

Lecture Notes for Week 3

Quantum Mechanics

In order to explain how quantum computers work, we will first need to provide a brief overview of quantum mechanics and the mathematical formalism that it uses. Our discussion of these topics will not be comprehensive, of course, but it will provide us with the necessary conceptual framework that is needed to describe quantum algorithms and the circuits that can implement them.

Schrödinger's Equation

One of the fundamental assumptions of quantum mechanics is that the state of a particle can be described by a complex-valued *wave function* (which is usually denoted by the Greek letter ψ). The temporal evolution of this function is governed by Schrödinger's equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad (1)$$

where \hat{H} represents a linear operator (the so-called Hamiltonian), and \hbar is Planck's constant divided by 2π .

Remark 1. Note that the Hamiltonian has nothing to do with the Hadamard operator (although they are both denoted by \hat{H}). This can be a source of confusion, so we will need to exercise some care when we use this symbol.

When interpreting what equation (1) means, it is important to keep in mind that operator \hat{H} is associated with the *total energy of the system*. This quantity is usually expressed as

$$E = E_k + E_p \quad (2)$$

where E_k represents the kinetic energy, and E_p corresponds to the potential energy. In the special case when we are dealing with a single particle, this expression takes the form

$$E = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2) + V(x, y, z, t) \quad (3)$$

where m is the particle mass, and $V(x, y, z, t)$ represents the potential energy that is due to an external field (which could be time-varying in general).

To keep our discussion as simple as possible, in the following we will assume that the particle moves only along the x -axis, in which case Schrödinger's equation has solutions of the form $\psi(x, t)$. In cases when the external field is *not* time varying, these solutions can be expressed as

$$\psi(x, t) = f(t)\varphi(x) \quad (4)$$

where $f(t)$ is a function of time, and $\varphi(x)$ depends on spatial coordinates. To see why this separation of variables is helpful, let us substitute (4) into equation (1). When we do so, we obtain

$$i\hbar \varphi(x) \frac{\partial f(t)}{\partial t} = f(t) \hat{H} \varphi(x) \quad (5)$$

which can be rewritten as

$$i\hbar \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = \frac{1}{\varphi(x)} \hat{H} \varphi(x) \quad (6)$$

after dividing both sides by $f(t)\varphi(x)$.

Expression (6) is convenient to work with, since its left hand side depends exclusively on t , while the right hand side depends only on x . In general, equations of this sort have a solution only if $f(t)$ and $\varphi(x)$ satisfy

$$i\hbar \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = E \quad (7)$$

and

$$\frac{1}{\varphi(x)} \hat{H} \varphi(x) = E \quad (8)$$

where E is a constant. Under such circumstances, (7) can be rewritten as an ordinary differential equation

$$\frac{df}{dt} = -\frac{i}{\hbar} E f(t) \quad (9)$$

whose solution is

$$f(t) = e^{-iEt/\hbar} \quad (10)$$

This allows us to represent $\psi(x, t)$ as

$$\psi(x, t) = \varphi(x) e^{-iEt/\hbar} \quad (11)$$

where the time varying portion of the wave function has a simple exponential form (in quantum mechanics, such states are known as *stationary states*).

When the system is in such a state, we need to focus our attention primarily on equation (8) and its solution $\varphi(x)$. Because of that, the function $\psi(x, t)$ is often expressed as $\psi(x)$, with the implicit understanding that the final result must be multiplied by $e^{-iEt/\hbar}$.

Quantum Operators and their Interpretation

The mathematical formalism of quantum mechanics is based on a fundamental postulate which allows us to relate operators and their eigenvalues to physical quantities. This postulate can be stated as follows.

Postulate 1. Every observable physical quantity q has an associated operator \hat{Q} , whose eigenvalues $\{q_i\}$ represent the *only* possible values of q that we can register.

One of the immediate implications of this postulate is that a measurement will produce $q = q_i$ if and only if $\psi(x) = \phi_i(x)$, where $\phi_i(x)$ is the eigenfunction of \hat{Q} that corresponds to q_i . This means (among other things) that we can find a particle only in states $\{\phi_1, \phi_2, \dots\}$ when an observation is made.

Schrödinger's equation provides us with a nice illustration of how this principle works in practice. Since this equation reduces to

$$\hat{H}\varphi(x) = E\varphi(x) \quad (12)$$

when the field is not time-varying, we can conclude that E represents *an eigenvalue of operator \hat{H}* , and that $\varphi(x)$ is the corresponding eigenfunction. Given the interpretation of this operator, it follows that the set of values $\{E_i\}$ for which (12) is satisfied determines the possible values that the total energy can take.

To get a sense for how quantum mechanics handles states that do *not* correspond to eigenfunctions, we first need to point out that Postulate 1 implicitly assumes that every quantum operator \hat{Q} satisfies the following two properties.

Property 1. Operator \hat{Q} must be *self-adjoint*, which means that all of its eigenvalues are *real* (see Theorem 1). This is important because it allows us to identify observable physical quantities with eigenvalues.

Property 2. The eigenfunctions $\{\phi_1(x), \phi_2(x), \dots\}$ of operator \hat{Q} form an *orthonormal basis* in the space of square integrable functions. As a result, *any* function $f(x)$ in this space can be expressed as

$$f(x) = \sum_i \beta_i \phi_i(x) \quad (13)$$

where β_i ($i = 1, 2, \dots$) are constant coefficients (which can be complex in general).

When $\psi(x)$ is *not* an eigenfunction of \hat{Q} , Property 2 allows us to express it as

$$\psi(x) = \sum_i \alpha_i \phi_i(x) \quad (14)$$

In such cases, we say that the particle is in a *state of superposition* (as opposed to a state where q has a definite value). What this means is that a measurement could produce *any* one of the possible values for q , but we cannot tell in advance which one. The following postulate tells us how we can determine the probabilities of different outcomes.

Postulate 2. If a particle is in state ψ , the probability of observing value q_i when we perform a measurement can be calculated as

$$P(q_i) = |\alpha_i|^2 \quad (15)$$

where α_i is the coefficient that corresponds to $\phi_i(x)$ in (14).

When invoking this postulate, there are two things that we have to bear in mind.

- (a) The physical quantity that we are interested in dictates what expression (14) will look like, because we have to use the eigenfunctions of the appropriate operator as our basis.
- (b) In order to treat the terms $|\alpha_i|^2$ as probabilities, coefficients α_i must satisfy

$$\sum_i |\alpha_i|^2 = 1 \quad (16)$$

This condition is guaranteed to hold if the wave function satisfies $\langle \psi(x), \psi(x) \rangle = 1$ (when this is the case, we say that $\psi(x)$ is *normalized*). A proof of this property is provided in the textbook.

Calculating Probabilities

To see how $P(q_i)$ can be computed from functions $\psi(x)$ and $\phi_i(x)$, we should first observe that

$$\langle \psi(x), \phi_i(x) \rangle = \left\langle \sum_j \alpha_j \phi_j(x), \phi_i(x) \right\rangle \quad (17)$$

Recalling that

$$\left\langle \sum_i \alpha_i f_i(x), g(x) \right\rangle = \sum_i \alpha_i^* \langle f_i(x), g(x) \rangle \quad (18)$$

expression (17) can be rewritten as

$$\langle \psi(x), \phi_i(x) \rangle = \sum_j \alpha_j^* \langle \phi_j(x), \phi_i(x) \rangle \quad (19)$$

Since functions $\{\phi_i(x)\}$ constitute an orthonormal basis, (19) becomes

$$\langle \psi(x), \phi_i(x) \rangle = \alpha_i^* \langle \phi_i(x), \phi_i(x) \rangle = \alpha_i^* \quad (20)$$

which allows us to compute $P(q_i)$ as

$$P(q_i) = |\alpha_i|^2 = |\alpha_i^*|^2 = |\langle \psi(x), \phi_i(x) \rangle|^2 \quad (21)$$

This relationship is very useful, because it provides us with a simple way to determine the probabilities of all possible outcomes if function $\psi(x)$ (i.e., the state of the particle) is known.

Quantum Measurements

Quantum measurements are always performed *with respect to a given basis*, which is associated with the physical quantity that we are interested in. If we have a particle in state ψ , for example, and choose $\{\psi_0, \psi_1\}$ as our measurement basis, then we will invariably find it in one of these two states after the observation is made. The probabilities of the possible outcomes can be obtained by expressing ψ as

$$\psi = \alpha_0 \psi_0 + \alpha_1 \psi_1 \quad (22)$$

and computing $|\alpha_0|^2$ and $|\alpha_1|^2$.

If we were to choose a different measurement basis (say, $\{\varphi_0, \varphi_1\}$), the situation would change, and we would be able to record only states φ_0 and φ_1 . To determine the corresponding probabilities, we would have to express ψ as

$$\psi = \beta_0 \varphi_0 + \beta_1 \varphi_1 \quad (23)$$

and compute $|\beta_0|^2$ and $|\beta_1|^2$.

In quantum computing, the measurement basis typically consists of states such as “spin up” and “spin down” or high and low energy levels, which have an obvious physical interpretation. For this reason, the corresponding functions $\{\psi_0, \psi_1\}$ are commonly referred to as the “standard” basis. Quantum mechanics asserts, however, that *any* orthonormal basis can be used for this purpose, so we need to examine what would change if we were to pick a basis that is different from the “standard” one.

To see this, suppose that basis $\{\psi_0, \psi_1\}$ corresponds to states of definite spin, but that we would like to make a measurement in basis $\{\varphi_0, \varphi_1\}$ whose constituents φ_0 and φ_1 needn't necessarily have an obvious physical meaning. A convenient way to distinguish between these two scenarios is to assume that the state of the system prior to the measurement is described by wave function ψ , whose representations in bases $\{\psi_0, \psi_1\}$ and $\{\varphi_0, \varphi_1\}$ are given by expressions (22) and (23), respectively. The question then becomes whether one can perform the measurement in such a way that the possible outcomes are states φ_0 and φ_1 .

To show how this can be done, let us introduce a *self-adjoint unitary* operator \hat{U} which is defined by

$$\hat{U}\varphi_0 = \psi_0 \quad (24)$$

and

$$\hat{U}\varphi_1 = \psi_1 \quad (25)$$

Note that this is a perfectly legitimate way to define \hat{U} , since we know how it acts on each basis function.

When this operator is applied to ψ , we obtain a new function ξ which can be expressed as

$$\xi = \hat{U}\psi = \beta_0\hat{U}\varphi_0 + \beta_1\hat{U}\varphi_1 = \beta_0\psi_0 + \beta_1\psi_1 \quad (26)$$

This transformation is useful for our purposes because it allows us to make a measurement in the “standard” basis $\{\psi_0, \psi_1\}$, and subsequently convert the result to basis $\{\varphi_0, \varphi_1\}$.

Before we describe how this process works, we should observe that expression (26) allows for two possible outcomes, ψ_0 and ψ_1 , whose probabilities are $|\beta_0|^2$ and $|\beta_1|^2$, respectively. It is important to recognize that these probabilities are *exactly the same* as the ones in equation (23), which relate to φ_0 and φ_1 . This implies that we can switch from one measurement basis to another without affecting the final result.

With that in mind, let us now consider what happens if the particle is in state ξ , and we perform a measurement in the standard basis. If we register state ψ_0 , we can easily recover φ_0 by applying operator \hat{U} to function ψ_0 , since

$$\hat{U}\psi_0 = \hat{U}(\hat{U}\varphi_0) = \hat{U}^2\varphi_0 = \varphi_0 \quad (27)$$

(recall that $\hat{U}^{-1} = \hat{U}$ for unitary self-adjoint operators). If the measurement happens to produce state ψ_1 , we can obtain φ_1 in a similar manner, using the fact that $\hat{U}\psi_1 = \varphi_1$.

From this, we can conclude that states φ_0 and φ_1 can be measured *indirectly*, using an appropriately chosen operator that converts the result from one basis to the other. A schematic representation of this procedure is shown in Fig. 1.

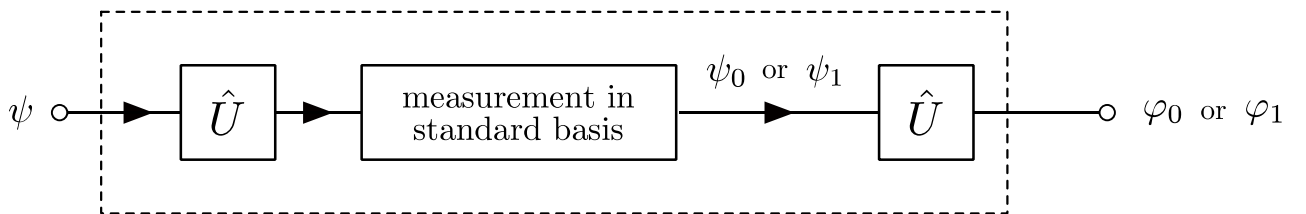


Figure 1: A general framework for quantum measurements.

Composite States and Quantum Entanglement

When two or more quantum particles form a larger system, their wave functions combine in a way that allows us to treat them as a unified whole. To understand what this means, let us consider a simple two particle system whose constituents were described by wave functions $\psi_a(x)$ and $\psi_b(x)$ prior to the interaction. We will assume that ψ_a is expressed as

$$\psi_a(x) = \sum_i \alpha_i \phi_i(x) \quad (28)$$

where functions $\{\phi_1, \phi_2, \dots\}$ represent an orthonormal basis in functional space S_1 , and are associated with measurable values of some physical quantity q . We will do something similar for ψ_b as well, and assume that it is expressed as

$$\psi_b(x) = \sum_i \beta_i \xi_i(x) \quad (29)$$

where functions $\{\xi_1, \xi_2, \dots\}$ are an orthonormal basis in functional space S_2 , and are associated with measurable values of some physical quantity p .

When these two particles interact, quantum mechanics postulates that the state of the resulting system can be described by a function that belongs to space $S_1 \otimes S_2$, whose elements have the form

$$\Psi = \sum_{i,j} \sigma_{ij} (\phi_i \otimes \xi_j) = \sum_{i,j} \sigma_{ij} \Psi_{ij} \quad (30)$$

In this expression, σ_{ij} represent constant coefficients and $\Psi_{ij} = \phi_i \otimes \xi_j$ denotes the *tensor product* of functions $\phi_i(x)$ and $\xi_j(x)$.

This definition implies (among other things) that functions $\Psi_{ij} = \phi_i \otimes \xi_j$ constitute an *orthonormal basis* in $S_1 \otimes S_2$, which is something that we will use extensively. These functions have a straightforward physical interpretation, because $\Psi_{ij} = \phi_i \otimes \xi_j$ corresponds to the case when the first particle is in state ϕ_i and the second one in state ξ_j . When a simultaneous measurements is performed on both particles, the composite system will necessarily collapse into one of these states, and the probabilities of the possible outcomes can be computed as $|\sigma_{ij}|^2$.

What do we mean by a “tensor product” of two functions? For our purposes, it will suffice to define it as a mathematical operation that has the following three properties.

Property 1. If functions ψ , φ and η belong to the same space S and α and β are complex numbers, the following identities hold true:

$$(\alpha\psi + \beta\varphi) \otimes \eta = (\alpha\psi) \otimes \eta + (\beta\varphi) \otimes \eta \quad (31)$$

$$\psi \otimes (\alpha\varphi + \beta\eta) = \psi \otimes (\alpha\varphi) + \psi \otimes (\beta\eta) \quad (32)$$

$$\alpha(\psi \otimes \varphi) = (\alpha\psi) \otimes \varphi = \psi \otimes (\alpha\varphi) \quad (33)$$

Property 2. Suppose that functions ψ_1 and φ_1 belong to space S_1 , and that functions ψ_2 and φ_2 belong to space S_2 . The scalar product of functions $\psi_1 \otimes \psi_2$ and $\varphi_1 \otimes \varphi_2$ (both of which belong to space $S = S_1 \otimes S_2$) is defined as

$$\langle \psi_1 \otimes \psi_2, \varphi_1 \otimes \varphi_2 \rangle = \langle \psi_1, \varphi_1 \rangle_{S_1} \cdot \langle \psi_2, \varphi_2 \rangle_{S_2} \quad (34)$$

Property 3. The scalar product in space $S = S_1 \otimes S_2$ satisfies

$$\begin{aligned} \langle \psi_1 \otimes \psi_2, \alpha(\varphi_1 \otimes \varphi_2) + \beta(\varphi_3 \otimes \varphi_4) \rangle &= \alpha \langle \psi_1 \otimes \psi_2, \varphi_1 \otimes \varphi_2 \rangle + \\ &+ \beta \langle \psi_1 \otimes \psi_2, \varphi_3 \otimes \varphi_4 \rangle \end{aligned} \quad (35)$$

and

$$\begin{aligned} \langle \alpha(\psi_1 \otimes \psi_2) + \beta(\psi_3 \otimes \psi_4), \varphi_1 \otimes \varphi_2 \rangle &= \alpha^* \langle \psi_1 \otimes \psi_2, \varphi_1 \otimes \varphi_2 \rangle + \\ &+ \beta^* \langle \psi_3 \otimes \psi_4, \varphi_1 \otimes \varphi_2 \rangle \end{aligned} \quad (36)$$

The following example illustrates how Property 1 is used in practice.

Example 1. Suppose that

$$\psi_a = \alpha_0 \psi_0 + \alpha_1 \psi_1 \quad (37)$$

and

$$\psi_b = \beta_0 \psi_0 + \beta_1 \psi_1 \quad (38)$$

What will the tensor product of these two functions look like? According to (31) and (32), function

$$\psi_a \otimes \psi_b = (\alpha_0 \psi_0 + \alpha_1 \psi_1) \otimes (\beta_0 \psi_0 + \beta_1 \psi_1) \quad (39)$$

can be expanded as

$$\begin{aligned} \psi_a \otimes \psi_b &= (\alpha_0 \psi_0 + \alpha_1 \psi_1) \otimes (\beta_0 \psi_0) + (\alpha_0 \psi_0 + \alpha_1 \psi_1) \otimes (\beta_1 \psi_1) = \\ &= (\alpha_0 \psi_0) \otimes (\beta_0 \psi_0) + (\alpha_1 \psi_1) \otimes (\beta_0 \psi_0) + (\alpha_0 \psi_0) \otimes (\beta_1 \psi_1) + (\alpha_1 \psi_1) \otimes (\beta_1 \psi_1) \end{aligned} \quad (40)$$

Using (33), this becomes

$$\psi_a \otimes \psi_b = \alpha_0 \beta_0 (\psi_0 \otimes \psi_0) + \alpha_0 \beta_1 (\psi_0 \otimes \psi_1) + \alpha_1 \beta_0 (\psi_1 \otimes \psi_0) + \alpha_1 \beta_1 (\psi_1 \otimes \psi_1) \quad (41)$$

Our next example shows how the properties of tensor products can be used to calculate the probabilities of different measurement outcomes.

Example 2. Suppose that S_1 and S_2 are *identical* two dimensional spaces, and that functions ψ_0 and ψ_1 represent the chosen orthonormal basis in both of them. We will additionally assume that our system consists of two particles whose wave functions belong to spaces S_1 and S_2 , respectively.

When these two particles interact, expression (30) tells us that the state of the the overall system can be described by function

$$\Psi = \sigma_{00}(\psi_0 \otimes \psi_0) + \sigma_{01}(\psi_0 \otimes \psi_1) + \sigma_{10}(\psi_1 \otimes \psi_0) + \sigma_{11}(\psi_1 \otimes \psi_1) \quad (42)$$

Setting $\Psi_{00} = \psi_0 \otimes \psi_0$, $\Psi_{01} = \psi_0 \otimes \psi_1$, $\Psi_{10} = \psi_1 \otimes \psi_0$ and $\Psi_{11} = \psi_1 \otimes \psi_1$, expression (42) can be rewritten in a more compact form as

$$\Psi = a_0 \Psi_{00} + a_1 \Psi_{01} + a_2 \Psi_{10} + a_3 \Psi_{11} \quad (43)$$

where $a_0 = \sigma_{00}$, $a_1 = \sigma_{01}$, $a_2 = \sigma_{10}$ and $a_3 = \sigma_{11}$. This type of representation is standard in quantum computing, and we will use it in all subsequent discussions.

Since functions Ψ_{00} , Ψ_{01} , Ψ_{10} and Ψ_{11} constitute an orthonormal basis in space $S = S_1 \otimes S_2$, the coefficients a_0 , a_1 , a_2 and a_3 that appear in expression (43) can be associated

with the probabilities of different outcomes. To illustrate how these probabilities should be computed, suppose that we are interested in determining the likelihood that state Ψ_{10} will be observed when a measurement is made on both particles. If we form a scalar product that involves Ψ and basis function Ψ_{10} , we obtain

$$\langle \Psi_{10}, \Psi \rangle = a_0 \langle \Psi_{10}, \Psi_{00} \rangle + a_1 \langle \Psi_{10}, \Psi_{01} \rangle + a_2 \langle \Psi_{10}, \Psi_{10} \rangle + a_3 \langle \Psi_{10}, \Psi_{11} \rangle \quad (44)$$

by virtue of Property 3. Observing that all scalar products in this expression are zero (except for $\langle \Psi_{10}, \Psi_{10} \rangle$, which equals 1), (44) reduces to

$$\langle \Psi_{10}, \Psi \rangle = a_2 \quad (45)$$

This means that the probability of registering state Ψ_{10} can be computed as $|\langle \Psi_{10}, \Psi \rangle|^2$.

Remark 2. The ideas that we introduced in this example can be easily extended to systems of n interacting particles, in which case Ψ has the general form

$$\Psi = a_0 \Psi_{00\dots 0} + a_1 \Psi_{00\dots 1} + \dots + a_{2^n-1} \Psi_{11\dots 1} \quad (46)$$

and coefficients a_i satisfy

$$\sum_{i=0}^{2^n-1} |a_i|^2 = 1 \quad (47)$$

(since they represent probabilities). The fact that function Ψ has 2^n components in this case suggests that the number of measurable states grows *exponentially* as the system size increases, which is a very important property from the standpoint of quantum computing.

Quantum Entanglement

An interesting question related to the structure of space $S = S_1 \otimes S_2$ is whether *all* of its elements can be represented as

$$\Psi = \psi_a \otimes \psi_b \quad (48)$$

where $\psi_a \in S_1$ and $\psi_b \in S_2$. On first glance, this seems like a reasonable assumption, since one would expect that the states of the overall system can be expressed in terms of the states of its constituents (as is the case in classical physics). It turns out, however, that arguments of this sort do not apply to quantum mechanics.

To see why, let us consider functions ψ_a and ψ_b in their most general form, which is

$$\psi_a = \alpha_0 \psi_0 + \alpha_1 \psi_1 \quad (49)$$

and

$$\psi_b = \beta_0 \psi_0 + \beta_1 \psi_1 \quad (50)$$

As we showed in Example 1, the tensor product

$$\psi_a \otimes \psi_b = (\alpha_0 \psi_0 + \alpha_1 \psi_1) \otimes (\beta_0 \psi_0 + \beta_1 \psi_1) \quad (51)$$

can then be expressed as

$$\Psi = \alpha_0 \beta_0 \Psi_{00} + \alpha_0 \beta_1 \Psi_{01} + \alpha_1 \beta_0 \Psi_{10} + \alpha_1 \beta_1 \Psi_{11} \quad (52)$$

In order for (52) to match (43) for a given set of coefficients $\{a_0, a_1, a_2, a_3\}$, the following four conditions must be satisfied:

$$\alpha_0\beta_0 = a_0 \quad (53)$$

$$\alpha_0\beta_1 = a_1 \quad (54)$$

$$\alpha_1\beta_0 = a_2 \quad (55)$$

$$\alpha_1\beta_1 = a_3 \quad (56)$$

Note, however, that dividing (53) by (54) and (55) by (56) produces

$$\frac{\beta_0}{\beta_1} = \frac{a_0}{a_1} \quad (57)$$

and

$$\frac{\beta_0}{\beta_1} = \frac{a_2}{a_3} \quad (58)$$

This means that equations (53) - (56) have a solution only if

$$\frac{a_0}{a_1} = \frac{a_2}{a_3} \quad (59)$$

Since condition (59) does not hold for all possible choices of coefficients $\{a_0, a_1, a_2, a_3\}$, there will obviously be many functions in space S that *cannot* be represented in the form (46). Such states are said to be *entangled*, because they are not reducible to the states of individual particles.

Operators in Composite Spaces

How are operators in space $S = S_1 \otimes S_2$ related to operators in spaces S_1 and S_2 ? The following definition provides a simple answer to this question.

Definition 1. Let \hat{A}_1 and \hat{A}_2 be linear operators in spaces S_1 and S_2 , respectively. We can then define operator $\hat{A}_1 \otimes \hat{A}_2$ in space $S = S_1 \otimes S_2$ as

$$\left(\hat{A}_1 \otimes \hat{A}_2\right)(\psi \otimes \varphi) = (\hat{A}_1\psi) \otimes (\hat{A}_2\varphi) \quad (60)$$

Since operator $\hat{A}_1 \otimes \hat{A}_2$ is linear, applying it to a composite function such as the one in (30) produces

$$\left(\hat{A}_1 \otimes \hat{A}_2\right)\Psi = \sum_{i,j} \sigma_{ij}(\hat{A}_1\phi_i) \otimes (\hat{A}_2\xi_j) \quad (61)$$

An important implication of this property is that we can simultaneously apply *different* operators to different particles in the system. This will prove to be very useful, because it allows us to efficiently manipulate the constituents of a multiparticle system. We could choose, for example, to perform a measurement on some of them but not on others, or we could transform the state of each particle in a different way.

Remark 3. If we want to leave particle i undisturbed, operator \hat{A}_i should be chosen as $\hat{A}_i = \hat{I}$, where \hat{I} is the identity operator.

Measurements on Multiparticle Systems

Suppose that we have a two particle system whose state is described by function

$$\Psi = a_0\Psi_{00} + a_1\Psi_{01} + a_2\Psi_{10} + a_3\Psi_{11} \quad (62)$$

where all a_i are nonzero. As we noted earlier, coefficients $|a_0|^2$, $|a_1|^2$, $|a_2|^2$ and $|a_3|^2$ can be interpreted as the probabilities of the four possible outcomes when *both* particles are measured simultaneously in basis $\{\psi_0, \psi_1\}$. To illustrate this point a bit more clearly, suppose that function Ψ collapsed into basis state Ψ_{10} after we performed such a measurement. This is equivalent to saying that the first particle was found in state ψ_1 , and the second one in state ψ_0 . The likelihood that this particular scenario will materialize is $|a_2|^2$, since a_2 is the coefficient next to Ψ_{10} in (62).

What would happen if we decided to perform a measurement *on just one of the particles* (say, the first one)? In order to see that, we should first observe that any function of the form (62) can be expressed as

$$\Psi = \psi_0 \otimes (a_0\psi_0 + a_1\psi_1) + \psi_1 \otimes (a_2\psi_0 + a_3\psi_1) \quad (63)$$

If we rewrite (63) as

$$\begin{aligned} \Psi = & \sqrt{|a_0|^2 + |a_1|^2} \cdot \psi_0 \otimes \left[\frac{a_0}{\sqrt{|a_0|^2 + |a_1|^2}} \cdot \psi_0 + \frac{a_1}{\sqrt{|a_0|^2 + |a_1|^2}} \cdot \psi_1 \right] + \\ & + \sqrt{|a_2|^2 + |a_3|^2} \cdot \psi_1 \otimes \left[\frac{a_2}{\sqrt{|a_2|^2 + |a_3|^2}} \cdot \psi_0 + \frac{a_3}{\sqrt{|a_2|^2 + |a_3|^2}} \cdot \psi_1 \right] \end{aligned} \quad (64)$$

and set

$$\begin{aligned} \rho_0 &= \sqrt{|a_0|^2 + |a_1|^2} \\ \rho_1 &= \sqrt{|a_2|^2 + |a_3|^2} \end{aligned} \quad (65)$$

together with

$$\begin{aligned} b_0 &= \frac{a_0}{\sqrt{|a_0|^2 + |a_1|^2}} \\ b_1 &= \frac{a_1}{\sqrt{|a_0|^2 + |a_1|^2}} \\ b_2 &= \frac{a_2}{\sqrt{|a_2|^2 + |a_3|^2}} \\ b_3 &= \frac{a_3}{\sqrt{|a_2|^2 + |a_3|^2}} \end{aligned} \quad (66)$$

expression (62) becomes

$$\Psi = \rho_0\Phi_0 + \rho_1\Phi_1 \quad (67)$$

where

$$\Phi_0 = \psi_0 \otimes (b_0\psi_0 + b_1\psi_1) \quad (68)$$

and

$$\Phi_1 = \psi_1 \otimes (b_2\psi_0 + b_3\psi_1) \quad (69)$$

It is easily verified that coefficients $\rho_0, \rho_1, b_0, b_1, b_2$ and b_3 satisfy

$$|\rho_0|^2 + |\rho_1|^2 = 1 \quad (70)$$

$$|b_0|^2 + |b_1|^2 = 1 \quad (71)$$

and

$$|b_2|^2 + |b_3|^2 = 1 \quad (72)$$

so we can interpret them as probabilities. It can also be shown that Φ_0 or Φ_1 are normalized and are orthogonal to each other, which means that they constitute an orthonormal basis in $S_1 \otimes S_2$ (a proof of this property is provided in the textbook)

Expression (67) tells us that the system will collapse into state Φ_0 or Φ_1 when a measurement is performed only on particle 1, and that the probabilities of these two outcomes are $|\rho_0|^2$ and $|\rho_1|^2$, respectively. These two states can be represented in more compact form as

$$\Phi_0 = b_0\Psi_{00} + b_1\Psi_{01} \quad (73)$$

and

$$\Phi_1 = b_2\Psi_{10} + b_3\Psi_{11} \quad (74)$$

which is a common practice in quantum computing.

To see what happens when a second measurement is made, let us assume that we found particle 1 in state ψ_0 once the initial measurement has been performed. At this point, the state of the overall system will be

$$\Phi_0 = b_0\Psi_{00} + b_1\Psi_{01} \quad (75)$$

which implies that the system will be in state Ψ_{00} or Ψ_{01} after a second measurement. The first scenario corresponds to finding particle 2 in state ψ_0 , and the second one corresponds to the case when particle 2 is in state ψ_1 . The probabilities of these outcomes are $|b_0|^2$ and $|b_1|^2$, respectively.

Similarly, if we happen to find particle 1 in state ψ_1 , the overall system will collapse into state

$$\Phi_1 = b_2\Psi_{10} + b_3\Psi_{11} \quad (76)$$

which tells us that a subsequent measurement on particle 2 could produce either ψ_0 or ψ_1 (with probabilities $|b_2|^2$ and $|b_3|^2$, respectively). Since the state of particle 2 remains *undetermined* in both scenarios, we can conclude that it will be in a state of superposition until a second observation is made.

Measurements on Bell States

In the scenario that we just considered, successive measurements on the two particles are obviously *independent*, because we don't know what state particle 2 will be in until the second measurement is performed. The question that we now need to ask is whether this is always the case. One would intuitively expect that it is, but it turns out that there are situations when the second measurement is actually influenced by the first one.

A typical example of this sort are so-called *Bell states*, which have the form

$$\Phi_{00} = \frac{1}{\sqrt{2}} (\Psi_{00} + \Psi_{11}) \quad (77)$$

$$\Phi_{01} = \frac{1}{\sqrt{2}} (\Psi_{01} + \Psi_{10}) \quad (78)$$

$$\Phi_{10} = \frac{1}{\sqrt{2}} (\Psi_{00} - \Psi_{11}) \quad (79)$$

$$\Phi_{11} = \frac{1}{\sqrt{2}} (\Psi_{01} - \Psi_{10}) \quad (80)$$

These states play an important role in quantum mechanics, and can be produced by certain types of quantum circuits (which we will describe shortly).

It is not difficult to show that Φ_{00} , Φ_{01} , Φ_{10} and Φ_{11} represent *entangled* states. To demonstrate this, let us consider function Φ_{00} and examine whether it can be decomposed as

$$\Phi_{00} = \psi_a \otimes \psi_b \quad (81)$$

where

$$\psi_a = \alpha_0 \psi_0 + \alpha_1 \psi_1 \quad (82)$$

and

$$\psi_b = \beta_0 \psi_0 + \beta_1 \psi_1 \quad (83)$$

Since

$$\psi_a \otimes \psi_b = \alpha_0 \beta_0 \Psi_{00} + \alpha_0 \beta_1 \Psi_{01} + \alpha_1 \beta_0 \Psi_{10} + \alpha_1 \beta_1 \Psi_{11} \quad (84)$$

matching (77) and (84) would require that

$$\alpha_0 \beta_1 = 0 \quad (85)$$

$$\alpha_1 \beta_0 = 0 \quad (86)$$

$$\alpha_0 \beta_0 = 1/\sqrt{2} \quad (87)$$

$$\alpha_1 \beta_1 = 1/\sqrt{2} \quad (88)$$

Note, however, that condition (85) implies either $\alpha_0 = 0$ or $\beta_1 = 0$. Consequently, (87) and (88) *cannot be satisfied simultaneously*. Proceeding in a similar manner, we can show that this conclusion applies to states Φ_{01} , Φ_{10} and Φ_{11} as well.

If a two particle system is in Bell state

$$\Phi_{00} = \frac{1}{\sqrt{2}} \Psi_{00} + \frac{1}{\sqrt{2}} \Psi_{11} \quad (89)$$

what will happen when we perform a measurement on the first particle? In that case, function Φ_{00} will collapse into either Ψ_{00} or Ψ_{11} , since these two states are the only available possibilities. Note, however, that both outcomes automatically place the second particle in the *same* state as the first one, although it was not disturbed in any way. What this tells us is that measurements on individual particles needn't always be independent, and can affect each other directly if the system is in a particular type of state. This unusual (and counterintuitive) property inspired Einstein to formulate his famous EPR paradox, and refer to quantum entanglement as “spooky action at a distance”.