115203 - Quantum Physics 1

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Abstract

1 Introduction

1.1 Stern–Gerlach experiment

Suppose particles can be either black or white and we have some tool which can measure a color of particles. Additional, suppose, particles have additional property ”hardness‘ ‘- and we can measure whether particles are hard or soft.
The properties are consistent - i.e. it doesn't matter how many times you measure it one after other, you get the same result.
Also, hardness and color are independent - if you measure hardness, you get either white or black with same probability.
The experiment itself is measuring color, then hardness, and then color again. Even though we input only white particles into hardness measuring tool, the output of second color measurement is either white or black with equal probability.

Principles of quantum mechanics

1. Particle is described with normalized vector in complex space of physical states.

   In our example, the space is 2D - black/white and hard/soft.

2. Given system in (normalized) state $\vec{v}_1$, probability that it will be in state $\vec{v}_2$ is

$$P = \left|\vec{v}_2 \cdot \vec{v}_1\right|^2$$

   So, in our example, suppose $\hat{w}$ and $\hat{b}$ are orthogonal basis of our space. Since we know that

$$\begin{cases} \left|\vec{w} \cdot \vec{s}\right|^2 = \frac{1}{2} \\ \left|\vec{b} \cdot \vec{s}\right|^2 = \frac{1}{2} \end{cases}$$

   We know that angle with both axis of $\vec{s}$ is $\frac{\pi}{4}$. We can choose any of 4 possibilities. Lets choose $\hat{s} = \frac{\hat{w}-\hat{b}}{\sqrt{2}}$ and since $\hat{h}$ is orthogonal, $\hat{h} = \frac{\hat{w}+\hat{b}}{\sqrt{2}}$.

3. Each measurement can be characterized with Hermitian operator, whose eigenvalues are outcomes of measurements and corresponding eigenvectors are states after the measuremnts.

Now we can predict the results of opposite experiment - if we measure hardness of white particle, it will be hard with probability $\frac{1}{2}$. Now the probability that resulting hard particle will be measured to be white, is also $\frac{1}{2}$.
In quantum mechanics we use bra ket notation: vector is denoted $|b\rangle$ (conjugate transposed vector is denoted as $\langle w|$):

$$|h\rangle = \frac{1}{\sqrt{2}}|b\rangle + \frac{1}{\sqrt{2}}|w\rangle$$

Example Suppose we have a particle

$$|\Psi\rangle = \frac{1}{\sqrt{3}}|w\rangle + \sqrt{\frac{2}{3}}|b\rangle$$

Then probability that it will be measured as white

$$P(w) = \left|\langle w|\Psi\rangle\right|^2 = \left|\frac{1}{\sqrt{3}}\langle w|w\rangle + \sqrt{\frac{2}{3}}\langle w|b\rangle\right|^2 = \frac{1}{3}$$

If measure hardness:

$$P(h) = |\langle h|\Psi\rangle|^2 = \left|\left(\frac{1}{\sqrt{2}}|b\rangle + \frac{1}{\sqrt{2}}|w\rangle\right)\left(\frac{1}{\sqrt{3}}|w\rangle + \sqrt{\frac{2}{3}}|b\rangle\right)\right|^2 = \left|\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}}\right| \approx 0.3$$

2 Linear algebra

Linear operator In quantum mechanics we write operators as multiplication of vectors. For example for

$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

we write

$$R = -|w\rangle\langle b| + |b\rangle\langle w|$$

And then

$$R|\Psi\rangle = -|w\rangle\langle b|\Psi\rangle + |b\rangle\langle w|\Psi\rangle = -\langle b|\Psi\rangle|w\rangle + \langle w|\Psi\rangle|b\rangle$$

For example

$$R|s\rangle = |b\rangle\langle w|s\rangle - |w\rangle\langle b|s\rangle = |b\rangle\frac{1}{\sqrt{2}} + |w\rangle\frac{1}{\sqrt{2}} = |h\rangle$$

Examples

- $$W = |w\rangle\langle b| + |w\rangle\langle w|$$
- $$T = |h\rangle\langle b| + |s\rangle\langle w|$$
- $$Q = 2|w\rangle\langle w| + 3|b\rangle\langle b|$$

  This is not unitary operator, since in doesn't conserves norm.

Basis change To change from basis to basis we just substitute the values of old basis in a new one:

$$T = |h\rangle\left(\frac{1}{\sqrt{2}}\langle h| - \frac{1}{\sqrt{2}}\langle s|\right) + |s\rangle\left(\frac{1}{\sqrt{2}}\langle h| + \frac{1}{\sqrt{2}}\langle s|\right) = \frac{1}{\sqrt{2}}|h\rangle\langle h| - \frac{1}{\sqrt{2}}|h\rangle\langle s| + \frac{1}{\sqrt{2}}|s\rangle\langle h| + \frac{1}{\sqrt{2}}|s\rangle\langle s|$$

Hermitian operators We want to build an operator C such that for state $|\psi\rangle$ it will return us the average of ψ:

$$\langle\psi|C|\psi\rangle = \langle\psi\rangle$$

If we give a value of -1 to white and value of 1 to black:

$$\langle\psi|C|\psi\rangle = -1\cdot P(\psi = w) + 1\cdot P(\psi = b) = -|\langle w|\psi\rangle|^2 + |\langle b|\psi\rangle|^2 = -\langle\psi|w\rangle\langle w|\psi\rangle + \langle\psi|b\rangle\langle b|\psi\rangle$$

Thus

$$C = -|w\rangle\langle w| + |b\rangle\langle b|$$

For example, for $\psi = \frac{1}{\sqrt{3}}|w\rangle + \sqrt{\frac{2}{3}}|b\rangle$:

$$\langle\psi|C|\psi\rangle = \langle\psi|\left(-|w\rangle\langle w| + |b\rangle\langle b|\right)\left(\frac{1}{\sqrt{3}}|w\rangle + \sqrt{\frac{2}{3}}|b\rangle\right) = \langle\psi|\left(-\frac{1}{\sqrt{3}}|w\rangle + \sqrt{\frac{2}{3}}|b\rangle\right) = \frac{1}{3}$$

Additional example Suppose we have two properties - color and temperature. Possible values are red, green, blue for color and hot, lukewarm, cold for temperature.
If we measure temperature of red or green particle we get lukewarm of hot with equal probability. If we measure temperature of blue particle we get cold surely.
How can we write $|b\rangle$, $|g\rangle$, $|r\rangle$ in basis of $|c\rangle$, $|l\rangle$, $|h\rangle$?
From first experiment

$$|r\rangle = \frac{1}{\sqrt{2}}|l\rangle + \frac{1}{\sqrt{2}}|h\rangle$$

$$|g\rangle = \frac{1}{\sqrt{2}}|l\rangle - \frac{1}{\sqrt{2}}|h\rangle$$

Note that we need minus since else we'd get $\langle g|r\rangle = 1$. From last experiment

$$|b\rangle = |c\rangle$$

Lets denote $h = 1$, $l = 0$, $c = -1$ and build temperature operator. It's characterized by

$$\begin{cases} T|h\rangle = |h\rangle \\ T|l\rangle = 0 \\ T|c\rangle = -|c\rangle \end{cases}$$

And thus an operator is

$$T = |h\rangle\langle h| - |c\rangle\langle c|$$

Now let's calculate temperature of state $|g\rangle$:

$$\langle g|T|g\rangle = \left(\frac{1}{\sqrt{2}}|l\rangle - \frac{1}{\sqrt{2}}|h\rangle\right)T\left(\frac{1}{\sqrt{2}}|l\rangle - \frac{1}{\sqrt{2}}|h\rangle\right) = \frac{1}{2}(|l\rangle - |h\rangle)T(|l\rangle - |h\rangle) = -\frac{1}{2}(|l\rangle - |h\rangle)|h\rangle = \frac{1}{2}$$

We can also calculate variance:

$$\sigma^2 = \langle g|T^2|g\rangle - \big(\langle g|T|g\rangle\big)^2$$

Example We have a particle can be at one of five points. So possible states are $|1\rangle$,$|2\rangle$,$|3\rangle$,$|4\rangle$,$|5\rangle$.
If we want to describe a particle on finite 1D interval, we'll divide it into N equal intervals of length a. We are interested in $a \to 0$, thus number of dimensions goes to infinity.

double slit experiment

3 Tons of linear algebra

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3.1 Fourier transform operator

Define space with basis $|x\rangle$ such that $\langle x|f\rangle = f(x)$ and $\langle x|x'\rangle = \delta(x - x')$ Define identity operator

$$I = \int |x\rangle\langle x| \,\mathrm{d}x$$

Define also operator K such that

$$\langle x|K|f\rangle = -i\frac{\partial f}{\partial x}$$

K is Hermitian if $f \cdot g\big|_a^b = 0$ for any f,g.
It's eigenvalues k are such that

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx}$$

Also for f

$$|f\rangle = \int f(x)\,|x\rangle \,\mathrm{d}x = \int \hat{f}(k)\,|k\rangle \,\mathrm{d}k$$

when

$$\langle k|f\rangle = \hat{f}(k)$$

Define operator X such that $X|x\rangle = x|x\rangle$. Obviously, X is Hermitian.

$$\langle x|X|f\rangle = \left(\langle f|X^\dagger|x\rangle\right)^* = \left(\langle f|X|x\rangle\right)^* = (x\langle f|x\rangle)^* = x^*\langle x|f\rangle = xf(x)$$

Lets calculate $[X, K]$:

$$\langle x|XK|f\rangle = \langle x|XIK|f\rangle = \int \langle x|X|x'\rangle \langle x'|K|f\rangle \,\mathrm{d}x' = \int x'\delta(x-x')\left(-i\frac{\partial f}{\partial x'}\right)\mathrm{d}x' = -ix\frac{\partial f}{\partial x}$$

Now

$$\langle x|KX|f\rangle = \int \langle x|K|x'\rangle \langle x'|X|f\rangle \,\mathrm{d}x' = \int -i\delta(x-x')\frac{\partial}{\partial x'}(x'f(x))\,\mathrm{d}x' = -i\frac{\partial}{\partial x}(xf(x)) = -if(x) - ix\frac{\partial f}{\partial x}$$

Thus

$$\langle x|[X,K]|f\rangle = -ix\frac{\partial f}{\partial x} - \left(-if(x) - ix\frac{\partial f}{\partial x}\right) = if(x) = i\langle x|I|f\rangle$$

i.e.

$$[X, K] = iI$$

We suppose that our space is complete (i.e. each Cauchy sequence converges). Complete inner product space is called Hilbert space.

4 Quantum mechanics principles

1. Physical state is described by vector $|\psi\rangle$ in Hilbert space
2. Given state $|\psi\rangle$, probability to measure it in state φ is

$$P = \frac{|\langle\varphi|\psi\rangle|^2}{\langle\varphi|\varphi\rangle\langle\psi|\psi\rangle}$$

3. Measurable quantities are described by Hermitian operator Ω:
   (a) Result of measurement is one of eigenvalues of Ω
   (b) A state corresponding to measurement of value ω is $|\omega\rangle$.
   (c) After measurements, the state will be corresponding eigenvector
4. Given state ψ at $t = 0$, a state at time t is given by following PDE:

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

which is called Schrödinger equation

Position and momentum operators Position operator is X and momentum operator $P = \hbar K$.

Consequences of principles

1. Particle on line is described with vector in infinite-dimensional space.
2. If $|\psi\rangle$ and $|\varphi\rangle$ are physical states, $|\varphi\rangle + |\psi\rangle$ is physical state too.
3. It's impossible to predict results of measurements, only probability of results.
4. Norm of the vector is not important, since we always can normalize them.
5. Results of measurements of Ω are only ω_i.
6. If $|\psi\rangle = |\omega\rangle$, such that $\Omega|\omega\rangle = \omega|\omega\rangle$ then measurement of Ω will always give ω.

7. Classical physical quantity which depends on x and p, its quantum analogue is same function of operators X and P:

$$\Omega(x, p) \Rightarrow \Omega(X, P)$$

The order is important, since $[X, P] \neq 0$. Some operators are defined only in quantum case, e.g. $\Omega = [X, P]$. Thus the right way to proceed is to define quantum quantities and then to check what happens in classical limit.

8. If there is degeneracy, i.e., some eigenvalue of the operator has multiple eigenvectors, the probability is a sum of probabilities:

$$P = |\langle \omega, 1|\psi\rangle|^2 + |\langle \omega, 2|\psi\rangle|^2$$

Expectation and variance of measurement Expectation of measurement can be calculated as

$$\langle \psi|\Omega|\varphi\rangle = \sum_i \omega_i P_\psi(\omega)$$

and variance

$$\Delta\Omega^2 = \langle \psi|(\Omega - \langle \psi|\Omega|\psi\rangle)^2|\psi\rangle$$

4.1 Schrödinger equation

Examples of Hamiltonian For free particle

$$H = \frac{P^2}{2m}$$

For harmonic oscillator

$$H = \frac{P^2}{2m} + \frac{1}{2}\omega^2 X^2$$

Suppose Hamiltonian is independent on time. We want to diagonalize Hamiltomnian.