Introduction to quantum mechanics, two-state systems and entanglement

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Outline

- Introduction to quantum mechanics
- Two-state systems and qubits
- Entanglement between two qubits
- Bell inequality

Some basics of quantum mechanics

1. Particles can be in one of many states. Each state is described by a wave function or amplitude ψ which is a function of space and time. Wave functions are complex numbers whose magnitude squared, $|\psi|^2$, gives the probability or probability density of finding the particle at that space-time point

If the states form a continuous set, like the position x of a particle moving in one dimension, then $|\psi|^2$ describes the probability density, i.e., $|\psi(x,t)|^2\,dx$ is the probability of finding the particle in the interval $[x, x+dx]$ at time t. We must have $\int dx\,|\psi(x,t)|^2 = 1$

If the states form a discrete set, like a particle in a finite-size box or in a simple harmonic potential or the hydrogen atom or the spin states of a particle (more on this latter), $|\psi_j|^2$ is the probability of finding the particle in a state j

Wave functions can be superposed; in general, one has to add up or integrate over many wave functions before calculating $|\psi|^2$

Some basics of quantum mechanics

2. Quantum mechanics is a probabilistic theory unlike classical mechanics where one can, in principle, measure any property (like position and momentum) of any particle with infinite accuracy, and one would always get the same values every time

In quantum mechanics, given a state, we only know the probabilities of getting different values of an observable. Every time we measure the value of an observable, say, R, we may get a different value, say, r_j. If we make the measurement a very large number of times, we find that the values r_j are found with a probability P_j which can be found from the wave function ψ. The expectation value of the observable is then denoted by $\langle\psi|R|\psi\rangle$, and is given by

$$E(R) = \sum_j r_j P_j$$

where the sum runs over all the possible values of r_j

Some basics of quantum mechanics

3. An electron has a spin angular momentum. Its magnitude has a fixed value given by $\hbar/2 \simeq 0.527 \times 10^{-34}$ Joule-sec. ($\hbar$ is called Planck's constant). The value of the component of the spin along any direction is quantized and can only take the values $\pm \hbar/2$.
This is unlike in classical mechanics where the component in any direction of a rotating object can take a continuous range of values (think of a rotating top)

Spin is a purely quantum property of the electron and it has no classical counterpart. For instance, the spin of an electron does not change with time. Also, as far as we know, an electron is a point particle (has no substructure), and a classical point particle cannot have a spin angular momentum

We call an electron a spin-1/2 particle. So the spin part has two possible states

Some basics of quantum mechanics

4. Photons (quanta of electromagnetic radiation) have spin-1. The component of the spin of a photon along the direction of its motion can only be $+\hbar$ or $-\hbar$. In terms of electromagnetic waves, these two possibilities correspond to left circularly polarized or right circularly polarized, respectively

So the polarization has two possible states

Some basics of quantum mechanics

5. The wave function ψ of a particle (or a system of particles) changes in time according to a first-order differential equation called the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi$$

where H is called the Hamiltonian

For a particle with a continuous set of states, such as states labeled by its position x, H is a differential operator, such as

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

where m is the mass of the particle

Some basics of quantum mechanics

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi$$

For a particle with a discrete set of states, say, only two states 1 and 2, the wave function is a column with two entries

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

where α, β denote the amplitudes for the particle to be in the states 1 and 2 respectively. We must have $|\alpha|^2 + |\beta|^2 = 1$ so that the probability of the particle to be in one of the two states is equal to 1

Then the Hamiltonian will be a 2×2 Hermitian matrix whose eigenvalues are real and correspond to the allowed energies of the particle, ϵ_1 and ϵ_2

Solving the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi$$

If ψ_j is an eigenvector of H with eigenvalue E_j, a particular solution of the Schrödinger equation is

$$\psi_j(t) = e^{-iE_j t/\hbar} \psi_j$$

Then the general solution of the Schrödinger equation is given by the superposition

$$\psi(t) = \sum_j c_j e^{-iE_j t/\hbar} \psi_j$$

where the c_j can be arbitrary complex numbers. Their values can be found if the initial wave function $\psi(0)$ is given

Combining continuous and discrete states

An electron can move in space (with a coordinate x) in one dimension and they also carry spin-$1/2$. To combine the continuous label x and the discrete label for spin, we write the wave function for an electron as

$$\psi = \begin{pmatrix} \alpha(x,t) \\ \beta(x,t) \end{pmatrix}$$

Here $|\alpha|^2$ is the probability density to find the electron at x with the component of its spin along the $\hat{z}$ direction being equal to $+\hbar/2$, and $|\beta|^2$ is the probability density to find the electron at x with the component of its spin along the $\hat{z}$ direction being equal to $-\hbar/2$. The choice of the $\hat{z}$ direction is arbitrary

We must have $\int dx\, (|\alpha|^2 + |\beta|^2) = 1$ to have the total probability of finding the electron somewhere and with some spin equal to 1

Spin wave function of an electron

We now ignore the motion of the electron in space and also ignore the time-evolution of its wave function. We then just have a spin-$1/2$ particle with the general wave function

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

As remarked earlier, α and β are the amplitudes to find the electron with the component of its spin along the $\hat{z}$ direction being equal to $+\hbar/2$ and $-\hbar/2$ respectively

Namely, ψ is the superposition

$$\psi = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

of two states in which the electron spin points in the $+\hat{z}$ and $-\hat{z}$ directions respectively

Spin wave function of an electron

To find the amplitudes for the electron with wave function $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

to have its spin components along an arbitrary direction, we have to do a unitary transformation

For instance, the amplitudes to find the electron with the component of its spin along the $\hat{x}$ direction being equal to $+\hbar/2$ and $-\hbar/2$ is given by the upper and lower components respectively of the column

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha + \beta \\ \alpha - \beta \end{pmatrix}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

is the unitary matrix which transforms from the spin $\hat{z}$ basis to the spin $\hat{x}$ basis. Where does this unitary matrix come from?

The mathematics of spin-1/2

The quantum mechanical description of a spin- $1/2$ electron requires us to define three 2×2 Hermitian matrices called the Pauli matrices

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

The spin operators for a spin- $1/2$ electron are given by

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}, \quad \text{i.e.,} \quad S_x = \frac{\hbar}{2}\sigma_x, \quad S_y = \frac{\hbar}{2}\sigma_y, \quad S_z = \frac{\hbar}{2}\sigma_z$$

Note that

$$S_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad S_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

This is why $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are called the wave functions of an electron with the $\hat{z}$ component of its spin being equal to $+\hbar/2$ and $-\hbar/2$ respectively

The mathematics of spin-1/2

Similarly,

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and we see that

$$S_x \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$S_x \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = -\frac{\hbar}{2}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Hence $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ are the wave functions of an electron with the $\hat{x}$ component of its spin being equal to $+\hbar/2$ and $-\hbar/2$ respectively

We now see that these wave functions are exactly the columns of the unitary matrix which transforms from spin $\hat{z}$ basis to the spin $\hat{x}$ basis

Electron spin pointing in a general direction

Consider a general direction $\hat{n}$ in three dimensions which is parametrized by the polar coordinates (θ, ϕ). Thus the three Cartesian coordinates of the unit vector $\hat{n}$ are given by $(n_x, n_y, n_z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. We can then define the quantity $\vec{n} \cdot \vec{S} = n_x S_x + n_y S_y + n_z S_z$

Then the wave function of an electron whose spin component in the direction $\hat{n}$ is equal to $+\hbar/2$ is given by the eigenvalue equation

$$\vec{n} \cdot \vec{S}\, \psi = \frac{\hbar}{2}\, \psi$$

We find that

$$\psi = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)\, e^{i\phi} \end{pmatrix}$$

Hence the probabilities that this state has its spin component in the $\hat{z}$ direction equal to $+\hbar/2$ and $-\hbar/2$ are given by $\cos^2(\theta/2)$ and $\sin^2(\theta/2)$ respectively

Some remarks about unitary transformations

Unitary transformations play a very useful role in quantum mechanics. Many transformations (such as the change of spin basis from one direction to another or, in general, rotating the coordinate axis of an arbitrary system, or evolving a wave function in time, or moving a particle from one position to another) can be described by unitary operators acting on the wave functions of the system

Unitary transformations preserve the total probability. If ψ is a wave function which has probability 1, then $U\,\psi$ will also have probability 1 if U is a unitary operator

Unitary transformations acting on operators do not change their eigenvalues. For instance, if H is the Hamiltonian of a system and its eigenvalues are the possible energies, then the unitary transformation gives a new Hamiltonian $U\,H\,U^{-1}$ which has the same eigenvalues and therefore the same energies

Qubit

A qubit (quantum bit) is a two-state quantum mechanical system. Denote the two basis states as

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The most general possible state of the system is a superposition

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

where we always fix $|\alpha|^2 + |\beta|^2 = 1$ so that the total probability to find the system in one of the two states is 1

Examples: a spin-1/2 object, where the two basis states correspond to the object having the component of its spin in the z direction being equal to $\hbar/2$ and $-\hbar/2$ respectively. Another example of a qubit is a photon which can have two possible spin states or polarizations

Two qubits

We now consider a system with two qubits (spin-1/2's).
The wave functions of this given by a direct product of the states of two separate qubits. We will work in the spin $\hat{z}$ basis as usual.
We will simplify the notation to

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle$$

to emphasize that these two states have components of the spin in the $\hat{z}$ direction being up and down respectively

The most general wave function of two qubits will be a linear superposition of the four states

$$|\uparrow\uparrow\rangle, \quad |\uparrow\downarrow\rangle, \quad |\downarrow\uparrow\rangle \quad \text{and} \quad |\downarrow\downarrow\rangle$$

There will be two sets of spin operators $\vec{S}_1$ and $\vec{S}_2$ which act only on the states of the first and second qubit respectively

A spin-singlet state

A particularly interesting state of two qubits is the state

$$|S\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

This is called a spin-singlet state since all the components of the total spin operator $\vec{S}_1 + \vec{S}_2$ give zero when they act on this state. Hence this state has total spin-0, and it is the unique state of two qubits which has this property

There are three other states of two qubits which have total spin-1. They are called spin-triplet states, and their wave functions are given by

$$|T_1\rangle = |\uparrow\uparrow\rangle, \quad |T_0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right) \quad \text{and} \quad |T_{-1}\rangle = |\downarrow\downarrow\rangle$$

Entanglement

$$|S\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

The spin-singlet state is an example of an entangled state

Suppose that there are two observers, A and B, who can only measure the $\hat{z}$ spin components, S_{1z} and S_{2z}, of qubits 1 and 2 respectively. If they are told that the two-qubit system is in a spin-singlet state, they would not be able to say with certainty what the spin state of their own qubit is. The best that observer A would be able to say is that their qubit has a probability of 1/2 of having spin $\uparrow$ and a probability of 1/2 of having spin $\downarrow$. And similarly for B.

However, suppose that observer A makes the measurement of S_{1z} and finds that it is in an $\uparrow$ state. Then they would immediately be able to say, without communicating in any way with B, that B's qubit will be in a $\downarrow$ state

Entanglement

$$|S\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

So we have the strange situation that initially the observers don't know the states of their qubits, but as soon as one of them makes a measurement and finds the state of their qubit, they instantaneously know the state of the other qubit. This holds even if the two qubits and their respective observers are very far apart and cannot communicate with each other

This strange feature which a quantum system consisting of more than particle can have is called entanglement. This has no classical counterpart at all

A single quantum mechanical particle with a continuous set of states, like position, has wave functions which are mathematically similar to waves in classical mechanics. But entanglement is a feature of multi-particle quantum mechanics alone, and it has no analogs in classical theories

An unentangled state

All two-qubit states are not necessarily entangled. An example of an unentangled state is one of the spin-triplet states

$$|T_1\rangle = |\uparrow\uparrow\rangle$$

If the observers are told that this is the state of their two qubits, each observer would immediately know the state of the qubit of the other observer even without making a measurement of their own qubit

An unentangled state like the one above is called a product state: the state of the two states is simply a direct product of the states of the two qubits separately. This is a classical kind of state

There is a quantitative way of defining the entanglement of an arbitrary state of two objects. This is called entanglement entropy

Entanglement entropy

A general two-qubit state can be written in the form

$$\psi = \sum_{S_{1z}=\uparrow,\downarrow} \sum_{S_{2z}=\uparrow,\downarrow} C_{S_{1z},S_{2z}} \, |S_{1z} S_{2z}\rangle$$

where C_{jk} are complex numbers which denote the amplitudes of the spin states j and k of qubits 1 and 2 respectively

We then define a reduced density matrix of qubit 1 by summing over the possible states of qubit 2 as

$$\rho_{jj'} = \sum_{k} C^*_{jk} C_{j'k}$$

One can show that ρ is a Hermitian matrix, its eigenvalues must lie in the range $[0, 1]$, and the sum of its eigenvalues is equal to 1

Entanglement entropy

If λ_1, λ_2 are the two eigenvalues of the reduced density matrix ρ, the entanglement entropy is defined as

$$s = -\lambda_1 \log \lambda_1 - \lambda_2 \log \lambda_2$$

where the base of the logarithm is often taken to be 2 in the quantum information community.

For an unentangled state, one finds that $s = 0$, while in an entangled state, we find that $s > 0$

For the spin-singlet state $|S\rangle$, we find that $s = 1$. This is, in fact, the largest possible value of the entanglement entropy that one can have for a two-qubit state. So the spin-singlet state is maximally entangled

Hidden-variable theories

We turn to another feature of quantum mechanics which is also motivated by the idea of entangled states. Given the singlet state

$$|S\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

we know that before making any measurements, neither observer can say with certainty what state of their own qubit is

But is it possible that there can be a hidden variable which leads to results similar to what observers A and B would find by making measurements on the above state?

For example, there may be a hidden person who decides randomly to either give a spin $\uparrow$ to A and a spin $\downarrow$ to B with probability $1/2$, or a spin $\downarrow$ to A and a spin $\uparrow$ to B with probability $1/2$

In each case, the state of the two qubits would be a product state

Hidden-variable theories

John Bell showed that such hidden-variable theories (which are essentially classical) would give results which are different from what quantum mechanics predicts

Consider again a two-qubit state ψ. Now suppose that each of the two observers A and B can make one of two possible measurements. We will call these measurements a_1 and a_2 for observer A, and b_1 and b_2 for observer B

So four possible joint measurements are possible, and the expectation values for the four possibilities are given by the expressions $E(a_1, b_1) = \langle\psi|a_1 b_1|\psi\rangle$, and similarly for $E(a_1, b_2)$, $E(a_2, b_1)$ and $E(a_2, b_2)$

A hidden-variable theory would predict that $E(a_1, b_1) = E(a_1)\,E(b_1)$, $E(a_1, b_2) = E(a_1)\,E(b_2)$, etc. since the measurements are being made on a product state which is a classical state with no entanglement

Bell inequality

Now suppose that each of the four quantities a_1, a_2, b_1 and b_2 can only take values in the range $[-1, 1]$. This means that the expectation values of each of these four quantities also lie in the range $[-1, 1]$

Using the properties that $E(a_1, b_1) = E(a_1)\, E(b_1)$, etc. and $-1 \leq E(a_i),\ E(b_j) \leq 1$, we can show that

$$\begin{aligned} & E(a_1, b_1) + E(a_1, b_2) + E(a_2, b_1) - E(a_2, b_2) \\ = \ & E(a_1)\,(E(b_1) + E(b_2)) + E(a_2)\,(E(b_1) - E(b_2)) \end{aligned}$$

has a magnitude which is less than or equal to 2

Bell inequality

Now suppose that the properties that the observers A and B are measuring are given by

$$\begin{aligned} & a_1 = \vec{a}_1 \cdot \vec{\sigma}_A, \quad a_2 = \vec{a}_2 \cdot \vec{\sigma}_A \\ \text{and} \quad & b_1 = \vec{b}_1 \cdot \vec{\sigma}_B, \quad b_2 = \vec{b}_2 \cdot \vec{\sigma}_B \end{aligned}$$

respectively, where $\vec{\sigma}_A$, $\vec{\sigma}_B$ are the Pauli spin operators for A and B, and $\vec{a}_1$, $\vec{a}_2$, $\vec{b}_1$ and $\vec{b}_2$ are some unit vectors

We then discover that if ψ is the spin-singlet state, we get
$E(\vec{a}_i, \vec{b}_j) = \langle\psi| \vec{a}_i \cdot \vec{\sigma}_A \, \vec{b}_j \cdot \vec{\sigma}_B |\psi\rangle = -\vec{a}_i \cdot \vec{b}_j$

This is clearly different from $E(\vec{a}_i)$ and $E(\vec{b}_j)$ which are both equal to zero in the spin-singlet state

Violation of Bell inequality

In the spin-singlet state, we have

$$E(\vec{a}_i, \vec{b}_j) \;=\; \langle\psi|\; \vec{a}_i \cdot \vec{\sigma}_A \; \vec{b}_j \cdot \vec{\sigma}_B \; |\psi\rangle \;=\; -\; \vec{a}_i \cdot \vec{b}_j$$

This gives

$$\begin{aligned} & E(a_1, b_1) \;+\; E(a_1, b_2) \;+\; E(a_2, b_1) \;-\; E(a_2, b_2) \\ = \;& -\; \vec{a}_1 \cdot (\vec{b}_1 \;+\; \vec{b}_2) \;-\; \vec{a}_2 \cdot (\vec{b}_1 \;-\; \vec{b}_2) \end{aligned}$$

Depending on the choices of $\vec{a}_1$, $\vec{a}_2$, $\vec{b}_1$ and $\vec{b}_2$, the magnitude of the quantity $E(a_1, b_1) + E(a_1, b_2) + E(a_2, b_1) - E(a_2, b_2)$ can exceed 2 which violates the Bell inequality

The violation of the Bell inequality has been confirmed in numerous experiments over the years, using photons, electrons and other two-state systems. This proves that quantum mechanics is not compatible with hidden-variable theories

Violation of Bell inequality

$$\begin{aligned} & E(a_1, b_1) + E(a_1, b_2) + E(a_2, b_1) - E(a_2, b_2) \\ = & -\vec{a}_1 \cdot (\vec{b}_1 + \vec{b}_2) - \vec{a}_2 \cdot (\vec{b}_1 - \vec{b}_2) \end{aligned}$$

To see that the magnitude of this can exceed 2, we choose $\vec{a}_1, \vec{b}_1, \vec{a}_2, \vec{b}_2$ to lie in a plane and rotated successively by 45^0

$$\begin{aligned} \vec{a}_1 &= (1,0,0), \quad \vec{b}_1 = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0) \\ \vec{a}_2 &= (0,1,0), \quad \vec{b}_2 = (-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0) \end{aligned}$$

Then $E(a_1, b_1) + E(a_1, b_2) + E(a_2, b_1) - E(a_2, b_2) = -2\sqrt{2}$ whose magnitude is clearly larger than 2

Interestingly, we can show that $2\sqrt{2}$ is the upper bound of the magnitude of the above quantity for any choice of the four vectors. This is called the Tsirelson bound

Summary

- Wave function and its interpretation
- The spin-$1/2$ nature of the electron which leads to a qubit
- Two-qubit wave functions and entanglement
- Bell inequality

References

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