QCOMP102: Quantum Systems

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Based on:

Yanofsky, N. & Mannucci, M. (2008). Quantum Computing for Computer Scientists.

Cambridge University Press

Lecture Outline: In this lecture, we will first introduce the basic quantum mechanics principles using graphs and matrices and then finally we will dive into the wonders of quantum theory. Needless to say that the understanding of basic quantum mechanics is fundamental to understand quantum computation.

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1 From Classical to Quantum

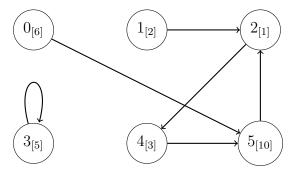
In this section, we will define the notion of system, its state and its dynamics, we will start with the deterministic systems we interact with in our everyday life then we shall introduce the probabilistic systems to introduce the notion of uncertainty and then finally we will discover the notion of quantum systems.

1.1 Classical Deterministic System

Notion goal 1.1. Understanding the representation of classical system is fundamental to be able to grasp the fundamental difference between classical and quantum systems.

We begin with a simple **system** described by a **directed graph** and some toy marbles. Imagine the identical marbles as being placed on the vertices of this graph. The **state** of a system is described by how many marbles are on each vertex.

Let us consider the graph G defined as follows:



We can then represent the state of this system with the vector $S = \begin{pmatrix} 6 \\ 2 \\ 1 \\ 5 \\ 3 \\ 10 \end{pmatrix} = \begin{pmatrix} 6 & 2 & 1 & 5 & 3 & 10 \end{pmatrix}^T$.

But we can also represent the **dynamics** of the system (which describe the flux of marbles between the vertices of our graph) using the Boolean adjacency matrix D (for "dynamics"). The only requirement is that each vertex have exactly one outgoing edge, which translates in the adjacency matrix having only one 1 per column.

Exercise 1.1. What would happen if we relaxed the requirement that exactly one edge leaves each vertex?

Notice that a Boolean adjacency matrix follows this property:

$$D[i,j] = 1 \iff \text{there is an edge going from vertex } j \text{ to vertex } i$$

$$\iff \text{there is a path of length 1 from vertex } j \text{ to vertex } i$$
(1)

Exercise 1.2. What would happen if we permitted not only 0's and 1's but also -1 in the adjacency matrix?

To summarize, D represents the dynamics of the system while S represents its state at current time step t. Thus we can obtain the state of the system at time step t+1 by calculating the product D * X:

Looking at the formula for Boolean matrix multiplication:

$$D^{2}[i,j] = \bigvee_{i=1}^{n-1} D[i,k] \wedge D[k,j]$$
(4)

We observe that there will be a path of length 2 from vertex j to vertex i if there exists (\bigvee) some vertex k such that there is an edge from vertex j to vertex k and (\land) an edge from vertex k to vertex i.

Then we can deduce the following property:

 $D^{2}[i,j] = 1 \iff$ there is a path of length 2 from vertex j to vertex i

and more generally for an arbitrary k we have:

 $D^{k}[i,j] = 1 \iff$ there is a path of length k from vertex j to vertex i

Consider the state $S_t = \begin{pmatrix} x_0 & x_1 & \dots & x_{n-1} \end{pmatrix}^T$ the state of the system of dynamics D at time step t, then the state of the system k time steps later is:

$$S_{t+k} = D^k * S_t = (x_0' \quad x_1' \quad \dots \quad x_{n-1}')^T$$
 (5)

In others words, x'_j is the state of the vertex j (or the number of marbles on this vertex) after k time steps in the future.

In quantum mechanics, if there are two or more matrices that manipulate the states of a system, then the action of one followed by another is described by their product.

What we have learned 1.1. In this section we defined the basic definitions of a system and described how deterministic systems works, and in particular that:

- The **states** of a system corresponds to **column vectors** (state vectors).
- The **dynamics** of a system corresponds to **matrices**.
- To progress from one state to another in one time step, we must multiply the state vector by the dynamics matrix.
- Multiple step dynamics are obtained via matrix multiplication.

1.2 Probabilistic Systems

Notion goal 1.2. In quantum mechanics, there is an inherent indeterminacy in our knowledge of a physical state and states change with probabilistic laws. We then need to first define and comprehend classical probabilistic systems before beginning to work with full-fledged quantum systems.

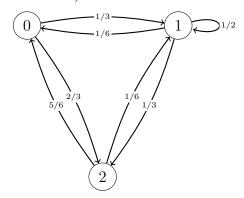
To modelize those probabilistic scenarios, we modify what we did in the last section: **instead of dealing with multiple marbles, we will work with a single marble**. The system's state will tell us the probabilities of the marble being on each vertex. A state vector of a probabilistic system is thus composed of **real-valued entries between 0 and 1 whose sum is equal to 1** since the marble must be somewhere on the graph at any time.

We must modify the constraints on the system dynamics as well, instead of having exactly one outgoing edge for each vertex, we will have several outgoing edges for each vertex with real numbers between 0 and 1 as weights whose sum for each vertex must be equal to 1. Those weights describe the probability of the marble moving from one vertex to another in one time step.

To summarize, we impose the following constraints on probabilistic systems dynamics:

- the sum of the weights of **outgoing edges** for one vertex is 1.
- the sum of the weights of **in-going edges** for one vertex is 1.

Let us consider a system represented by the following graph (we take a general view of it and do not assign to it specific vertex states):



The adjacency matrix describing the dynamics of such system is then:

$$D = \begin{pmatrix} 0 & \frac{1}{6} & \frac{5}{6} \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix} \tag{6}$$

Note that the matrix D have real entries between 0 and 1 where the sum of the rows and the sum of the columns are all 1. Such matrices are called **doubly stochastic**.

Suppose the current state of this system is $S_t = \begin{pmatrix} \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \end{pmatrix}^T$ that express an indeterminacy about the position of the marble in the system at time t. Then the state of the system at the next time step simply corresponds to:

$$S_{t+1} = D * S_t = \begin{pmatrix} 0 & \frac{1}{6} & \frac{5}{6} \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix} * \begin{pmatrix} \frac{1}{6} \\ \frac{1}{6} \\ \frac{2}{3} \end{pmatrix} = \begin{pmatrix} \frac{21}{36} \\ \frac{9}{36} \\ \frac{6}{36} \end{pmatrix}$$
 (7)

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Thus in the same way as the previous section we have $D^k S_t = S_{t+k}$ with $D^k[i,j]$ the probability of the marble going from vertex j to vertex i in k time steps.

 $D^{k}[i,j]$ = the probability of going from vertex j to vertex i in k time steps

Notice that we are not constrained to multiply D by itself. We may also multiply D by another doubly stochastic matrix. Let D and D' be two n-by-n doubly stochastic matrices corresponding to the two directed weighted graphs G and G'. The n-vertices graph represented by the product of D and D':

$$(D*D')[i,j] = \sum_{k=0}^{n-1} D[i,k]D'[k,j]$$
(8)

corresponds to the sum of the probabilities of the marble to shift from vertex j to some vertex k in G' and then to shift from vertex k to vertex i in G. If D and D' describe some probability of transition during a single time step, then D*D' describes the probability of transition from time t to t+1 and then to t+2.

Let us consider as an example of **probabilistic double-slit experiment**.

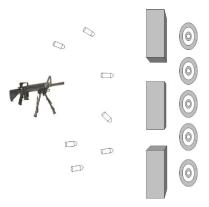
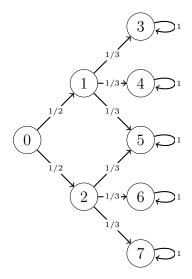


Figure 1: The double-slit experiment with bullets.

There are two slits on the wall, the shooter is good enough to always hit one of the two slits with equal probability (0.5 each). Additionally, once a bullet has passed one of the two slits, it can then hit one of three targets with equal probability, note that the middle target can be hit by bullets coming either from the above slit or the bottom slit.

We can then represent such system as the following graph:



It is assumed that it takes one time step for the bullet to travel from the gun to one of the slits and that it takes an additional time step for it to travel from a slit to its target. Notice that the vertex marked 5 can receive bullets from either of the two slits. Also notice that once a bullet has reached its target (vertices 3 through 7), it will stay there with a probability of 1.

Let us describe the dynamics of this system using the adjacency matrix B (for "bullets"):

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(9)$$

B describes the way a bullet will move after one time step but is not a doubly stochastic matrix. In order to convert it in a doubly stochastic matrix, the bullet would be required to be able to go from the right to the left through some kind of ricochet. For the sake of clarity we will not consider such a complicated scenario.

After two time steps, we then have:

Thus B^2 indicates the probabilities of the bullet's position after two time steps. If the bullet starts at vertex 0 then we have:

$$S_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}^T \tag{11}$$

and after two time steps we have:

$$S_2 = B^2 * S_0 = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & \frac{1}{6} \end{pmatrix}^T$$
 (12)

The key idea to notice is that $B^2[5,0] = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$ because the gun shoots the bullet from the vertex 0, hence, there are two possible ways for the bullet to the vertex 5, the probabilities then sum to $\frac{1}{3}$. This is what we expect, we will revisit this example in the next part where strange things start happening!

What we have learned 1.2. In this section we discovered probabilistic systems and introduced the classical probabilistic implementation of the double-slit experiment, and in particular we saw that:

- The vectors that represent state of a probabilistic physical system express a type of in**determinacy** about the exact physical state of the system.
- The matrices that represent the dynamics also express a type of indeterminacy about the way the physical system evolves over time. Their entries allow to compute the likelihood of transitioning from one state to the next.
- The way in which the indeterminacy progresses over time is modelized by matrix multiplication, just like deterministic systems.

1.3 Quantum Systems

Notion goal 1.3. We shall now begin to explore quantum principles using the graph-based model we built during the last two section, doing so will allow us to comprehend more easily the quantum theory later in this lecture.

We are now leaving the world of classical probabilities to now the quantum world. Quantum mechanics works with complex numbers, a weight on our graph will no longer be given by a real number p between 0 and 1 but rather by a complex number c such that $|c|^2$ is a real number between 0 and 1.

What difference does it make? The difference lies at the core of quantum theory and is that while real valued probabilities can only increase when added, complex numbers can cancel each other and lower the probabilities they represent. For example, if $p_1, p_2 \in \mathbb{R}$ between 0 and 1, then $(p_1 + p_2) \ge p_1$ and $(p_1 + p_2) \ge p_2$. Now let us consider two complex numbers c_1 and c_2 with associated squared moduli/amplitudes $|c_1|^2$ and $|c_2|^2$, then $|c_1 + c_2|^2$ is not necessarily bigger than $|c_1|^2$ or $|c_2|^2$.

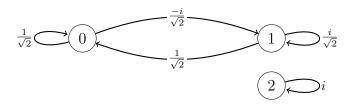
Example 1.1. Let $c_1 = 5 + 3i$ and $c_2 = -3 - 2i$, then $|c_1|^2 = 34$ and $|c_2|^2 = 13$ but $|c_1 + c_2|^2 = 34$ 5.5 which is less than 34 or 13.

The fact that complex numbers may cancel each other out when added has a well defined meaning in quantum mechanics and it is referred to as **interference** which is a key concept in quantum theory.

If we generalize the graphs and state vectors we studied previously, let us define the state vector S_t such as:

$$S_t = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{2i}{\sqrt{15}} & \sqrt{\frac{2}{5}} \end{pmatrix}^T \tag{13}$$

corresponding to the system represented by the following graph:



With the corresponding adjacency matrix representing the quantum system's dynamics:

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0\\ 0 & 0 & i \end{pmatrix}$$
 (14)

The dynamics (adjacency) matrix of a quantum system is **not required to be doubly stochastic** but is **required to be unitary**.

Unitary matrices are related to stochastic matrices as follows: the squared modulus of all the complex entries in U forms a doubly stochastic matrix. The i, j^{th} element of U is denoted U[i, j] and its squared modulus denoted $|U[i, j]|^2$. By abuse of notation, we will denote the entire matrix of squared moduli as $|U[i, j]|^2$.

$$|U[i,j]|^2 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0\\ \frac{1}{2} & \frac{1}{2} & 0\\ 0 & 0 & 1 \end{pmatrix}$$
 (15)

It is easy to see that this matrix is doubly stochastic.

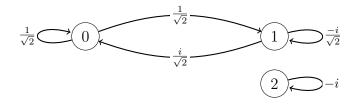
Let us show how unitary matrices act in state vectors. Calculating $U * S_t = S_{t+1}$ we get:

$$U * S_{t} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0\\ 0 & 0 & i \end{pmatrix} * \begin{pmatrix} \frac{1}{\sqrt{3}}\\ \frac{2i}{\sqrt{15}}\\ \sqrt{\frac{2}{5}} \end{pmatrix} = \begin{pmatrix} \frac{5+2i}{\sqrt{30}}\\ \frac{-2-\sqrt{5}i}{\sqrt{30}}\\ \sqrt{\frac{2}{5}i} \end{pmatrix} = S_{t+1}$$
 (16)

The matrix U^{\dagger} then represents the system with **reverted dynamics**, meaning the direction of the edges of the graph have been reverted:

$$U^{\dagger} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0\\ 0 & 0 & -i \end{pmatrix}$$
 (17)

corresponds to



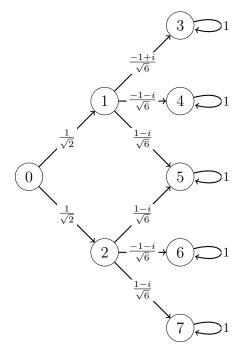
Since U is unitary, $U^{\dagger}U = I_3$ thus if $S_{t+1} = US_t$ then $U^{\dagger}S_{t+1} = U^{\dagger}US_t = I_3S_t = S_t$. We can then **reverse time to previous time steps** in a quantum system as easily as we go forward in time, such notions of reversibility and time symmetry are very important in quantum computing.

Note that I_3 corresponds to the dynamics of the system represented by the graph:



This means that if you perform some operation and then "undo" it, you will find yourself (with probability 1) in the same state you started.

In order to see the interference phenomenon more clearly, we revisit the **double-slit experiment**, except this time the examined subject will not be macroscopic objects like bullets that follow the laws of classical physics, but rather microscopic objects like **photons** that follow the laws of quantum mechanics. We have thus the following graph representing our system:



The squared modulus of $\frac{1}{\sqrt{2}}$ is $\frac{1}{2}$, which corresponds to a **50-50** chance of the photon passing through either slit.

Similarly $\left|\frac{\pm 1 \pm i}{\sqrt{6}}\right|^2 = \frac{1}{3}$, which corresponds to the fact that once a photon passed a slit, there is a $\frac{1}{3}$ chance of it hitting any of the 3 targets on the right of that slit.

We then have the corresponding adjacency matrix P (for "photons"):

$$P = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1+i}{\sqrt{6}} & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1-i}{\sqrt{6}} & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \frac{1-i}{\sqrt{6}} & \frac{-1+i}{\sqrt{6}} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{-1-i}{\sqrt{6}} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{1-i}{\sqrt{6}} & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(18)$$

Since we didn't represented all the possible photon transitions (e.g. bounce right to left) in order to keep our model from becoming overly complicated, the matrix P is not unitary. We are simply trying to demonstrate the phenomenon of interference in quantum systems.

The squared modulus of the P matrix is exactly the same as the B matrix we saw during the bullet experiment:

$$|P[i,j]|^{2} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(19)$$

This means that **nothing** "strange" happens after one time step. Let us see what happens if we calculate the system's dynamics after two time steps:

 $|P^2[i,j]|^2$ is almost exactly the same as B^2 , the matrix describing the dynamics of the bullet experiment after two time steps. However there is **one major difference**: in B^2 we have $B^2[5,0]=\frac{1}{3}=\frac{1}{6}+\frac{1}{6}$ since the bullet can hit the middle target (vertex 5) from both slits starting from vertex 0, however with a photon that follows the laws of quantum mechanics, the complex numbers are added as opposed to their probabilities.

$$P^{2}[5,0] = \frac{1}{\sqrt{2}}(\frac{-1+i}{\sqrt{6}}) + \frac{1}{\sqrt{6}}(\frac{1-i}{\sqrt{6}}) = \frac{-1+i}{\sqrt{12}} + \frac{1-i}{\sqrt{12}} = \frac{0}{\sqrt{12}} = 0$$
 (21)

Thus resulting in $|P^2[i,j]|^2 = 0$. In other words, although there are two ways for a photon to travel from vertex 0 to vertex 5, there will be no photons at vertex 5. How to understand this phenomenon?

In the past centuries, physicists had a simple explanation for interference: waves. Indeed if we take the analogy of waves on water, we can see that they sometime reinforce each other or cancel each other. Thus the double-slit experiment points to the wave-like nature of light. At the same time, another crucial experiment in quantum mechanics, namely the photoelectric effect points toward a different direction: light is absorbed and emitted in discrete quantities, photons.

It is like light had a **double nature**: sometimes it acts as a **beam of particles**, and at other times it acts like a **wave**. Note that this **experiment can be reproduced with a single photon shot from vertex 0. Even in this scenario, inferences will still occur**. What is going on here?

The naive probabilistic interpretation of the position of the photon using the bullet metaphor is not entirely accurate. Let the state of the system be given by $X = \begin{pmatrix} c_0 & c_2 & \dots & c_{n-1} \end{pmatrix}^T \in \mathbb{C}^n$, then it is in fact incorrect to say that the probability of the photon's being at position k is $|c_k|^2$.

Rather, to be in state X means that **the particle is in all positions simultaneously**. The photon passes through the top slit and the bottom slit simultaneously and then **interferes with itself!**

The photon is not a single particle, rather it is in many positions simultaneously, such particle is said to be in **superposition**. How can this be? Our every day experience tells us that things can only be at a single position at the same time. the reason we see particles in one particular position is because we have performed a **measurement** on them.

When we measure something at the quantum level, the quantum object that we have measured is no longer in a superposition of states, rather it collapses to a single classical state.

We have to redefine what the state of a quantum state is: a system is in a state X means that after measuring it, it will be found in position i with a probability of $|c_i|^2$. What are we to make of those strange ideas? Are we really to believe them? Richard Feynman, in discussing the double slit experiment, wrote:

"We chose to examine a phenomenon which is impossible, absolutely impossible to explain in any classical way, and which has in it the heart of quantum mechanics. In reality, it contains the only mystery. We cannot make the mystery go away by explaining why it works in such manner. We will just tell you how it works."

It is exactly this superposition of states that is the real power behind quantum computing. Classical computers are in one state at every moments. **Imagine putting a computer in many different classical states simultaneously and then processing with all the states at once**. This is the holy grail of parallel processing!

What we have learned 1.3. In this section we introduced the strange world of quantum mechanics and quantum systems, in particular, we saw that:

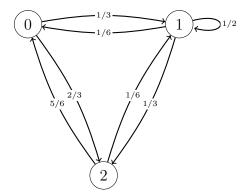
- States in a quantum system are represented by **column vectors of complex numbers** whose sum of squared moduli is 1.
- The dynamics of a quantum system is represented by a **unitary matrix and is therefore reversible**. The "undoing" is obtained by the inverse matrix which is equal to the adjoint matrix of the unitary matrix representing forward evolution.
- The probabilities of a quantum system to collapse to a specific classical state are always given by the square moduli of complex numbers.
- Quantum states can be in **superposition**, a physical system can be in more than one basic state simultaneously.

1.4 Assembling Systems

Notion goal 1.4. Quantum mechanics also deals with composite systems, systems that have more than one part. In this part, we will learn how to combine several systems.

For the sake of clarity, we will only assemble classical probabilistic systems in this section, however, whatever is stated about probabilistic systems in this section is also true for quantum systems.

Consider two different marbles. The **red marble** which follows the probabilities of a system represented by the graph G_M :



whose dynamics are described by the adjacency matrix M:

$$M = \begin{pmatrix} 0 & \frac{1}{6} & \frac{5}{6} \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix} \tag{22}$$

And the **blue marble** that follows the probabilities of a system represented by the graph G_N :

$$1/3$$
 $2/3$ b $1/3$

whose dynamics are described by the adjacency matrix N:

$$N = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} \tag{23}$$

How does a state for two marbles looks? Because the red marble can be on one of three vertices and the blue marble can be on one of two vertices, **there are** $3 \times 2 = 6$ **possible states for the combined system**. This corresponds to a tensor product of the state of system M and the state of system N:

$$S = S_{M} \otimes S_{N} = \begin{pmatrix} x_{0} \\ x_{1} \\ x_{2} \end{pmatrix} \otimes \begin{pmatrix} x_{a} \\ x_{b} \end{pmatrix} = \begin{pmatrix} x_{0} \\ x_{b} \\ x_{1} \\ x_{b} \\ x_{2} \\ x_{2} \\ x_{b} \end{pmatrix} = \begin{pmatrix} x_{0}x_{a} \\ x_{0}x_{b} \\ x_{1}x_{a} \\ x_{1}x_{b} \\ x_{2}x_{a} \\ x_{2}x_{b} \end{pmatrix}$$

$$(24)$$

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With each entry $x_i x_j$ corresponding to the probability of the red marble being in vertex i in the graph G_M and the blue marble being in vertex j in graph G_N at the same time, this state is then referred as ij.

A typical state might look like this:

$$S = \begin{cases} 0a & \left(\frac{1}{18}\right) \\ 0b & 0 \\ 1a & \left(\frac{2}{18}\right) \\ 1b & \left(\frac{1}{3}\right) \\ 2a & 0 \\ 2b & \left(\frac{1}{2}\right) \end{cases}$$

$$(25)$$

What does the dynamics of such combined system looks like? For a system to go from state ij to state i'j' we must multiply the probability of going from state i to state i' with the probability of going from state j to state j'. That gives us the following relation:

$$ij \xrightarrow{M[i',j] \times N[j',i]} i'j'$$
 (26)

In order to do that for every possible combinations of states, we need to perform a tensor product of the two systems' dynamics matrices:

$$M \otimes N = \begin{pmatrix} 0 & \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & \frac{1}{6} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & \frac{1}{6} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} \\ \frac{1}{3} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & \frac{1}{2} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & \frac{1}{6} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} \\ 2 \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & \frac{1}{3} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} & 0 \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} \end{pmatrix} \end{pmatrix}$$

$$(27)$$

which upon development gives us:

$$0a \quad 0b \quad 1a \quad 1b \quad 2a \quad 2b$$

$$0a \quad \begin{pmatrix} 0 & 0 & \frac{1}{18} & \frac{2}{18} & \frac{5}{18} & \frac{10}{18} \\ 0b & 0 & \frac{2}{18} & \frac{1}{18} & \frac{10}{18} & \frac{5}{18} \\ 0 & 0 & \frac{2}{18} & \frac{1}{18} & \frac{10}{18} & \frac{5}{18} \\ 0 & \frac{1}{9} & \frac{2}{9} & \frac{1}{6} & \frac{2}{6} & \frac{1}{18} & \frac{2}{18} \\ 0 & \frac{2}{9} & \frac{1}{9} & \frac{2}{6} & \frac{1}{6} & \frac{2}{18} & \frac{1}{18} \\ 0 & \frac{2}{9} & \frac{1}{9} & \frac{2}{6} & \frac{1}{6} & \frac{2}{18} & \frac{1}{18} \\ 0 & \frac{2}{9} & \frac{4}{9} & \frac{1}{9} & \frac{2}{9} & 0 & 0 \\ 0 & \frac{4}{9} & \frac{2}{9} & \frac{2}{9} & \frac{1}{9} & 0 & 0 \end{pmatrix}$$

$$(28)$$

The graph that corresponds to the matrix $M \otimes N$, the graph $G_M \times G_N$, is called the **Cartesian product** of two weighted graphs and has 28 directed edges.

In quantum mechanics, there are many more possible states than just states that can be combined from smaller ones. In fact, the states that are not the tensor product from smaller states are the most interesting ones, they are called **entangled states**. We will see them later in this lecture. Also note that there are more actions on a combined quantum system than simply that of the tensor product of the individual system's actions/dynamics.

In general, the Cartesian product of a n-vertex graph with a n'-vertex graph is a $(n \times n')$ -vertex graph. If we have an n-vertex graph G and we are interested in m different marbles moving in this system, we would consider the graph:

$$G^{m} = \underbrace{G \times G \times \dots \times G}_{\text{m times}} \tag{29}$$

which will have n^m vertices. If M_G is the associated adjacency matrix, then:

$$M_G^{\otimes m} = \underbrace{M_G \otimes M_G \otimes \dots M_G}_{\text{m times}} \tag{30}$$

which will be a n^m -by- n^m matrix.

We could represent a bit as a 2-vertex graph with a marble on the vertex 0 or on the vertex 1. If we wanted to represent m bits, we would need a 2^m -vertex graph, or equivalently, a 2^m -by- 2^m matrix. Thus there is an exponential growth of the resources needed for the number of bits under discussion. This exponential growth is actually one of the main reasons Richard Feynman started talking about quantum computing. He realized that it would be hard for a classical computer to simulate such complex systems, then wondered if whether a prospective quantum computer, with its ability to perform massive parallel processing, might be able to accomplish such a task.

What we have learned 1.4. In this section we learned about composite systems and the computational challenges related to them, in particular we saw that:

- A composite system is represented by the **Cartesian product** of the transition/dynamics matrix of its subsystems.
- If two matrices act on the subsystems independently, then their **tensor product** acts on their combined system.
- There is an **exponential growth** in the amount of resources needed to describe larger and larger composite systems.

2 Basic Quantum Theory

In the beginning of this lecture we acquired the necessary mathematical requirements and developed some heuristics that gently led us to the threshold of the quantum world. Now it is time to open the door in order to continue our journey toward quantum computing.

2.1 Quantum States

Notion goal 2.1. Quantum states will be our basic building blocks in quantum computation, we already introduced the notion of state vectors, now it is time to integrate this notion into quantum mechanics.

Consider a subatomic particle on a line, let us suppose that this particle can only be detected at one of equally spaced points $\{x_0, x_1, ..., x_{n-1}\}$ where $x_i = x_{i-1} + \delta x$ with δx some fixed increment.

$$x_0$$
 x_1 \cdots x_i \cdots x_{n-1}

We assume that δx is sufficiently small to give us a decent approximation, of course in real life a particle could be at any point on the line but representing such a continuous model would require significantly larger mathematical prerequisites and is not needed in the scope of this lecture.

We associate to the current **state** of the particle an n-dimensional column vector $\begin{pmatrix} c_0 & c_1 & \dots & c_{n-1} \end{pmatrix}^T$. the particle being at point x_i shall be denoted $|x_i\rangle$ using the Dirac's **ket**, don't worry about this notation, it will be fully explained soon enough.

To each of those n basic states, we shall associate a column vector:

$$|x_{0}\rangle \longrightarrow \begin{pmatrix} 1 & 0 & \dots & 0 \end{pmatrix}^{T}$$

$$|x_{1}\rangle \longrightarrow \begin{pmatrix} 0 & 1 & \dots & 0 \end{pmatrix}^{T}$$

$$\vdots$$

$$|x_{n-1}\rangle \longrightarrow \begin{pmatrix} 0 & 0 & \dots & 1 \end{pmatrix}^{T}$$
(31)

Observe that those vectors form the **canonical basis** of \mathbb{C}^n . In classical mechanics, those basic states would be all that we would need, however that is not the case in quantum mechanics, indeed experimental evidences show that the particle can be in some "fuzzy blending" of those basic states.

We thus have to incorporate all the basic states to represent the physical state of the particle. This state, that we shall denote $|\psi\rangle$, is a **linear combination of basic states** $|x_0\rangle$, $|x_1\rangle$,..., $|X_{n-1}\rangle$, by suitable complex weights $c_0, c_1, \ldots, c_{n-1}$, known as **amplitudes**.

$$|\psi\rangle = c_0 |x_0\rangle + c_1 |x_1\rangle + \dots + c_{n-1} |x_{n-1}\rangle$$
 (32)

Every state of the system can be represented by a column state vector of \mathbb{C}^n such as:

$$|\psi\rangle \longrightarrow \begin{pmatrix} c_0 & c_1 & \dots & c_{n-1} \end{pmatrix}^T$$
 (33)

The state $|\psi\rangle$ is then said to be in **superposition** of the basic states. Thus $|\psi\rangle$ represents the particle being simultaneously in all $\{x_0, x_1, ..., x_{n-1}\}$ locations. The squared norm/modulus of the complex number divided by the squared norm of the state vector $|\psi\rangle$ will give us

probability that, after observing the particle, we will detect it at point x_i:

$$p(x_i) = \frac{|c_i|^2}{||\psi\rangle|^2} = \frac{|c_i|^2}{\sum_{j=0}^{n-1} |c_j|^2}$$
(34)

When $|\psi\rangle$ is **observed**, it will **collapse** in one of the basic states. We will write this process with the following notation:

$$|\psi\rangle \sim |x_i\rangle$$
 (35)

Let us take a look at the Dirac's **ket** notation and describe its properties. Let $|\psi\rangle$ and $|\psi'\rangle$ be two distinct quantum states such as:

$$|\psi\rangle = c_0 |x_0\rangle + c_1 |x_1\rangle + \dots + c_{n-1} |x_{n-1}\rangle$$
 (36)

and

$$|\psi'\rangle = c_0' |x_0\rangle + c_1' |x_1\rangle + \dots + c_{n-1}' |x_{n-1}\rangle$$
 (37)

then

$$|\psi\rangle + |\psi'\rangle = (c_0 + c'_0)|x_0\rangle + (c_1 + c'_1)|x_1\rangle + \dots + (c_{n-1} + c'_{n-1})|x_{n-1}\rangle$$

= $(c_0 + c'_0 \ c_1 + c'_1 \ \dots \ c_{n-1} + c'_{n-1})^T$ (38)

What happens if we add a ket to itself?

$$|\psi\rangle + |\psi\rangle = 2 |\psi\rangle = (c_0 + c_0 \quad c_1 + c_1 \quad \dots c_{n-1} + c_{n-1})^T$$

= $(2c_0 \quad 2c_1 \quad \dots \quad 2c_{n-1})^T$ (39)

Let S be the sum of squared moduli of $2|\psi\rangle$ such as:

$$S = |2c_0|^2 + |2c_1|^2 + \dots + |2c_{n-1}|^2$$

= $2^2 (|c_0|^2 + |c_1|^2 + \dots + |c_{n-1}|^2)$ (40)

Thus for the state $2|\psi\rangle$, the chance that the particle will be found in position x_j after measurement is:

$$p(x_j) = \frac{|2c_j|^2}{S} = \frac{2^2 |c_j|^2}{2^2 (|c_0|^2 + |c_1|^2 + \dots + |c_{n-1}|^2)}$$

$$= \frac{|c_j|^2}{|c_0|^2 + |c_1|^2 + \dots + |c_{n-1}|^2}$$
(41)

In other words, the ket $2 | \psi \rangle$ describes the same system as $| \psi \rangle$. Notice that we could replace 2 by any $c \in \mathbb{C}$ and get the same result, it works for all the scalar multiples of $| \psi \rangle$. The **length** of $| \psi \rangle$ does not matter from the physical point of view.

As we can multiply (or divide) a ket by any complex number and still have the representation of the same physical state, we may as well work with a **normalized** $|\psi\rangle$ such as:

$$\frac{|\psi\rangle}{||\psi\rangle|} \tag{42}$$

which as a length of 1. From now on, we will only work with normalized kets.

In order to continue our journey to the quantum world, we need to introduce a property of subatomic particles called **spin**. In fact spin will play a major role in our story because it is the prototypical way to implement quantum bits of information (qubits).

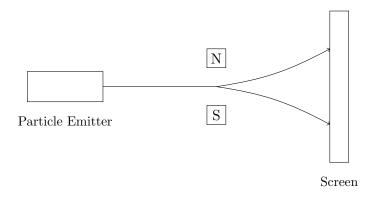


Figure 2: The Stern-Gerlach experiment

What is spin? The Stern-Gerlach experiment (first performed in 1922) showed that an electron in the presence of a magnetic field will behave as if it were a charged spinning top: it will act as a small magnet and strive to align itself to the external field while spinning. the experiment consists of shooting a beam of electrons through a non-homogeneous magnetic field oriented vertically (z axis). The field then splits the beam into two streams with opposite spins, some will be found spinning in one way, and the other spinning in the opposite way.

There are two striking differences between the observed phenomenon and a classical spinning top:

- First, the electron does not appear to have an internal structure by itself it is just a charged point. Spin is therefore a **new property of the quantum world**, without classical analog.
- Secondly, and quite surprisingly, all our electrons can be found **either at the top of the screen or at the bottom but not in between**. When a particle is measured in a given direction, it can only be found in two states: it spins either **clockwise** or **counter-clockwise**.

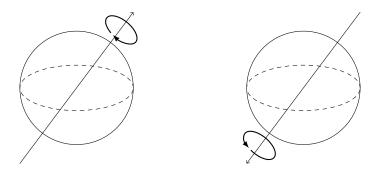


Figure 3: Particles with spin

For each given direction in space there are **only two basic spin states**. For the vertical axis, those states are named spin **up** $|\uparrow\rangle$ and spin **down** $|\downarrow\rangle$. The generic state will then be a superposition of up and down such as:

$$|\psi\rangle = c_0 |\uparrow\rangle + c_1 |\downarrow\rangle \tag{43}$$

Just like before, c_0 is the amplitude of finding the particle in the up state and c_1 is the amplitude of finding the particle in the down state.

Exercise 2.1. Consider a spinning electron which current state is defined by $|\psi\rangle = 3i |\uparrow\rangle - 2 |\downarrow\rangle$.

Find the probability that the state collapses to the up state upon measurement and normalize the ket.

Let us now investigate the physical meaning of the **inner product**. The inner product of the state space (vector space representing the quantum system under discussion) gives us a tool to compute complex numbers known as **transition amplitudes**, which in turn allows us to determine how likely the state of the system **before** a specific measurement (start state) will collapse to another (end state) **after** measurement has been performed. Let:

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{n-1} \end{pmatrix} \text{ and } |\psi'\rangle = \begin{pmatrix} c'_0 \\ c'_1 \\ \vdots \\ c'_{n-1} \end{pmatrix}$$
 (44)

be two normalized state vectors. We can extract the transition amplitude between state $|\psi\rangle$ and state $|\psi'\rangle$ using the following method: $|\psi\rangle$ will be our start state, the end state will be **row** vector whose coordinates will be complex conjugates of $|\psi'\rangle$ coordinates.

Such a state is called a **bra** in Dirac's notation, and will be denoted $\langle \psi' |$, or equivalently:

$$\langle \psi' | = |\psi' \rangle^{\dagger} = (\overline{|\psi' \rangle})^T = (\overline{c_0'} \quad \overline{c_1'} \quad \dots \quad \overline{c_{n-1}'})$$
 (45)

To find the transition amplitude, we multiply $\langle \psi' |$ and $| \psi \rangle$ as matrices, notice that we put them side-by-side, forming what is called a bra-ket, their inner product:

$$\langle \psi' | \psi \rangle = \left(\overline{c'_0} \quad \overline{c'_1} \quad \dots \quad \overline{c'_{n-1}} \right) \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{n-1} \end{pmatrix} = \overline{c'_0} c_0 + \overline{c'_1} c_1 + \dots + \overline{c'_{n-1}} c_{n-1} \in \mathbb{C}$$
 (46)

We can represent the start state and the end state with the transition amplitude of one collapsing into the other as the following decorated arrow:

$$|\psi\rangle \sim |\psi'\rangle$$
 (47)

This method is none other than the inner product of complex vector spaces we introduced in the last lecture, what we have done is simply split the product into the bra-ket form.

Note that the transition amplitude between two states may be zero. In fact, this happens precisely when the two states are **orthogonal** to one another. This indicates the physical meaning of orthogonality: orthogonal are as far apart as they can possibly be. We can think of them as **mutually exclusive alternatives**, for instance, an electron could be in arbitrary superposition of spin up and spin down, but after we measure it in the vertical direction (z-axis) it will always be either up **or** down but never both up **and** down.

Assume we are given a normalized start state $|\psi\rangle$ and an orthogonal basis $\{|b_0\rangle, |b_1\rangle, \dots, |b_{n-1}\rangle\}$ representing a maximal list of mutually exclusive end states. We know that the result of our measurement will be one of the states in the basis, but never a superposition of them.

We can then express $|\psi\rangle$ in the basis $\{|b_0\rangle, |b_1\rangle, \dots, |b_{n-1}\rangle\}$ as:

$$|\psi\rangle = \langle b_0 | \psi \rangle |b_0\rangle + \langle b_1 | \psi \rangle |b_1\rangle + \dots \langle b_{n-1} | \psi \rangle |b_{n-1}\rangle$$

$$= c_0 |b_0\rangle + c_1 |b_1\rangle + \dots + c_{n-1} |b_{n-1}\rangle$$
(48)

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with $c_i = \langle b_i | \psi \rangle$ corresponding to the length of the projection of vector $|\psi\rangle$ on basis vector $|b_i\rangle$ and $|c_0|^2 + |c_1|^2 + \cdots + |c_{n-1}|^2 = 1$. Thus each $|c_i|^2 = |\langle b_i | \psi \rangle|^2$ is the **probability** of ending in the state $|b_i\rangle$ after measurement.

What we have learned 2.1. In this part we have applied the mathematical tools we learned to modelize physical states of quantum systems and studied their properties, in particular, we saw that:

- We associate a **vector space** (more precisely an Hilbert space) to a quantum system and is often called a state space, the dimension of this space reflects the amount of basic states of the system (which constitute its basis).
- States can be **superposed** by adding their representing vector through linear combination.
- A physical state is left **unchanged** if its representing vector is multiplied by a complex **scalar**.
- The state space has a **geometry** given by its inner product. This geometry has a physical meaning: it tells us the **likelihood** for a given state to transition to another one after being measured. States that are **orthogonal** to one another are **mutually exclusive**.
- In quantum mechanics, we use the **Dirac notation**, where the **ket** $|\psi\rangle$ express a complex column vector representing a quantum state and the **bra** $\langle\psi|=(|\overline{\psi}\rangle)^T=|\psi\rangle^{\dagger}$ which expresses the **adjoint** of $|\psi\rangle$, in other words, it is the row vector corresponding to to the transpose of $|\overline{\psi}\rangle$ whose coordinates are the complex conjugates of the coordinates of $|\psi\rangle$.

2.2 Observables

Notion goal 2.2. Observables constitute a fundamental notion in physics, it is required to understand the subtleties of quantum systems measurement.

The field of physics is mostly about observation, physical quantities like mass, momentum, velocity, etc, make sense only so far as they can be observed in a quantifiable way. We can think of a physical as a collection of **two sets**: on one hand, the **state space** corresponding to the set of all states it can be possibly found in, and in the other hand, the set of its **observables** corresponding to the **physical quantities that can be observed** in each state of the state space.

Each observable may be thought of as a **specific question we pose to the system**: if the system is currently in some given state $|\psi\rangle$, which values can we possibly observe? We need to introduce the mathematical analog of an observable:

Postulate 2.1. To each physical observable there corresponds a hermitian operator.

What does it implies? First of all, an **observable is a linear operator**, which means that it maps states to states. If we apply an observable $\Omega \in \mathbb{C}^{n \times n}$ to the state vector $|\psi\rangle \in C^n$, then the result is the state $\Omega |\psi\rangle \in \mathbb{C}^n$.

Example 2.1. Let $|\psi\rangle = \begin{pmatrix} -1 & -1-i \end{pmatrix}^T$ be the start state in the two-dimensional spin state space. Now let:

$$\Omega = \begin{pmatrix} -1 & -i \\ i & 1 \end{pmatrix}$$

This matrix acts as an operator on \mathbb{C}^2 . Therefore, we can apply it to $|\psi\rangle$. The result is $\Omega |\psi\rangle = (i, -1 - 2i)^T$, note that $|\psi\rangle$ and $\Omega |\psi\rangle$ are not scalar multiples of one another, and thus they do not represent the same state: Ω has modified the state of the system.

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Secondly, as we saw in the last lecture, the **eigenvalues of a hermitian operator are all real**. The physical meaning of this fact is established by the following postulate:

Postulate 2.2. The eigenvalues of a hermitian operator Ω associated with a physical observable are the only possible values observable can take as a result of measuring it on any given state. Furthermore, the eigenvectors of Ω form a basis for the state space.

To summarize, an observable $\Omega \in \mathbb{C}^{n \times n}$ is an hermitian operator, it corresponds to a question, its normalized eigenvectors (also called eigenstates) $\{|e_0\rangle, |e_1\rangle, \dots, |e_{n-1}\rangle\}$ forming its **eigenbasis** correspond to the possible answers, thus the basic states that the system collapses on upon measurement of the observable **depends of the measured observable** (they form the eigenbasis of Ω).

The application of this observable on $|\psi\rangle$ corresponds to the product $\Omega |\psi\rangle$, since $|\psi\rangle$ is a linear combination of the eigenvectors e_i of distinct eigenvalues $\lambda_i \in \mathbb{R}$, then $\Omega |\psi\rangle = \Omega c_0 |e_0\rangle + \Omega c_1 |e_1\rangle + \cdots + \Omega c_{n-1} |e_{n-1}\rangle$ and since the **scalar multiple of an eigenvector is equivalent to** the original eigenvector then we can write $\Omega |\psi\rangle = \lambda_0 c_0 |e_0\rangle + \lambda_1 c_1 |e_1\rangle + \cdots + \lambda_{n-1} c_{n-1} |e_{n-1}\rangle$ which is not a scalar multiple of $|\psi\rangle$ and thus represents a different physical state.

Meaning that once you have measured an observable on a specific quantum state (eg. position), the state collapses into a whole new state and you cannot measure another observable (eg. momentum) on the state you wanted to measure since it doesn't exist anymore.

When we arbitrarily describe a state, its basic states form the eigenbasis of a predefined observable, in the case of our previous example, the most obvious observable is **position**, $\{|x_0\rangle, |x_1\rangle, \ldots, |x_{n-1}\rangle\}$ then are the eigenvectors of the position observable forming its eigenbasis. The position observable corresponds to the question "Where the particle can be found after measurement?". Then we have to define the **position observable** Ω_P , its eigenvalues form the possible position vector such as $(\lambda_0 \ \lambda_1 \ \ldots \ \lambda_{n-1})^T$, let see how to act on a basic state:

$$\Omega_P |x_i\rangle = \lambda_i |x_i\rangle \tag{49}$$

In other words, Ω_P acts as the multiplication by position, the only remaining basic state being the one being equal to $\begin{pmatrix} \lambda_0 & \lambda_1 & \dots & \lambda_{n-1} \end{pmatrix}^T$, those eigenvalues are determined at the instant of **measurement** in a non-deterministic fashion. As eigenvectors form the basis of $|\psi\rangle$ we can extend the above equation to:

$$\Omega_P |\psi\rangle = \Omega_P \sum_{i=0}^{n-1} c_i |x_i\rangle = \sum_{i=0}^{n-1} \Omega_P c_i |x_i\rangle = \sum_{i=0}^{n-1} \lambda_i c_i |x_i\rangle$$
(50)

Hence the representation of the position operator in the standard basis:

$$\Omega_{P} = \begin{pmatrix}
\lambda_{0} & 0 & \dots & 0 \\
0 & \lambda_{1} & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \dots & \lambda_{n-1}
\end{pmatrix} = \begin{pmatrix}
x_{j}[0] & 0 & \dots & 0 \\
0 & x_{j}[1] & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \dots & x_{j}[n-1]
\end{pmatrix}$$
(51)

Where the eigenvalues forming position vector $(\lambda_0 \ \lambda_1 \ \dots \ \lambda_{n-1})^T$ corresponds to the basic state/position vector $|x_j\rangle$ with $0 \le j \le n-1$ determined in a non-deterministic way during measurement. The observable Ω_P is the **question**, the basic states of $|\psi\rangle$ are the set of **possible answers**, the product $\Omega_P |\psi\rangle$ representing the measurement then returns the **definitive answer** λ_j to the question (nullifying the other possible final states), collapsing the system into the corresponding state $|x_j\rangle$.

A second example of observable comes from the spin system we saw previously. Given a specific direction in space, in which way is the particle spinning? We can ask, for instance: is the particle spinning...

- ...up or down in the z direction?
- ...in or out in the y direction?
- ...left or right in the x direction?

The three spin operators corresponding to those questions (observables) are based on matrices called the **Pauli operators** normalized by the value $\frac{\hbar}{2}$ and are expressed as:

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 (52)

Where \hbar (pronounced "h bar") represents a universal constant in quantum mechanics known as **reduced Planck constant**, we can safely ignore it given the scope of our lecture.

We have already met $\mathbf{up} \mid \uparrow \rangle$ and $\mathbf{down} \mid \downarrow \rangle$, the eigenbasis of S_z . Similarly, S_y has the eigenbasis $\{ \mid \swarrow \rangle, \mid \nearrow \rangle \}$ called \mathbf{in} and \mathbf{out} , and S_x has the eigenbasis $\{ \mid \leftarrow \rangle, \mid \rightarrow \rangle \}$, called \mathbf{left} and \mathbf{right} .

Exercise 2.2. Consider a particle in initial spin up. Apply S_x to it and determine the resulting state after measurement.

By definition, for an hermitian matrix Ω and a state $|\psi\rangle$, the quantity $\langle\psi|\Omega|\psi\rangle = \langle\Omega\psi,\psi\rangle$ is real and is denoted as $\langle\Omega\rangle_{\psi}$, this number corresponds to the **expected value** of observing Ω repeatedly on the same state ψ .

Let us conduct an experiment: assume we have a quantum system at state $|\psi\rangle$. We want the value of an observable Ω of eigenvalues $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$. By definition, we will observe one of its eigenvalues. Let us now repeat this n times, at the end of the experiment, λ_i has been seen p_i times, where $0 \leq p_i \leq n$ (in statistical vocabulary, the **frequency** of λ_i is $\frac{p_i}{n}$). If we compute:

$$\lambda_0 \frac{p_0}{n} + \lambda_1 \frac{p_1}{n} + \dots + \lambda_{n-1} \frac{p_{n-1}}{n} \tag{53}$$

If n is sufficiently large, this number (known in statistics as **estimated expected value**) will be very close to $\langle \Omega \rangle_{\psi}$.

What we have learned 2.2. We omitted a lot about the notion of observables to keep only the essentials given the scope of our lecture, we should remember, in particular, that:

- Observables are represented by **hermitian operators**. The result of an observation is always an **eigenvalue** of the hermitian.
- The expression $\langle \Omega \rangle_{\psi} = \langle \psi | \Omega | \psi \rangle = \langle \Omega \psi, \psi \rangle$ represents the **expected value** of observing Ω on $|\psi\rangle$.
- Observables in general do not commute. This means that the order of observation does matter.

2.3 Measurement

Notion goal 2.3. Measurement is a fundamental notion in quantum mechanics since it allows to collapse superposed states into one classical state and extract this information. Let us dive deeper into the quantum world.

The act of performing an observation on a given physical system is called **measuring**. Just as a single observable represents a specific question asked to the system, measuring is **the process** of asking a specific question and receiving a definite answer.

In classical physics we assumed that:

- The act of measuring would leave the system **unchanged** in whatever state it was.
- The result of measurement on a well defined state is **predictable**, in other words, if we know the state with absolute certainty, we can anticipate the value of the observable on that state.

Both those assumptions proved wrong, as research in subatomic scale proved repeatedly that measurement is an inherently non-deterministic process. We currently know that an observable can only assume one of its eigenvalues as the result of an observation (the other being zero), but we don't know the likelihood of seeing a specific eigenvalue λ nor what happens to the state vector if λ is observed. That is why we need the following postulate:

Postulate 2.3. Let Ω be an observable and $|\psi\rangle$ be a state. If the result of measuring Ω is the eigenvalue λ , the state after after measurement will always be an eigenvector of Ω corresponding to λ .

The **probability** of collapsing from the normalized starting state $|\psi\rangle$ to a specific eigenvector $|e\rangle$ is given by the **squared transition amplitude** $|\langle e|\psi\rangle|^2$ which corresponds to the squared projection length of $|\psi\rangle$ on $|e\rangle$.

Since the normalized eigenvectors $\{e_0, e_1, \dots, e_{n-1}\}$ of Ω constitute an orthonormal basis of the state space, we can write $|\psi\rangle$ as a linear combination in this basis:

$$|\psi\rangle = \langle e_0 | \psi \rangle | e_0 \rangle + \langle e_1 | \psi \rangle | e_1 \rangle + \dots + \langle e_{n-1} | \psi \rangle | e_{n-1} \rangle$$

= $c_0 | e_0 \rangle + c_1 | e_1 \rangle + \dots + c_{n-1} | e_{n-1} \rangle$ (54)

Let us compute the expected value:

$$\langle \Omega \rangle_{\psi} = \langle \Omega \psi, \psi \rangle = |c_0|^2 \lambda_0 + |c_1|^2 \lambda_1 + \dots + |c_{n-1}|^2 \lambda_{n-1} = |\langle e_0 | \psi \rangle|^2 \lambda_0 + |\langle e_1 | \psi \rangle|^2 \lambda_1 + \dots + |\langle e_{n-1} | \psi \rangle|^2 \lambda_{n-1}$$
(55)

As we can see $\langle \Omega \rangle_{\psi}$ is the **expected value** of the probability distribution:

$$(\lambda_0, p_0), (\lambda_1, p_1), \dots, (\lambda_{n-1}, p_{n-1})$$
 (56)

where each $p_i = |\langle e_i | \psi \rangle|^2$ is the square of the amplitude of the collapse of $|\psi\rangle$ to eigenvector $|e_i\rangle$. What if we perform measurement with **more than one observable**? The answer depends on which order we ask our questions, in other words, it depends on which observable we measure first.

Assume that we are at a state $|\psi\rangle$ and we ask a specific question (observable). We get as an answer the eigenvalue λ . Also, by our discussion so far, the system will collapse to the

corresponding eigenvector. Assume now that we asked the same question again. What would then happen? The answer will still be λ , since the current state (eigenvector of the observable) is orthogonal to all eigenvectors, except itself. Now, how do we get out of this state? By asking a different question (observable). Asking many questions in a different order might lead to different intermediate and final states.

What we have learned 2.3. In this part we have finished our exploration of the notion of measurement and observables, in particular, we learned that:

- The end state of the measurement of an observable is always one of its **eigenvector**.
- The probability of an initial state $|\psi\rangle$ to collapse into a eigenvector $|e\rangle$ of the observable is given by the **squared projection length** (or squared transition amplitude) of $|\psi\rangle$ on $|e\rangle$.
- When we measure several observables, the **order of measurement matters**.

2.4 Quantum Dynamics

Notion goal 2.4. Time wait for no one. Until now we have studied quantum systems frozen in a single time tick. Now it is time to see how they evolve over time.

So far in this section, we only studied static quantum systems, that does not evolve over time. Of course changes could still occur upon measurements but the system itself was not time dependent. In the real world, quantum systems **do evolve over time**, and thus we need to introduce the notion of **quantum dynamics**.

Just as hermitian operators represent physical observables, **unitary operators** introduce dynamics in the quantum world.

Postulate 2.4. The evolution of a quantum system (that is not a measurement) is given by a unitary operator or transformation.

This means that if U is a unitary matrix that represents a unitary operator and $|\psi(t)\rangle$ is a state of the quantum system at time t, then:

$$|\psi(t+1)\rangle = U|\psi(t)\rangle \tag{57}$$

will represent the system at time t + 1. An important feature of unitary transformations are that they are **closed under composition and inverse**, meaning that the product of two unitary matrices is also a unitary matrix and that the inverse of a unitary transformation is also unitary. Finally there is a multiplicative identity for unitary transformation (in fact it is simply the identity matrix which is trivially unitary), thus we can say that the set of unitary transformations constitutes a **group of transformations** with respect to composition.

Let us see how dynamics is determined by unitary transformations, assume we associate each time steps $t_0, t_1, \ldots, t_{n-1}$ with unitary operators $U_0, U_1, \ldots, U_{n-1}$. Let us start with a initial state vector $|\psi\rangle$. We can apply U_0 to $|\psi\rangle$, then apply U_1 to the result and so on. We will thus obtain the following sequence of vectors:

$$U_{0} | \psi \rangle$$

$$U_{1}U_{0} | \psi \rangle$$

$$\vdots$$

$$U_{n-1}U_{n-2} \dots U_{0} | \psi \rangle = \prod_{i=0}^{n-1} U_{i} \cdot | \psi \rangle$$
(58)

Such a sequence is called the **orbit** of $|\psi\rangle$ under the action of U_i at time steps $t_0, t_1, \ldots, t_{n-1}$.

Observe that we can **go back in time** by applying the inverse (reminder: if U is unitary then $U^{\dagger} = U^{-1}$), we can thus say that the evolution of a quantum system is **time symmetric** and that unitary operators are revertible.

We can now preview how quantum computation will work. A quantum computer shall be placed into an initial state $|\psi\rangle$ and we shall then apply a sequence of unitary operators to the state, when we are done, we will measure the outputs and get a final state.

But how is the sequence of unitary transformations actually determined? The answer of how the system dynamics are determined lies in the **Schrödinger equation** (the discretized version in our case):

$$\frac{|\psi(t+\delta t)\rangle - |\psi(t)\rangle}{\delta t} = -i\frac{2\pi}{h}H|\psi(t)\rangle \tag{59}$$

With h corresponding to the **Planck constant** (the reduced Planck constant we saw before corresponds to $\hbar = \frac{h}{2\pi}$). Let us discuss this equation for a bit: **energy is an observable**, and therefore for a quantum system it is possible to define a hermitian matrix to represent it, this observable is called the **hamiltonian** of the system, indicated by H in the equation above.

The Schrödinger equation states that the rate of variation of the state vector $|\psi(t)\rangle$ with respect to time at the instant t is proportional to $|\psi(t)\rangle$ multiplied by the operator -i*H. By solving this equation with some initial conditions, we are able to determine the evolution of the system over time.

In other words, we know that the global energy is preserved in an isolated system, throughout its evolution. Energy is an observable and, for a quantum system, we can use a hermitian matrix to represent it. This matrix is also known as the hamiltonian matrix. Then, the Schrodinger equation describes that the rate of variation from a state to another is proportional to the energy expressed via the hamiltonian matrix.

What we have learned 2.4. We should remember, in particular that:

- Quantum dynamics are given by unitary transformations.
- Unitary transformations are **revertible**, thus all closed systems dynamics are reversible in time as long as no measurement is performed.
- The concrete dynamics is given by the Schrödinger equation, which determines the evolution of a quantum system whenever its hamiltonian is specified,

2.5 Assembling Quantum Systems

Notion goal 2.5. Now that we are beginning to grasp quantum systems, let us show how we can build more complex composite systems from them. It will also allow us to introduce the notion of entanglement, which will be used extensively in the next parts of our lectures for algorithm design, quantum cryptography and quantum teleportation.

Let us suppose that we are dealing with two subatomic particles, each one moving in a confined one-dimensional grid. The first particle can be found in the set of points $\{x_0, x_1, \ldots, x_{n-1}\}$ in one grid while the second particle can be found in the set of points $y_0, y_1, \ldots, y_{m-1}$ in the other grid.



Postulate 2.5. Let Q and Q' be two independent quantum systems represented respectively by the vector spaces \mathbb{V} and \mathbb{V}' . The quantum system obtained by merging Q and Q' will be represented by the tensor product $\mathbb{V} \otimes \mathbb{V}'$.

Note that we can assemble as many systems as we like, the tensor product is **associative**, so we can **incrementally build larger and larger systems** as demonstrated below:

$$\mathbb{V}_0 \otimes \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_k \tag{60}$$

Let us go back to our example, we can observe that there are $n \times m$ basic states such as:

$$|x_i\rangle \otimes |y_i\rangle$$
, $0 \le i < n$ and $0 \le j < m$ (61)

This state describes that the position of the first particle is x_i and the position of the second particle is y_j . We can then represent the system before measurement as a generic state vector representing the the superposition of basic states of both subsystems:

$$|\psi\rangle = c_{0,0} \cdot |x_0\rangle \otimes |y_0\rangle + \dots + c_{i,j} \cdot |x_{i'}\rangle \otimes |y_{j'}\rangle + \dots + c_{n-1,m-1} \cdot |x_{n-1}\rangle \otimes |y_{m-1}\rangle$$
 (62)

which is a vector in the $(n \times m)$ -dimensional complex space $\mathbb{C}^{n \times m}$. The quantum amplitude $|c_{i,j}|$ squared will give us the probability of finding two particles at positions x_i and y_j respectively.

Example 2.2. Assume n = 2 and m = 2 in the example above. We are thus dealing with the state space \mathbb{C}^4 whose standard (canonical) basis is:

$$\{|x_0\rangle \otimes |y_0\rangle, |x_0\rangle \otimes |y_1\rangle, |x_1\rangle \otimes |y_0\rangle, |x_1\rangle \otimes |y_1\rangle\}$$
(63)

Suppose the state vector for the two-particles system is given by:

$$|\psi\rangle = i|x_0\rangle \otimes |y_0\rangle + (1-i)|x_0\rangle \otimes |y_1\rangle + 2|x_1\rangle \otimes |y_0\rangle + (-1-i)|x_1\rangle \otimes |y_1\rangle \tag{64}$$

What is the probability of finding the first particle in position x_1 and the second one at y_1 ?

$$p(x_1, y_1) = \frac{|-1 - i|^2}{|i|^2 + |1 - i|^2 + |2|^2 + |-1 - i|^2} \approx 0.2222$$
(65)

Exercise 2.3. Redo the steps of the last example when n = m = 4 and $c_{0,0} = c_{0,1} = \cdots = c_{3,3} = 1 + i$.

Now that we are a bit familiar with quantum assemblages, we are ready for the final surprise of quantum mechanics: **entanglement**. Entanglement will force us to abandon one last comforting faith, namely, that assembled complex systems can be understood completely in term of its constituents.

Example 2.3. Let us work the simplest non-trivial two-particle system: each particle is allowed only two points. Consider the state:

$$|\psi\rangle = |x_0\rangle \otimes |y_0\rangle + |x_1\rangle \otimes |y_1\rangle \tag{66}$$

In order to clarify what is left out, we might write this as:

$$|\psi\rangle = 1 \cdot |x_0\rangle \otimes |y_0\rangle + 0 \cdot |x_1\rangle \otimes |y_0\rangle + 0 \cdot |x_0\rangle \otimes |y_1\rangle + 1 \cdot |x_1\rangle \otimes |y_1\rangle \tag{67}$$

Let us see if we can write $|\psi\rangle$ as the tensor product of two states coming from the two subsystems. Any vector representing the first particle on the line can be written as:

$$c_0 |x_0\rangle + c_1 |x_1\rangle \tag{68}$$

Similarly, any vector representing the second particle on the line can be written as:

$$c_0' |y_0\rangle + c_1' |y_1\rangle \tag{69}$$

Therefore, if $|\psi\rangle$ came from the tensor product of the two subsystems, we would have:

$$|\psi\rangle = (c_0 \cdot |x_0\rangle + c_1 \cdot |x_1\rangle) \otimes (c_0' \cdot |y_0\rangle + c_1' \cdot |y_1\rangle)$$

$$= c_0c_0' \cdot |x_0\rangle \otimes |y_0\rangle + c_0c_1' \cdot |x_0\rangle \otimes |y_1\rangle + c_1c_0' \cdot |x_1\rangle \otimes |y_0\rangle + c_1c_1' \cdot |x_1\rangle \otimes |y_1\rangle$$
(70)

For our $|\psi\rangle$ in Equation 66, the Equation 70 imply that $c_0c'_0 = c_1c'_1 = 1$ and $c_0c'_1 = c_1x'_0 = 0$ which is impossible. Thus those two equations have no solution: we cannot use the basic states and the tensor product to generate the state. In this case, we say that the two particles are **entangled**.

What does it physically means? What would happen if we measured the first particle? A quick calculation show that the first particle has a 50-50 chance of being found at the position x_0 or at x_1 . So what if it is, in fact, found at position x_0 ? Because the term $|x_0\rangle \otimes |y_1\rangle$ has 0 coefficient, we know that there is no chance that the second particle will be found in position y_1 . We must then conclude that that the second particle can only be found at position y_0 .

Similarly, if the first particle is found in position x_1 then the second particle must be in position y_0 . Note that the situation is perfectly **symmetrical** with respect to the two particles, it would be the same if we measured the second one first.

The individual states of the two particles are intimately related to one another, or **entangled**. the amazing side of this story is that the x_i 's can be light years away from the y_j 's. Regardless of their actual distance in space, a measurement's outcome will always determine the measurement's outcome for the other one.

The state $|\psi\rangle$ is in sharp contrast with state $|\psi'\rangle$ corresponding to:

$$|\psi'\rangle = 1 \cdot |x_0\rangle \otimes |y_0\rangle + 1 \cdot |x_1\rangle \otimes |y_0\rangle + 1 \cdot |x_1\rangle \otimes |y_0\rangle + 1 \cdot |x_1\rangle \otimes |y_1\rangle \tag{71}$$

Here, finding the first particle at a particular position does not provide any clue as to where the second particle will be found. States that can be broken into the tensor product of states from the constituent subsystems (like $|\psi'\rangle$) are called **separable states**, whereas states that are unbreakable (like $|\psi\rangle$) are referred to as **entangled states**.

Exercise 2.4. Assume the same scenario as the example above and let:

$$|\phi\rangle = |x_0\rangle \otimes |y_1\rangle + |x_1\rangle \otimes |y_1\rangle$$

Is this state separable?

To illustrate entanglement with a concrete physical case, let us go back to the spin system. Just as there are laws of conservation of momentum, angular momentum, energy-mass, and other physical properties, so too there is a **law of conservation of total spin** of a quantum system.

This means that in an isolated system, the total amount of spin must stay the same. Let us fix a specific direction, say, the vertical one (z-axis), and the corresponding spin basis, up and down. Consider the case of a quantum system such as a composite particle, whose total spin is zero. This particle might split up at some point in time into two other particles that do have spin:

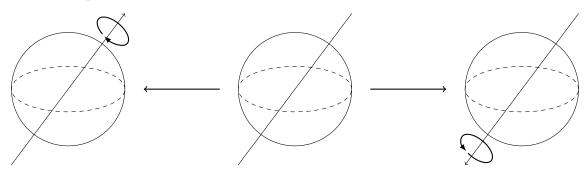


Figure 4: Composite system where the total spin is zero

The spin state of the two particles will now be **entangled**. The law of conservation of spin stipulates that because we began with a total spin zero, **the sum of spins of the two particles must cancel each other out**. This amounts to the fact that if we measure the spin of the left particle on along the z-axis in the state $|\uparrow_L\rangle$ (where L describes which particle we are dealing with), then the spin of the other particle must be $|\downarrow_R\rangle$. Similarly, if the state of the left particle is $|\downarrow_L\rangle$, then the spin of the right particle must be $|\uparrow_R\rangle$.

We can describe this in term of vector spaces, the basis that describe the left particle is $B_L = \{\uparrow_L, \downarrow_L\}$ and the basis that describes the right particle is $B_R = \{\uparrow_R, \downarrow_R\}$. The basis elements of the composite system are:

$$\{\uparrow_L \otimes \uparrow_R, \uparrow_L \otimes \downarrow_R, \downarrow_L \otimes \uparrow_R, \downarrow_L \otimes \downarrow_R\} \tag{72}$$

In such a vector space, our entangled particles can be described by:

$$|\beta\rangle = \frac{1}{\sqrt{2}}(|\uparrow_L \otimes \downarrow_R\rangle + |\downarrow_L \otimes \uparrow_R\rangle) \tag{73}$$

With $\frac{1}{\sqrt{2}}$ being the normalization term (so the length of $|\beta\rangle$ is 1). As we said before, the combinations $|\uparrow_L \otimes \uparrow_R\rangle$ and $|\downarrow_L \otimes \downarrow_R\rangle$ cannot occur because of the law of conservation of spin. When one measures the left particle and it collapses to the state $|\uparrow_L\rangle$ then **instantaneously** the right particle will collapse to the state $|\downarrow_R\rangle$, **even if the particles are millions of light-years away**.

What we have learned 2.5. From this part, we should remember that:

- We can use **tensor product** to build complex quantum systems out of simpler ones.
- The new system cannot be analyzed simply in terms of states belonging to its subsystems. An entire set of new states has been created, which cannot be resolved into their constituents.
- Subsystems can be **entangled** or **separable**.

3 Exercise Corrections

3.1 From Classical to Quantum

3.1.1 Exercise 1.1

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The marbles in each vertex would "magically" multiply themselves and the many copies of the marbles would go to each vertex that has an edge connecting them. That would be non-determinism!

3.1.2 Exercise 1.2

The marbles would "magically" disappear.

3.2 Basic Quantum Theory

3.2.1 Exercise 2.1

$$|\psi\rangle = 3i |\uparrow\rangle - 2 |\downarrow\rangle$$

The norm of the state vector $(3i -2)^T$ corresponding to the ket $|\psi\rangle$ is:

$$||\psi\rangle| = \sqrt{|3i|^2 + |-2|^2} = \sqrt{9+4} = \sqrt{13}$$

Therefore, the probability of detecting the particle in the up state is:

$$p(\uparrow) = \frac{|3i|^2}{||\psi\rangle|^2} = \frac{|3i|^2}{(\sqrt{13})^2} = \frac{9}{13} \approx 0.6923$$

Thus we obtain the normalized ket by dividing it by the norm of its corresponding vector:

$$|\psi\rangle = \frac{1}{\sqrt{13}} * \begin{pmatrix} 3i & -2 \end{pmatrix}^T \approx \begin{pmatrix} 0.8321i & 0.5547 \end{pmatrix}^T \longrightarrow |\psi\rangle = 0.8321i |\uparrow\rangle + 0.5547 |\downarrow\rangle$$

We can verify that it is a normalized vector by checking if its length is equal to 1:

$$||\psi\rangle| \approx \sqrt{|0.8321i|^2 + |0.5547|^2} \approx 1$$

3.2.2 Exercise 2.2

Let the state $|\uparrow\rangle = 1 \times |\uparrow\rangle + 0 \times |\downarrow\rangle$ be the state of the particle in spin up initial state. Let us multiply it by S_x (we can ignore $\frac{\hbar}{2}$):

$$S_x |\psi\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

It flips it! $S_x |\uparrow\rangle = |\downarrow\rangle$

3.2.3 Exercise 2.3

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If n = m = 4 then the basis of our state space would be:

$$\{|x_0\rangle\otimes|y_0\rangle, |x_1\rangle\otimes|y_0\rangle, |x_0\rangle\otimes|y_1\rangle, \dots, |x_3\rangle\otimes|y_3\rangle\}$$

Therefore the state $|\alpha\rangle$ of our composite two-particles system would be:

$$|\alpha\rangle = (1+i)\cdot|x_0\rangle\otimes|y_0\rangle + (1+i)\cdot|x_1\rangle\otimes|y_0\rangle + (1+i)\cdot|x_0\rangle\otimes|y_1\rangle + \dots, (1+i)\cdot|x_3\rangle\otimes|y_3\rangle$$

As all the coefficients are equals and the system contains the superposition of 16 basicstates in total, then the system collapses in each possible basic states share the same probability which is trivially:

$$p(x_i, y_j) = \frac{|1+i|^2}{\sum_{k=1}^{16} |1+i|^2} = \frac{(\sqrt{2})^2}{16 \cdot (\sqrt{2})^2} = \frac{2}{32} = \frac{1}{16} = 0.0625$$

3.2.4 Exercise 2.4

So, is $|\phi\rangle$ separable? Let us take a look at it:

$$|\phi\rangle = |x_0\rangle \otimes |y_1\rangle + |x_1\rangle \otimes |y_1\rangle = 0 \cdot |x_0\rangle \otimes |y_0\rangle + 1 \cdot |x_0\rangle \otimes |y_1\rangle + 0 \cdot |x_1\rangle \otimes |y_0\rangle + 1 \cdot |x_1\rangle \otimes |y_1\rangle$$

So if it was separable, it would satisfies the equation:

$$|\psi\rangle = (c_0 \cdot |x_0\rangle + c_1 \cdot |x_1\rangle) \otimes (c'_0 \cdot |y_0\rangle + c'_1 \cdot |y_1\rangle)$$

= $c_0c'_0 \cdot |x_0\rangle \otimes |y_0\rangle + c_0c'_1 \cdot |x_0\rangle \otimes |y_1\rangle + c_1c'_0 \cdot |x_1\rangle \otimes |y_0\rangle + c_1c'_1 \cdot |x_1\rangle \otimes |y_1\rangle$

Those two equations have a solution: $\begin{cases} c_0 = 1 \\ c'_0 = 0 \\ c_1 = 1 \\ c'_1 = 1 \end{cases}$

Thus the states of the two subsystems of $|\phi\rangle$ are separable.