Chapter 3.
Basic Concepts of Quantum Theory

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In the previous chapters we develop the necessary mathematical apparatus and presented the terminology that will be used throughout this course. It is now time to open the door and introduce the basic concepts and tools of the quantum theory to continue our study of quantum computing.

At the beginning of 1900 the classical physics dominate in the scene with its double-pronged approach: particle and wave. Matter is considered to be composed of macroscopic particles, and, in contrast, the light is thought of as continuous electromagnetic waves propagating in space. The dichotomy - particle versus waves - was proven false by several groundbreaking experimental discoveries. The photoelectric effect observed by Hertz in 1887 is the emission of electrons when light falls on a material. According to classical electromagnetic theory, this effect can be attributed to the transfer of energy from the light to an electron. However, the classical electromagnetic theory fails to explain why the energy of emitted electron does not depend of the intensity of the light. To make sense of the fact that light can eject electrons even if its intensity is low, Albert Einstein proposed that a beam of light is not a wave propagating through space, but rather a collection of discrete wave packets called later photons, each with energy hf. This shed light on Max Planck's previous discovery of the Planck relation $E = hf$ linking energy E and frequency f via the factor h is known as the Planck constant, arising from quantization of energy. French physicist Louis De Broglie formulated hypothesis that predicts that a beam of subatomic particle hitting the slit diffract following a wave-like pattern, entirety similar to the diffraction pattern of the light itself. In 1927 George Thomson passed a beam of electrons through a thin metal film and observed the predicted interference patterns. Independently around the same time Davisson and Germer guided their beam through a crystalline grid and observed the interference patterns for electrons. Therefore experimentally it was confirmed that particle diffract following a wave-like pattern. Further experimental evidence from many quarters accumulated over time strongly suggesting that classical particle and wave approach must be replaced by a new theory of the microscopic world in which both matter and light manifest a new particle-like and wave-like behavior. Time was ripe for the conceptual framework of quantum mechanics.

Let us formulate the main postulates of quantum mechanics.

1) Microscopic system can be described by the wave function or state function $\Psi(\mathbf{r},t)$. The physical meaning has $|\Psi(\mathbf{r},t)|^2$, which is the probability of the state and $|\Psi(\mathbf{r},t)|^2$ is integrable function. The wave function $\Psi(\mathbf{r},t)$ is

i) generally a complex function;

ii) continues function;

iii) differentiable function;

iv) the derivative of the wave function is the continue function.

An arbitrary quantum state $\Psi(\mathbf{r},t)$ we denote using Dirac notation as $|\psi\rangle$.

2) Principle of superposition.

If he quantum system can be in the state $\Psi_1(\mathbf{r},t)$ and in state $\Psi_2(\mathbf{r},t)$ than means the system can be in the state $\Psi(\mathbf{r},t) = c_1\Psi_1(\mathbf{r},t) + c_2\Psi_2(\mathbf{r},t)$, where c_1 and c_2 are any complex numbers known as a complex amplitudes. In Dirac notations $|\psi\rangle = c_1 |\psi\rangle + c_2 |\psi\rangle$. The latter means that the state $\Psi(\mathbf{r},t)$ is the linear combination of the the states $\Psi_1(\mathbf{r},t)$ and $\Psi_2(\mathbf{r},t)$. Moreover, from principle of superposition it is follow that state function $\Psi_1(\mathbf{r},t)$ must satisfy the linear equation.

3) To each physical quantity corresponds the operator: $A \to \widehat{A}$. The average value of the operator is the physical value that can be measured experimentally. Therefore this value must be real.

$$\langle A\rangle = \int \Psi^* \widehat{A}\Psi d\mathbf{r}dt \equiv \langle\psi| \widehat{A} |\psi\rangle . \tag{1}$$

From postulate Average Value immediately follows that operator $\widehat{A}$ should be the Hermitian operator: $\langle\psi| \widehat{A} |\psi\rangle = \langle\psi| \widehat{A}^\dagger |\psi\rangle$.

4) When the operator $\widehat{A}$ acts on the state function Ψ it transforms this state to a new state $\Psi^{'}$ so that $\Psi^{'} = \widehat{A}\Psi$. The following two conditions must be satisfied to keep the principle of superposition: $\widehat{A}c\Psi = c\widehat{A}\Psi$ and $\widehat{A}\Psi = \widehat{A}c_1\Psi_1 + \widehat{A}c_2\Psi_2$ for any complex numbers c, c_1, and c_2.

By introducing a computation basis 2^n ket vectors as

$$\begin{aligned}
|x_0\rangle &= \begin{bmatrix} 1 & 0 & ... & 0 \end{bmatrix}^T && (2)\\
|x_1\rangle &= \begin{bmatrix} 0 & 1 & ... & 0 \end{bmatrix}^T && (3)\\
&...\\
|x_{n-1}\rangle &= \begin{bmatrix} 0 & 0 & ... & 1 \end{bmatrix}^T
\end{aligned}$$

based on the principle of superposition an arbitrary state $|\psi\rangle$ can be presented in this basis as

$$|\psi\rangle = c_0 |x_0\rangle + c_1 |x_1\rangle + ...c_{n-1} |x_{n-1}\rangle . \tag{4}$$

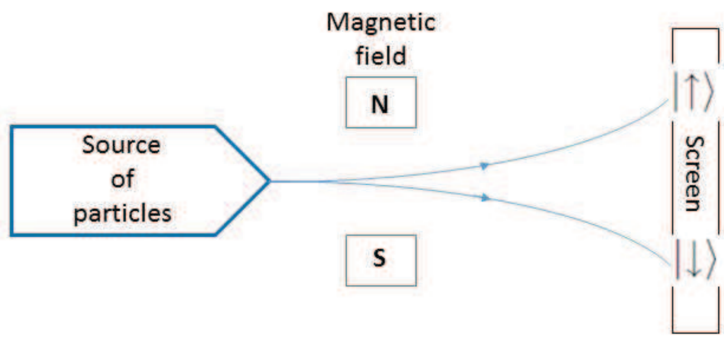

Figure 1: (Color online) The schematics of the Stern-Gerlach experiment.

where $c_0, c_1, ...c_{n-1}$ are the amplitude of the states. Thus, we say that the state $|\psi\rangle$ is a superposition of the basis states and represents the particle as being simultaneously in all states $|x_0\rangle, |x_1\rangle, ... |x_{n-1}\rangle$. The complex numbers $c_0, c_1, ...c_{n-1}$ tell us precisely which superposition the particle is currently in. The norm square of the complex number c_i, $|c_i|^2$, gives the probability that after observing the particle, it will be detected in state $|x_i\rangle$ Thus , every state of the system can be represented by an elements of complex C^n as

$$|\psi\rangle \longmapsto \begin{bmatrix} c_0, & c_1, & ... & c_{n-1} \end{bmatrix}^T. \tag{5}$$

Let us now introduce the property of subatomic system called spin. As it turns out, spin will play a major role in quantum computing because it is a prototypical way to implement quantum bit or qubit. What is spin? Two types of experimental evidence which arose in the 1920s suggested an additional property of the electron. One was the closely spaced splitting of the hydrogen spectral lines, called fine structure. The other was the Stern-Gerlach experiment which showed in 1922 that a beam of silver atoms directed through a nonhomogeneous magnetic field would be forced into two beams and observed their deflection. Both of these experimental situations were consistent with the possession of an intrinsic angular momentum and a magnetic moment by individual electrons. Classically this could occur if the electron were a spinning ball of charge, and this property was called electron spin. The results show that particles possess an intrinsic angular momentum that is closely analogous to the angular momentum of a classically spinning object, but that takes only certain quantized values. If we consider the beam of electrons which goes through a nonhomegeneous magnetic field oriented in certain direction it happens that the field splits the beam into two streams with opposite spins. Certain electrons will be found spinning in one way and certain others the opposite way. With respect of classical spinning top there are two striking differences. First, the electron has no any internal structure and just a charged point particle. It acts as a spinning top but it is no top. Therefore, spin is a new property of the electron with no classical analog. Secondly, which is quite surprisingly, electrons can be found in either in the top of the screen or at the bottom, none between. We did not prepared the "spinning" electrons in any way before letting them interact with magnetic field. The latter means that this property electron has by itself.

For each given direction in space there are only two basic spin states. For the vertical axis, these states have name: spin up $|\uparrow\rangle$ and spin down $|\downarrow\rangle$. Therefore the generic state will then be a superposition of up and down states

$$|\psi\rangle = c_0 |\uparrow\rangle + c_1 |\downarrow\rangle . \tag{6}$$

In this expression c_0 is the amplitude of finding the particle in the spin up state and similarly c_2 is the amplitude of finding the particle in the spin down state.

We introduce the inner product as an abstract mathematical idea. The physical meaning of the inner product is the following: the inner product of the state space gives us a tool to compute *a transition amplitude,* that are the complex numbers, which in turn will enable to determine how likely the state of the system before the specific measurement (*initial state*) will change to another state (*final state*), after measurement has been carried out. Graphically we can present the inner product as it is shown below

$$\langle\psi\,|\phi\rangle$$

$$|\psi\rangle \qquad\qquad\qquad\qquad |\phi\rangle$$

Let say in the initial state system is described by Eq. (4) which is expressed in the basis $\{|x_0\rangle, |x_1\rangle, ... |x_{n-1}\rangle\}$. It is easy to show that the inner product of $|x_i\rangle$ and $|\psi\rangle$ is $c_i = \langle x_i\,|\psi\rangle$ and that $|c_0|^2 + |c_1|^2 + |c_2|^2 + ... + |c_{n-1}|^2 = 1$. Thus it is obvious to read Eq. (4) in the following way: each $|c_i|^2$ is a probability of transition from the initial state $|\psi\rangle$ to the final state $|x_i\rangle$.

$$
|\psi\rangle \qquad
\begin{array}{c}
\langle x_0 \, |\psi\rangle \\
\langle x_1 \, |\psi\rangle \\
\\
\\
\langle x_{n-2} \, |\psi\rangle \\
\langle x_{n-1} \, |\psi\rangle
\end{array}
\qquad
\left.
\begin{array}{c}
|x_0\rangle \\
|x_1\rangle \\
. \\
. \\
. \\
|x_{n-2}\rangle \\
|x_{n-1}\rangle
\end{array}
\right\} 2^n,
$$

We introduce the tensor product as an abstract mathematical idea as well and now let us provide the physical meaning of the tensor product. For this purpose we consider the system of two particles one in basis $\{|x_0\rangle, |x_1\rangle, ... |x_{n-1}\rangle\}$ and the other in basis $\{|y_0\rangle, |y_1\rangle, ... |y_{m-1}\rangle\}$. Let us find the way of assembling more complex quantum system staring from simpler ones. This procedure lies in very core of modern quantum physics and enable to model multiparticle quantum system. First, let introduce the definition. Assume we have two independent quantum system Q_1 and Q_2 represented by the Hilbert spaces H_1 and H_2, respectively. The quantum system Q obtained by merging Q_1 and Q_2 will have a state space H, which is defined by the tensor product $H = H_1 \otimes H_2$. Therefore, one can build the assemble of two particles. If $n = 2$ and $m = 2$ we have $\{|x_0\rangle, |x_1\rangle\}$ and $\{|y_0\rangle, |y_1\rangle\}$ and we deal with the state space C^4 with basis

$$\{|x_0\rangle \otimes |y_0\rangle, |x_0\rangle \otimes |y_1\rangle, |x_1\rangle \otimes |y_0\rangle, |x_1\rangle \otimes |y_1\rangle\}. \tag{7}$$

Let us consider the state vector for the two particle system in this basis

$$|\psi\rangle = i\,|x_0\rangle \otimes |y_0\rangle + (1-i)\,|x_0\rangle \otimes |y_1\rangle + 2\,|x_1\rangle \otimes |y_0\rangle + (-1-i)\,|x_1\rangle \otimes |y_1\rangle. \tag{8}$$

The norm of this state vector can be calculated using the corresponding amplitude: $||\psi\rangle|^2 = |i|^2 + |1-i|^2 + |2|^2 + |-1-i|^2 = 1+2+4+2 = 9$. Now let's determine the probability to find two particles one in the state $|x_1\rangle$ and the other in the state $|y_1\rangle$,which is $\frac{|-1-i|^2}{||\psi\rangle|^2} = \frac{2}{9} = 0.2222$, while the probability to find two particles one in the state $|x_0\rangle$ and the other in the state $|y_0\rangle$ is $\frac{|2|^2}{||\psi\rangle|^2} = \frac{4}{9} = 0.4444$. The same machinery can be applied to any quantum system. This approach enable to us to assemble as many system as we like, because the tensor product of vector space is associate, so we can progressively build larger and larger systems. Finally, we can conclude that the physical meaning of the tensor product is ability assembling the quantum system.

Now we are ready to introduce the puzzling surprise of quantum mechanics: *entanglement.* The basic state of the assembled system is just a tensor product of the basic states of its constituents. However, not always each generic state vector can be rewritten a the tensor product of two states, one coming from the first quantum subsystem and the other one from the second quantum system. We will illustrate this using the following example. The state $|\psi\rangle = |x_0\rangle \otimes |y_0\rangle + |x_1\rangle \otimes |y_1\rangle$ can be rewritten as $|\psi\rangle = 1\,|x_0\rangle \otimes |y_0\rangle + 0\,|x_0\rangle \otimes |y_1\rangle + 0\,|x_1\rangle \otimes |y_0\rangle + 1\,|x_1\rangle \otimes |y_1\rangle$. Let us see if this state comes from most general representation of the first particle state $|\phi_1\rangle = c_0\,|x_0\rangle + c_1\,|x_1\rangle$ and the second particle state $|\phi_2\rangle = d_0\,|y_0\rangle + d_1\,|y_1\rangle$. Does the state $|\psi\rangle$ came from the tensor product $|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$? Let's see

$$
\begin{aligned}
|\psi\rangle \;\; = \;\; & (c_0\,|x_0\rangle + c_1\,|x_1\rangle) \otimes (d_0\,|y_0\rangle + d_1\,|y_1\rangle) = \\
& c_0 d_0\,|x_0\rangle \otimes |y_0\rangle + c_0 d_1\,|x_0\rangle \otimes |y_1\rangle + \\
& c_1 d_0\,|x_1\rangle \otimes |y_0\rangle + c_1 d_1\,|x_1\rangle \otimes |y_1\rangle\,.
\end{aligned} \tag{9}
$$

To obtain our state $c_0 d_0 = 1$, $c_0 d_1 = 0$, $c_1 d_0 = 0$, and $c_1 d_1 = 1$. However, this equations have no solutions at all and we can conclude that $|\psi\rangle$ cannot be rewritten as a tensor product. Let us understand what this physically means. The state $|\psi\rangle = |x_0\rangle \otimes |y_0\rangle + |x_1\rangle \otimes |y_1\rangle$ means that the first particle can be in the state $|x_0\rangle$ or $|x_1\rangle$ with the 50-50 chance. However, because the term $|x_0\rangle \otimes |y_1\rangle$ has a 0 coefficient there is no chance to find the second particle in state $|y_1\rangle$. Therefore we must conclude that the second particle is in the state $|y_0\rangle$. The same logic is applicable for the states $|x_1\rangle$ and $|y_1\rangle$ for the first and second particle. Thus the individual states of two particle are intimately related to one other or one can say the states are entangled. The amazing site of the entangled state is that regardless of the actual distance in space a measurement's outcome for one particle will always determine the measurement's outcome of the other one. We can conclude with the following definition: states that can be broken into the tensor product of states from the constituent subsystem are referred to as *separable states*, whereas states that are unbreakable are called *entangled states.*

1 Homework

1. Find the probability of the state $|\uparrow\rangle$ and $|\downarrow\rangle$

$$|\psi\rangle = (1-2i)\,|\uparrow\rangle + 3i\,|\downarrow\rangle\,. \tag{10}$$

2. Find the probability of each state

$$|\psi\rangle = 3i\,|x_0\rangle \otimes |y_0\rangle + (1-2i)\,|x_0\rangle \otimes |y_1\rangle + 3\,|x_1\rangle \otimes |y_0\rangle + (-1+i)\,|x_1\rangle \otimes |y_1\rangle\,. \tag{11}$$

$$|\psi\rangle = 2i\,|x_0\rangle \otimes |y_0\rangle + (-1+2i)\,|x_1\rangle \otimes |y_1\rangle\,. \tag{12}$$