Wave Function

Before we discuss what wave function is, we might need to think of a simpler thing. In this case, we want to remind you about three dimensional space. This is the space that we usually see in our life. In this space, we can describe a position with three bases ($\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$). Suppose $\vec{r}$ is a position of an object, an equation like

$\vec{r} = 2\hat{\imath} + 3\hat{\jmath} + 4\hat{k}$, …(1)

means that, from the origin, we need to "walk" as far as 2 steps along x-axis, 3 steps y-axis, and 4 steps along z-axis. See? We can express a physical system with an equation that consists of some bases. Note that this is a classical system (not a quantum mechanical system).

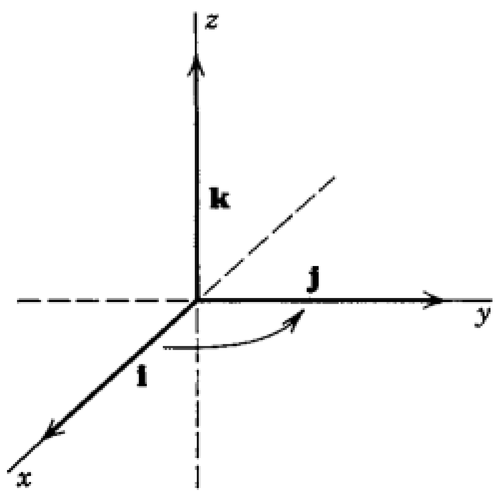

Figure 1. A representation of a three-dimensional Cartesian coordinate system

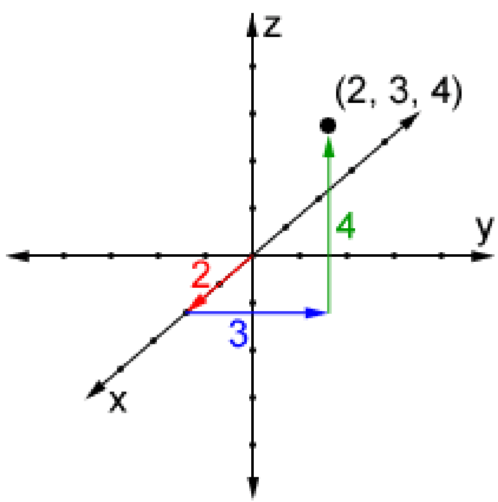

Figure 2. Position of $\vec{r}$

What about a quantum system? We can express this system with a wave function. Different from our usual dimension that we have discussed before, this space can consist of many dimensions (let's say D is the number of the dimension).

We will make this explanation more sense with this example. In a system of a polarized photon, polarization state of a photon can be horizontal or vertical polarization expressed as $|h\rangle$ and $|v\rangle$. It means that $D = 2$ and we can write the polarization state as

$|\psi\rangle = c_h|h\rangle + c_v|v\rangle$, ...(2)

with $|c_h|^2$ is the probability of getting $|h\rangle$ and $|c_v|^2$ is the probability of getting $|v\rangle$. Furthermore, $|c_h|^2 + |c_v|^2 = 1$ because the total probability must be 1. As you can see, the equation (2) expresses the quantum system and the system has two bases, $|h\rangle$ and $|v\rangle$. We also can measure the state with rotated bases, for example

$$|\nearrow\rangle = \frac{1}{\sqrt{2}}(|h\rangle + |v\rangle),$$
$$|\nwarrow\rangle = \frac{1}{\sqrt{2}}(|h\rangle - |v\rangle).$$
...(3)

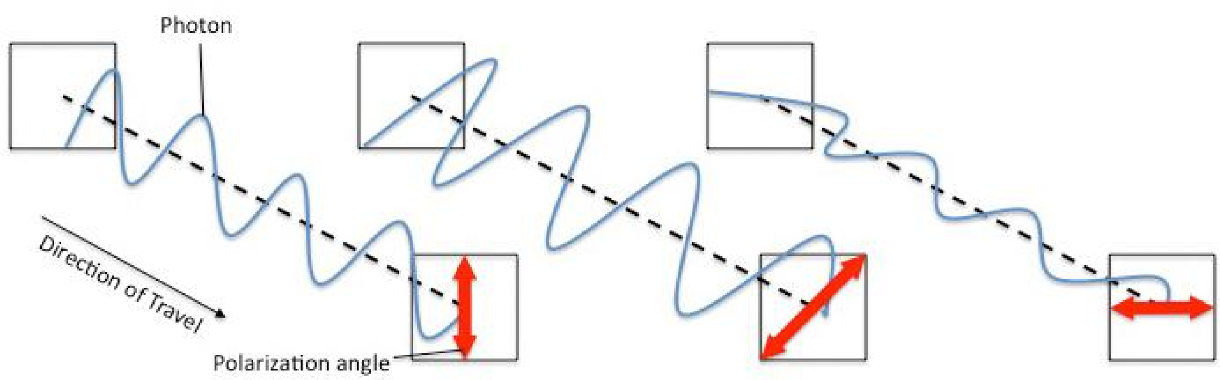

Figure 3. Polarization of a photon

This system is in two-dimensional space represented by two unit vectors called state vectors. You may be curious about what limits the number of dimensions of the quantum system. The answer is actually there is no limit and depends on the system. The space where quantum systems can be represented by a unit vector (or unit vectors), called Hilbert space, doesn't limit the number of the dimension. It's different from a vector in three-dimensional space that consists of just three bases ($\hat{i}$, $\hat{j}$, and $\hat{k}$).

There is another difference between quantum systems and classical systems. You may notice that in equation (2), we actually didn't represent a physical property of the system. However, equation (1) has a physical meaning because it represents a position of an object (which is real). It means that wave function is not something that we can observe directly. We need an observable (represented by an operator) included in our calculation so that we can get meaningful information related to the experiment. We will learn more about operators in another section.

By changing the name of the bases in equation (2) to $|0\rangle$ and $|1\rangle$, this equation also describes a qubit (quantum bit). Qubits is a "quantum version" of classical bits. As we already knew, bits can be represented as either "0" or "1". However, equation (2) is a superposition of the $|0\rangle$ and $|1\rangle$ state. This superposition is one of the keys that makes quantum computers better than classical computers in some cases.

Qubits also can be represented as column vectors. Suppose

$$|h\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |v\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \text{...(4)}$$

We will get

$$|\psi\rangle = \begin{pmatrix} c_h \\ c_v \end{pmatrix} \text{...(5)}$$

Evolution of the Wave Function

You may wonder, the real world is dynamic and always changing. The position of an object can change for whatever reason. It means a quantum system can also change, right?

That's right! If you have learned about classical mechanics, you may know that we can describe the time evolution of a system by using Newton's Law so that we can determine the system's position. In quantum mechanics, however, we can use the Schrödinger equation to describe the time evolution of a quantum system so that we can determine the system's wave function. This equation can be applied if the system is closed (doesn't interact with its environment). Suppose H is the Hamiltonian (an operator related to the energy) of the system and $\hbar$ is the reduced Planck constant, the time evolution can be described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = -i\hbar H\psi(t) \text{...(6)}$$

Let $\hbar = 1$ and suppose H is not time-dependent. By calculating this equation further, we will get

$\psi(t) = U\psi(0)$, ...(7)

with $U = e^{-iHt}$. It means, by this equation, we have already determined the wave function.

Eigenstate
Suppose an equation

$M\vec{r} = \vec{r}$ ...(8)

with M as an operator, $\vec{r}$ as a vector. λ is a number. As you can see from equation (8), operating M to a vector results in the same vector multiplied by a number, λ. This number (λ) is called the eigenvalue of the operator (in this case, M) and $\vec{r}$ is called eigenfunction or eigenstate of M.

For example,

$M = \begin{pmatrix} 5 & -2 \\ -2 & 2 \end{pmatrix}$, ...(9)

so that equation (8) becomes

$\begin{pmatrix} 5 & -2 \\ -2 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \lambda x \\ \lambda y \end{pmatrix}$ . ...(10)

Then, by calculating

$$\begin{vmatrix} 5-\lambda & -2 \\ -2 & 2-\lambda \end{vmatrix} = 0.$$

We get $\lambda = 1$ or $\lambda = 6$. Therefore, $M\vec{r} = \vec{r}$ or $M\vec{r} = 6\vec{r}$

In the context of quantum mechanics, we can see this kind of equation at the Schrödinger equation. Suppose H is the Hamiltonian of the system, we can write

$H|\psi\rangle = E|\psi\rangle$ ...(11)

With E is a real number. E is called eigenvalue and $|\psi\rangle$ is the eigenstate of the operator.

Composite Quantum System and Entanglement

Composite quantum system is a system which consists of subsystems (let's say the number of the subsystems is N). Its vector space is expressed by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \mathcal{H}_N$, with $\otimes$ is a tensor product. If a subsystem is described by a wave function ψ_i in Hilbert space $\mathcal{H}_i$, the wave function of the total system is $\psi = \psi_1 \otimes \psi_2 \otimes \cdots \otimes \psi_N$

A wave function that can be described as

$$\psi = \sum_{i,j} \psi_i \otimes \psi_j$$
, …(12)

is called a separable state. Whereas the entangled state is a state that can't be described as a separable state. This state represents a phenomenon called entanglement. A simple representation of entanglement can be done by Bell states. For example, one of the Bell states is

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle_{\mathrm{A}} \otimes |0\rangle_{\mathrm{B}} + |1\rangle_{\mathrm{A}} \otimes |1\rangle_{\mathrm{B}})$$
. …(13)

See equation (2) again. We know that $|c_h|^2$ is the probability of getting $|h\rangle$ and $|c_v|^2$ is the probability of getting $|v\rangle$. This kind of understanding also can be used to understand equation (13). From equation (13), we can know that the probability of getting $|0\rangle_{\mathrm{A}} \otimes |0\rangle_{\mathrm{B}}$ is ½ and the probability of getting $|1\rangle_{\mathrm{A}} \otimes |1\rangle_{\mathrm{B}}$ is ½. It means that if we measure and get $|0\rangle_{\mathrm{A}}$, we automatically also get $|0\rangle_{\mathrm{B}}$. If we measure and get $|1\rangle_{\mathrm{A}}$, we automatically also get $|1\rangle_{\mathrm{B}}$. This is one of the key phenomena that makes quantum computers better compared to classical computers.

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