Computational Physics
Set 3

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Problem 1 : 1D Heisenberg chain

In this problem we are dealing with 1D Heisenberg chain with 12 spins, with nearest neighbor interaction of strength $J_1 = 1.0$ and next nearest interaction with $J_2 = 0.3$. We also assume periodic boundary condition. The hamiltonian in this case is:

$$H = J_1(\sum_{i=1}^{n-1} \vec{S}_i.\vec{S}_{i+1} + \vec{S}_n.\vec{S}_1) + J_2(\sum_{i=1}^{n-2} \vec{S}_i.\vec{S}_{i+2} + \vec{S}_{n-1}.\vec{S}_1 + \vec{S}_n.\vec{S}_2) \quad (1)$$

The spin operators in site-n can be constructed as below:

$$S^{(n)}_{x,y,z} = \mathbb{1}_{n-1} \otimes (\frac{\hbar}{2}\sigma_{x,y,z}) \otimes \mathbb{1}_{L-n} \quad (2)$$

A) **At the end of the report.**

B) In this part, we first project the hamiltonian in a subspace with $S_{z,tot} = 0$, then diagonalize projected hamiltonian and obtain the 20 lowest energy eigenvalues, that can be seen in Figure 1.

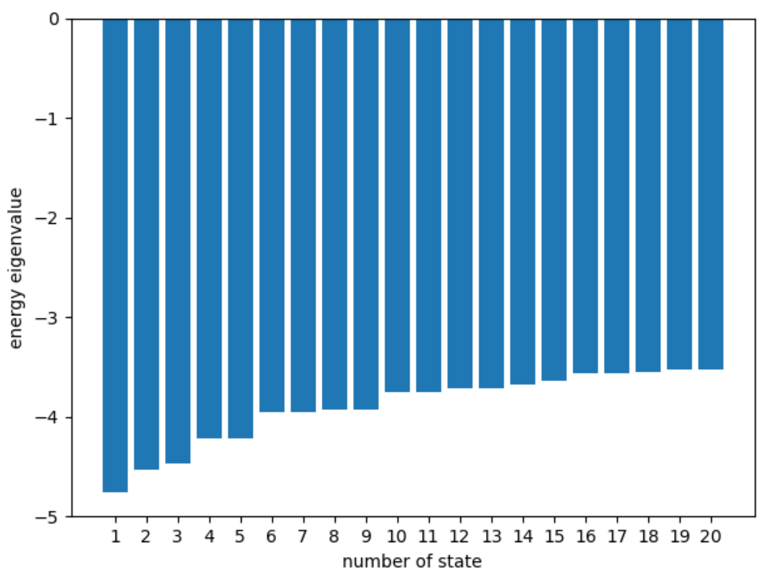


Figure 1: 20 lowest energy eigenvalues

The values for eigenenergies that obtained by the running the code are: [-4.76303164, -4.5285588, -4.46505456, -4.21822193, -4.21822193, -3.95576514, -3.95576514, -3.93188563, -3.93188563, -3.75118283, -3.75118283, -3.72020866, -3.72020866, -3.67408807, -3.63300302, -3.56160843, -3.56160843, -3.55043673, -3.53041809, -3.53041809]

C) in this part we have to calculate spin-spin correlation function that is obtained by equation (3):

$$Corr(\vec{S}_i, \vec{S}_j) = \langle \psi | \vec{S}_i . \vec{S}_j | \psi \rangle \tag{3}$$

To obtain the correlation function, first we have to convert the ground state wave-function in $S_{z,tot} = 0$ to the original Hilbert space, then sandwich desired operators between them. Note that because of translational symmetry, the correlation function between site-i and site-j is only function of the difference of i and j, or in other words, the **distance**. In Figure 2 you can see the spin-spin correlation function with respect to distance.

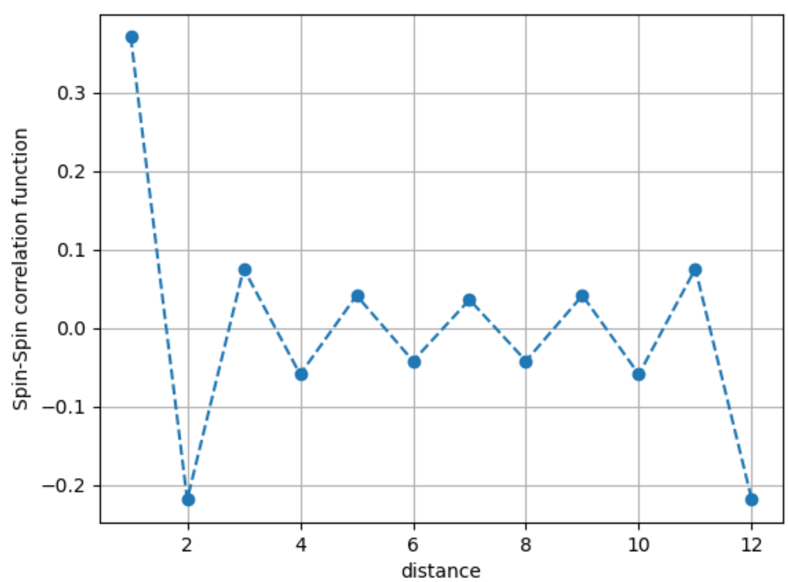


Figure 2: Spin-Spin correlation function

D) In this part, I have to calculate entanglement entropy of n spins in the left hand side, with L-n spins in the right hand side (n= 0, 1, 2, 3, ..., 12). First, I assume that the total system is in the ground state, and thus is a pure state. The density matrix is obtained by:

$$\rho_{tot} = |\psi\rangle\langle\psi| \tag{4}$$

Instead of calculating partial traces to obtain ρ_L and ρ_R, I use the method of reshaping to obtain them by this formulas:

$$\tilde{\psi} = reshape(\psi,\ dim_R,\ dim_L) \tag{5}$$

$$\rho_L = (\tilde{\psi}^\dagger \tilde{\psi})^* \tag{6}$$

$$\rho_R = \tilde{\psi}\tilde{\psi}^\dagger \tag{7}$$

Entanglement entropy is plotted in Figure 3 for n = 0, 1, 2, ..., 12 particles in the left hand side. Note the symmetry around n=6 (half left, half right). In n = 0 and n = 12 the subsystem is actually the total system and is pure, so its entanglement entropy is zero.

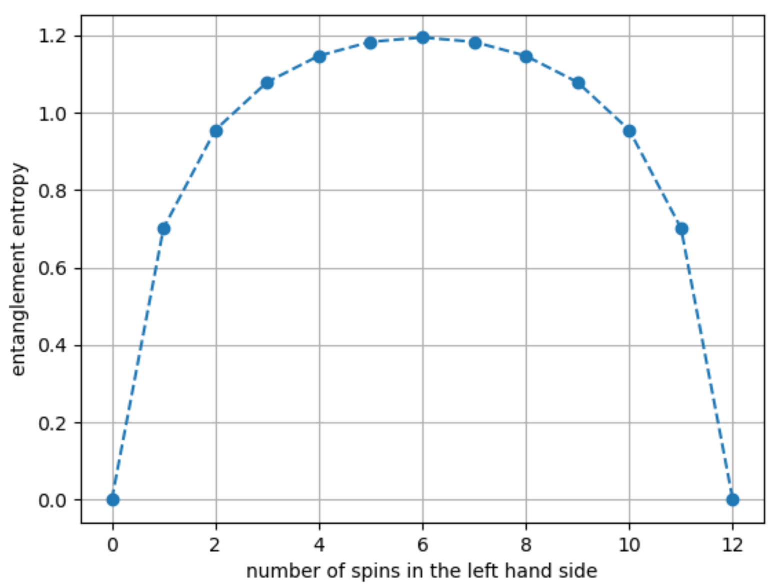


Figure 3: Entanglement entropy of n = 0, 1, 2, ..., 12 spins in left, with L - n in right

Problem 2 : 2D Heisenberg chain

In this problem, we are dealing with similar problem as problem 1, but in 2D, and we have a 3 (vertical) $\times$ 4 (horizontal) rectangular configuration. In this 2D Heisenberg chain, first we have to label all point by i and j, and also ij index. The later is turning a 2D problem to a 1D one by relabeling points by one label "ij" instead of two "i and j"in this way (discussed in the class):

$$ij = (i-1) \times N_y + j \tag{8}$$

All relations are similar to the previous problem, except that we have to apply periodic boundary condition in x and y axes, and also we have to use $\vec{S}_{ij}$. This periodic boundary condition implies that for each column (fixed i), i gets the values 1, 2, 3 and after that, again 1, 2, 3. For each row (fixed j), i gets the values 1, 2, 3, 4 and after that, again 1, 2, 3, 4.

A) This part is exactly similar to part A in problem 1, after relabeling.

B) Again as in problem 1, I project the hamiltonian in a subspace with $S_{z,tot} = 0$, then diagonalize it. The resulting 20 lowest energy eigenvalues are plotted in Figure 4.

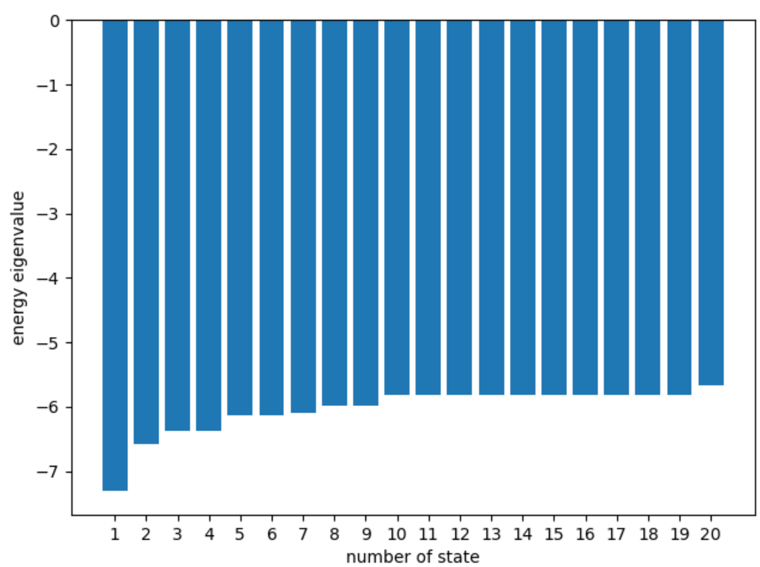


Figure 4: 20 lowest energy eigenvalues of 2D system

Their values are:
[-7.30920839, -6.57965484, -6.37543542, -6.37543542, -6.12574653, -6.12574653, -6.10228709, -5.97269863 -5.97269863, -5.82214587, -5.82214587, -5.81896608 -5.81896608, -5.81896608, -5.81896608, -5.80688998, -5.80688998, -5.80688998, -5.80688998, -5.66670484]

C) Then for calculating correlation function, I have to convert the ground state wave-function in the projected Hilbert space to the original Hilbert space. For plotting the correlation function, assuming translational symmetry, I calculate and plot the real part of spin-spin correlation function against the **difference in ij s**, or **ij(n) - ij(1)**. The resulting plot can be seen in Figure 5.

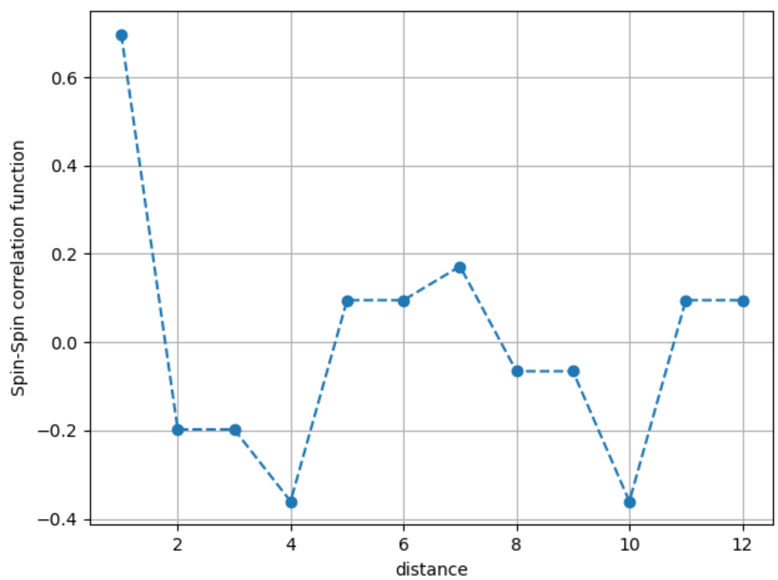


Figure 5: Spin-Spin correlation function of 2D system

D) For computing the entanglement entropy, I divide the system to two parts and use the **ij labeling system** and continue as part D of problem 1. The resulting plot is shown in figure 6.

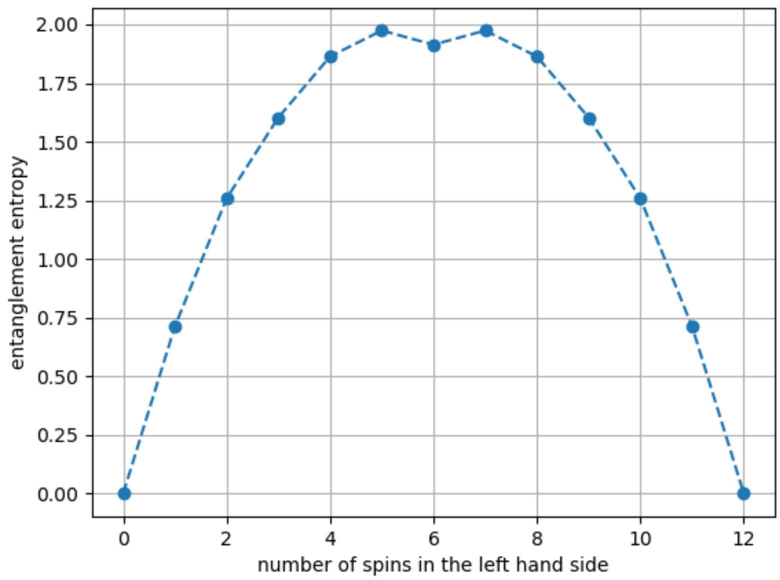


Figure 6: Entanglement entropy of 2D system n = 0, 1, 2, ..., 12 spins in left, with L - n in right

Problem 3 : Time evolution in alternating 1D Heisenberg chain

In this problem, again we have a 1D chain of 12 spins. At t=0, the Heisenberg interaction is between 1 and 2, 3 and 4, ... For t¿0, the conventional Heisenberg interaction turned one between all spins and periodic boundary condition imposed on the system.

A) **At the end of the report.**

For numerical computation, I again use similar hamiltonian as equation (1), but i jumps 2 steps instead of 1. The Energy of the ground state is -4.5000 and ground state wave function is plotted in Figure 7.

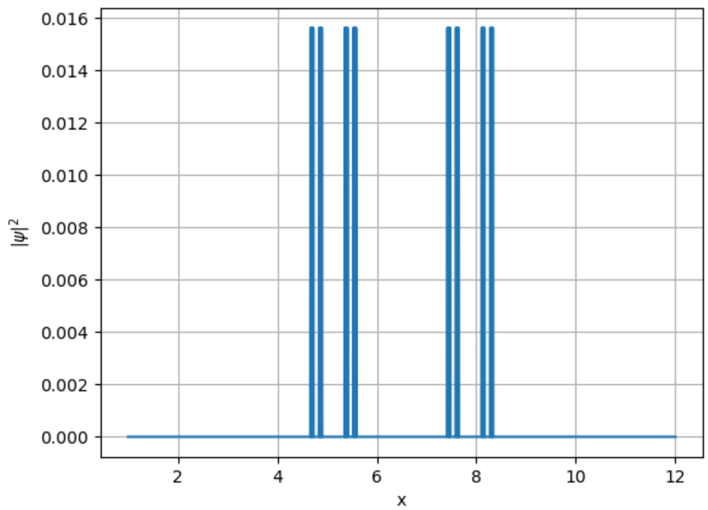


Figure 7: Probability distribution for ground state at t=0

B) The time evolution of the initial state is obtained by the formula:

$$|\psi(t)\rangle = \exp(-\frac{iH_{(t)}\Delta t}{\hbar})\exp(-\frac{iH_{(t-\Delta t)}\Delta t}{\hbar})...\exp(-\frac{iH_{(\Delta t)}\Delta t}{\hbar})|\psi(0)\rangle \quad (9)$$

This has been evaluated in the code and its result is used in the next two parts. C) Using the result of part B, the spin-spin correlation function as a function of time for each distance is plotted in Figure 8.

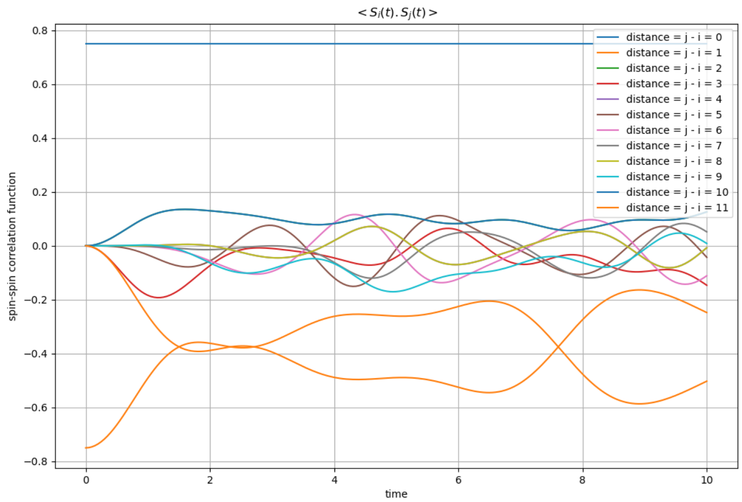


Figure 8: Spin-Spin correlation function as function of time for each distance

Now if we take account of one spin's time evolution, but consider the other spin in t=0, the resulting spin-spin correlation function is plotted in Figure 9.

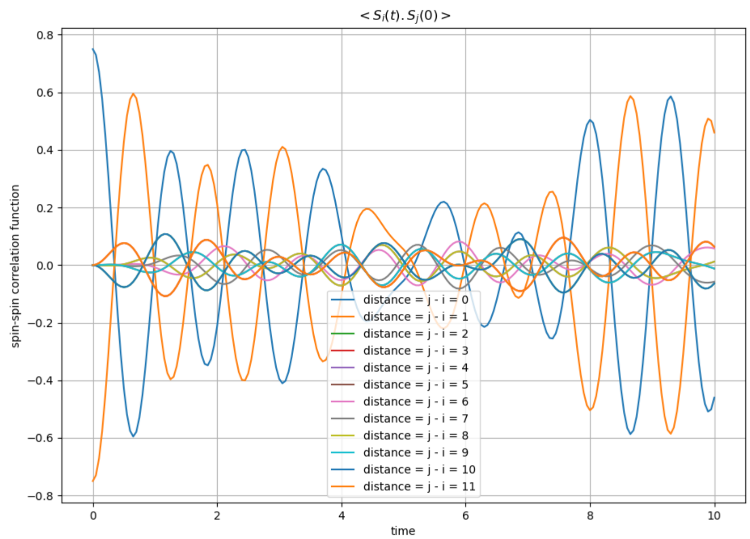


Figure 9: Spin-Spin correlation function as function of time for each distance, if left spin evolves in time but right spin is considered at t=0

D) In this part, we examine the time evolution of entanglement entropy of one half of the system with the other half. At t=0, there is no interaction between 6th and 7th spins, and two groups must be unentangled. But as time passes, the entanglement entropy increase to a certain valued, but after that oscillate with time (if the time interval was between 0 and 100 instead of 0 and 10 it could be easily observes). This observation can be seen in the numerical solution in Figure 10.

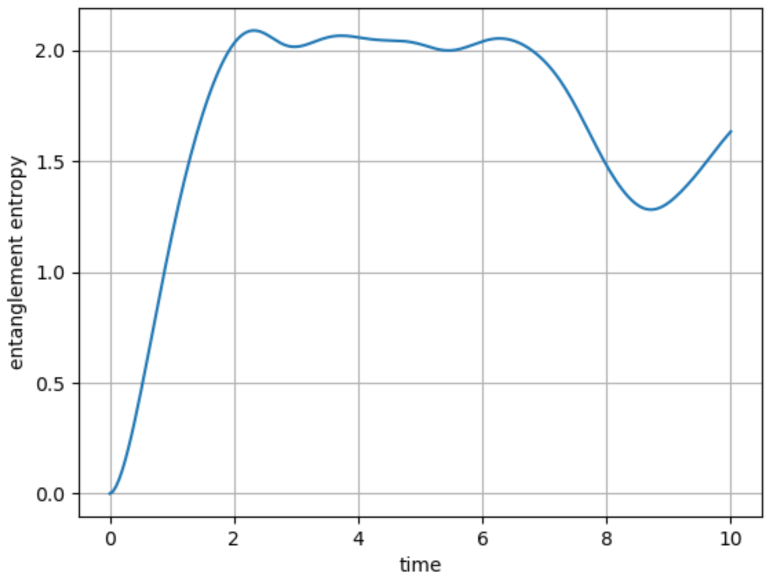
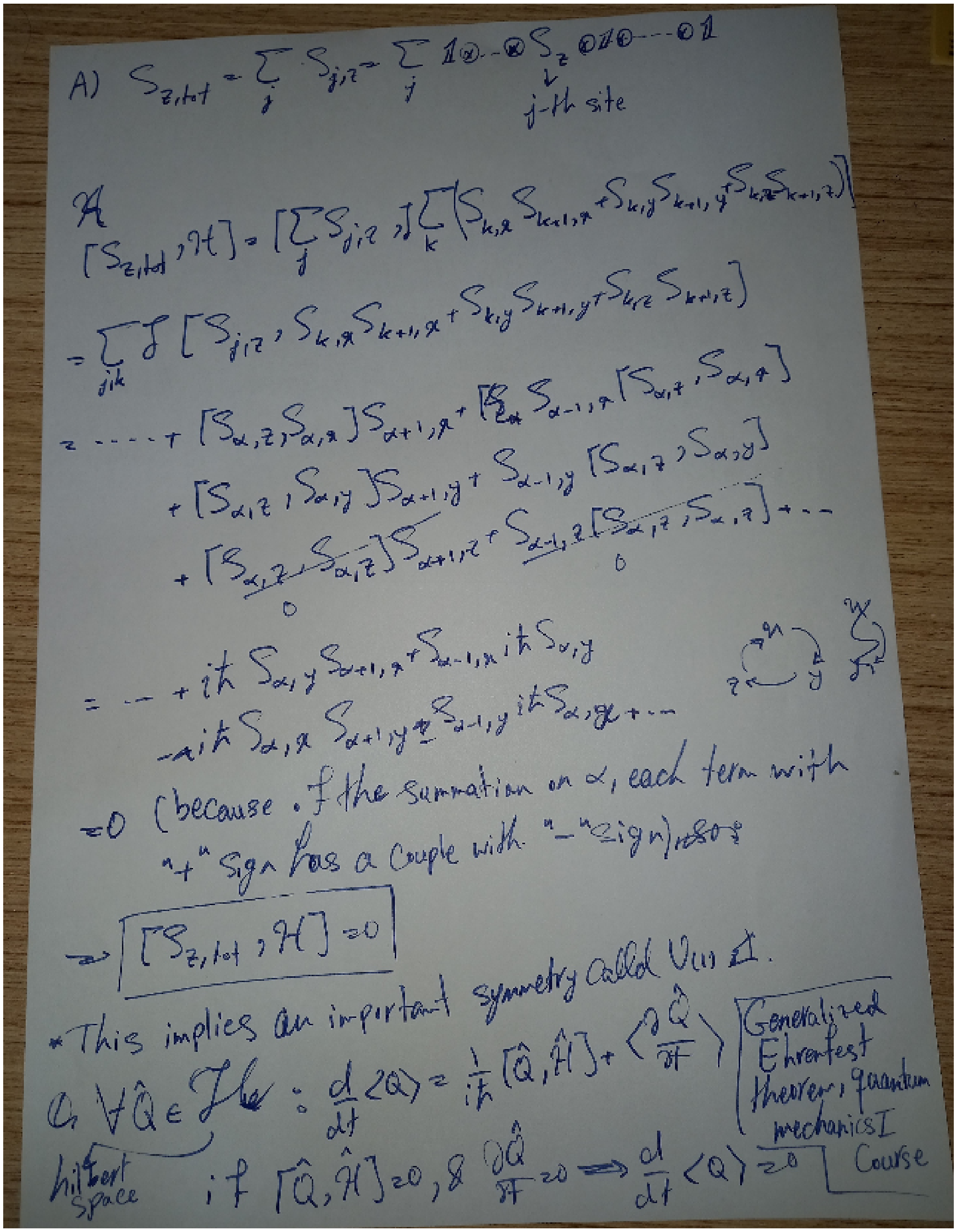


Figure 10: Entanglement entropy of left half of the system with the right half, as a function of time

Analytical parts of problems



A) $S_{z,tot} = \sum_j S_{j,z} = \sum_j \mathbb{1} \otimes \cdots \otimes \underset{j\text{-th site}}{S_z} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$

$$[S_{z,tot}, \mathcal{H}] = [\sum_j S_{j,z}, J \sum_k (S_{k,x} S_{k+1,x} + S_{k,y} S_{k+1,y} + S_{k,z} S_{k+1,z})]$$

$$= \sum_{jk} J [S_{j,z}, S_{k,x} S_{k+1,x} + S_{k,y} S_{k+1,y} + S_{k,z} S_{k+1,z}]$$

$$= \cdots + [S_{\alpha,z}, S_{\alpha,x}] S_{\alpha+1,x} + S_{\alpha-1,x} [S_{\alpha,z}, S_{\alpha,x}]$$
$$+ [S_{\alpha,z}, S_{\alpha,y}] S_{\alpha+1,y} + S_{\alpha-1,y} [S_{\alpha,z}, S_{\alpha,y}]$$
$$+ \underbrace{[S_{\alpha,z}, S_{\alpha,z}]}_{0} S_{\alpha+1,z} + S_{\alpha-1,z} \underbrace{[S_{\alpha,z}, S_{\alpha,z}]}_{0} + \cdots$$

$$= \cdots + i\hbar S_{\alpha,y} S_{\alpha+1,x} + S_{\alpha-1,x} i\hbar S_{\alpha,y}$$
$$- i\hbar S_{\alpha,x} S_{\alpha+1,y} - S_{\alpha-1,y} i\hbar S_{\alpha,x} + \cdots$$

$= 0$ (because of the summation on α, each term with "+" sign has a couple with "−" sign)

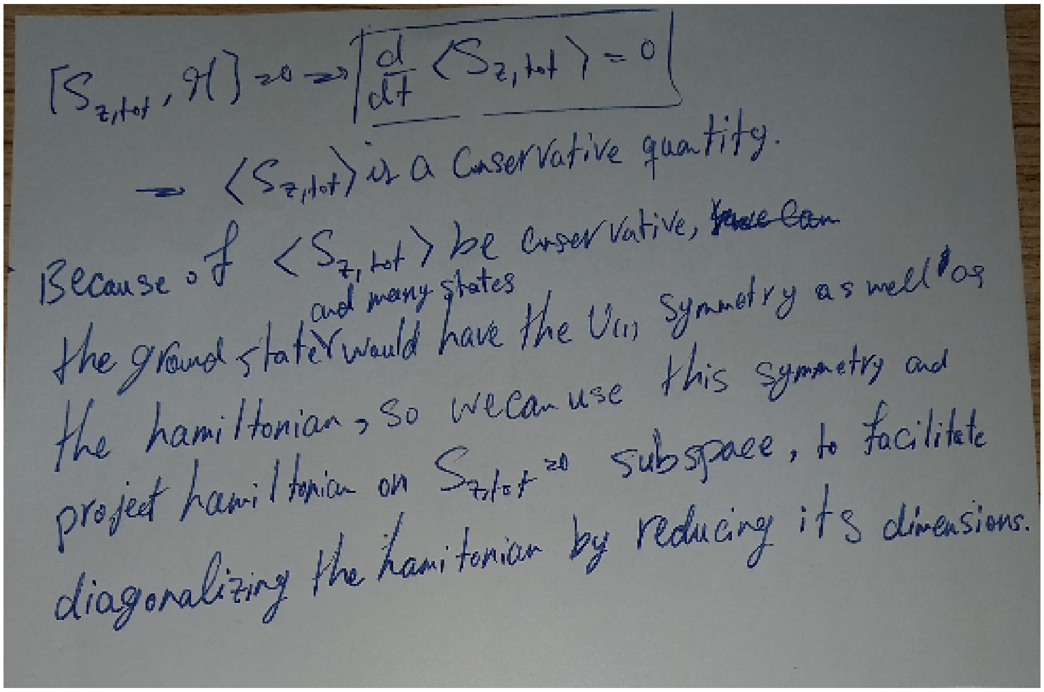
$\Rightarrow \boxed{[S_{z,tot}, \mathcal{H}] = 0}$

* This implies an important symmetry called $U(1)$.

$\hookrightarrow \forall \hat{Q} \in \underbrace{\mathcal{H}}_{\text{hilbert space}}$: $\frac{d}{dt}\langle Q \rangle = \frac{1}{i\hbar}[\hat{Q}, \hat{H}] + \langle \frac{\partial \hat{Q}}{\partial t} \rangle$ [Generalized Ehrenfest theorem, quantum mechanics I Course]

if $[\hat{Q}, \hat{H}] = 0$, & $\frac{\partial \hat{Q}}{\partial t} = 0 \Longrightarrow \frac{d}{dt}\langle Q \rangle = 0$

Figure 11: Problem 1 and 2; Part A



$[S_{z,tot}, \mathcal{H}] = 0 \Rightarrow \boxed{\frac{d}{dt}\langle S_{z,tot}\rangle = 0}$

$\Rightarrow \langle S_{z,tot}\rangle$ is a Conservative quantity.

Because of $\langle S_{z,tot}\rangle$ be Conservative, ~~we can~~ the ground state and many states would have the $U(1)$ Symmetry as well as the hamiltonian, so we can use this symmetry and project hamiltonian on $S_{z,tot}=0$ subspace, to facilitate diagonalizing the hamitonian by reducing its dimensions.

Figure 12: Problem 1 and 2; Part A

A) Each pair is disconneted from the surrounding, so we can find the ground state for each pair, and because of being disconnected, the total energy would be sum of energyies and the total ground state would be tensor product of each pair's groud state:

$$E_{tot} = \sum_{\langle ij \rangle} E_{ij} \,,\, |\Psi_{tot}\rangle = |\Psi_{12}\rangle \otimes |\Psi_{34}\rangle \otimes \cdots \otimes |\Psi_{11,12}\rangle$$

$$= E_{12} + E_{34} + \cdots + E_{11,12}$$

$$= 6E_{12}$$

two-body problem $\mathcal{H} = J \vec{S}_1 \cdot \vec{S}_2 \quad J$

$$(\vec{S}_1 + \vec{S}_2)^2 = (S_1)^2 + (S_2)^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

$$\rightarrow \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left[(\vec{S}_1 + \vec{S}_2)^2 - (S_1)^2 - (S_2)^2\right]$$

$$= \frac{1}{2}\left[(S_{tot})^2 - (S_1)^2 - (S_2)^2\right]$$

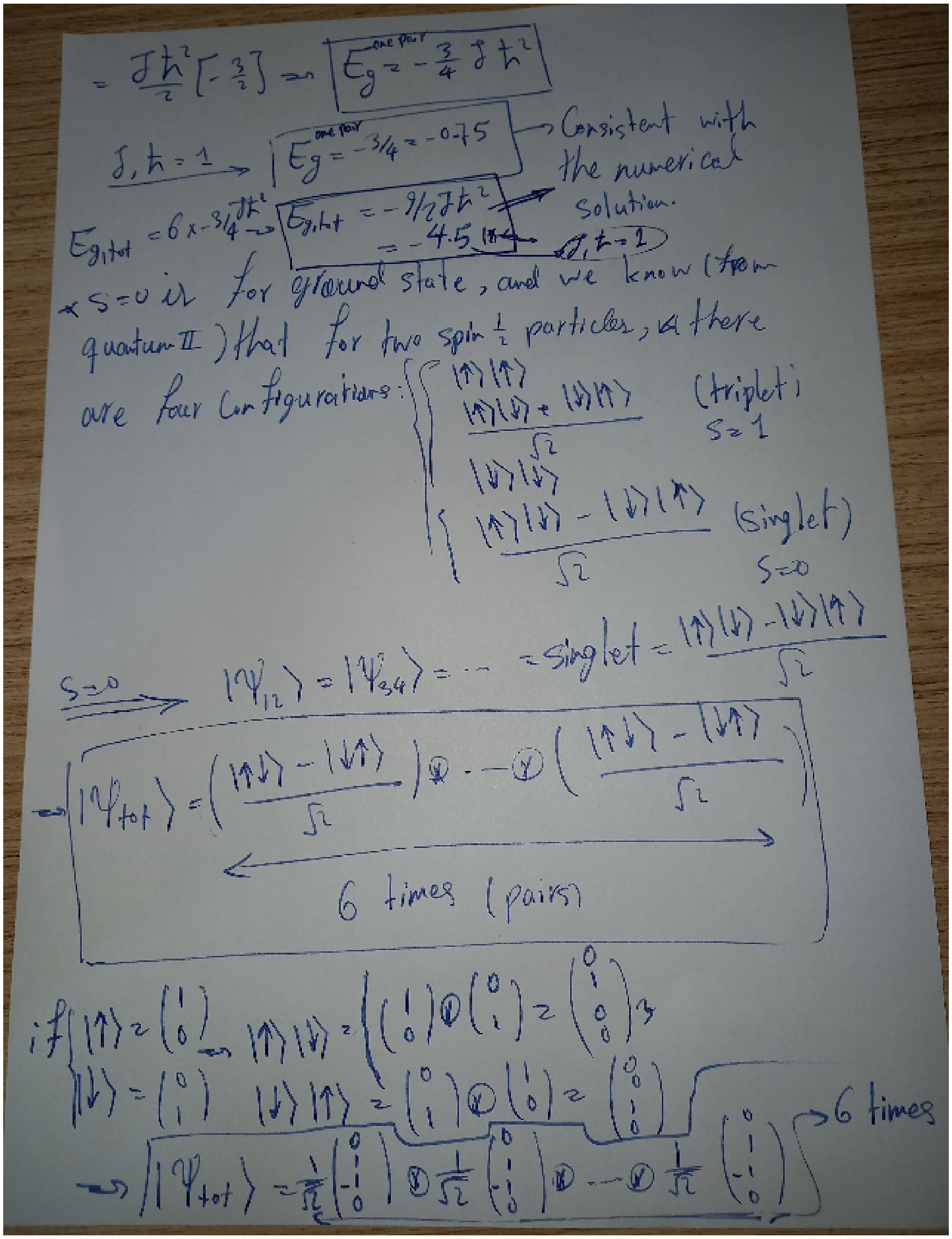
$$S^2 |s,m\rangle = \hbar^2 s(s+1)|s,m\rangle$$

$$\boxed{\mathcal{H} = \frac{J}{2}\left[(S_{tot})^2 - (S_1)^2 - (S_2)^2\right]} \xrightarrow{\text{in } (S_{tot})^2 \text{ basis}} \boxed{E = \frac{J\hbar^2}{2}\left[s(s+1) - s_1(s_1+1) - s_2(s_2+1)\right]}$$

$$\text{spin-}\tfrac{1}{2} \oplus \text{spin-}\tfrac{1}{2} = \begin{cases} \text{spin-}0 \rightarrow \text{ground state} \\ \text{spin-}1 \end{cases} \,,\, s_1 = s_2 = \frac{1}{2}$$

$$J=1, \hbar=1 \rightarrow E_g = \frac{J\hbar^2}{2}\left[0 - \left(\tfrac{1}{2}\right)\left(\tfrac{3}{2}\right) - \left(\tfrac{1}{2}\right)\left(\tfrac{3}{2}\right)\right]$$

Figure 13: Problem 3; Part A



$$= \frac{J\hbar^2}{2}\left[-\frac{3}{2}\right] \Rightarrow \boxed{E_g^{\text{one pair}} = -\frac{3}{4}J\hbar^2}$$

$J,\hbar=1 \rightarrow \boxed{E_g^{\text{one pair}} = -3/4 = -0.75}$ → Consistent with the numerical solution.

$E_{g,tot} = 6\times -3/4\, J\hbar^2 \rightarrow \boxed{E_{g,tot} = -9/2\, J\hbar^2 = -4.5}$ $(J,\hbar=1)$

* S=0 is for ground state, and we know (from quantum II) that for two spin $\frac{1}{2}$ particles, there are four configurations:

$|\uparrow\rangle|\uparrow\rangle$, $\frac{|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle}{\sqrt{2}}$, $|\downarrow\rangle|\downarrow\rangle$ (triplet; $S=1$)

$\frac{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle}{\sqrt{2}}$ (singlet) $S=0$

$$S=0 \Longrightarrow |\psi_{12}\rangle = |\psi_{34}\rangle = \cdots = \text{singlet} = \frac{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle}{\sqrt{2}}$$

$$\rightarrow \boxed{|\psi_{tot}\rangle = \underbrace{\left(\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}\right)\otimes\cdots\otimes\left(\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}\right)}_{6 \text{ times (pairs)}}}$$

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

$$\rightarrow \boxed{|\psi_{tot}\rangle = \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\otimes\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\otimes\cdots\otimes\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}}_{6 \text{ times}}}$$

Figure 14: Problem 3; Part A