Saha Institute of Nuclear Physics
UGA Project Report

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Aim:
To model a simple quantum mechanical system, such as a Heisenberg spin chain, and study its properties.

Work done:

I wrote a program to model a chain of electrons using the $S = \frac{1}{2}$ Heisenberg spin chain model with Hamiltonian:

$H = J \sum_{n=0}^{N-1} S_i \cdot S_{i+1}$

where $S_i \cdot S_{i+1}$ can be expanded as a diagonal term $S_i^z \cdot S_{i+1}^z$ plus an off-diagonal term $\frac{1}{2}(S_i^+ \cdot S_{i+1}^- + S_i^- \cdot S_{i+1}^+)$. Here $S = S_x + iS_y$ and we use the periodic boundary condition. S_i^+, S_i^- and S_i^z are the spin $= \frac{1}{2}$ operators acting on the i^{th} site and $S_m^j (m = x, y, z)$ are related to the Pauli spin matrices as: $S_m^j = \frac{1}{2}\sigma_m^j$. They satisfy the following relations:

$$\left[S_j^z, S_{j'}^{\pm}\right] = \pm\delta_{jj'} \cdot S_j^{\pm} \quad , \quad [S_j^a, S_{j'}^b] = \delta_{jj'} \cdot \epsilon_{abc} S_j^c \quad , \quad a, b, c \in \{x, y, z\}$$

$$\{S_j^+, S_j^-\} = \mathbf{1} \quad , \quad \left[S_j^+, S_{j'}^-\right] = 0 \quad \text{for} \quad j \neq j' .$$

We can now operate the hamiltonian on any state using the relations that tell us the eigen vectors and eigen values of the $S^+, S^- S^z$ operators:

$S^+|\uparrow\rangle = 0, \quad S^-|\uparrow\rangle = |\downarrow\rangle, \quad S^z|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle$

$S^+|\downarrow\rangle = |\uparrow\rangle, \quad S^-|\downarrow\rangle = 0, \quad S^z|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle.$

The hamiltonian is generated by incorporating the contribution of both diagonal and off-diagonal terms after which it is diagonalized exactly as is later described and obtain its eigen vectors and eigenvalues from which numerous quantities of interest can be calculated.

The hamiltonian for an N electron long chain consists of a $2^N X 2^N$ matrix. The basis states can simply be labelled by a going from 0 to 2^{N-1}. These integers when represented in binary form the basis states where we use 1 and 0 to represent up and down spin respectively. The diagonal contribution of the hamiltonian is easily determined as:

$$\langle a|S_i^z S_{1+1}^z|a\rangle = \pm 1/4$$

where +0.25 is if corresponding bit pairs for a[i] and a[i+1] match; if they are different then the contribution is -0.25. The off- diagonal part of the hamiltonian operator, $\frac{1}{2}(S_i^+ \cdot S_{i+1}^- + S_i^- \cdot S_{i+1}^+)$, acts on some state $|a\rangle$ only if a[i] and a[i+1] don't match, to give a state $|b\rangle$ which has these two bits flipped: the matrix element is then:

$$\langle b|H|a\rangle = 1/2.$$

If, however a[i] matches a[i+1] there is no off-diagonal contribution at all. It is to be noted that as per the periodic boundary condition when we compare a[i] with a[i+1] the addition is modulo N, i.e a[N-1] is compared to a[0]. The code to generate the hamiltonian is given below:

```
//generates the hamiltonian matrix:
//written in java on bluej IDE
public class Hamiltonian
{ public void main(int n){
     int x=(int)Math.pow(2,n);
     double h[][]=new double[x][x];
     int arr[]=new int[n],b=0,k,a,i,c,t,sum=0;
     for(a=0;a<x;a++){
      c=a;
      for(i=0;i<n;i++){
           arr[n-1-i]=c%2;
           c/=2;}
      for(i=0;i<n-1;i++){
         b=(i+1)%n;
         if(arr[i]==arr[b])
         h[a][a]+=0.25;
         else
         h[a][a]-=0.25;}
      for(i=0;i<n;i++){
           b=(i+1)%n;
           k=arr[i];arr[i]=arr[b];arr[b]=k;
           for(t=0;t<n;t++){
    sum=sum+ (int)(Math.pow(2,n-1-t)*arr[t]);}
           if(sum!=a)
           {h[a][sum]=0.5;}
           sum=0;k=arr[i];arr[i]=arr[b];arr[b]=k;}}
     for(a=0;a<x;a++){
         for(b=0;b<x;b++){
             System.out.print(h[a][b]+", ");}
            System.outprintln();}}}
```

I wrote a program to generate the hamiltonian of the system and diagonalize it exactly thus finding the exact eigen vectors and eigen values. Using this it was possible to calculate and study the variation of several thermodynamic parameters such as specific heat of the chain.
We first perform the exact diagonalization of the hamiltonian matrix. Exact diagonalization of H can be done by finding a matrix U such that:

$$U^{-1}HU = E$$

where E is the exact diagonalized hamiltonian. Then U is the matrix whose column vectors are the eigenvalues of H. The expectation value of some operator (for any observable) A in an eigen state of H is given by the diagonal element of the corresponding matrix transformed to the energy basis:

$$\langle n|A|n\rangle = [U^{-1}AU]_{nn}.$$

Now the expectation value for any operator A can be found for example:

$$\begin{aligned} C &= \frac{d\langle H\rangle}{dt} = \frac{1}{T^2}\left(\langle H^2\rangle - \langle H\rangle^2\right) \\ \chi &= \frac{d\langle m_z\rangle}{dh} = \frac{1}{T}\left(\langle m_z^2\rangle - \langle m_z\rangle^2\right) \end{aligned}$$

which can be derived from the general expression:

$$\langle A\rangle = \frac{1}{Z}\sum_j \sum_{n=1}^{M_j} \mathrm{e}^{-\beta E_{j,n}}[U_j^{-1}A_jU_j]_{nn}, \quad Z = \sum_j \sum_{n=1}^{M_j} \mathrm{e}^{-\beta E_{j,n}}$$

Examples and Illustrations

We illustrate the above procedure for a 2 electron 'chain'. Considering an up spin to be represented by 1 and a down spin by 0, then we have 4 basis elements for the system: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$
now the hamiltonian matrix was generated by operating our hamiltonian: $H = J\sum_{n=0}^{N-1} S_i \cdot S_{i+1}$ as $\langle\psi_m|H|\psi_n\rangle$ for the cell at the m^{th} row and n^{th} column of the matrix representation of the hamiltonian; where ψ is a basis state.

Doing these operations, after expanding the hamiltonian into diagonal and off-diagonal terms, and putting the results into each of H[m,n] , gives us the following matrix:

$$\begin{pmatrix} 0.25 & 0 & 0 & 0 \\ 0 & -0.25 & 0.5 & 0 \\ 0 & 0.5 & -0.25 & 0 \\ 0 & 0 & 0 & 0.25 \end{pmatrix}$$

This is the matrix representation on the hamiltonian of the system. Now we can diagonalize this matrix, in principle by finding it's eigenvalues and eigen vectors by solving the equation: det[H-λ I]=0. However for large matrices this proves to be computationally inefficient and iterative algorithms to find some diagonalizing matrix U such that:

$$U^{-1}HU = E$$

exist, where E is the diagonalized hamiltonian and U is the matrix of eigen vectors. In the present case we diagonalize H using such a routine, giving E as:

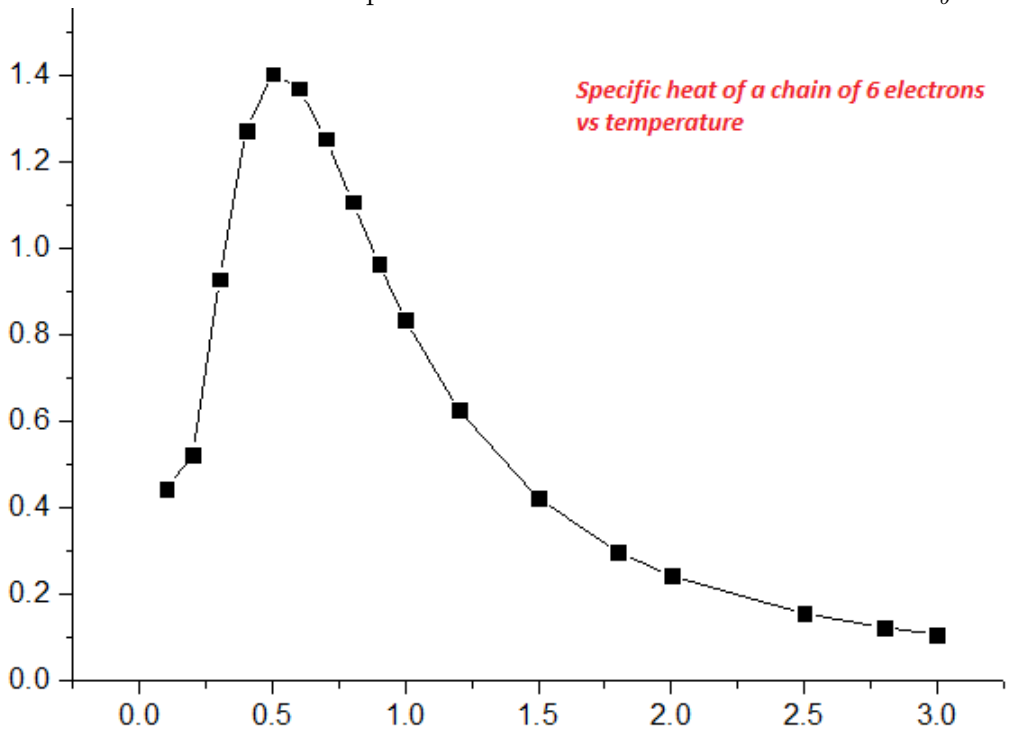
$$\begin{pmatrix} -0.75 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0.25 \end{pmatrix}$$

and we get 4 eigenstates: Three triplets $|00\rangle, |11\rangle, \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$ and one singlet state: $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ We can now show that these really are the eigenstates. as is expected we have got 3 states with S=1, because we have m=+1,0,-1 as allowed states but only 1 eigen state with S=0 (m=0 only allowed). We see that these eigenstates are built out of linear combinations of the basis states and we now verify analytically that they are indeed the eigenstates and determine their eigen values using the earlier stated formulae describing the action of the S_i^+, S_i^- and S_i^z operators. Here, as it is a two electron chain, i is just 1 and i+1 is just 2.

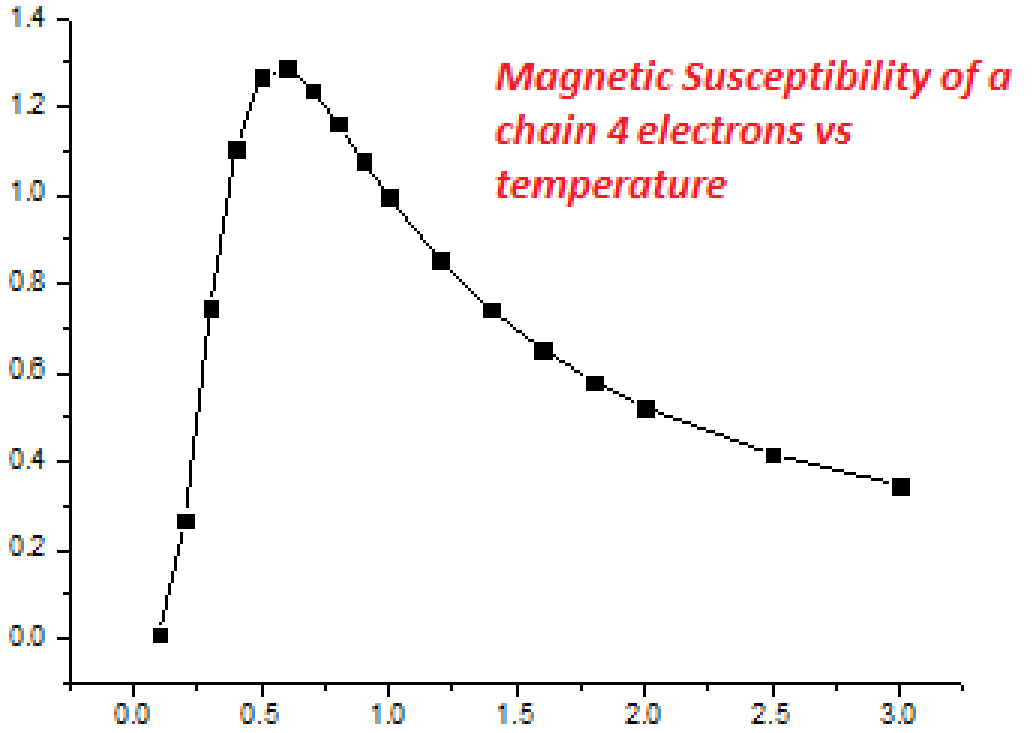
$H|11\rangle$
$= S_i \cdot S_{i+1}|11\rangle$
$= S_i^z \cdot S_{i+1}^z|11\rangle + \frac{1}{2}(S_i^+ \cdot S_{i+1}^-|11\rangle + S_i^- \cdot S_{i+1}^+|11\rangle)$
$= \frac{1}{2} \cdot 12|11\rangle + \frac{1}{2}(0+0)$

$= \frac{1}{4}|11\rangle$ Thus we have $|11\rangle$ as an eigen state with eigen value as $\frac{1}{4}$.

$H|00\rangle$
$= S_i \cdot S_{i+1}|00\rangle$
$= S_i^z \cdot S_{i+1}^z|00\rangle + \frac{1}{2}(S_i^+ \cdot S_{i+1}^-|00\rangle + S_i^- \cdot S_{i+1}^+|00\rangle)$
$= \frac{-1}{2} \cdot \frac{-1}{2}|00\rangle + \frac{1}{2}(0+0)$
$= \frac{1}{4}|00\rangle$
Thus we have $|00\rangle$ as an eigen state with eigen value as $\frac{1}{4}$.
Similarly one can calculate H $|01\rangle$ and H $|10\rangle$ to be $-0.25|01\rangle + 0.5|10\rangle$ and $-0.25|01\rangle + 0.5|10\rangle$ respectively. Thus $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ and $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ are shown to be eigen states too.
As discussed earlier, given the diagonalized hamiltonian we can calculate the expectation value for any operator. For example, some thermodynamic properties of the system were calculated, such as the specific heat of the chain. As an example we show the plot for a spin $= \frac{1}{2}$ Heisenberg chain where we have taken J = 1 in the expression for hamiltonian in units where $k_b = 1$:



Similarly the magnetic susceptibility of such chains could also be calculated. For example, we show below the plot of magnetic susceptibility vs temperature for a spin $= \frac{1}{2}$ Heisenberg chain where we have taken J $= 1$ in the expression for hamiltonian in units where $k_b = 1$:



It was noticed that both susceptibility and specific heat show peaks at the same temperature for the same chain. This can be rationalized as fluctuations in the system increase with temperature but after a critical temperature co-relation between measurements starts being lost causing any property related to a measure of fluctuations to fall off with increasing temperature.

Pseudocode:

Pseudocode for the program I wrote in Java on BlueJ IDE to generate the hamiltonian matrix for an n electron chain:textbf
DEF::
int flip(a,i,j,n): takes an integer a and flips the i'th and j'th bit in it's n bit

binary representation to return the resulting integer.
int bit(a,i,n): returns the i'th bit of the n bit binary representation of the integer a
H[,]: is a 2^n by 2^n matrix in which the hamiltonian will be stored

for a from 0 to $2^n - 1$

for i from 0 to n-1

j=(i+1) mod n

if bit(a,i,n) equals bit(a,j,n)
increment H[a,a] by 0.25

else
decrement H[a,a] by 0.25
set H[a,flip(a,i,j,n)]=0.5

For diagonalizing the output i.e the hamiltonian matrix, the eigen() routine of the statistical software package R was used.

Sources, References and Materials:

Under the guidance of my mentor I studied the initial chapters of *Modern Quantum Mechanics* by *J.J. Sakurai* as well as some statistical mechanics from *Statistical Mechanics* by *Kerson Huang*. Apart from these texts I studied a paper by Rigol and Dunjko, *Thermalization and it's Mechanism for Generic Isolated Quantum Systems*; that appeared in Nature vol.452, 17th April, 2008. I also referred to a set of notes provided by my mentor of Anders.W.Sandvik, Department of Physics, Boston University for the numerical work regarding programs to model the system using a Heisenberg spin chain.

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