Quantum Computing (量子计算)

Get ready to grasp the leading edge technologies

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Light: photons & particles[1]

Einstein believed light is a particle (photon) and the flow of photons is a wave (**电磁波**).

Einstein: 1905

- Its energy is given by

$$E = h\nu = \hbar\omega$$

where $h = 6.626 \times 10^{-34} Js$ (joule-seconds) is the Planck constant, $\hbar = \frac{h}{2\pi}$ and $2\pi\nu = \omega$.

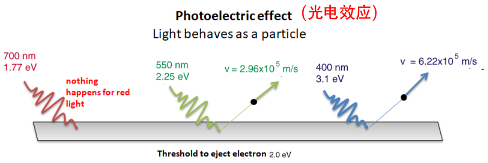
- Light has also a momentum (**动量**)

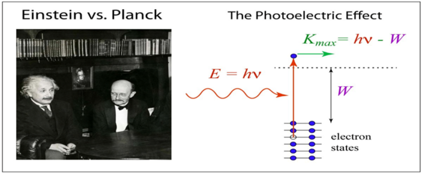
$$p = \frac{\hbar}{\lambda}$$

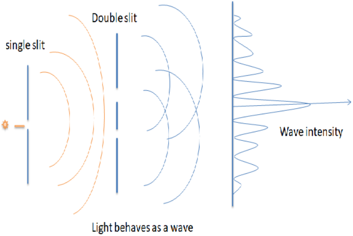
Where λ is wave length.

[1] 光的波粒二象性

Light: photons & particles

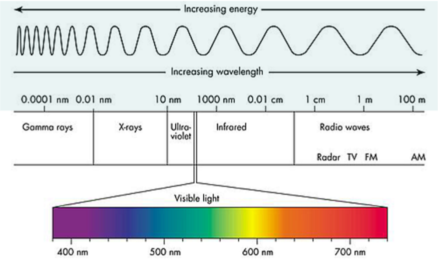


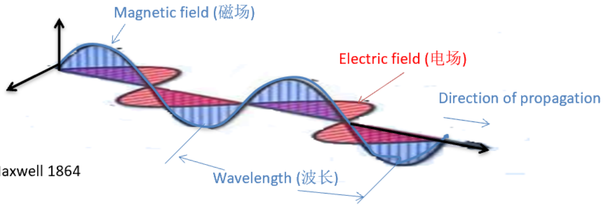




https://galileo-unbound.blog/2020/01/13/who-invented-the-quantum-einstein-vs-planck/

Light: photons & particles

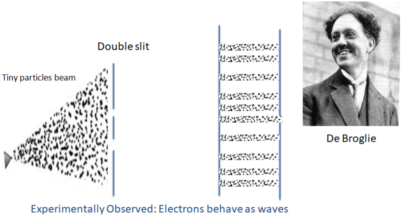




Maxwell 1864

Light travels carried by an electromagnetic waves.

Tiny particle waves



De Broglie: The tiny bits of matter(微小的物质), such as electrons (电子), behave like particles in some situations and like waves in others: wave-particle duality (波粒二象性).

De Broglie in his 1924 PhD thesis

- Tiny particle has a wave length $\lambda = \frac{\hbar}{p} = \frac{\hbar}{mv}$ where $p = mv$ is the momentum(动量) of the particle.
- Its energy is given by : $E = h\nu = \hbar\omega$

The Schrödinger equation

The wave function of a particle can be described as follows:

$$\psi(x,t) = e^{i(kx-\omega t)}$$

where the momentum is $p = \hbar k$ with $k = \frac{1}{\lambda}$ and energy $E = \hbar\omega = \frac{p^2}{2m} + V(x)$. Therefore, by applying the momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ to ψ we obtain

$$-i\hbar\frac{\partial}{\partial x}\psi = p\psi$$

thus ψ is an eigenstate (eigenfunction 特征函数) of the operator $\hat{p}$ with the momentum p as eigenvalue (特征值).

The Schrödinger equation

Moreover, if we apply $i\hbar\frac{\partial}{\partial t}$ to the wave function we get

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

because $\hbar\omega$ is the total energy $E = E_K + E_P = \frac{p^2}{2m} + V(x)$. Therefore if we apply the operator $\hat{p}^2 = -\hbar^2\frac{\partial^2}{\partial^2 x}$, we get the time independent Schrödinger equation given by:

$$\hat{H}\psi = E\psi, \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

Combine the above equations, we get the time depending Schrödinger equation:

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

Quantum postulates[2] 1, 2

Postulate 1

A quantum system is describe by a wave function $\psi(x,t)$ that contain everything known about a system that depends upon on position and time. It has the property that $\|\psi(x,t)\|dx$ represents the density probability the particle lies in an interval element dx at time t. Therefore, it must fulfill: $\int_{-\infty}^{+\infty} \|\psi(x,t)\|^2 dx = 1$

Postulate 2

Each observable (**可观察量**) A (measurement) on a wave function (system) is an eigenvalue of an operator $\hat{A}$. As the measurement are real the operators associated with the observable are Hermitian. If the outcome of a measurement of an operator $\hat{A}$ is a real number a then $\hat{A}\psi = a\psi$ where ψ is an eigenstate (eigenfunction).

[2] **量子力学公设**

Quantum postulate 3

If a quantum system is describe by a wave function ψ then the expectation value (期望值) of any observable A is given

$\langle A \rangle = \left\langle \psi \middle| \hat{A} \middle| \psi \right\rangle$, if $\hat{A}\psi = a\psi$ then $\langle A \rangle = a$.

If $\psi = \sum\limits_{i=1}^{n} c_i \psi_i$, where $\hat{A}\psi_i = a_i \psi_i$ and then the expectation is given by

$$\langle A \rangle = \langle \psi | \widehat{A} | \psi \rangle = \left\langle \sum_{i=1}^{n} c_i \psi_i \middle| \widehat{A} \middle| \sum_{i=1}^{n} c_i \psi_i \right\rangle = \sum_{i=1}^{n} a_i \left| c_i \right|^2$$

.

Therefore we measure a_i with probability $P(a_i) = \left| c_i \right|^2$ and the wave function collapses (波函数坍缩) into ψ_i.

Quantum postulate 4

The time evolution of the wave function(波函数) is given by the time dependent Schrodinger equation:

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

where $\hat{H}$ is the hamiltonian of the system (kinetic energy(动能) + potential energy(势能)). If ψ is an eigenstate of $\hat{H}$ then

$$\psi = \psi(x, 0)e^{\frac{-iEt}{\hbar}}$$

where $\hat{H}\psi = E\psi$.

Some quantum operators

1. Position operator : $\hat{x}$ that acts on a state (wave function)

$$\hat{x}\psi = x\psi(x)$$

2. Momentum operator (动量算符) :

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

3. The Hamiltonian operator(哈密顿算符) :

$$\hat{H} = -\hbar\frac{\partial^2}{\partial x^2} + V(x)$$

4. The angular momentum operators (角动量算符) :

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

5. Position operator : $\hat{x}$ that acts on a state (wave function)

Operators : commutation

1. The commutator operator of the $\hat{X}$ and $\hat{p}$ is defined by

$$\left[\hat{X}, \hat{p}\right] = \hat{X}\hat{p} - \hat{p}\hat{X} = i\hbar\mathbf{1} \neq 0$$

2. Properties of angular momentum operator:

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \quad \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x, \quad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

3. One of the three angular momentums ($\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$) can be measured with $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$\left[\hat{L}_x, \hat{L}^2\right] = \left[\hat{L}_y, \hat{L}^2\right] = \left[\hat{L}_z, \hat{L}^2\right] = 0$$

Schrödinger equation : harmonic oscillator[3]

$$i h \frac{\partial \psi(x,t)}{\partial t} = \widehat{H} \psi(x,t), \quad \widehat{H} = \frac{\widehat{p}^2}{2m} + \frac{m}{2}\omega^2 \widehat{x}^2$$

$$\hat{H} = \frac{m\omega^2}{2}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) - \frac{\hbar\omega}{2}$$

Then it can be written as

$$\hat{H} = \hbar\omega\left(N - \frac{1}{2}\right) = \hbar\omega\left(N^\dagger + \frac{1}{2}\right)$$

$$N = aa^\dagger, \; a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

[3] 量子谐振子

harmonic oscillator: ladder operator concept

The lowering and raising operators as
$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$. we have

$$\left[a, a^\dagger\right] = 1.$$

Let recall the following formula: $\left[\hat{A}\hat{B}, \hat{C}\right] = \hat{A}\left[\hat{B}, \hat{C}\right] + \left[\hat{A}, \hat{C}\right]\hat{B}$, then we have $[N, a] = -a$ and $\left[N, a^\dagger\right] = a^\dagger$. There for if ψ is an eigenstate of the operator N with the eigenvalue n then $a\psi$ is also an eigenstate with the eigenvalue $n - 1$ indeed

$$Na\psi = aN\psi - a\psi.$$

Thereby if $\hat{H}\psi = E\psi$ we have $N\psi = (\frac{1}{\hbar\omega}E + \frac{1}{2})\psi$

$$\hat{H}a\psi = (E - \hbar\omega)a\psi$$

Thus the operator decreases the energy by an integer amount (-1).

harmonic oscillator: ladder operator concept

Therefore, if ψ_0 is a state of minimal energy then

$$\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{i}{m\omega}\hat{p}\right)\psi_0=0,$$

therefore

$$\frac{i}{m\omega}\hat{p}\psi_0=-\hat{x}\psi_0 \quad \Rightarrow \quad \frac{\partial}{\partial x}\psi_0=\frac{-m\omega x}{\hbar}\psi_.0$$

we obtain

$$\psi_0(x)=Ke^{\frac{-\hbar x^2}{2m\omega}}$$

where $k=\sqrt{\frac{\hbar}{2\pi m\omega}}$ is the constant normalization.

Schrödinger equation : harmonic oscillator

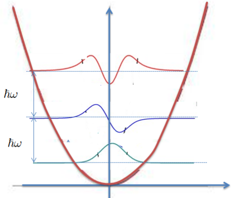
Now, using the raising operator $a^\dagger$ to obtain the highest of energies: the solutions of the Schrödinger's equation

$$\psi_1 = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\psi_0 = K_1 2x\psi_0$$

The general form is

$$\psi_n = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\psi_0 = K_n P_n(x)\psi_0$$

where P_n is called a Hermite polynomial and has n zeros.



Solution of harmonic oscillator

The Hamiltonian operator is

$$\hat{H} = \frac{m\omega^2}{2}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) - \frac{\hbar\omega}{2}$$

$$\hat{H} = \hbar\omega\left(N - \frac{1}{2}\right) = \hbar\omega\left(N^\dagger + \frac{1}{2}\right)$$

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + \frac{m}{2}\omega^2\widehat{x}^2$$

Then the time independent schrödinger equation is given by

$$\begin{aligned} \hat{H}\psi &= E\psi \\ -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{m}{2}\omega^2 x^2\psi &= E\psi \end{aligned}$$

Solution of harmonic oscillator

First the time independent schrödinger equation can be simplified by setting : $y = \sqrt{\frac{m\omega}{\hbar}}x$

$$\begin{aligned}\frac{\partial^2 \psi}{\partial y^2} + (\varepsilon - y^2)\psi &= 0 \\ \varepsilon &= \frac{2E}{\hbar\omega}\end{aligned}$$

We know that $\psi \to 0$ as $|y| \to +\infty$, therefore the equation $\frac{\partial^2 \psi}{\partial y^2} + (\varepsilon - y^2)\psi = 0$ become $\frac{\partial^2 \psi}{\partial y^2} - y^2\psi = 0$ near ∞.

Solution of harmonic oscillator

$$\begin{aligned} \frac{\partial^2\psi}{\partial y^2} &= y^2\psi \\ \psi &= Ce^{-\frac{y^2}{2}} \end{aligned}$$

Let plug this solution in the differential equation to get $\frac{\partial\psi}{\partial y} = -Cye^{-\frac{y^2}{2}}$ and $\frac{\partial^2\psi}{\partial y^2} = Cy^2e^{-\frac{y^2}{2}} - Ce^{-\frac{y^2}{2}}$

$$\begin{aligned} Cy^2e^{-\frac{y^2}{2}} - Ce^{-\frac{y^2}{2}} + C(\varepsilon - y^2)e^{-\frac{y^2}{2}} &= 0 \\ \varepsilon - 1 &= 0 \\ E &= \frac{\hbar\omega}{2} \end{aligned}$$

But we can chose $\psi = P(y)e^{-\frac{y^2}{2}}$ where $P(y) = \sum_{k=0}^{+\infty} a_k y^k$

Solution of harmonic oscillator

$$
\begin{aligned}
\frac{\partial \psi}{\partial y} &= P'(y)e^{-\frac{y^2}{2}} - yP(y)e^{-\frac{y^2}{2}} \\
\frac{\partial^2 \psi}{\partial y^2} &= P''(y)e^{-\frac{y^2}{2}} - 2yP'(y)e^{-\frac{y^2}{2}} + (y^2-1)P(y)e^{-\frac{y^2}{2}}
\end{aligned}
$$

where

$$P'(y) = \sum_{k=0}^{+\infty} k a_k y^{k-1} \Longrightarrow -2yP'(y) = -2\sum_{k=0}^{+\infty} k a_k y^k$$

$$P''(y) = \sum_{k=2}^{+\infty} k\,(k-1)\,a_k y^{k-2} = \sum_{k=0}^{+\infty} (k+1)\,(k+2)\,a_{k+2} y^k$$

Solution of harmonic oscillator

Let plug above terms in the differential equation to get

$$\sum_{k=0}^{+\infty}(k+1)(k+2)\,a_{k+2}y^k - 2\sum_{k=0}^{+\infty}k a_k y^k + (\varepsilon-1)\sum_{k=0}^{+\infty}a_k y^k = 0$$

$$\sum_{k=0}^{+\infty}\left[(k+1)(k+2)\,a_{k+2} + (\varepsilon-2k-1)\,a_k\right]y^k = 0$$

where

$$\begin{aligned}
a_{k+2} &= \frac{(\varepsilon-2k-1)}{(k+1)(k+2)}a_k \\
\varepsilon &= 2k+1 \Longrightarrow E_k = (2k+1)\frac{\hbar\omega}{2} = E_0 + k\hbar\omega \\
E_{k+1} &= E_k + \hbar\omega
\end{aligned}$$