Computational Physics
Set 6

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Problem 1 : Hopping model with second and first quantization

Second Quantization

In this problem, we have a chain of L=8 sites and N=3 electrons (fermions). The hamiltonian for the hopping model in second quantization is:

$$\mathcal{H} = V \sum_{i=1}^{L} n_i n_{i+1} - t \sum_{i=1}^{L} \left[c_{i+1}^{\dagger} c_i + c_i^{\dagger} c_{i+1} \right] \tag{1}$$

The numerical values are $V = 1.0$ and $t = 1.0$. The creation operator is defined as:

$$c_i^{\dagger} := \sigma_z \otimes ... \otimes \sigma_z \otimes \sigma_- \otimes \mathbb{1} \otimes ... \otimes \mathbb{1} \tag{2}$$

In which there are i-1 σ_z in left, then putting σ_- in i-th site, then adding L-i $\mathbb{1}$ in the right. σ_z, σ_- , $\mathbb{1}$ and n_0 are:

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, n_0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

(3)

We can also construct n_i as:

$$n_i := \mathbb{1} \otimes ... \otimes \mathbb{1} \otimes n_0 \otimes \mathbb{1} \otimes ... \otimes \mathbb{1} \tag{4}$$

By putting n_0 in i-th site. Now by considering these operators and constructing the hamiltonian, we can diagonalize it. But before this, note that we have N=3 electrons, so instead of diagonalizing full hamiltonian, I can project it to the subspace with $N_{tot} = 3$ electrons. N_{tot} can be constructed as:

$$\hat{N}_{tot} = \sum_{i=1}^{L} \hat{n}_i \tag{5}$$

Note that dimension of this subspace is $\binom{8}{3} = 56$, but dimension of our original Hilbert space was $2^8 = 256$! This is much easier to diagonalize!

After diagonalizing the projected hamiltonian, we obtain the ground-state energy:

$$E_{gs} = -4.4939592074 \tag{6}$$

The ground-state wave function (in original Hilbert space) is plotted in Figure 1.

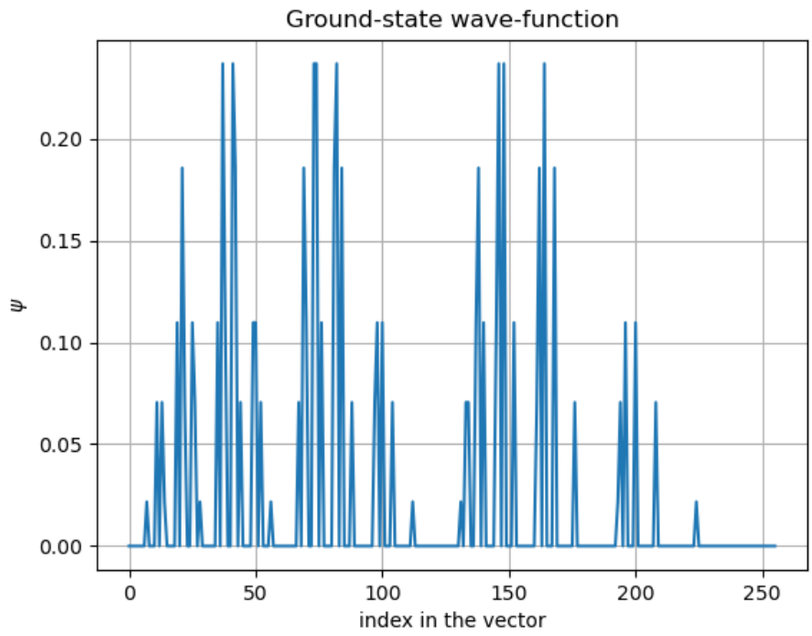

Figure 1: Ground-state wave-function in the original Hilbert space

The density-density correlation function $\langle n_i n_j \rangle = \langle \psi_{gs} | n_i n_j | \psi_{gs} \rangle$ is plotted in Figure 2. Note that because of transnational symmetry it is only function of distance j-i.

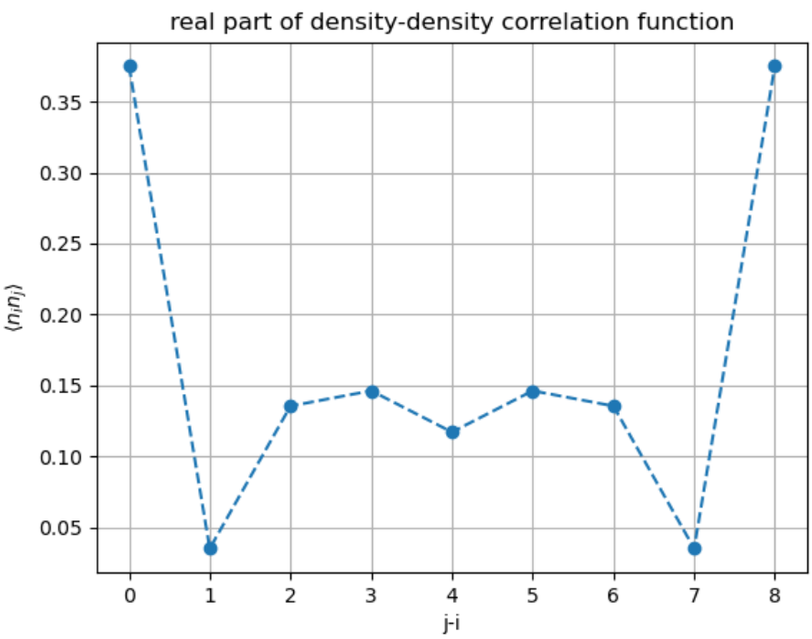

Figure 2: Density-density correlation function by second quantization

First Quantization

The first quantization answer for this problem was provided in HW2. I've prepare an appendix ".py" file, from the main code in HW2, but with numerical parameters of this problem. In first quantization we had to construct permutation operators and apply fermionic symmetry with it. By this method, the value for ground-state energy would be:

$$E_{gs} = -4.4939592074 \tag{7}$$

Exactly same as the answer from second quantization at least to 10 digits!

The density-density correlation function from the first quantization is plotted in Figure 3

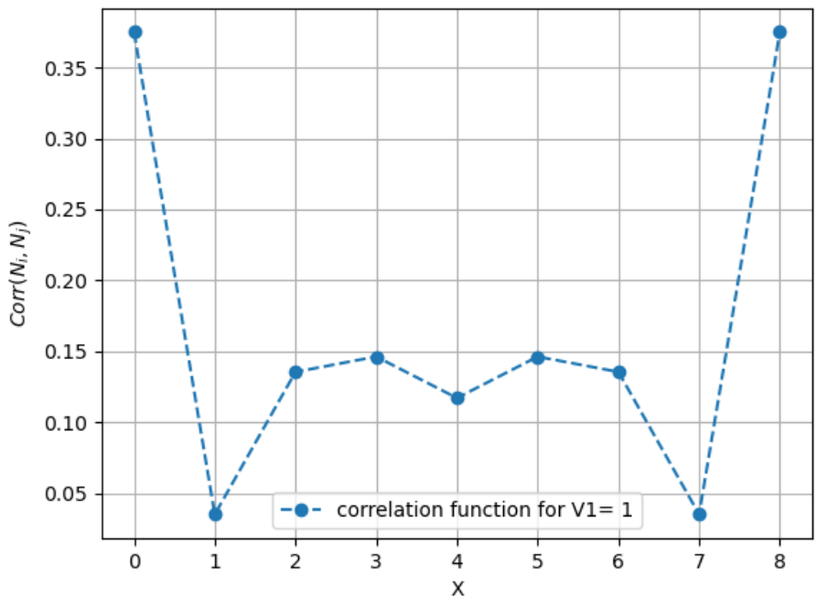

Figure 3: Density-density correlation function by first quantization

Again, similar to one obtained by second quantization approach! Here, "X" is the distance. Note the symmetry around the center, as a consequence of periodic boundary condition.

Problem 2 : NRG (Numerical Renormalization Group) for 1D quantum Ising chain

In this problem, we have a 1D Ising chain, consists of L=60 spins. The hamiltonian is of the form:

$$\mathcal{H} = \sum_{i=1}^{L} \vec{S}_i.\vec{S}_{i+1} \tag{8}$$

For NRG algorithm, we have to do the truncation of the Hilbert space; considering bond dimension m = 32 (it was given 30, but we have spin-$\frac{1}{2}$ particles and nearest power of 2 to 30 is 5, so I consider m=32). Until we get to this point, everything is exact; I construct the hamiltonian and all spin matrices by doing tensor products, but until I get to the point of 5 particles; after that, dimension of the Hilbert space will be more than $2^5 = 32$ and we have to truncate.

In NRG method, our truncation is due to energy eigenvalues. In each step, I construct a 64×64 hamiltonian, diagonalize it, keeping the 32 lowest energy eigenvalues and their corresponding eigenvectors, and thus constructing truncation matrix T:

$$\hat{T} = (|v_1\rangle, |v_2\rangle, ..., |v_{32}\rangle) \tag{9}$$

Now truncating all of operators as follows:

$$\tilde{O} = T^{\dagger} O T \tag{10}$$

In each truncation, our spin matrices be truncated as above, for example:

$$\tilde{S}_{x,2}^{(L=5)} = T^{\dagger} S_{x,2}^{(L=5)} T \tag{11}$$

When we add a site, we have to expand the Hilbert space in this fashion:

$$S_{x,i}^{(L+1)} = \tilde{S}_{x,i}^{(L)} \otimes \mathbb{1} \tag{12}$$

$$\mathcal{H}^{L+1} = \tilde{\mathcal{H}}^{L} \otimes \mathbb{1} + \tilde{S}_{x,L}^{(L)} \otimes \frac{\hbar}{2}\sigma_x + \tilde{S}_{y,L}^{(L)} \otimes \frac{\hbar}{2}\sigma_y + \tilde{S}_{z,L}^{(L)} \otimes \frac{\hbar}{2}\sigma_z \tag{13}$$

After that, we can again truncate according to equation (6). Note that for the last spin in the chain, we **don't** truncate the hamiltonian! We just diagonalize the 64×64 hamiltonian to obtain the eigenstates and eigenenergies.

The ground-state energy by this method is

$$E_{gs} = -26.161434807205225 \tag{14}$$

For average values, I use the following formula:

$$\langle S_{x,i} \rangle = \langle \psi_{gs} | S_{x,i} | \psi_{gs} \rangle \tag{15}$$

In which ψ_{gs} denotes the ground-state wave-function in the truncated Hilbert space. The plot for $\langle S_{x,i} \rangle$ is shown in Figure 4.

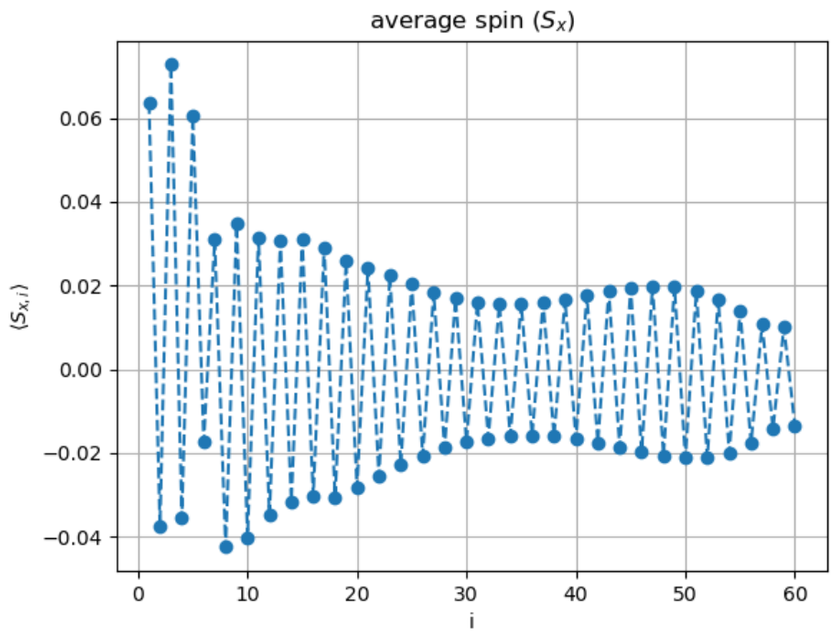

Figure 4: $\langle S_{x,i} \rangle$ with NRG method

And its average value in the whole chain is:

$$\overline{\langle S_{x,i} \rangle} = \frac{1}{L} \sum_{i=1}^{L} \langle S_{x,i} \rangle = 0.0009925913 \tag{16}$$

The same equations exist for y and z directions; For average spin in y direction:

$$\langle S_{y,i} \rangle = \langle \psi_{gs} | S_{y,i} | \psi_{gs} \rangle \tag{17}$$

The plot for $\langle S_{y,i} \rangle$ is shown in Figure 5.

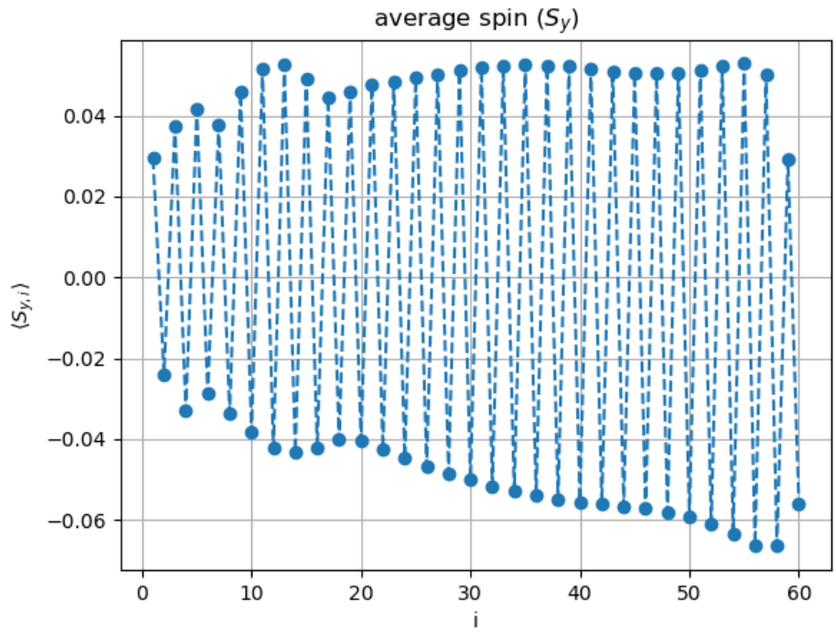

Figure 5: $\langle S_{y,i} \rangle$ with NRG method

And its average value in the whole chain is:

$$\overline{\langle S_{y,i} \rangle} = \frac{1}{L} \sum_{i=1}^{L} \langle S_{y,i} \rangle = -0.0005613300 \tag{18}$$

The spin spin-spin correlation function is defined as (for $S_x S_x$ correlation function):

$$\langle S_{x,i} S_{x,j} \rangle = \langle \psi_{gs} | S_{x,i} S_{x,j} | \psi_{gs} \rangle \tag{19}$$

And for $S_z S_z$ correlation function:

$$\langle S_{z,i} S_{z,j} \rangle = \langle \psi_{gs} | S_{z,i} S_{z,j} | \psi_{gs} \rangle \tag{20}$$

Because of translation symmetry, it only depends on the distance (j-i). $S_x S_x$ correlation function is shown in Figure 6.

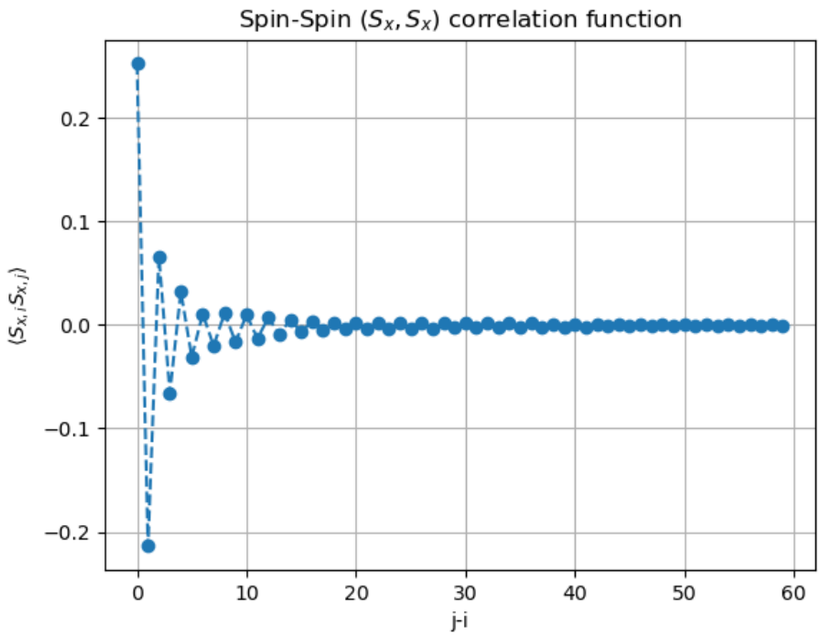

Figure 6: Correlation function $\langle S_{x,i} S_{x,j} \rangle$ with NRG method

And $S_z S_z$ correlation function is shown in Figure 7.

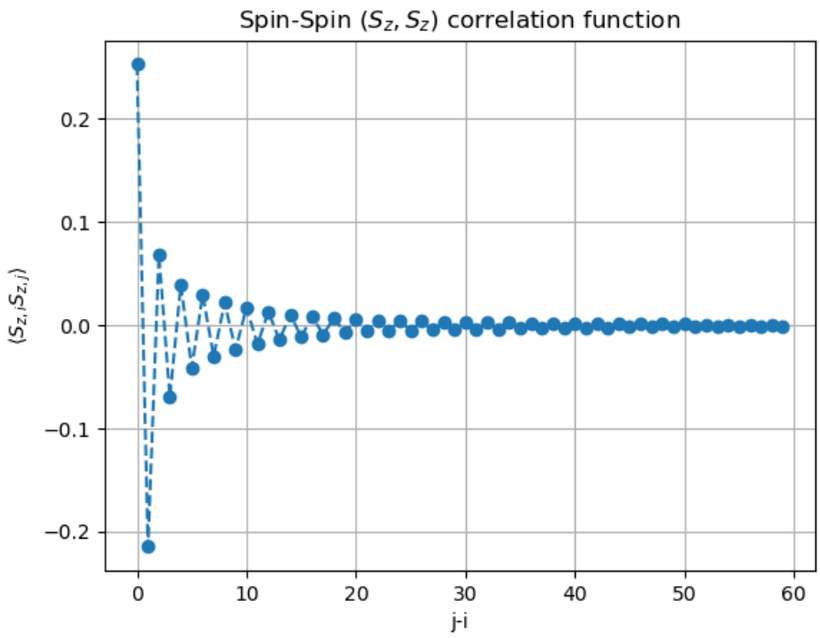

Figure 7: Correlation function $\langle S_{z,i} S_{z,j} \rangle$ with NRG method

Problem 3 : DMRG (Density Matrix Renormalization Group) for 1D quantum Ising chain

In this problem we are dealing with exactly the same chain as problem 2, but instead of NRG, I use DMRG algorithm to deal with it. In this problem, I set bond dimension 6 (dimension of matrices becomes 64 instead of 32) to obtain better answers. If we have

two blocks, any wave-function of this bipartite space can be written as

$$|\Psi\rangle = \sum_{i=1}^{D_L} \sum_{j=1}^{D_R} \psi_{ij} |i\rangle |j\rangle \tag{21}$$

We can obtain reduced density matrices for left and right blocks by taking partial traces:

$$\rho_L = Tr_R \left(|\Psi\rangle\langle\Psi| \right) = \psi\psi^\dagger \tag{22}$$

$$\rho_R = Tr_L \left(|\Psi\rangle\langle\Psi| \right) = \psi^T\psi^* \tag{23}$$

Now we add one site at a time similar to what we did in NRG, but here we add one site to **both blocks** simultaneously. The constructing the left and right block's hamiltonians as following:

$$\mathcal{H}_{l+1}^L = \tilde{\mathcal{H}}_l^L \otimes \mathbb{1}_2 + \tilde{S}_{x,l}^L \otimes \frac{\hbar}{2}\sigma_x + \tilde{S}_{y,l}^L \otimes \frac{\hbar}{2}\sigma_y + \tilde{S}_{z,l}^L \otimes \frac{\hbar}{2}\sigma_z \tag{24}$$

$$\mathcal{H}_{l+1}^R = \mathbb{1}_2 \otimes \tilde{\mathcal{H}}_l^R + \frac{\hbar}{2}\sigma_x \otimes \tilde{S}_{x,l}^R + \frac{\hbar}{2}\sigma_y \otimes \tilde{S}_{y,l}^R + \frac{\hbar}{2}\sigma_z \otimes \tilde{S}_{z,l}^R \tag{25}$$

And the super-block hamiltonian is:

$$\mathcal{H}_{l+l} = \mathcal{H}_l^L \otimes \mathbb{1}^R + \mathbb{1}^L \otimes \mathcal{H}_l^R + S_{x,l}^L \otimes S_{x,l}^R + S_{y,l}^L \otimes S_{y,l}^R + S_{z,l}^L \otimes S_{z,l}^R \tag{26}$$

Note that my labeling is in a way that the most left spin in the left block is 1, right of that 2, then 3 and ... . The most right spin in the right block is 1, left of that 2, then 3 and ... .

For operators $O = O_L \otimes O_R$, expectation values can be obtained by:

$$\langle O \rangle = \langle \psi | O_L \otimes O_R | \psi \rangle = Tr(\psi^\dagger O_L \psi O_R^T) \tag{27}$$

If $O_L = \mathbb{1}_L$ equation (27) reduces to:

$$\langle O \rangle = Tr(O_R \rho_R) \tag{28}$$

And if $O_R = \mathbb{1}_R$ equation (27) reduces to:

$$\langle O \rangle = Tr(\rho_L O_L) \tag{29}$$

By this method (that called **Infinite DMRG**), the ground-state wave function is obtained as:

$$H_{gs} = -26.7953632366 \tag{30}$$

It is really close to the energy obtained by NRG in equation (14).

Average spin in x and y directions are plotted in Figures 8 and 9, respectively.

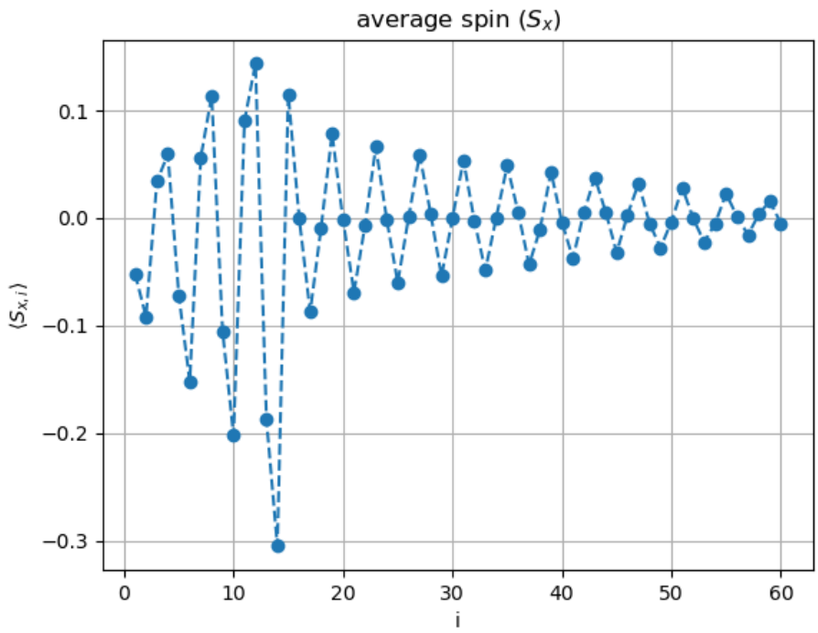

Figure 8: $\langle S_{x,i} \rangle$ with infinite DMRG method

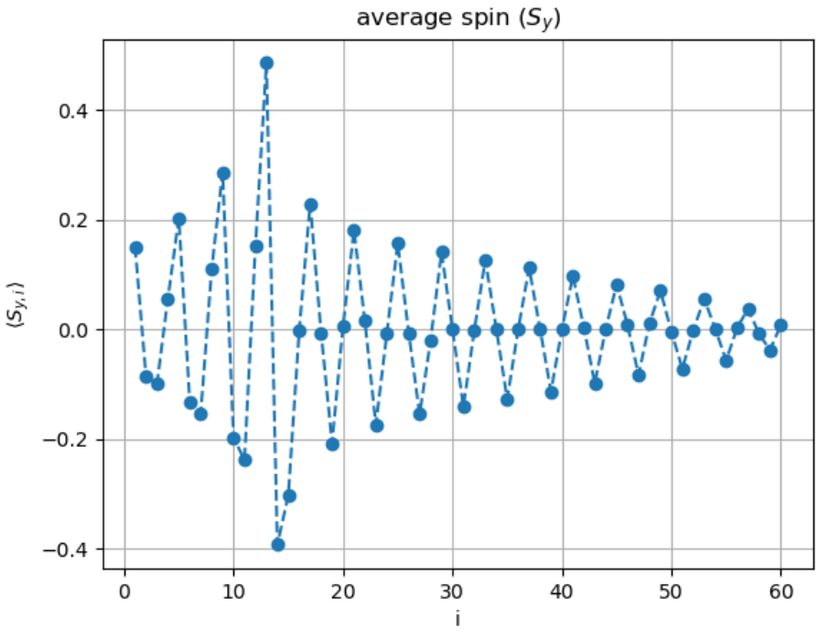

Figure 9: $\langle S_{y,i} \rangle$ with infinite DMRG method

Note there is more error near the first few sites, because by DMRG method, the error is larger near the edges, and smaller near the center of the system. The average value for spins can be evaluated as:

$$\overline{\langle S_{x,i} \rangle} = \frac{1}{L} \sum_{i=1}^{L} \langle S_{x,i} \rangle = -0.0097546829 \tag{31}$$

$$\overline{\langle S_{y,i} \rangle} = \frac{1}{L} \sum_{i=1}^{L} \langle S_{x,i} \rangle = -0.0019683567 \tag{32}$$

The spin-spin correlation functions are plotted in Figure 10 and 11, respectively.

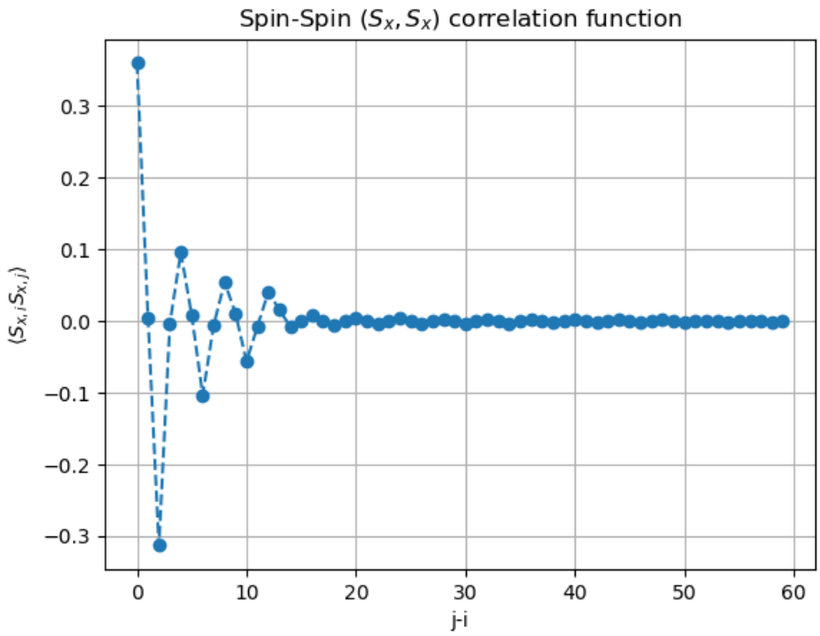

Figure 10: Correlation function $\langle S_{x,i} S_{x,j} \rangle$ with infinite DMRG method

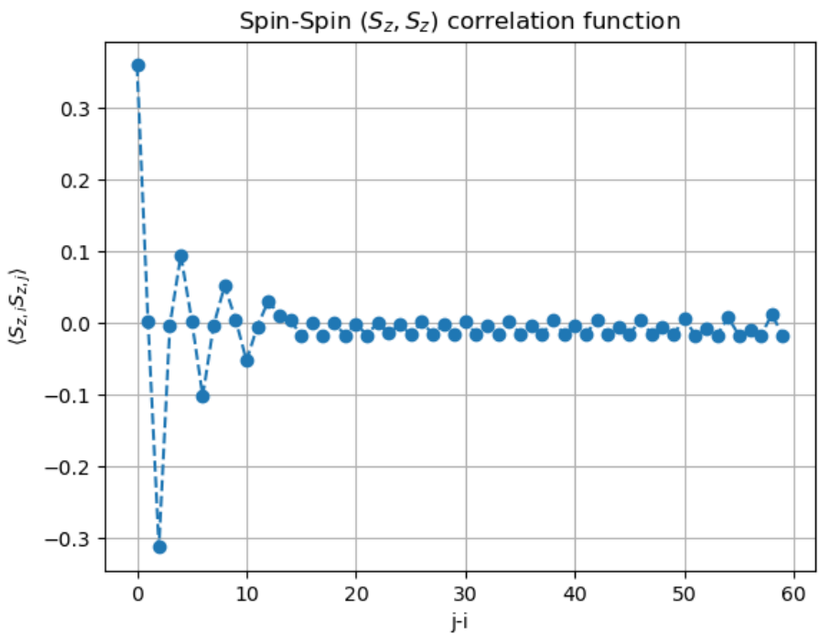

Figure 11: Correlation function $\langle S_{z,i} S_{z,j} \rangle$ with infinite DMRG method

The graphs for correlation function are really similar with Figures 6 and 7, obtained by NRG.

*Note that in my code, wherever I had an operator that i know in theory is hermitian, I made it hermitian make numerical errors less by considering $O_{new} = (O + O^{\dagger})/2$