Algorithm Overview

I am using Suzuki-Trotter Product-Formula Algorithm for evolution of the system. The details are also present in paper [1].

Hamiltonian of the spin system is given by

$$H(t) = -\sum_{i,j=1}^{L} \sum_{\propto=x,y,z} J_{i,j}^{\propto}(t) S_i^{\propto} S_j^{\propto} - \sum_{i,j=1}^{L} \sum_{\propto=x,y,z} h_i^{\propto}(t) S_i^{\propto}$$

The evolution can be split into two different type of terms – single-spin and double-spin terms.

Single-spin is given by

$$e^{itS_j h_j} = \begin{pmatrix} \cos\frac{th_j}{2} + \frac{ih_j^z}{h_j}\sin\frac{th_j}{2} & \frac{ih_j^x + h_j^y}{h_j}\sin\frac{th_j}{2} \\ \frac{ih_j^x - h_j^y}{h_j}\sin\frac{th_j}{2} & \cos\frac{th_j}{2} - \frac{ih_j^z}{h_j}\sin\frac{th_j}{2} \end{pmatrix}$$

- (1)

Where $h_j = \|\boldsymbol{h}_j\|$

Double-spin term is given by

$$e^{it\left(J_{j,k}^x S_j^x S_k^x + J_{j,k}^y S_j^y S_k^y + J_{j,k}^z S_j^z S_k^z\right)} = \begin{pmatrix} e^{iat}\cos bt & 0 & 0 & e^{iat}\sin bt \\ 0 & e^{-iat}\cos ct & e^{-iat}\sin ct & 0 \\ 0 & e^{-iat}\sin ct & e^{-iat}\cos ct & 0 \\ e^{iat}\sin bt & 0 & 0 & e^{iat}\cos bt \end{pmatrix}$$

- (2)

Where $a = \frac{J_{j,k}^z}{4}$, $b = \frac{J_{j,k}^x - J_{j,k}^y}{4}$, $c = \frac{J_{j,k}^x + J_{j,k}^y}{4}$

The algorithm is as follows

1. The wavefunction is initialized to all “x” direction.
2. The h-values are initialized to provide a bias in x-direction.
3. The h-values and J-values are read from files
4. The single-spin operator (1) is applied to wave function for a timestep.
5. The double-spin is operated (2) is applied to wave function for a timestep.
6. Normalize the step function.

7. Calculate energy of the system so that we can plot and ensure the progress of the system.
8. Repeat the steps-4, 5 and 6 for each time until the final values of h and J is reached.

[1] H. De Raedt and K. Michielsen. Computational Methods for Simulating Quantum Computers. In M. Rieth and W. Schommers, editors, Handbook of Theoretical and Computational Nanotechnology, volume 3, chapter 1, page 248. American Scientific Publisher, Los Angeles, 2006.