Solving Heisenberg Spin-$\frac{1}{2}$ Chain using Lanczos Algorithm

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Abstract

In this project I am going to study one-dimensional Heisenberg Spin-$\frac{1}{2}$ chain for N lattice sites and solve for its ground state and first excited state. For this I am going to use *Lanczos algorithm* which transforms a big symmetric sparse matrix to small symmetric tri-diagonal matrix such that its smallest eigenvalues converges to that of our actual matrix. We shall see this problem for both open and periodic chain.

Contents

1 Introduction

Spin Chains are used to model magnetic system having its particle with spin magnetic moment in fixed lattice sites. In absence of magnetic field the electric interaction between the particles does not depend on their spins. However we can see materials with their spins ordered to achieve their ground states. It is because of indistinguishibility of the particles. As an example if we consider a system of spin-$\frac{1}{2}$ particles (electrons) the total wave function of the system must be anti-symmetric. Depending on its spin configuration, its spatial part can be symmetric or anti-symmetric to maintain that the system have a preferred energy state. For one dimensional chain the Hamiltonian which parameterize the ground state of the magnetic system is

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \vec{B} \cdot \sum_{i=1} \vec{S}_i \qquad ; i \neq j \tag{1}$$

where J is the exchange interaction strength, $\vec{B}$ is the external magnetic field and $\vec{S_i}$ (S_i^x S_i^y S_i^z) is the spin operator (Pauli operators multiplied by $\frac{\hbar}{2}$) acting on ith site. This is the *Heisenberg Spin-$\frac{1}{2}$ model*.

1.1 Heisenberg Spin-$\frac{1}{2}$ Chain

In absence of magnetic field and for the nearest spin interaction the spin Hamiltonian for N-site Heisenberg spin half Chain is

$$\mathcal{H} = \sum_{i=1}^{N-1} [J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z] \tag{2}$$

For a periodic chain $\vec{S}_N = \vec{S}_1$. If $J_x = J_y = 0$ the model is *Ising Model*. Here above Hamiltonian (2) is known as XYZ model as $J_x \neq J_y \neq J_z$. If $J_x = J_y \neq J_z$, it is XXZ model. We shall study XXX model where $J_x = J_y = J_z = J$ which is just the equation (1) with $\vec{B} = 0$. This model is particularly geared for magnetic insulators like the 3d-,4d-,4f-,5f-systems. For convenience we rewrite this in terms of hopping terms S^+,S^-.

$$\mathcal{H} = J \sum_{i=1}^{N-1} [\frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z] \tag{3}$$

where $S^{\pm} = (S^x \pm iS^y)$.

We see for $J > 0$ nearest particles having opposite spins give ground state. So the particle spins tend to be anti-parallel to their neighbours. The system is called *anti-ferromagnet*. It tends to the limit of half-filling state.($N_\uparrow = N_\downarrow = N/2$). However, the perfectly ordered neel state $|\uparrow\downarrow\uparrow\downarrow\rangle$ is not the ground state of the system. For $J < 0$ particle with same spin of neighbour give lower energy and the particle spins tend to be parallel with neighbour to achieve ground state. Then the system is *ferromagnet*. There is other class of material called *ferrimagnet* where spins are aligned anti-parallel but do not cancel each other.

1.2 Background of the problem

To find the ground and first excited state energy of N-site spin chain we need to find the eigenenergies of the Hamiltonian. For $N = 2$ the possible spin configurations of the chain are

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$$

and the Heisenberg Hamiltonian is :

$$\mathcal{H} = \begin{bmatrix} 0.25 & 0 & 0 & 0 \\ 0 & -0.25 & 0.5 & 0 \\ 0 & 0.5 & -0.25 & 0 \\ 0 & 0 & 0 & 0.25 \end{bmatrix}$$

with eigenvalues : 0.25 -0.75 0.25 0.25 (in units of J). We also considered $\hbar = 1$.

Thus for N site there are 2^N spin configurations and the Hamiltonian matrix $\mathcal{H}$ becomes $2^N \times 2^N$ dimensional. Only for few sites the matrix becomes so large that finding its eigenvalues becomes very tedious and time-consuming. However the matrix will be sparse and symmetric. By using *Lanczos algorithm* we convert the matrix to a symmetric tridiagonal matrix T which has very small

dimension compared to actual matrix. Lanczos algorithm guarantees that the low lying eigenvalues of T does converge to that of $\mathcal{H}$. This task may be long but definitely less time-consuming than to find the eigenvalues directly from $\mathcal{H}$. Then finding the eigenvalues of T is easy and I have done it by QR method.

2 Computational methodology

There are three parts for the computation of ground state and first excited state of N-site spin-$\frac{1}{2}$ chain discussed below.

2.1 Forming Heisenberg Hamiltonian

Heisenberg spin Hamiltonian (1) can be calculated by calculating its matrix elements $\mathcal{H}_{mn} = \langle m|\,\mathcal{H}\,|n\rangle$. Main problem is to construct the bases $\{|m\rangle\}$.
STEPS:

1. Input number of lattice sites N and value of J.
2. Calculate all possible spin configurations of N spins by converting 0 to 2^N-1 decimal numbers to binary numbers. Here $|1\rangle$ represents spin up and $|0\rangle$ represents spin down. As an example for $N=3$ the possible spin configurations are

$$\begin{array}{llll} |000\rangle \equiv 0 & |010\rangle \equiv 2 & |100\rangle \equiv 4 & |110\rangle \equiv 6 \\ |001\rangle \equiv 1 & |011\rangle \equiv 3 & |101\rangle \equiv 5 & |111\rangle \equiv 7 \end{array}$$

3. Represent $|1\rangle$ by $\begin{pmatrix}1\\0\end{pmatrix}$ and $|0\rangle$ by $\begin{pmatrix}0\\1\end{pmatrix}$. They will be called chains. So each chain is $2^N \times N \times 2$ dimensional.
4. Initial bases is constructed by taking Kronecker product of all N spins in each chain. Then the bases are $\{|i_m\rangle_{2^N}\}$ where $m = 0, 1, 2, \cdots, 2^N-1$.
5. Define operator functions $S^zS^z(\text{chain}, j), S^+S^-(\text{chain}, j)$ and $S^+S^-(\text{chain}, j)$ where they act on chain such that first operator act on j^{th} (j starting from 0) spin and second operator act on $(j+1)^{th}$ spin with all other spins unaltered. Output of them will be resultant basis. For example

$$\begin{aligned} &S^zS^z(|0100\rangle, 1) \to \big(\frac{1}{2}\big)\big(-\frac{1}{2}\big) \times \text{ basis form of } |0100\rangle \\ &S^+S^-(|0110\rangle, 1) \to \text{ basis form of } |0000\rangle \\ &S^-S^+(|0110\rangle, 2) \to \text{ basis form of } |0001\rangle \end{aligned}$$

   where

$$S^z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad S^+ = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \qquad S^- = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$$

6. For periodic chain if $j = N-1$ (last spin) $(j+1)^{th}$ spin will be the first spin $(j=0)$.

7. Calculate the resultant bases $|r_m\rangle = \mathcal{H}\,|i_m\rangle$ where $m = 0, 1, 2, \cdots, 2^N - 1$.

For $m = 0 \to 2^N - 1$
$|r_m\rangle = |0\rangle$
  For $j = 0 \to N - 2$ (for open chain) or $N - 1$ (for periodic chain)
    $|r_m\rangle = |r_m\rangle + S^z S^z(|i_m\rangle, j) + \frac{1}{2}[S^+ S^-(|i_m\rangle, j) + S^- S^+(|i_m\rangle, j)]$
  $j = j + 1$
$m = m + 1$

8. Compute the matrix elements

$$\mathcal{H}_{mn} = J\,\langle i_m | r_n\rangle \qquad \text{where } m, n = 0 \to 2^N - 1$$

2.2 Employing Lanczos Algorithm to convert $\mathcal{H}$ to T

Lanczos is an iterative method, devised by *Cornelius Lanczos* to find most usefull eigenvalues and eigenvectors of a big $n \times n$ Hermitian Matrix $\mathcal{H}$. We first take a random normalized vector $|v_0\rangle$ of size n. We then use Lanczos iteration to get our next vector $|v_1\rangle$ which is orthonormal to $|v_0\rangle$. If we do $m - 1$ iterations we get m orthonormal vectors $|v_i\rangle$ where $i = 1, 2, \cdots, m - 1$. They form orthogonal *Krylov basis matrix* $\mathcal{V}$ of $n \times m$ dimension. In that basis $\mathcal{H}$ transforms to tridiagonal matrix T of $m \times m$ dimension.

$$T = \mathcal{V}^T \mathcal{H} \mathcal{V} \tag{4}$$

STEPS:

1. Input randomly generated $|\tilde{v_0}\rangle \in \mathbb{C}^n$. Normalize $|v_0\rangle = \dfrac{|\tilde{v_0}\rangle}{\|\tilde{v_0}\|}$

2. Initial iteration to find $|v_1\rangle$

$$\begin{aligned} a_0 &= \langle v_0|\,\mathcal{H}\,|v_0\rangle \\ |\tilde{v}_1\rangle &= \mathcal{H}\,|v_0\rangle - a_0\,|v_0\rangle \\ b_1 &= \|v_1\| \\ |v_1\rangle &= \frac{|\tilde{v}_1\rangle}{b_1} \end{aligned}$$

3. Higher order iteration to find $|v_i\rangle$ where $i = 2, 3, \cdots, m - 1$

$$\begin{aligned} a_{i-1} &= \langle v_{i-1}|\,\mathcal{H}\,|v_{i-1}\rangle \\ |\tilde{v}_i\rangle &= \mathcal{H}\,|v_{i-1}\rangle - a_{i-1}\,|v_{i-1}\rangle - b_{i-1}\,|v_{i-2}\rangle \\ b_i &= \langle v_{i-1}|\,\mathcal{H}\,|\tilde{v}_i\rangle = \|\tilde{v}_i\| \\ |v_i\rangle &= \frac{|\tilde{v}_i\rangle}{b_i} \end{aligned}$$

4. Symmetric tridiagonal matrix T is formed.

$$\mathcal{V} = [|v_0\rangle, |v_1\rangle, \cdots, |v_{m-1}\rangle]$$

$$T = \mathcal{V}^T \mathcal{H} \mathcal{V} = \begin{bmatrix} a_0 & b_1 & 0 & 0 & \cdots & 0 \\ b_1 & a_1 & b_2 & 0 & \cdots & 0 \\ 0 & b_2 & a_2 & b_3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & b_{m-1} \\ 0 & 0 & \cdots & \cdots & b_{m-1} & a_{m-1} \end{bmatrix}$$

5. We calculate eigenvalues of T by QR method described in section 2.3. Sorting and taking unique values of T's eigenvalues we get ground and first exited state energy which is same as of $\mathcal{H}$ after some value of m.

6. We iterate the whole procedure from step 2 to step 4 for different value of m, started from $m = 1$ and calculate T's smallest eigenvalue (or $\mathcal{H}$'s ground state energy) for each m. If we see after certain m the ground state energy is not changing much, we break the iteration and get our final T matrix.

7. We shall see the eigenvalues of T matches with actual important eigenvalues (small and large ones) of $\mathcal{H}$.

2.3 Employing QR method to find eigenvalues of T

Lanczos algorithm guarantees the extreme eigenvalues of T converges to that of $\mathcal{H}$ with increasing dimensions. Upto some tolerance level (e.g $\epsilon = 10^{-7}$) of smallest eigenvalue (ground state energy), we terminate the m-value. The eigenvalues of T for each m are calculated using QR method. Here we decompose T in Q and R matrix. The diagonal representation of T will be $D = Q^T T Q$ with all its eigenvalues as the diagonal elements.
STEPS:

1. Let $T = [|t_1\rangle, |t_2\rangle, \cdots, |t_m\rangle]$.

2. Use Gram-Schimdt orthogonalization to construct m orthonormal vectors $\{|e_i\rangle\}$ from $\{|t_i\rangle\}$ where $i = 1, 2, \cdots, m$. We initialize this by taking

$$|u_1\rangle = |t_1\rangle$$
$$|e_1\rangle = \frac{|u_1\rangle}{\|u_1\|}$$

3. For higher order iteration $k = 2, 3, \cdots, m$

$$|u_k\rangle = |t_k\rangle - \sum_{j=1}^{k-1} \frac{\langle t_k | u_j \rangle}{\langle u_j | u_j \rangle} |u_j\rangle$$
$$|e_k\rangle = \frac{|u_k\rangle}{\|u_k\|}$$

4. Q and D matrices are formed as

$$Q = [|e_1\rangle, |e_2\rangle, \cdots, |e_m\rangle]$$
$$D = Q^T T Q$$
$$T = D \qquad \text{and repeat from step 2}$$

5. After sufficient iterations, say 100, D is diagonal enough to contain all of T's eigenvalues as diagonal elements of D.

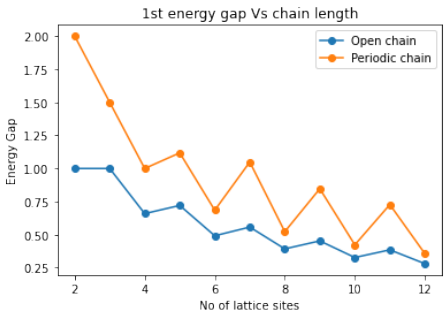
3 Result & discussion

Following are the ground state and first excited state for different number of lattice sites calculated with our program . It is to be noted that for $N = 3$ in open chain the QR method cannot work as there is an eigenvalue 0. There, we just use inbuilt eigenvalue function. For large $N(N > 3)$ the algorithm works perfectly well.

No of lattice sites	Open chain			Periodic chain		
	Ground state energy	1st excited state energy	Energy gap	Ground state energy	1st excited state energy	Energy gap
2	-0.75	0.25	1	-1.5	0.5	2
3	-1	0	1	-0.75	0.75	1.5
4	-1.6160	-0.9571	0.6589	-2	-1	1
5	-1.9279	-1.2071	0.7208	-1.8680	-0.75	1.1180
6	-2.4936	-2.0020	0.4916	-2.8028	-2.1180	0.6848
7	-2.8362	-2.2789	0.5573	-2.8552	-1.8063	1.0489
8	-3.3749	-2.9822	0.3927	-3.6511	-3.1284	0.5227
9	-3.7363	-3.2833	0.4530	-3.7830	-2.9361	0.8469
10	-4.2580	-3.9306	0.3274	-4.5154	-4.0922	0.4232
11	-4.6321	-4.2467	0.3854	-4.7189	-3.9917	0.7272
12	-5.1421	-4.8611	0.2810	-5.3874	-5.0315	0.3559

From the above table following conclusions can be drawn

1. With increasing number of lattice sites the ground state energy and first excited state energy is decreasing.
2. With increasing length of chain the first energy gap is decreasing. For periodic chain the gap decreases faster than open chain.



3. There is clear differences in energy in open and periodic chain.

4. We found for $N = 12$ lattice sites the ground states energy -5.3873909 for antiferromagnetic periodic chain.

5. Another thing I noticed. For $J < 0$ (say, -1) the ground state are following.

No of lattice sites	2	3	4	5	6	7	8	9	10	11	12
Open chain ground state energy	-0.25	-0.5	-0.75	-1	-1.25	-1.5	-1.75	-2	-2.25	-2.5	-2.75
Periodic chain ground state energy	-0.5	-0.75	-1	-1.25	-1.5	-1.75	-2	-2.25	-2.5	–2.75	-3

6. For open-ended chain $E_0 = -\frac{N-1}{4}$ and for periodic chain $E_0 = -\frac{N}{4}$.

7. So, $|\uparrow\uparrow \ldots\rangle$ (ferromagnetic system) is a ground state, but $|\uparrow\downarrow\uparrow\downarrow \ldots\rangle$ (anti-ferromagnetic system) is not a ground state.

8. This is because there is the hopping terms in the Hamiltonian.

4 Summary

The problem discussed in this project is a typical manybody Hamiltonian problem. Main challenge comes to diagonalizing those Hermitian matrices. Even for a few number of particles the size of the Hamiltonian becomes very large. However those matrices typically sparse and number of non-zero elements are typically $O(N)$. Usual scheme is to utilise this sparseness and to concatenate on ground state only. *Power method* is most popular method in doing so. Lanczos is modified version of it which gives us most usefull eigenvalues (tending to lowest or highest ones) and also it gives less error than power method.

In our antiferromagnetic chain problem the dimension of Hamiltonian increases in $O(2^N)$ order. So instead directly calculating its eigenvalues we convert it to *less dimensional symmetric tri-diagonal form* by *Lanczos Algorithm* and calculate its eigenvalues. This tridiagonal matrix eigenvalues converges to original matrix eigenvalues with its increasing dimension. It does not show the degeneracy but is able to get all of the important eigenvalues. By employing this procedure we can verify many important properties of magnetic systems. For a given J we can compute its ground state configurations. We have seen the energy gap is decreasing with increasing spin length. So, for infinite chain there is no energy gap. Also there is clear energy differences for open and periodic chain and for periodic chain the energy gap falls faster.