

UNIVERSITY OF OSLO

Project 1

FYS5419 – Project1

Hishem Kløvnes

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1 a)

In this project, there are a few matrices that will be used repeatedly. So before doing anything, I will formulate them here first. The three Pauli matrices:

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

The Hadamard and Phase gate

$$\begin{aligned}H &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ S &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix},\end{aligned}$$

and the CNOT gate

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

In this part of the project, the goal was to take a one qubit basis, apply the right gates to it - creating a Bell state - and then measure the state. The states we use are simply $|0\rangle = [1, 0]$ and $|1\rangle = [0, 1]$. The Bell state is given by

$$\begin{aligned}|\Phi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |\Phi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |\Psi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)\end{aligned}$$

where $|00\rangle$ is the state where both qubits are in the state $|0\rangle$, and $|11\rangle$ is the state where both qubits are in the state $|1\rangle$.

The first thing I did was to apply the Hadamard gate and the Phase gate to the one qubit basis to see what happens.

$$\begin{aligned}H|0\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ H|1\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}\end{aligned}$$

This means that after applying the Hadamard gate to the one-qubit basis, we get a pair of new states which are defined as superpositions of the original states. Here the new superpositioned states are almost identical. The only difference is the sign of the second state, which represents that the state points along $-X$ axis on the Bloch sphere, in contrast to the first state which points along the X axis.

The next step was to apply the Phase gate to the one-qubit basis.

$$S|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$S|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix}$$

This means that the Phase gate does not change the state of the qubit in the $|0\rangle$ state, but it changes the state of the qubit in the $|1\rangle$ state. The $|1\rangle$ state still points to the south pole of the block sphere, but has acquired a phase factor of i .

The next step was to define Bell states. To do this, I first defined them explicitly, and then I created the Bell states by applying the right gates to each state. As I mentioned earlier there are four Bell states, and to create them I applied the CNOT and Hadamard gates to different tensor products of the one-qubit basis.

$$CNOT \cdot (H|0\rangle) \otimes |0\rangle = \frac{1}{\sqrt{2}}[1, 0, 0, 1]$$

$$CNOT \cdot (H|1\rangle) \otimes |0\rangle = \frac{1}{\sqrt{2}}[0, 1, 1, 0]$$

$$CNOT \cdot (H|0\rangle) \otimes |1\rangle = \frac{1}{\sqrt{2}}[1, 0, 0, -1]$$

$$CNOT \cdot (H|1\rangle) \otimes |1\rangle = \frac{1}{\sqrt{2}}[0, 1, -1, 0]$$

I double checked these states with the definition of the Bell states, and they are correct. The next step was to apply the Hadamard gate and thereafter the CNOT gate to the Bell states. Let's take the first Bell state as an example.

$$CNOT \cdot (H \otimes I) |\Phi^+\rangle =$$

$$CNOT \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} |\Phi^+\rangle =$$

$$CNOT \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} |\Phi^+\rangle =$$

$$CNOT \cdot \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ 1 \end{pmatrix}$$

When repeating this process for all our Bell states, we notice that all of them are superpositions of all states: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. This means that it does not matter which of the modified Bell states we use to measure, because the outcome should be the same.

In 1 I have compared the measurement of the Bell states using the method described above with the measurement of the Bell states using Qiskit. I did $n = 10000$ measurement on both methods, and the results are practically identical, which is what we would expect. For a system like this, we would expect the results to be around 25% for each state. If we were to do even more measurements, $n = 100000, 1000000 \dots$ we would expect the results to be even closer to 25% for each state.

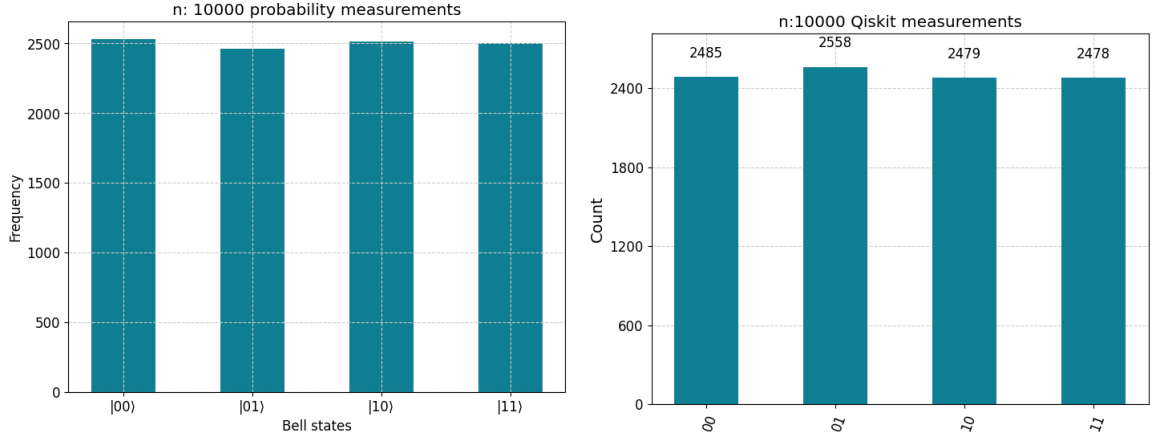


Figure 1: The left figure shows the measurement of the Bell states using the method described above. The right figure shows the measurement of the Bell states using Qiskit.

2 b)

For this part of the problem, we have the same one-qubit basis as in the previous problem. Now we have a Hamiltonian $H = H_0 + \lambda H_I$, where

$$H_0 = \mathcal{E}I + \Omega\sigma_z, \quad \mathcal{E} = \frac{E_1 + E_2}{2}, \quad \Omega = \frac{E_1 - E_2}{2}$$

and

$$H_I = cI + \omega_z\sigma_z + \omega_x\sigma_x$$

where $c = (V_{11} + V_{22})/2$, $\omega_z = (V_{11} - V_{22})/2$, $\omega_x = V_{12} = V_{21}$. We have a set of given values for our parameters: $E_1 = 0, E_2 = 4, V_{11} = V_{-22} = 3, V_{12} = V_{21} = 0.2$.

In this section we want to find the eigenvalues of the Hamiltonian when acted on the one-qubit basis, as a function of the parameter λ . This was solved numerically. I computed the eigenvalues of the Hamiltonian as a function of λ , as shown in 2. At λ the energy levels of $|0\rangle$ and $|1\rangle$ are separated by $2\Omega = 4$. As λ increases, the interaction term H_I modifies the energy levels, causing them to converge. At $\lambda = \frac{2}{3}$, the eigenvalues cross, which indicates degeneracy where the ground state and excited state have the same energy. When λ continues to increase, energy levels starts to separate again.

The crossing is a level crossing, which occurs when the energy levels of the two states become degenerate. The physical interpretation of this result is that the system undergoes a transition at $\lambda = \frac{2}{3}$, where the ground state and excited states exchanges.

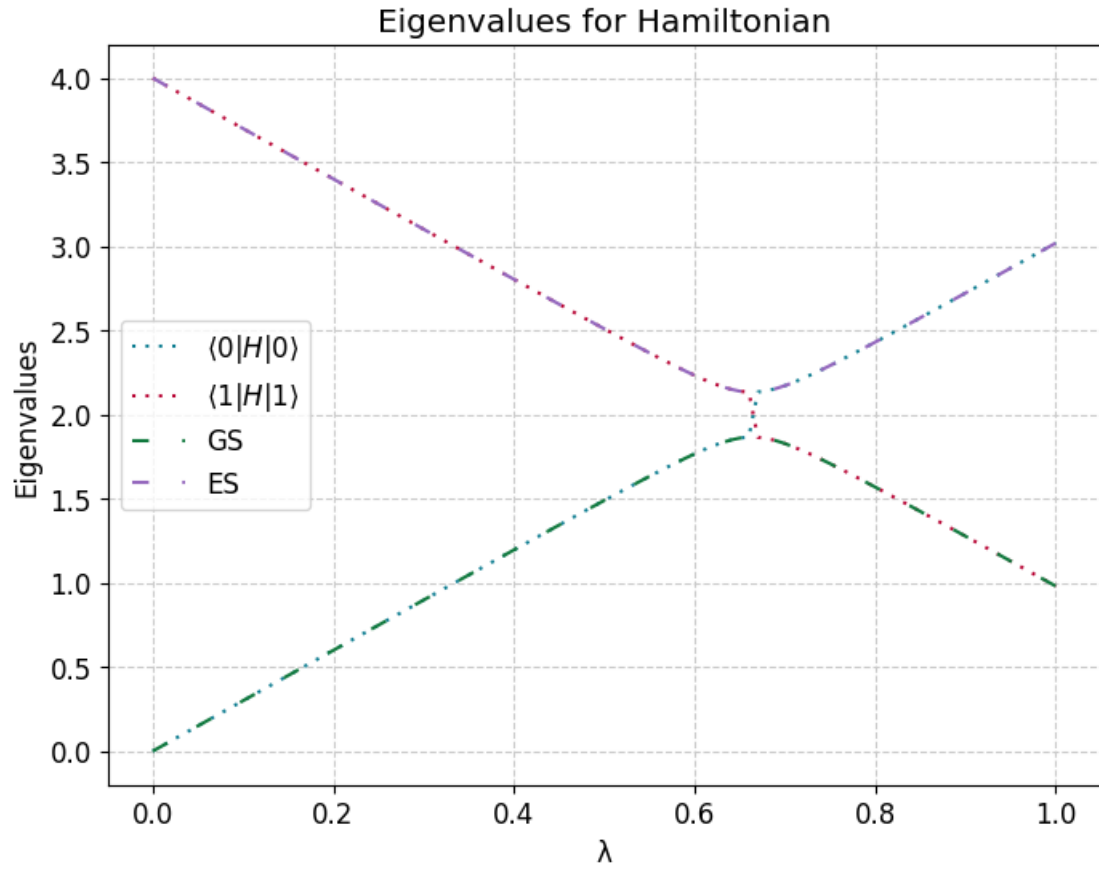


Figure 2: The eigenvalues of the Hamiltonian as a function of the parameter λ . ES represents the excited state, and GS represents the ground state.

3 c)

In this section we want to attempt to implement the variational Quantum eigensolver (VQE) for the above Hamiltonian system.

To do this I begun by defining the state $|0\rangle = [1, 0]$. I also defined two rotation matrices $R_x(\theta)$ and $R_y(\phi)$, which are given by

$$R_x(\theta) = \cos\left(\frac{\theta}{2}\right) \cdot I - i \sin\left(\frac{\theta}{2}\right) \cdot \sigma_x$$

$$R_y(\phi) = \cos\left(\frac{\phi}{2}\right) \cdot I - i \sin\left(\frac{\phi}{2}\right) \cdot \sigma_y$$

where θ and ϕ are the angles of rotation around the x and y axis, respectively, and I is the identity matrix.

The process of the VQE method is to first prepare the state $|0\rangle$, then apply the rotation matrices $R_x(\theta)$ and $R_y(\phi)$ to the state, with some arbitrary angles θ and ϕ . After this, we measure the expectation value of the Hamiltonian, which is given by

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | H_0 | \psi \rangle + \lambda \langle \psi | H_I | \psi \rangle$$

where $|\psi\rangle$ is the state after applying the rotation matrices. To find the optimal parameters for the rotation matrices, I used a gradient descent method, which is a method that minimizes a function by iteratively moving in the direction of the negative gradient. The gradient is calculated by

$$\partial\theta = \frac{\partial \langle H \rangle}{\partial \theta},$$

$$\partial\phi = \frac{\partial \langle H \rangle}{\partial \phi}$$

And the parameters are updated by

$$\theta_{new} = \theta_{old} - \eta \partial\theta,$$

$$\phi_{new} = \phi_{old} - \eta \partial\phi$$

where η is the learning rate. This method was performed a number of times for each λ , to find the optimal parameters.

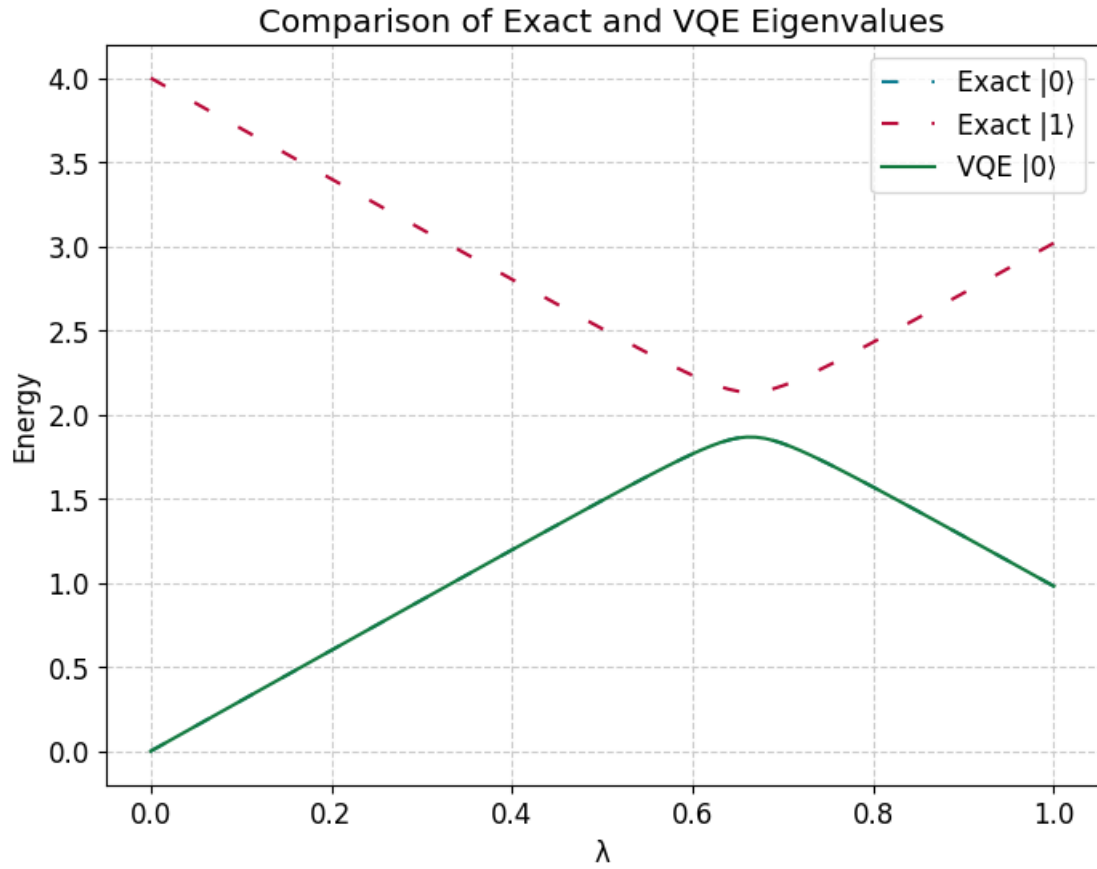


Figure 3: The figure shows a plot of the expectation value of the Hamiltonian as a function of the parameter λ . The plot shows that the VQE method aligned perfectly with the ground state energy of the Hamiltonian.

In figure 3 I have plotted the expectation value of the Hamiltonian as a function of the parameter λ . The plot shows that the VQE method aligned perfectly with the ground state energy of the Hamiltonian. Meaning that the VQE method was successful in finding the ground state energy of the Hamiltonian. The method of using gradient descent seemed to be a very effective and accurate method for the VQE of this simple system.

4 d)

In this section we expand to a two-qubit system, where our many-body computational basis is given by $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, defined as:

$$\begin{aligned} |00\rangle &= |0\rangle_A \otimes |0\rangle_B = [1 \ 0 \ 0 \ 0]^T \\ |01\rangle &= |0\rangle_A \otimes |1\rangle_B = [0 \ 1 \ 0 \ 0]^T \\ |10\rangle &= |1\rangle_A \otimes |0\rangle_B = [0 \ 0 \ 1 \ 0]^T \\ |11\rangle &= |1\rangle_A \otimes |1\rangle_B = [0 \ 0 \ 0 \ 1]^T \end{aligned}$$

These basis states also define the eigenstates of the non-interacting Hamiltonian:

$$\begin{aligned} H_0 |00\rangle &= \epsilon_{00} |00\rangle \\ H_0 |10\rangle &= \epsilon_{10} |10\rangle \\ H_0 |01\rangle &= \epsilon_{01} |01\rangle \\ H_0 |11\rangle &= \epsilon_{11} |11\rangle \end{aligned}$$

And the interacting part of the Hamiltonian is given by

$$H_I = H_x \sigma_x \otimes \sigma_x + H_z \sigma_z \otimes \sigma_z$$

Thus our Hamiltonian matrix is given by

$$\begin{pmatrix} \epsilon_{00} + \lambda H_z & 0 & 0 & \lambda H_x \\ 0 & \epsilon_{10} - \lambda H_z & \lambda H_x & 0 \\ 0 & \lambda H_x & \epsilon_{01} - \lambda H_z & 0 \\ \lambda H_x & 0 & 0 & \epsilon_{11} + \lambda H_z \end{pmatrix}$$

To find the energy eigenvalues we have a set of parameters $H_x = 2.0, H_z = 3.0, \epsilon_{00} = 0.0, \epsilon_{10} = 2.5, \epsilon_{01} = 6.5, \epsilon_{11} = 7.0$. I found the eigenvalues to this Hamiltonian by diagonalizing the matrix.

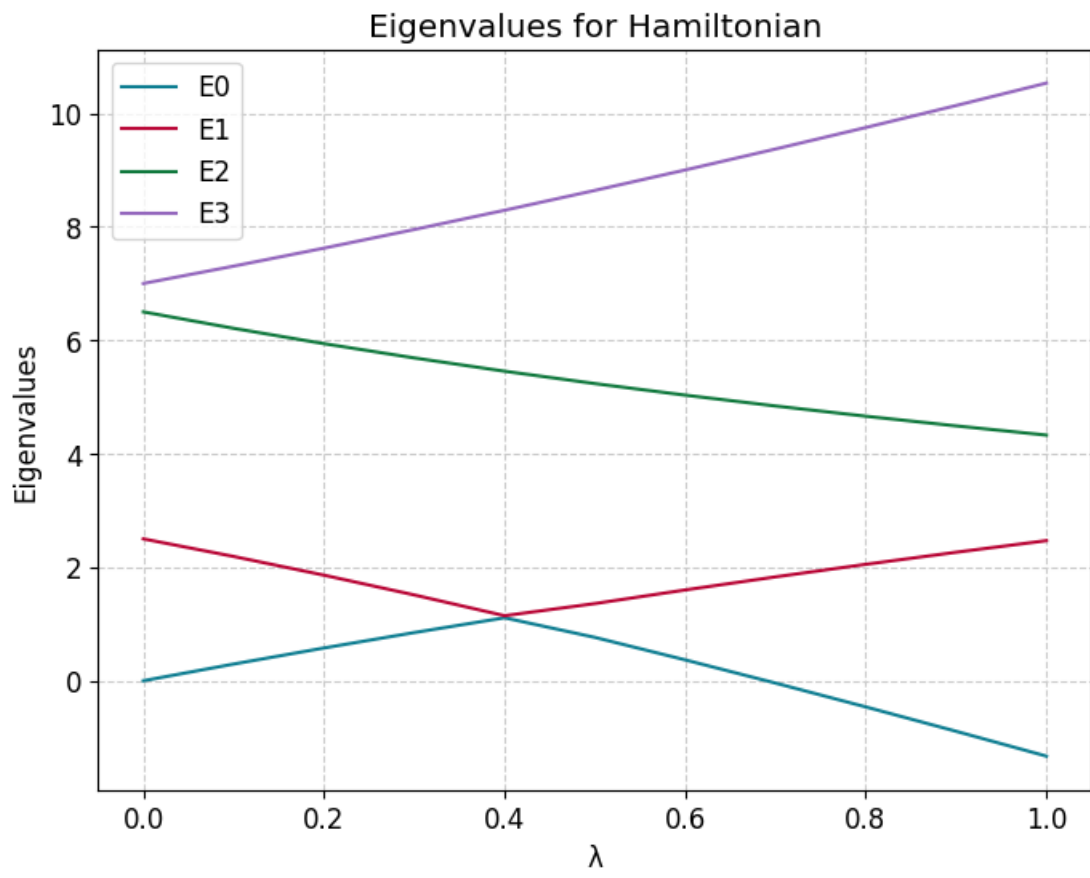


Figure 4: The figure shows the eigenvalues of the Hamiltonian as a function of the parameter λ .

In figure 4 we see the energy eigenvalues of the Hamiltonian, as a function of the interaction parameter λ . At $\lambda = 0.4$ we can, as in section b, see a level crossing where the ground state and excited state exchange. This shows how entanglement can be created in a system, by the Hamiltonian itself, due to the strength of the interaction.

The next step is to calculate the von Neumann entropy of the same system. This is done by first defining the density matrix of the lowest energy eigenstate.

$$\rho_0 = (\alpha_{00} |00\rangle \langle 00| + \alpha_{10} |10\rangle \langle 10| + \alpha_{01} |01\rangle \langle 01| + \alpha_{11} |11\rangle \langle 11|)$$

We can then define the density matrices for the subsets A and B , which are given by

$$\begin{aligned}\rho_A &= \text{Tr}_B(\rho_0) = \langle 0| \rho_0 |0\rangle_B + \langle 1| \rho_0 |1\rangle_B \\ \rho_B &= \text{Tr}_A(\rho_0) = \langle 0| \rho_0 |0\rangle_A + \langle 1| \rho_0 |1\rangle_A\end{aligned}$$

To find the von Neumann entropy, we will use the formula:

$$S(A, B) = -\text{Tr}(\rho_{A,B} \log_2(\rho_{A,B}))$$