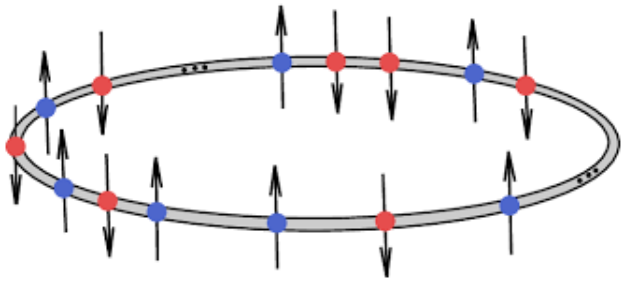
In this Homework we are going to simulate Heisenberg spin chain and investigate the properties of these systems specially correlation function and entanglement.

Theory :

Heisenberg spin chain

The Heisenberg spin chain was proposed by Werner Heisenberg in 1928 as a toy model to study magnetism. This is a one-dimensional model of magnetism or simply of spin $\frac{1}{2}$ particles that have a spin-spin interaction. Actually, this is not just a nice toy model. In some metals and crystals where this is some one-dimensional isotropy these spin chain actually appear and describe the dominant physical behaviour.



The spin chain simply consists of N sites, where on each site we consider a spin $\frac{1}{2}$ particle(for example an electron). This electron can have spin up or down and, consequently, any electron is in a linear state $a\langle\uparrow| + b|\downarrow\rangle$ generating a two-dimensional Hilbert space (local).

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix},\ |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

The spin operators for 1 particle are :

$$S_x = \frac{\hbar}{2}\sigma_x,\ S_y = \frac{\hbar}{2}\sigma_y,\ S_z = \frac{\hbar}{2}\sigma_z, S_+ = \hbar\sigma_p, S_- = \hbar\sigma_m$$

where :

$$\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix},\ \sigma_y = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix},\ \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix},\ \sigma_+ = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix},\ \sigma_- = \begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}$$

and they satisfy local commutation relations in the sense that :

$$[S_i, S_j] = i\epsilon_{ijk}S_k \qquad i \neq j$$

Hilbert space

As we said in the previous section, each spin is a linear space $V = \mathbb{C}^2$ Accordingly, a spin chain is the direct product of all the spins, namely

$$\mathcal{V} = V_1 \otimes V_2 \otimes V_3 \otimes \cdots \otimes V_L$$

where V_k is the linear space at site k. We call the space $\mathcal{V}$ the $Hilbert$ space of the spin chain. From basic linear algebra, we know that $\mathcal{V}$ is a linear space of dimension 2^L. A convenient basis for this space is given by states of the following type :

$$|\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes \cdots \otimes |\uparrow\rangle_L , \qquad |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes \cdots \otimes |\uparrow\rangle_L , \qquad \dots$$

Hamiltonian

The interactions among the spins is specified by a Hamiltonian. The Hamiltonian of the Heisenberg spin chain is given by:

$$\mathcal{H} = J \sum_{i,j} \vec{S}_i . \vec{S}_j$$

When :

$$S_x^i = \frac{\hbar}{2}(\mathbb{I}^{\otimes j-1} \times \sigma_x \times \mathbb{I}^{\otimes n-j})$$

And we consider only nearest and next nearest interactions between spins in this problem. So we have :
Nearest interactions (the boundary condition is periodic) :

$$\mathcal{H}_1 = J_1([S_x^1 S_x^2 + S_y^1 S_y^2 + S_z^1 S_z^2] + [S_x^2 S_x^3 + S_y^2 S_y^3 + S_z^2 S_z^3] + \dots)$$

Next nearest interactions :

$$\mathcal{H}_2 = J_2([S_x^1 S_x^3 + S_y^1 S_y^3 + S_z^1 S_z^3] + [S_x^2 S_x^4 + S_y^2 S_y^4 + S_z^2 S_z^4] + \dots)$$

Symmetries

As we saw the size of our Hamiltonian is 2^L and it's hard to solve eigen-value problem of this Hamiltonian even for computer. One way of reducing the effective size of the Hamiltonian is by looking at symmetries of the system. Consider the operator

$$S_z^{total} = \frac{\hbar}{2} \sum \frac{\sigma_z^i + \mathbb{I}}{2}$$

which measures the total number of up or down spins. It is quickly checked that it commutes with the Hamiltonian. This means that we can restrict to subsets of a fixed number of spins up (or down). We should consider that because of degeneracy we can't say their eigen-states are the same. We deal with this problem in Problem number 1.

Problem 1

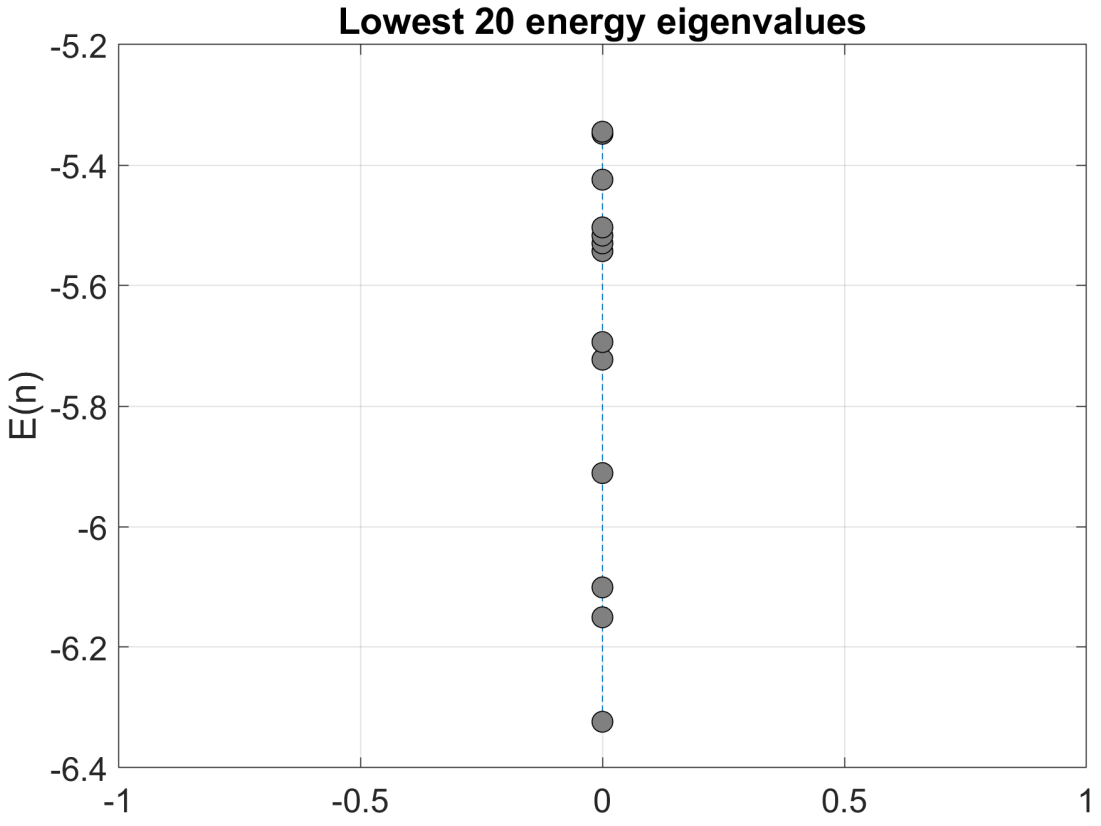
In this program we will simulate spin chain with $L = 16, J_1 = 1, J_2 = 0.3$ using $U_{(1)}$ symmetry we talked about and find :
a) Energy of 20 lowest energies.
b) Spin-spin correlation function.
c) Entanglement entropy for different partitions of system.

Results

To use $U_{(1)}$ symmetry, we first construct *number* operator(n_i) and find N_{tot} by summation in all n_i. This operator is a diagonal matrix with eigen values from 0 to L.
The number associated to $S_z^t = 0$ is $N_0 = \frac{\hbar}{2} \times \frac{L}{2}$.
Then we define F as :

$$F = N_{tot}(diag) == N_0$$

which is a boolean matrix.
After that we can separate the part we need from Hamiltonian $\widetilde{\mathcal{H}} = \mathcal{H}(F, F)$ and finally find 20 lowest eigen values of it.

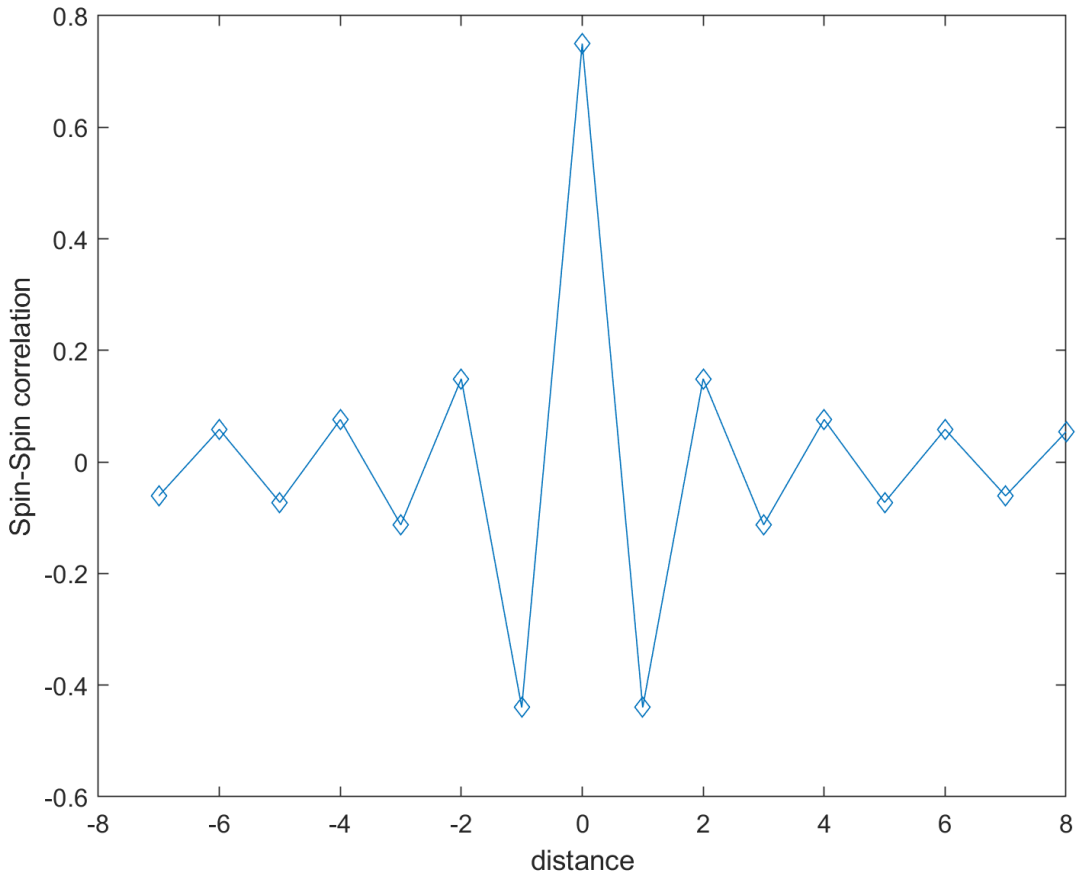


To find spin-spin correlation function, we first find the state with lowest energy from previous section and name it as $|\psi\rangle$.
Then we move back to original space by defining

$$U = sparse(2^L, 2^L), \quad U[F, F] = |\psi\rangle$$

And finally calculate correlation function of $\langle S_i.S_j\rangle$ as :

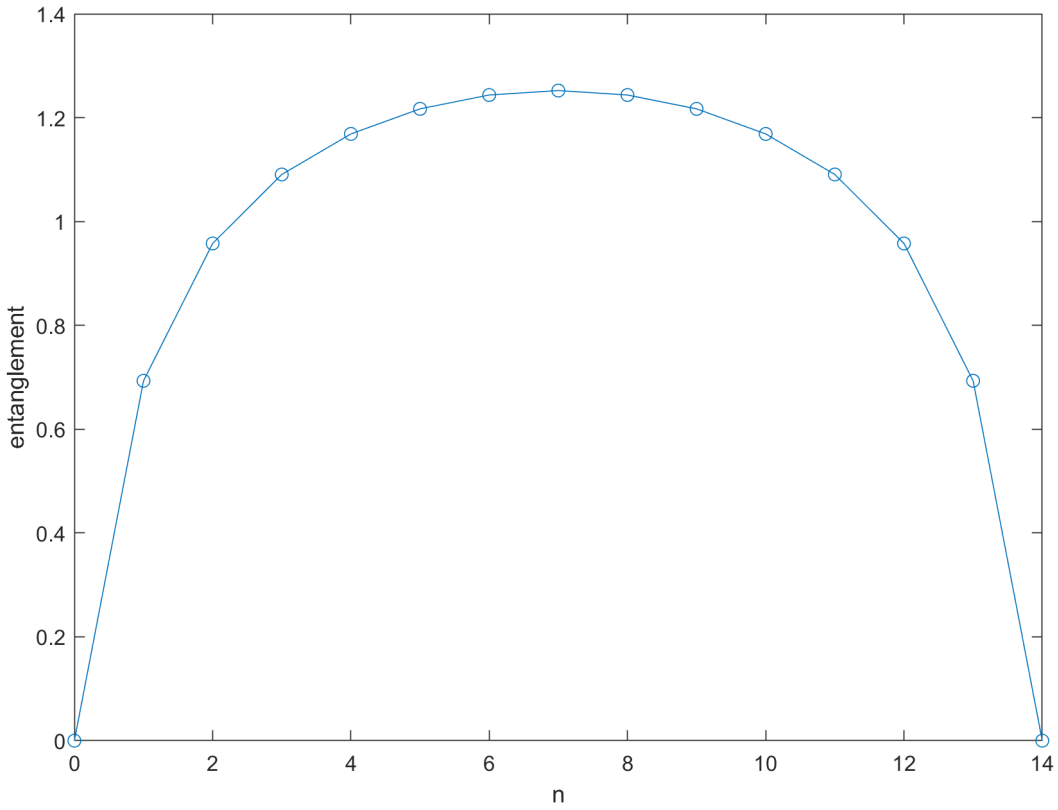
$$\langle S_i.S_j\rangle = \langle\psi|S_i.S_j|\psi\rangle$$



To calculate entanglement entropy we divide our system to 2 different parts, then reshape ψ as:

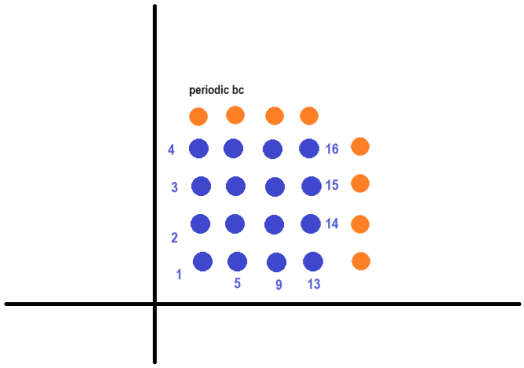
$$\widetilde{\psi} = reshape(\psi, 2^n, 2^{L-n})$$

Then we can find density matrix of left part and its eigen values by $\rho_L = conj(\widetilde{\psi}^T * \widetilde{\psi})$. Finally we use Neumann formula to calculate entanglement entropy.
(In this part because of memory problems I calculated entanglement entropy for 14 particles.)



Problem 2

In this section we solve the spin chain in 2Dimensional system. The Hamiltonian for this 2d lattice with periodic condition is different from the previous one :

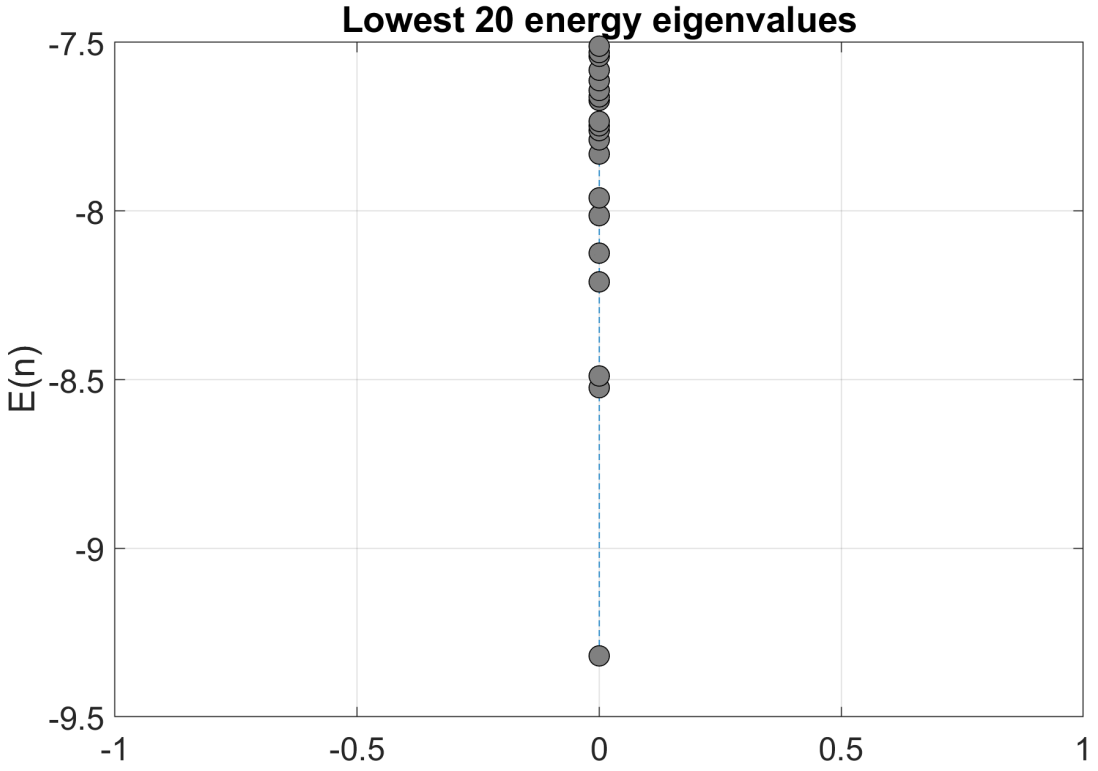


There are another 2 differences between 2D and 1D problem :
1 -The spin-spin correlation is now between vectors $S_{(x_1,x_2)}.S_{(y_1,y_2)}$ and because of transnational invariance we can fix $(x_1, x_2) = (1, 1)$.
2 -For an arbitrary numbering we have to first reshape ψ and then use permutation operator to rearrange the indices.(here we don't have to do that.)

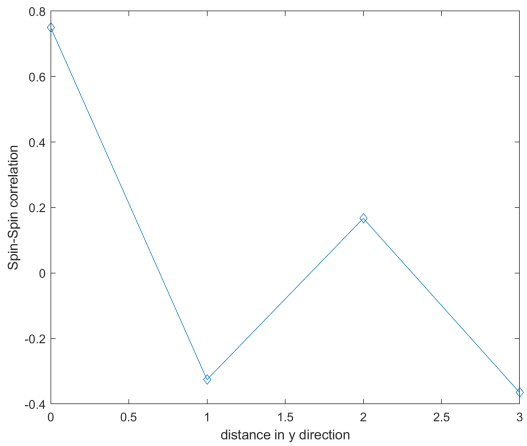
$$\widetilde{\psi} = reshape(\widetilde{\psi}, 2, 2, \dots)$$

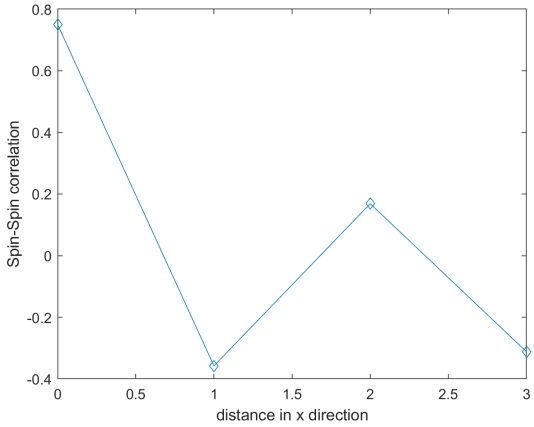
$$\widetilde{\psi} = permute(\widetilde{\psi}, [13, 9, 14, 10, ...])$$

The result for 20 lowest energies :

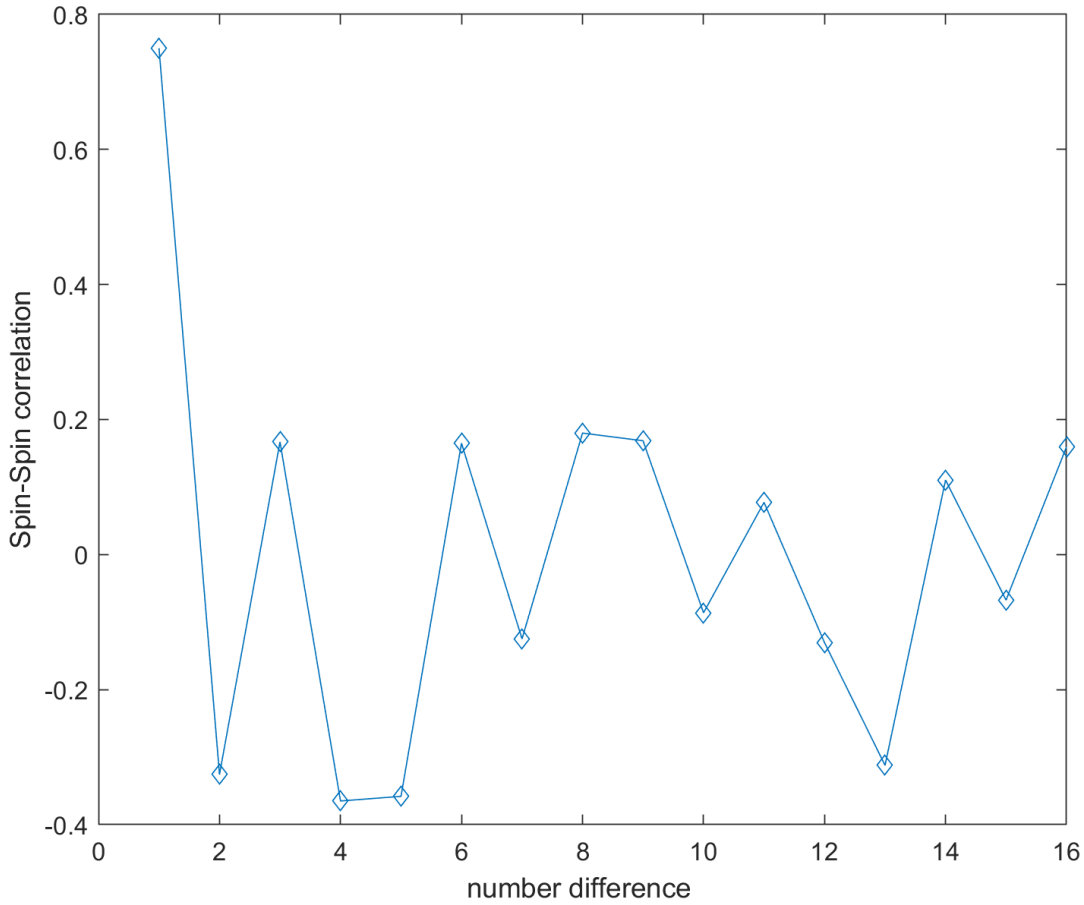


The result for correlation function $\langle S_{1,1}, S_{i,j} \rangle$ in x and y direction is:

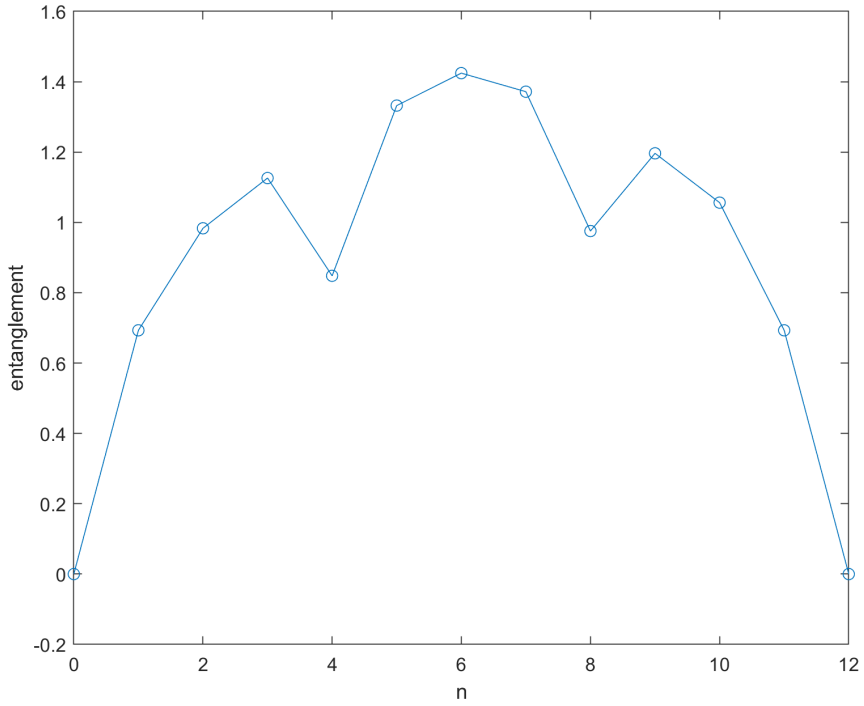




And for all particles from 1 to 16 is :



And entanglement is : (In this part because of memory problems I calculated entanglement entropy for 4×3 system.)



Problem 3

In this part we are going to simulate time evolution of a Heisenberg spin chain.
First consider there is only interaction between 2 neighbors (1,2),(3,4),... , that means we have $L/2$ systems each of consists 2 spin and they are all independent, So if we show the singlet state of 2 spin with :

$$|O\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{2}$$

Then the ground state of our chain will be :

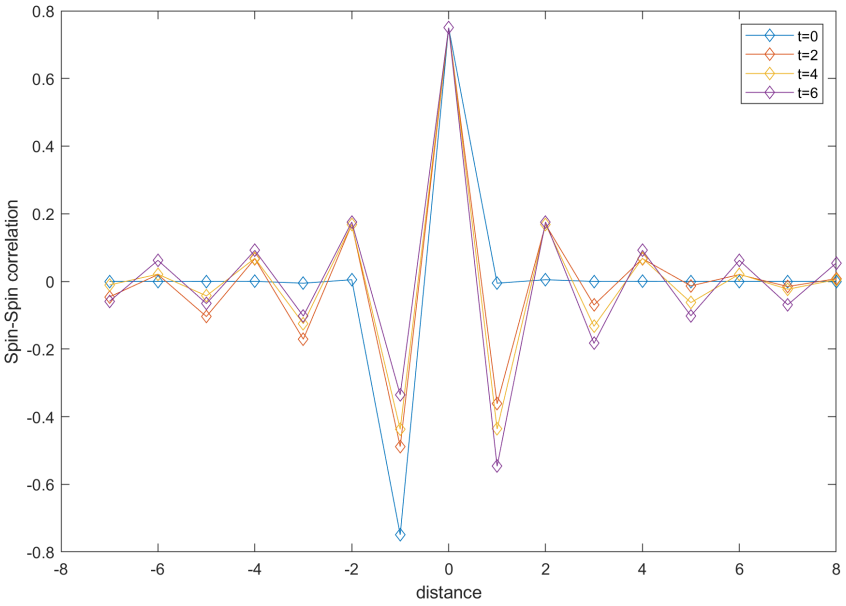
$$|O\rangle_1 \otimes |O\rangle_2 \otimes \cdots \otimes |O\rangle_{L/2}$$

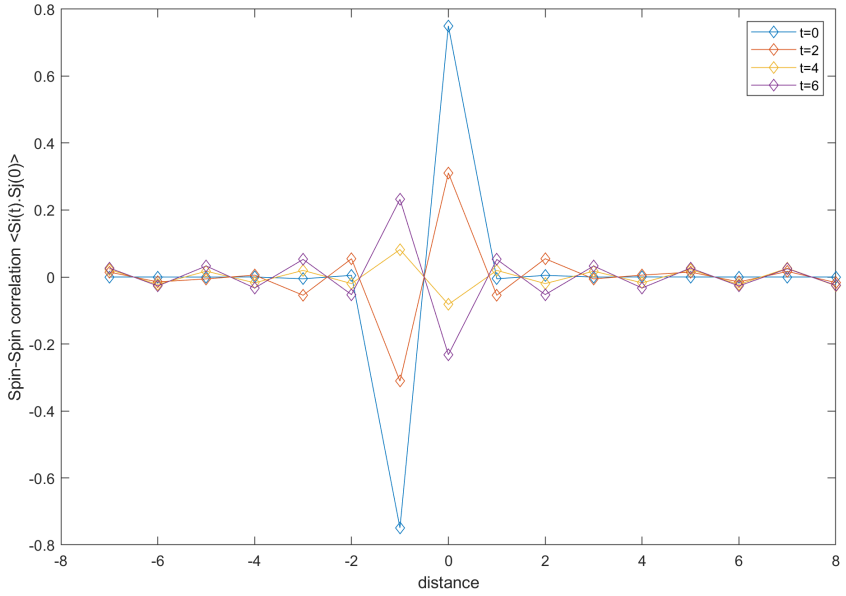
This result matches the one obtained from numerical calculations.
Now for time evolution we use below formula and notice we have to normalize ψ in every step.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \mathcal{H}(t) |\psi(t)\rangle$$

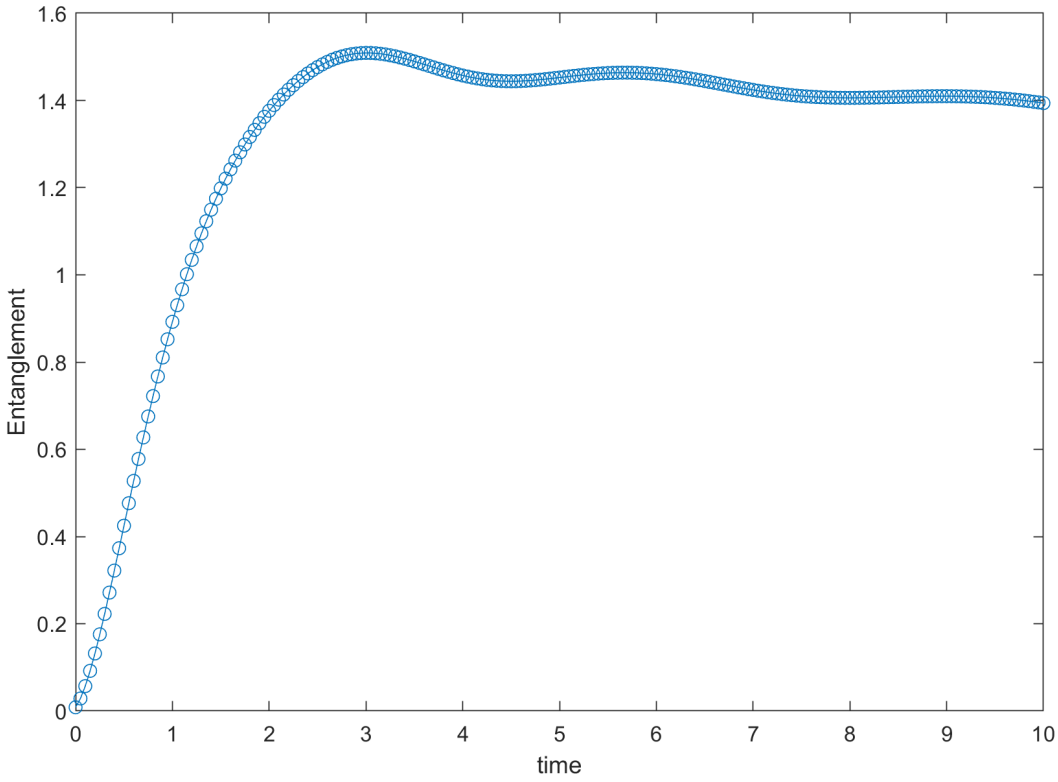
$$\psi(t') = (\mathbb{I} - i\frac{\epsilon}{\hbar}\mathcal{H}(t)) |\psi(t)\rangle$$

As we said because of translation invariance we fix i and for correlation function of $\langle S_i(t).S_j(t)\rangle$ and $\langle S_i(t).S_j(0)\rangle$ for (t=0,2,4,6) we have :





And for entanglement of half partition of system we have :


Entanglement
time
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
0
1
2
3
4
5
6
7
8
9
10