Numerical Solution of Quantum Spin Heisenberg Chain

Khagendra Adhikari

Department of Physics and Astronomy
The University of Mississippi
University, MS 38677

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Introduction

Quantum spin Heisenberg chain is a simple one dimensional model of the magnetism that captures various complex physical phenomena. In this model, mutually interacting quantum spins are arranged with a regular spacing along a line at fixed positions.

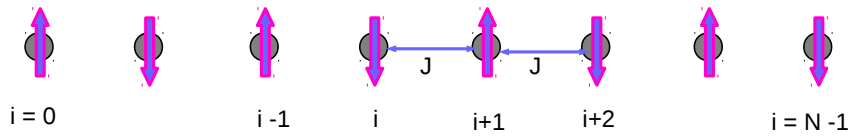

Figure 1: Quantum Spin $\frac{1}{2}$ Heisenberg Chain.

In Figure 1, the dark sphere and the pink arrow head represent the spin $\frac{1}{2}$ particle at the site i and its orientation respectively for finite system size $N = 8$. The strength of exchange interaction J is isotropic, i.e. $J = (J_x, J_y, J_z) = J(1, 1, 1)$. The nature of the interaction is *antiferromagnetic* ($J > 0$), meaning that the minimum energy configuration of the system favors the opposite alignment of the spins. The interaction is limited to nearest-neighbour spins as shown by the horizontal blue coloured double-headed arrows.

The Hamiltonian is

$$\begin{aligned}\hat{\mathbf{H}} &= J\sum_{i=0}^{N-1}\left[\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_{i+1}\right] \\ &= J\sum_{i=0}^{N-1}\left[\hat{\mathbf{S}}_i^x\hat{\mathbf{S}}_{i+1}^x+\hat{\mathbf{S}}_i^y\hat{\mathbf{S}}_{i+1}^y+\hat{\mathbf{S}}_i^z\hat{\mathbf{S}}_{i+1}^z\right] \\ &= J\sum_{i=0}^{N-1}\left[\frac{1}{2}\left(\hat{\mathbf{S}}_i^+\hat{\mathbf{S}}_{i+1}^-+\hat{\mathbf{S}}_i^-\hat{\mathbf{S}}_{i+1}^+\right)+\hat{\mathbf{S}}_i^z\hat{\mathbf{S}}_{i+1}^z\right]\end{aligned} \tag{1}$$

Where, $\hat{\mathbf{S}}^{\pm}=\hat{\mathbf{S}}^x\pm j\hat{\mathbf{S}}^y$ are ladder operators.

For spin S, ladder and cartesian operators are square matrices of dimensions $2S+1$. They can be represented in the basis of the form $|S,m\rangle$ with $m=-S,....,S$.

$$\hat{\mathbf{S}}_{\pm}|S,m\rangle=\sqrt{S(S+1)-(m(m\pm1)}\quad|S,m\pm1\rangle \tag{2}$$

$$\hat{\mathbf{S}}^z|S,m\rangle=m|S,m\rangle \tag{3}$$

In 1931, the model was solved analytically by Bethe [1] for any finite system size. Using Bethe's result, the exact ground state energy per site, $E_0=\frac{1}{4}-\log_e(2)$ in the limit of infinitely long chain was evaluated by Hulthen [2] in 1938.

Example for $N=2$

For this system, equation 1 becomes

$$\hat{\mathbf{H}}=J\hat{\mathbf{S}_1}\cdot\hat{\mathbf{S}_2}$$

Classical energy depends on the angle between the spins. So, the energy is

$$\begin{aligned}E_{\text{classical}} &= JS_1S_2\cos\theta \\ &= \frac{1}{4}J\cos\theta \qquad \text{using} \quad S_1=S_2=\frac{1}{2}\end{aligned} \tag{4}$$

and since $-1\leq\cos\theta\leq1$, all energies lie between $-\frac{J}{4}$ to $+\frac{J}{4}$.

Quantum mechanically, we need to construct a Hamiltonian matrix in a complete set of basis states and diagonalize it. We have four ($2^2=4$) basis states with $m=\pm\frac{1}{2}$.

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

Where, $|S_1,m_1\rangle|S_2,m_2\rangle=|m_1m_2\rangle=|\frac{1}{2},-\frac{1}{2}\rangle=|+-\rangle$ means S_1 is spin up and S_2 is spin down. From equation 1,

$$\hat{\mathbf{H}}=J\left[\frac{1}{2}\left(\hat{\mathbf{S}}_1^+\hat{\mathbf{S}}_2^-+\hat{\mathbf{S}}_1^-\hat{\mathbf{S}}_2^+\right)+\hat{\mathbf{S}}_1^z\hat{\mathbf{S}}_2^z\right]$$

Let us apply Hamiltonian on the basis using equations 2 and 3. Use $J = 1$ and $\hbar = 1$ for simplicity.

$$\hat{\mathbf{H}}|++\rangle = 0 + 0 + \frac{1}{4}|++\rangle$$
$$\hat{\mathbf{H}}|+-\rangle = 0 + \frac{1}{2}|-+\rangle - \frac{1}{4}|+-\rangle$$
$$\hat{\mathbf{H}}|-+\rangle = \frac{1}{2}|+-\rangle + 0 - \frac{1}{4}|-+\rangle$$
$$\hat{\mathbf{H}}|--\rangle = 0 + 0 + \frac{1}{4}|--\rangle$$

In this basis, Hamiltonian can be written in the matrix form

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

Diagonalization gives eigenvalues $E = (-\frac{3}{4}, \quad \frac{1}{4}, \quad \frac{1}{4}, \quad \frac{1}{4})$. The first one is singlet and the last three of these form triplet. The maximum eigenvalue $\frac{1}{4}$ is same as that of classical, but the minimum eigenvalue $-\frac{3}{4}$ is much lower. This is clearly a new quantum effect. This is due to the quantum fluctuation, where the first two terms in the Hamiltonian flips the spin when acted on basis state.

Numerical Method

The goal of this project is to solve the isotropic quantum spin $\frac{1}{2}$ Heisenberg Chain. The meaning of solving the model is finding all of the eigenstates of the Hamiltonian and its corresponding eigenvalues.The electron can have spin up or down. So, any electron is in the linear state $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$ generating a two-dimensional *Hilbert space*. Therefore, the size of the Hamiltonian for N electrons system is $2^N \times 2^N$.

Hamiltonian matrix is generated for a finite system size using spin matrices. Hamiltonian matrix is sparse, a matrix in which most of the elements are zero. So, taking the advantage of the sparsity, the computation is carried out using a large sparse real symmetric square matrix solver. The eigenvalues represent the energy spectrum. Since the basis size increases exponentially with system size N, it is impossible to diagonalize it for large system size. Here, the computation is carried out for the finite system of increasing size, and the results are extrapolated to an infinite system size (thermodynamic limit). For this, ground state energy per site versus square of inverse chain length $\frac{1}{N^2}$ is graphed as shown in Figure 2. The linear fit does best match for this plot. When $N \to \infty$, $\frac{1}{N^2} \to 0$. Here, y-intercept is the ground state energy per site for the infinite system size.

Result

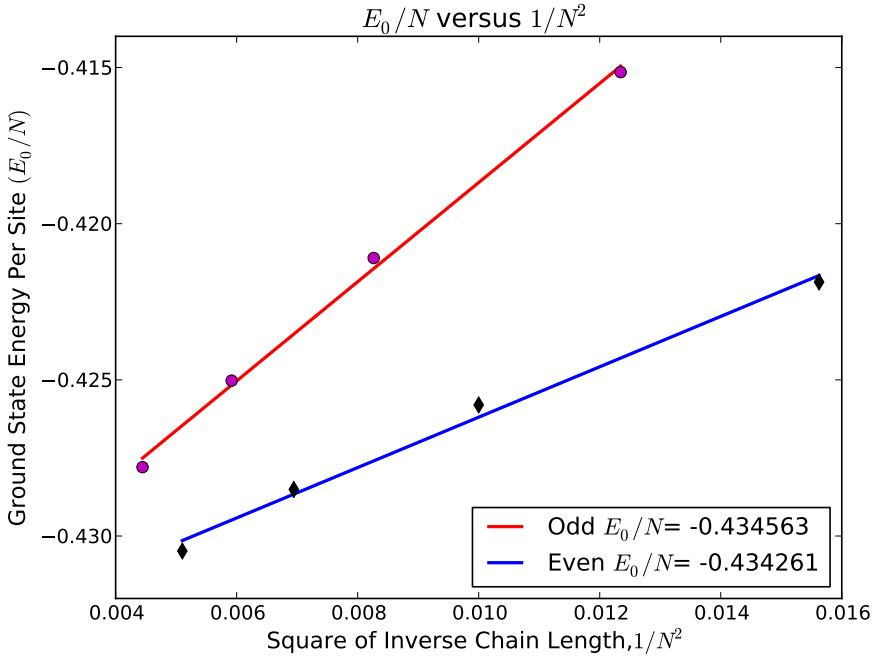

Figure 2: Extrapolation of the ground state energy for thermodynamics limit.

Known Result	**Odd N**	**Even N**
−0.443147	**−0.434563**	**−0.434261**

Table 1: Result table

From the plot, we can see that the ground state energy per site is linear with square of inverse chain length [3]. For finite system size N, there are different energies for the chain with odd ($N = 9, 11, 13, 15$) and even ($N = 8, 10, 12, 14$) number of sites represented by circle and diamond markers respectively. The data points are more linear for bigger system size. When the results are extrapolated to thermodynamic limit, both converge close to the exact value $\frac{1}{4} - \log_e(2)$.

Conclusion

The ground state energy extrapolated for the infinite system size is in agreement with the known result as shown in table 1. Although the analytical solution is available, this model gives the testing ground to validate the algorithm. So, it can be used for the *non-integrable* system with a slight modification. In my final project, I am planning to expand the interaction between the spins upto next-nearest neighbours.

In order to improve the result, computation should be carried out for bigger system size. But, exact diagonalization studies are limited to rather small lattices, few tens of spins, because of exponential increase of basis size $(2S+1)^N$ with system size N. So, we should either reduce the basis size or look for alternative method that can solve large matrix. The Hamiltonian can be block-diagonalized by taking the advantage of symmetry in the system. Each block matrix with dimension lower than that of a full Hamiltonian matrix, can be solved separately and the lowest eigenvalue overall is the ground state energy. Since we are interested in the ground state and a few low-lying excited states, computation can be carried out for bigger system size by using *Lanczos algorithm*, one of the elegant iterative methods for solving the eigenvalue problem of a large real symmetric square matrix.

References

[1] H.A Bethe,*Z. Phys.* **71**, 205 (1931)

[2] L.Hulthen,*Ark. Mater. Astron. Fys. A* **26**, 1 (1938)

[3] Bonner, J.C., Fisher, M.E., *Phys. Rev.* **135**, A640 - A658 (1964)