

# Solutions to problem set 6

## 6.1 Pure and mixed states

- a) A pure state is the most accurate description possible of a quantum system. It is represented by a state vector  $|\psi\rangle$  in Hilbert space. A mixed state is used when we do not know the exact quantum state, but only the probabilities  $p_i$  for a set of possible states  $|\psi_i\rangle$ . It is represented by a density matrix  $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ . Mixed states also occur for composite systems in pure states. The reduced density matrix of one component is then a mixed state when there is entanglement between this component and the rest of the system.
- b) We measure the spin in the  $x$ -direction.  $|\rightarrow\rangle$  is an eigenstate of  $\sigma_x$  with eigenvalue  $+1$ , which means that we will measure spin up in  $x$  for all particles in ensemble A. For ensemble B we will measure spin up and spin down randomly with equal probabilities.
- c) We prove that the density matrices are the same:

$$\begin{aligned}\rho_B &= \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow| \\ \rho_C &= \frac{1}{2} |\rightarrow\rangle\langle\rightarrow| + \frac{1}{2} |\leftarrow\rangle\langle\leftarrow| \\ &= \frac{1}{4} (|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|) + \frac{1}{4} (|\uparrow\rangle - |\downarrow\rangle)(\langle\uparrow| - \langle\downarrow|) \\ &= \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow|\end{aligned}$$

Since the density matrices are the same we will get the same statistics for all possible measurements, and we can distinguish the ensembles.

- d) The state is  $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ . It is clear that if we measure the first particle along the  $z$ -axis we have equal probabilities of measuring up or down, and the second particle will collapse to the opposite state, generating ensemble B. Ensemble C is generated by measuring the first particle in the  $x$ -direction. To see this we rewrite  $|\psi\rangle$  in terms of the states  $|\rightarrow\rangle$  and  $|\leftarrow\rangle$ . We have

$$\begin{aligned}|\uparrow\rangle &= \frac{1}{\sqrt{2}} (|\rightarrow\rangle + |\leftarrow\rangle) \\ |\downarrow\rangle &= \frac{1}{\sqrt{2}} (|\rightarrow\rangle - |\leftarrow\rangle)\end{aligned}$$

which we use to get

$$\begin{aligned}|\psi\rangle &= \frac{1}{2\sqrt{2}} (|\rightarrow\rangle + |\leftarrow\rangle)(|\rightarrow\rangle - |\leftarrow\rangle) - \frac{1}{2\sqrt{2}} (|\rightarrow\rangle - |\leftarrow\rangle)(|\rightarrow\rangle + |\leftarrow\rangle) \\ &= \frac{1}{\sqrt{2}} (|\leftarrow\rightarrow\rangle - |\rightarrow\leftarrow\rangle)\end{aligned}$$

- e) Consider the case where person 1 measures spin along the  $z$ -axis and therefore prepares ensemble B. If person 2 also measures along the  $z$ -axis, the outcomes of the two measurements will always be perfectly anticorrelated. If instead person 1 measures  $x$ -spin and prepares ensemble C while person 2 still measures  $z$ -spin, the results will be uncorrelated. Nothing changes if person 1 measures after person 2.

## 6.2 Entanglement

a)

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|++\rangle + |--\rangle)$$

This state is a pure state, and thus has the density matrix:

$$\begin{aligned}\hat{\rho} &= \frac{1}{2} (|++\rangle\langle++| + |--\rangle\langle--| + |++\rangle\langle--| + |--\rangle\langle++|) \\ &= \frac{1}{2} \sum_{n,m \in \{+,-\}} |nn\rangle\langle mm|\end{aligned}$$

The entropy is then given by:

$$S_{\mathcal{A}} = S_{\mathcal{B}} = -\text{Tr}_{\mathcal{A}} (\hat{\rho}_{\mathcal{A}} \log \hat{\rho}_{\mathcal{A}}) = -\text{Tr}_{\mathcal{B}} (\hat{\rho}_{\mathcal{B}} \log \hat{\rho}_{\mathcal{B}})$$

where  $\hat{\rho}_{\mathcal{A}} = \text{Tr}_{\mathcal{B}} (\hat{\rho})$ . The trace of a matrix in the product space is:

$$\begin{aligned}\hat{\rho}_{\mathcal{A}} &= \text{Tr}_{\mathcal{B}} \left( \frac{1}{2} \sum_{n,m \in \{+,-\}} |nn\rangle\langle mm| \right) = \frac{1}{2} \sum_{n,m \in \{+,-\}} \text{Tr}_{\mathcal{B}} (|nn\rangle\langle mm|) \\ &= \frac{1}{2} \sum_{n,m \in \{+,-\}} \text{Tr}_{\mathcal{B}} ((|n\rangle_{\mathcal{A}} \otimes |n\rangle_{\mathcal{B}}) (\langle m|_{\mathcal{A}} \otimes \langle m|_{\mathcal{B}})) \\ &= \frac{1}{2} \sum_{n,m \in \{+,-\}} \text{Tr}_{\mathcal{B}} ((|n\rangle\langle m|)_{\mathcal{A}} \otimes (|n\rangle\langle m|)_{\mathcal{B}}) \\ &= \frac{1}{2} \sum_{n,m \in \{+,-\}} ((|n\rangle\langle m|)_{\mathcal{A}} \otimes \text{Tr}(|n\rangle\langle m|)_{\mathcal{B}}) \\ &= \frac{1}{2} \sum_{n,m \in \{+,-\}} ((|n\rangle\langle m|)_{\mathcal{A}} \otimes \delta_{mn})\end{aligned}$$

Due to the trace only sums the diagonal elements ( $\text{Tr}(|n\rangle\langle m|) = \langle m|n\rangle = \delta_{mn}$ ). Since  $\delta_{mn}$  is a number, the tensor product reduces down to simple multiplication:

$$\hat{\rho}_{\mathcal{A}} = \frac{1}{2} \sum_{n,m \in \{+,-\}} (\delta_{mn} |n\rangle\langle m|)$$

Thus,

$$\hat{\rho}_{\mathcal{A}} = \frac{1}{2} (|+\rangle\langle+| + |-\rangle\langle-|)$$

This is a matrix with both eigenvalues  $\frac{1}{2}$ , thus we find the entropy:

$$S_A = S_B = -\frac{1}{2} \ln \frac{1}{2} - \frac{1}{2} \ln \frac{1}{2} = \log 2 \quad (1)$$

Thus, they are maximally entangled.

b) The operation  $\hat{U}_B = \mathbb{1} \otimes \hat{U}_B$ , and  $\hat{U}_A = \hat{U}_A \otimes \mathbb{1}$ , thus, applying both yields:

$$\hat{U}_A \hat{U}_B = (\hat{U}_A \otimes \mathbb{1}) (\mathbb{1} \otimes \hat{U}_B) = \hat{U}_A \otimes \hat{U}_B$$

Applying this as a transformation, we get:

$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{U}_A \otimes \hat{U}_B |\psi\rangle$$

$$\hat{\rho} \rightarrow \hat{\rho}' = (\hat{U}_A \otimes \hat{U}_B) \hat{\rho} (\hat{U}_A \otimes \hat{U}_B)^\dagger$$

Then:

$$\begin{aligned} \hat{\rho}'_A &= \text{Tr}_B \left[ (\hat{U}_A \otimes \hat{U}_B) \hat{\rho} (\hat{U}_A \otimes \hat{U}_B)^\dagger \right] \\ &= \text{Tr}_B \left[ (\hat{U}_A \otimes \hat{U}_B) \left( \frac{1}{2} \sum_{n,m \in \{+, -\}} (|n\rangle_A \otimes |n\rangle_B) (\langle m|_A \otimes \langle m|_B) \right) (\hat{U}_A \otimes \hat{U}_B)^\dagger \right] \\ &= \text{Tr}_B \left[ \frac{1}{2} \sum_{n,m \in \{+, -\}} \left( [\hat{U}_A |n\rangle_A] \otimes [\hat{U}_B |n\rangle_B] \right) \left( [\langle m|_A \hat{U}_A^\dagger] \otimes [\langle m|_B \hat{U}_B^\dagger] \right) \right] \\ &= \frac{1}{2} \text{Tr}_B \left[ \sum_{n,m \in \{+, -\}} \left( [\hat{U}_A |n\rangle_A \langle m|_A \hat{U}_A^\dagger] \otimes [\hat{U}_B |n\rangle_B \langle m|_B \hat{U}_B^\dagger] \right) \right] \\ &= \frac{1}{2} \left[ \sum_{n,m \in \{+, -\}} \left( [\hat{U}_A |n\rangle_A \langle m|_A \hat{U}_A^\dagger] \otimes \text{Tr} [\hat{U}_B |n\rangle_B \langle m|_B \hat{U}_B^\dagger] \right) \right] \end{aligned}$$

From problem set 1, we showed that  $\text{Tr} (\hat{U} A \hat{U}^\dagger) = \text{Tr} (A)$  by

$$\text{Tr} (\hat{U} A \hat{U}^\dagger) = \text{Tr} (\hat{U} [A \hat{U}^\dagger]) = \text{Tr} ([A \hat{U}^\dagger] \hat{U}) = \text{Tr} (A)$$

We arrive at

$$\hat{\rho}'_A = \frac{1}{2} \left[ \sum_{n,m \in \{+, -\}} \hat{U}_A |n\rangle \langle m| \hat{U}_A^\dagger \delta_{mn} \right] = \left[ \sum_{n \in \{+, -\}} \hat{U}_A |n\rangle \langle n| \hat{U}_A^\dagger \right] = \hat{U}_A \hat{\rho}_A \hat{U}_A^\dagger$$

The entropy is then given as:

$$S'_A = -\text{Tr} (\hat{\rho}'_A \log (\hat{\rho}'_A))$$

Since  $\hat{\rho}'_A = \hat{U}_A \hat{\rho}_A \hat{U}_A^\dagger$ , they have the same eigenvalues, and therefore the entropy is the same.

- c) After the measurement, part A of the system is projected on one of the eigenstates of the operator being measured (it does not matter which operator this is). It is then in a well defined pure state and not entangled with part B any more. The entropy of entanglement after the measurement is 0.

### 6.3 Matrix representation of tensor products

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

$$|c\rangle = |a\rangle \otimes |b\rangle \Rightarrow |c\rangle = \sum_{ij} a_i b_j |ij\rangle, \quad |ij\rangle = |i\rangle_A \otimes |j\rangle_B$$

- a) We have

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix} = \begin{pmatrix} a_1 \mathbf{b} \\ a_2 \mathbf{b} \end{pmatrix} \quad (2)$$

For the basis vectors, we can assume

$$|1\rangle_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle_A = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

And similarly in the  $B$  space. We can use the result (2), to have:

$$|ij\rangle = |i\rangle_A \otimes |j\rangle_B = \begin{pmatrix} i_1 \mathbf{j} \\ i_2 \mathbf{j} \end{pmatrix}$$

Then:

$$|11\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |12\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |21\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |22\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

- b) We have

$$\mathbf{C} = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix} = \begin{pmatrix} A_{11}\mathbf{B} & A_{12}\mathbf{B} \\ A_{21}\mathbf{B} & A_{22}\mathbf{B} \end{pmatrix}$$

- c)

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We show three examples

$$\begin{aligned}\sigma_1 \otimes \sigma_2 &= \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix} \\ \sigma_1 \otimes \sigma_3 &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \\ \sigma_2 \otimes \sigma_3 &= \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i\sigma_3 \\ i\sigma_3 & 0 \end{pmatrix}\end{aligned}$$

d) We have

$$\mathbf{C}\mathbf{c} = \begin{pmatrix} A_{11}\mathbf{B} & A_{12}\mathbf{B} \\ A_{21}\mathbf{B} & A_{22}\mathbf{B} \end{pmatrix} \begin{pmatrix} a_1\mathbf{b} \\ a_2\mathbf{b} \end{pmatrix} = \begin{pmatrix} A_{11}a_1\mathbf{B}\mathbf{b} + A_{12}a_2\mathbf{B}\mathbf{b} \\ A_{21}a_1\mathbf{B}\mathbf{b} + A_{22}a_2\mathbf{B}\mathbf{b} \end{pmatrix}$$

We use that  $\hat{A} \otimes \hat{B}|a\rangle \otimes |b\rangle = \hat{A}|a\rangle \otimes \hat{B}|b\rangle$  and that the matrix representing  $\hat{A}|a\rangle$  is

$$\mathbf{A}\mathbf{a} = \begin{pmatrix} A_{11}a_1 + A_{12}a_2 \\ A_{21}a_1 + A_{22}a_2 \end{pmatrix}$$

Then the matrix representing  $\hat{A} \otimes \hat{B}|a\rangle \otimes |b\rangle$  is

$$\begin{pmatrix} (A_{11}a_1 + A_{12}a_2)\mathbf{B}\mathbf{b} \\ (A_{21}a_1 + A_{22}a_2)\mathbf{B}\mathbf{b} \end{pmatrix}$$

which is the same as  $\mathbf{C}\mathbf{c}$

## 6.4 Schmidt decomposition 1

We have a system consisting of two spin- $\frac{1}{2}$  particles. For each of the following states, study the reduced density matrix of one of the particles and determine if the state is entangled or not. For the states which are not entangled, find a factorization of the state as a tensor product of one state for each particle. For the entangled states, find the Schmidt decomposition of the state.

$$\begin{aligned}|\psi_1\rangle &= \frac{1}{2} (|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle) \\ |\psi_2\rangle &= \frac{1}{2} (|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle) \\ |\psi_3\rangle &= a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + a_-|\downarrow\uparrow\rangle + a_+|\downarrow\downarrow\rangle \\ |\psi_4\rangle &= a_-|\uparrow\uparrow\rangle + a_+|\uparrow\downarrow\rangle + a_+|\downarrow\uparrow\rangle + a_-|\downarrow\downarrow\rangle\end{aligned}$$

where

$$a_{\pm} = \frac{\sqrt{3} \pm 1}{4}$$

$$|\psi_1\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle):$$

The density matrix

$$\rho_1 = |\psi_1\rangle\langle\psi_1| = \frac{1}{4}(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle)(\langle\uparrow\uparrow| - \langle\uparrow\downarrow| + \langle\downarrow\uparrow| - \langle\downarrow\downarrow|)$$

$$\rho_1^A = \text{Tr}_B \rho_1 = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

The eigenvalues are 0 and 1, which shows that  $|\psi_1\rangle$  is not entangled. To find the factorization of the state we need the eigenvectors of the reduced density matrix  $\rho_1^A$ . The one with eigenvalue 1 is  $|1\rangle_A = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ , while the one with eigenvalue 0 is  $|0\rangle_A = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$  (since this has eigenvalue 0 it will not appear in the factorization). We can now express the state  $|\psi_1\rangle$  in terms of these eigenvectors and find that

$$|\psi_1\rangle = |1\rangle_A \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$$

$$|\psi_2\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle):$$

The density matrix

$$\rho_2 = |\psi_2\rangle\langle\psi_2| = \frac{1}{4}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle)(\langle\uparrow\uparrow| + \langle\uparrow\downarrow| + \langle\downarrow\uparrow| - \langle\downarrow\downarrow|)$$

$$\rho_2^A = \text{Tr}_B \rho_2 = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

This is not a pure state, so  $|\psi_2\rangle$  is entangled. The eigenvalues are both  $\frac{1}{2}$  and all vectors are eigenvectors. Because of that we can choose which basis to use for part A, and the Schmidt decomposition is not unique. Let us take the basis to be  $|\uparrow\rangle$  and  $|\downarrow\rangle$  for simplicity, and we find

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) + \frac{1}{\sqrt{2}}|\downarrow\rangle \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$$

$$|\psi_3\rangle = a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + a_-|\downarrow\uparrow\rangle + a_+|\downarrow\downarrow\rangle:$$

The density matrix

$$\rho_3 = |\psi_3\rangle\langle\psi_3| = (a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + a_-|\downarrow\uparrow\rangle + a_+|\downarrow\downarrow\rangle)(a_+\langle\uparrow\uparrow| + a_-\langle\uparrow\downarrow| + a_-\langle\downarrow\uparrow| + a_+\langle\downarrow\downarrow|)$$

$$\rho_3^A = \text{Tr}_B \rho_3 = (a_+^2 + a_-^2)|\uparrow\rangle\langle\uparrow| + 2a_+a_-|\uparrow\rangle\langle\downarrow| + 2a_+a_-|\downarrow\rangle\langle\uparrow| + (a_+^2 + a_-^2)|\downarrow\rangle\langle\downarrow| = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{pmatrix}$$

Diagonalizing we find the eigenvalues  $p^+ = \frac{3}{4}$  with eigenvector  $|\uparrow_x\rangle$  and  $p^- = \frac{1}{4}$  with eigenvector  $|\downarrow_x\rangle$ . This is not a pure state, so  $|\psi_3\rangle$  is entangled. Expressing the state in terms of the eigenvectors we find

$$|\psi_3\rangle = \frac{\sqrt{3}}{2}|\uparrow_x\uparrow_x\rangle + \frac{1}{2}|\downarrow_x\downarrow_x\rangle$$

$$|\psi_4\rangle = a_-|\uparrow\uparrow\rangle + a_+|\uparrow\downarrow\rangle + a_+|\downarrow\uparrow\rangle + a_-|\downarrow\downarrow\rangle:$$

The density matrix

$$\rho_4 = |\psi_4\rangle\langle\psi_4| = (a_-|\uparrow\uparrow\rangle + a_+|\uparrow\downarrow\rangle + a_+|\downarrow\uparrow\rangle + a_-|\downarrow\downarrow\rangle)(a_- \langle\uparrow\uparrow| + a_+ \langle\uparrow\downarrow| + a_+ \langle\downarrow\uparrow| + a_- \langle\downarrow\downarrow|)$$

$$\rho_4^A = \text{Tr}_B \rho_4 = (a_+^2 + a_-^2)|\uparrow\rangle\langle\uparrow| + 2a_+a_-|\uparrow\rangle\langle\downarrow| + 2a_+a_-|\downarrow\rangle\langle\uparrow| + (a_+^2 + a_-^2)|\downarrow\rangle\langle\downarrow| = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{pmatrix}$$

which is the same as we found for  $\rho_3^A$ . Thus we get the same eigenvalues and eigenvectors and we find

$$|\psi_4\rangle = \frac{\sqrt{3}}{2}|\uparrow_x\uparrow_x\rangle - \frac{1}{2}|\downarrow_x\downarrow_x\rangle.$$

## 6.5 Schmidt decomposition 2

- a) The Schmidt decomposition rewrites a general state in the product space, as a sum of states expressed in an orthonormal basis for each Hilbert space:

$$\Psi(x) = c_1\chi_1\phi_1(x) + c_2\chi_2\phi_2(x) \quad (3)$$

Thus, the spinors and wavefunctions must satisfy the orthonormality conditions

$$\chi_i^\dagger \chi_j = \int dx \phi_i^* \phi_j = \delta_{ij}$$

- b) The normalization factor is given by  $\langle\Psi|\Psi\rangle = 1$ .

$$\begin{aligned} \langle\Psi|\Psi\rangle &= \int_{-\infty}^{\infty} |\Psi(x)|^2 dx \\ &= \int_{-\infty}^{\infty} dx |\psi_1(x)|^2 + \int_{-\infty}^{\infty} dx |\psi_2(x)|^2 \\ &= |N|^2 \left( \int_{-\infty}^{\infty} e^{-2\lambda(x-x_0)^2} dx + \int_{-\infty}^{\infty} e^{-2\lambda(x+x_0)^2} dx \right) \end{aligned}$$

Substituting  $y = x \pm x_0$  in the first and second integral respectively yields :

$$\begin{aligned} \langle\Psi|\Psi\rangle &= 2|N|^2 \int_{-\infty}^{\infty} e^{-2\lambda y^2} dy \\ &= 2|N|^2 \sqrt{\frac{\pi}{2\lambda}} \\ \Rightarrow N &= \sqrt[4]{\frac{\lambda}{2\pi}}, \quad \text{when choosing } N \in \mathbb{R} \end{aligned}$$

Then it follows:

$$\begin{aligned}
 \Delta &= \langle \psi_1 | \psi_2 \rangle \\
 &= N^2 \int_{-\infty}^{\infty} e^{-\lambda(x-x_0)^2} e^{-\lambda(x+x_0)^2} dx \\
 &= N^2 \int_{-\infty}^{\infty} e^{-2\lambda(x^2+x_0^2)} dx \\
 &= N^2 e^{-2\lambda x_0^2} \int_{-\infty}^{\infty} dx e^{-2\lambda x^2} \\
 &= N^2 e^{-2\lambda x_0^2} \sqrt{\frac{\pi}{2\lambda}} \\
 \Delta &= \frac{1}{2} e^{-2\lambda x_0^2}
 \end{aligned}$$

- c) To find the Schmidt decomposition, we have to find the eigenstates of the reduced density matrix for at least one of the subsystems (spin or position). It is simplest to work with spin, since it has the smallest Hilbert space. Therefore we will trace over the position

$$\rho_{spin} = \int dx \langle x | \Phi \rangle \langle \Phi | x \rangle = \int dx \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \begin{pmatrix} \psi_1^* & \psi_2^* \end{pmatrix} = \int dx \begin{pmatrix} \psi_1 \psi_1^* & \psi_1 \psi_2^* \\ \psi_2 \psi_1^* & \psi_2 \psi_2^* \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \Delta \\ \Delta & \frac{1}{2} \end{pmatrix}$$

The eigenvalues of this are

$$p_1 = \frac{1}{2} (1 + e^{-2\lambda x_0^2}) \quad p_2 = \frac{1}{2} (1 - e^{-2\lambda x_0^2})$$

with the corresponding eigenvectors

$$\chi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \chi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The coefficients in the Schmidt decomposition are the square roots of the eigenvalues,  $c_i = \sqrt{p_i}$  and we get from Eq (3) that

$$\begin{aligned}
 \psi_1 &= \frac{1}{\sqrt{2}} c_1 \phi_1 + \frac{1}{\sqrt{2}} c_2 \phi_2 \\
 \psi_2 &= \frac{1}{\sqrt{2}} c_1 \phi_1 - \frac{1}{\sqrt{2}} c_2 \phi_2
 \end{aligned}$$

which we can solve to find

$$\begin{aligned}
 \phi_1 &= \frac{1}{\sqrt{2}c_1} (\psi_1 + \psi_2) = \frac{N}{\sqrt{1 + e^{-2\lambda x_0^2}}} (e^{-\lambda(x-x_0)^2} + e^{-\lambda(x+x_0)^2}) \\
 \phi_2 &= \frac{1}{\sqrt{2}c_2} (\psi_1 - \psi_2) = \frac{N}{\sqrt{1 - e^{-2\lambda x_0^2}}} (e^{-\lambda(x-x_0)^2} - e^{-\lambda(x+x_0)^2})
 \end{aligned}$$

## 6.6 Coupled two-level systems

$$\hat{H} = \frac{\epsilon}{2} (3\sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_z) + \lambda (\sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+)$$

$$\sigma_{\pm} = \frac{1}{2} (\sigma_x \pm i\sigma_y)$$

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

a)

$$\begin{aligned} \sigma_+ &= \frac{1}{2} \begin{pmatrix} 0 & 1+1 \\ 1-1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \sigma_- &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

$$\hat{H} = \frac{\epsilon}{2} \left[ \begin{pmatrix} 3 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0 \\ 0 & -3 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} + \begin{pmatrix} 1 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0 \\ 0 & 1 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix} \right] \quad (4)$$

$$\begin{aligned} &+ \lambda \left[ \begin{pmatrix} 0 & 1 \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & 0 \end{pmatrix} \right] \\ &= \begin{pmatrix} 2\epsilon & 0 & 0 & 0 \\ 0 & \epsilon & \lambda & 0 \\ 0 & \lambda & -\epsilon & 0 \\ 0 & 0 & 0 & -2\epsilon \end{pmatrix} \end{aligned} \quad (5)$$

The eigenvalue equation becomes:

$$\begin{aligned} |\hat{H} - \mathbb{1}e| &= 0 \\ \begin{vmatrix} 2\epsilon - e & 0 & 0 & 0 \\ 0 & \epsilon - e & \lambda & 0 \\ 0 & \lambda & -\epsilon - e & 0 \\ 0 & 0 & 0 & -2\epsilon - e \end{vmatrix} &= 0 \\ (2\epsilon - e) \begin{vmatrix} \epsilon - e & \lambda & 0 \\ \lambda & -\epsilon - e & 0 \\ 0 & 0 & -2\epsilon - e \end{vmatrix} &= 0 \\ (2\epsilon - e)(-2\epsilon - e) [(\epsilon - e)(-\epsilon - e) - \lambda^2] &= 0 \end{aligned}$$

From here, we immediately see the value of the first two eigenvalues, the rest is determined by:

$$\begin{aligned} -(\epsilon^2 - e^2) - \lambda^2 &= 0 \\ e &= \pm \sqrt{\epsilon^2 + \lambda^2} \end{aligned}$$

The eigenvalues are thus:

$$e_1 = 2\epsilon, \quad e_2 = -2\epsilon, \quad e_3 = \sqrt{\epsilon^2 + \lambda^2}, \quad e_4 = -\sqrt{\epsilon^2 + \lambda^2}$$

We see that  $e_1$  and  $e_2$  are independent of  $\lambda$ , and from the hamiltonian (5), it is easy to see that the eigenvectors are:

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Then setting  $\epsilon = \mu \cos \theta$  and  $\lambda = \mu \sin \theta$ , we get:

$$e_1 = 2\mu \cos \theta, \quad e_2 = -2\mu \cos \theta, \quad e_3 = \mu, \quad e_4 = -\mu$$

The hamiltonian takes the form:

$$\hat{H} = \begin{pmatrix} 2\mu \cos \theta & 0 & 0 & 0 \\ 0 & \mu \cos \theta & \mu \sin \theta & 0 \\ 0 & \mu \sin \theta & -\mu \cos \theta & 0 \\ 0 & 0 & 0 & -2\mu \cos \theta \end{pmatrix}$$

For the remaining subspace, the eigenvector equation is:

$$\begin{pmatrix} \mu \cos \theta & \mu \sin \theta \\ \mu \sin \theta & -\mu \cos \theta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \pm \mu \begin{pmatrix} a \\ b \end{pmatrix}$$

Then:

$$\begin{aligned} a \cos \theta + b \sin \theta &= \pm a \\ a \cos \theta - b \sin \theta &= \pm b \end{aligned}$$

Starting with the first equation:

$$a \cos \theta + b \sin \theta = \pm a \Rightarrow b = a \frac{\pm 1 - \cos \theta}{\sin \theta}$$

Then, if  $a = \sin \theta$ , we get the following eigenvectors:

$$\mathbf{e}'_3 = \begin{pmatrix} 0 \\ \sin \theta \\ 1 - \cos \theta \\ 0 \end{pmatrix}, \quad \mathbf{e}'_4 = \begin{pmatrix} 0 \\ \sin \theta \\ -1 - \cos \theta \\ 0 \end{pmatrix}$$

I marked them as to say that they are not the final eigenvectors, they need to be normalized first:

$$\begin{aligned} \sqrt{\mathbf{e}'_3 \cdot \mathbf{e}'_3} &= \sqrt{\sin^2 \theta + (1 - \cos \theta)^2} = \sqrt{\sin^2 \theta + 1 - 2 \cos \theta + \cos^2 \theta} = \sqrt{2 - 2 \cos \theta} \\ \sqrt{\mathbf{e}'_4 \cdot \mathbf{e}'_4} &= \sqrt{\sin^2 \theta + (1 + \cos \theta)^2} = \sqrt{\sin^2 \theta + 1 + 2 \cos \theta + \cos^2 \theta} = \sqrt{2 + 2 \cos \theta} \end{aligned}$$

Then:

$$\mathbf{e}_3 = \frac{1}{\sqrt{2-2\cos\theta}} \begin{pmatrix} 0 \\ \sin\theta \\ 1-\cos\theta \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \\ 0 \end{pmatrix}, \quad \mathbf{e}_4 = \frac{1}{\sqrt{2+2\cos\theta}} \begin{pmatrix} 0 \\ \sin\theta \\ -1-\cos\theta \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \\ 0 \end{pmatrix}$$

Just to summarize, the eigenvectors are:

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{e}_3 = \begin{pmatrix} 0 \\ \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \\ 0 \end{pmatrix}, \quad \mathbf{e}_4 = \begin{pmatrix} 0 \\ \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \\ 0 \end{pmatrix}$$

The energies are:

$$E_1 = 2\mu \cos\theta, \quad E_2 = -2\mu \cos\theta, \quad E_3 = \mu, \quad E_4 = -\mu$$

b) The two interesting eigenstates are  $\mathbf{e}_3$  and  $\mathbf{e}_4$

$$\hat{\rho}_3 = \mathbf{e}_3 \mathbf{e}_3^T = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2} & 0 \\ 0 & \cos\frac{\theta}{2}\sin\frac{\theta}{2} & \sin^2\frac{\theta}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{\rho}_4 = \mathbf{e}_4 \mathbf{e}_4^T = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \sin^2\frac{\theta}{2} & -\cos\frac{\theta}{2}\sin\frac{\theta}{2} & 0 \\ 0 & -\cos\frac{\theta}{2}\sin\frac{\theta}{2} & \cos^2\frac{\theta}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Before considering the partial traces, let's look at how this works out in the matrix representation. A general 4x4 matrix can be written as a sum over tensor products between 2x2 matrices (also called "Kronecker product"):

$$\begin{aligned} C &= \sum_{ij} c_{ij} A_i \otimes B_j \\ &= \sum_{ij} c_{ij} \begin{pmatrix} A_{11}^i & A_{21}^i \\ A_{12}^i & A_{22}^i \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}_j \\ &\equiv \sum_{ij} c_{ij} \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}_{ij} \end{aligned}$$

Then the partial traces become:

$$\begin{aligned} \text{Tr}_A C &= \sum_{ij} c_{ij} (C_{11} + C_{22})_{ij} \\ \text{Tr}_B C &= \sum_{ij} c_{ij} \begin{pmatrix} \text{Tr} C_{11} & \text{Tr} C_{12} \\ \text{Tr} C_{21} & \text{Tr} C_{22} \end{pmatrix}_{ij} \end{aligned}$$

And since  $\text{Tr}(A + B) = \text{Tr}A + \text{Tr}B$ , we see that in our case:

$$\begin{aligned}\hat{\rho}_3^A = \text{Tr}_B \hat{\rho}_3 &= \begin{pmatrix} \cos^2 \frac{\theta}{2} & 0 \\ 0 & \sin^2 \frac{\theta}{2} \end{pmatrix} \\ \hat{\rho}_3^B = \text{Tr}_A \hat{\rho}_3 &= \begin{pmatrix} \sin^2 \frac{\theta}{2} & 0 \\ 0 & \cos^2 \frac{\theta}{2} \end{pmatrix} \\ \hat{\rho}_4^A = \text{Tr}_B \hat{\rho}_4 &= \begin{pmatrix} \sin^2 \frac{\theta}{2} & 0 \\ 0 & \cos^2 \frac{\theta}{2} \end{pmatrix} \\ \hat{\rho}_4^B = \text{Tr}_A \hat{\rho}_4 &= \begin{pmatrix} \cos^2 \frac{\theta}{2} & 0 \\ 0 & \sin^2 \frac{\theta}{2} \end{pmatrix}\end{aligned}$$

c) We see that all the reduced density matrices have the same eigenvalues, and the von Neuman entropy is thus the same and given by:

$$S = -\cos^2 \frac{\theta}{2} \ln \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \ln \sin^2 \frac{\theta}{2}$$

The entropy is maximal when  $\cos^2 \frac{\theta}{2} = \sin^2 \frac{\theta}{2} = \frac{1}{2}$ , which means

$$\theta = \frac{\pi}{2} + n\pi, \quad n \in \mathbb{Z}$$