. This result presaged the more recent picture of stripe formation which represents a more subtle, partial form of phase separation. And it is, of course, methods like DMRG which have been among our most powerful approaches to attacking this problem.

It is true too that exact diagonalization codes are vital stepping stones to other numerical methods like the Quantum Monte Carlo approaches to be described in the next two lectures. Exact diagonalization both provides hints as to the interesting physics to uncover, and also very valuable checks on the QMC codes themselves.

The weakness of exact diagonalization, on the other hand, is in the really quite small lattices, typically 10-20 sites, which one can study. For this reason, exact diagonalization is really only useful for problems in one and two dimensions. Even so, the accessible lattices are so limited in size, that scaling to extract the behavior in the thermodynamic limit is essentially hopeless. Quantum Monte Carlo simulations increase accessible lattice sizes by one or two orders of magnitude, and do much to alleviate this problem.