Lecture 4 Particle Waves and Schrodinger's Wave Mechanics

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Topics

1. Particle waves
2. Erwin Schrodinger and his wave mechanics
3. Particle wave function
4. Quantum statistics
5. Wave packet and uncertainty principle

Particle Waves

Max Plank was proposed the idea of *photon* as a particle of EM wave, with energy and momentum of

$$E = \frac{hc}{\lambda}, \; p = \frac{E}{c} = \frac{h}{\lambda}, \; E = pc$$

Louise de Broglie though that if wave can be particle so do particle can be wave. For a particle with momentum p, its wave should has a wavelength of

$$\lambda = \frac{h}{p} - de\ Broglie's\ wavelength$$

where $h = 6.626 \times 10^{-34}[J \cdot s] = 4.135 \times 10^{-15}[eV \cdot s]$ is Plank's constant. ($hc = 12.4 \times 10^{-7} eV \cdot m$) ($1.0eV = 1.6 \times 10^{-19} J$)

Example:

An electron is accelerated to get the kinetic energy of $50eV$, its de Broglie wavelength will be

$$K = \frac{p^2}{2m} = 50eV \mapsto p = \sqrt{2m_c K}, \;\; pc = \sqrt{2m_e c^2 K}$$

$$m_e c^2 = 0.512 MeV \mapsto pc = 7.16[keV] \;\; ([p] = eV/c)$$

$$\mapsto \lambda = \frac{hc}{pc} = \frac{12.4 \times 10^{-7}[eV \cdot m]}{71.6 \times 10^3 [eV]} = 0.17 \times 10^{-10}[m]$$

$$= 0.17^0 A$$

Max Plank

Louise de Broglie

Erwin Schrodinger

Erwin Schrodinger and his wave mechanics

In his PhD thesis, Erwin Schrodinger want to write wave equation of particle wave, in order to know its wave function. He started from free particle with constant momentum p, this corresponds to monochromatic wave with wavelength $\lambda = h/p$. We know its wave function, for $+x$ propagation we have

$$\psi(x,t) = Ae^{ikx - i\omega t},\ k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar},\ \hbar = \frac{h}{2\pi} \tag{1}$$

As we know that the wave function will tell us everything about the wave, and it is also true for the particle wave.

So we can ask the wave function about the energy conservation between particle and its wave-particle, i.e.,

$$\begin{aligned}(E_{particle} - E_{wave-particle})\psi(x,t) &= 0 \\ \mapsto \left(\frac{p^2}{2m} - \hbar\omega\right)\psi(x,t) &= 0\end{aligned} \tag{2}$$

when $E_{wave-particle} = hf = \hbar\omega,\ \omega = 2\pi f$.

Correspondence principle:

From the fact that $p = \hbar k$, let us consider

$$
\begin{aligned}
0 &= \left(\tfrac{\hbar^2 k^2}{2m} - \hbar\omega\right) e^{ikx - i\omega t} \\
&\equiv \left(\tfrac{1}{2m}\left(-i\hbar\tfrac{\partial}{\partial x}\right)^2 - \left(i\hbar\tfrac{\partial}{\partial t}\right)\right) e^{ikx - i\omega t} \\
&\mapsto p = -i\hbar\tfrac{d}{dx},\ E = i\hbar\tfrac{d}{dt}
\end{aligned} \tag{3}
$$

Let us denote $H_0 = \frac{p^2}{2m}$, it is the total free particle energy (it is called Hamiltonian). The particle wave equation will be

$$H_0\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{4}$$

This is known as *Schrodinger's equation* for free particle.

- It is complex equation with complex wave function, i.e., we cannot directly observe this wave but its square.
- Extension for particle with potential energy $U(x)$ can be done by replacing $H_0 \mapsto H = \frac{p^2}{2m} + U(x)$, without any operation by the position x

Particle wave function

Schrodinger's equation in full form is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{5}$$

This is a kind of second order partial differential equation, it is really hard to find solution even for mathematicians.
Actually we don't need to use this full form, physicists interest to describe particle wave existing *here*, not propagating wave from to anywhere like solution from equation (5).
Not propagating wave is known in form of *standing wave*, described by a wave function in which space and time functions are *separated*, so that we need particle wave function in the form

$$\psi(x,t) = \varphi(x)f(t) \tag{6}$$

where $\varphi(x)$ is *stationary particle wave* we need. This kind of particle is said to be in its *stationary state*.

Insertion (6) into (5), we get

$$f(t)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\varphi(x)=\varphi(x)\left(i\hbar\frac{d}{dt}f(t)\right)$$

$$\mapsto \frac{1}{\varphi(x)}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\varphi(x)=\frac{1}{f(t)}\left(i\hbar\frac{d}{dt}f(t)\right)=\alpha \quad (7)$$

$$\frac{1}{f(t)}\left(i\hbar\frac{d}{dt}f(t)\right)=\alpha\mapsto\frac{df(t)}{f(t)}=-i\frac{\alpha}{\hbar}dt$$

$$\ln f(t)=-i\frac{\alpha t}{\hbar}\mapsto f(t)=e^{-i\alpha t/\hbar} \quad (8)$$

When compare to the case of free particle, we observe that

$$\frac{\alpha}{\hbar}=\omega\mapsto\alpha=\hbar\omega=E$$

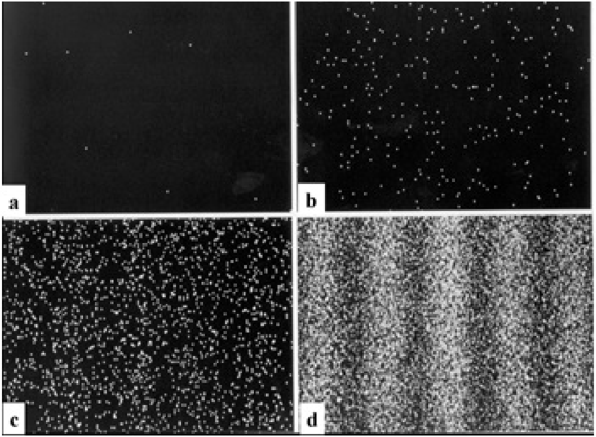
It is the particle energy. From (7) we can have

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\varphi(x)=E\varphi(x) \quad (9)$$

This is the reduced (time-independent) Schrodinger equation for particle wave in its stationary state, *we need to pay attention to*.

Quantum statistics

Do particle really behave like a wave?
Reference to: A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki, and H. Ezawa. American Journal of Physics 57, 117 (1989), *demonstration of electron interference from double slit*.



We observe that a few electrons cannot construct interference pattern but a number of them.
So that observation of particle wave is a kind of statistical measurement. According to fact, Max Born was interpret particle wave function as a *statistical amplitude of its measurement*

$$|\varphi(x)| = \text{a probability density amplitude} \quad (10)$$

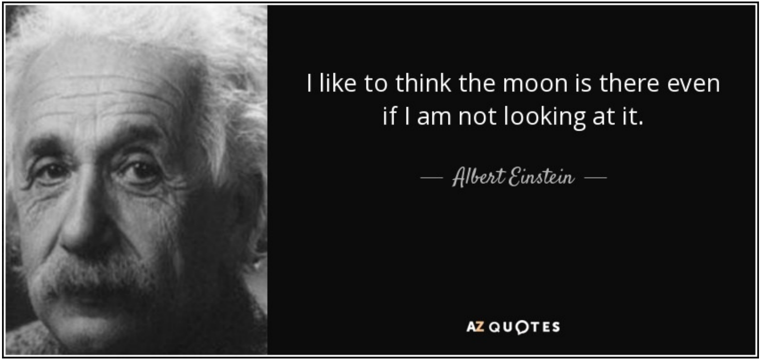
$$|\varphi(x)|^2 = \text{a probability density} \quad (11)$$

$$|\varphi(x)|^2 dx = \text{a probability (chance)} \quad (12)$$

of finding particle between x to $x + dx$.
This requires the *normalization condition* of the particle wave function

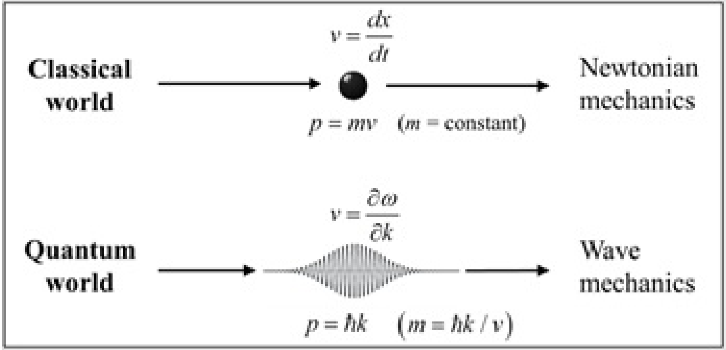
$$\int_a^b |\varphi(x)|^2 dx = 1, \; x \in [a, b] (13)$$

This makes Einstein refuse to believe in quantum physics up to the end of his life.

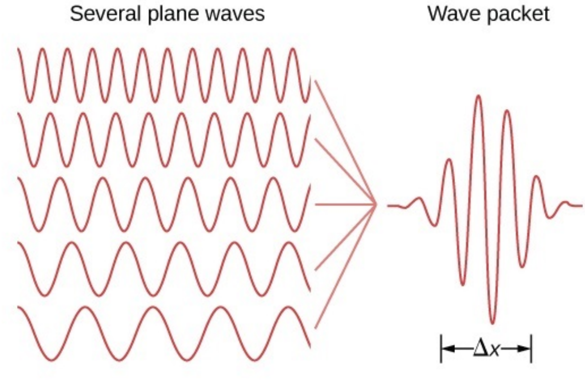


Wave packet and uncertainty principle

At the last step, we have to make a connection between particle wave to the existing point particle at any point or region.



The wave packet can be constructed by superposition of number of plane waves of wave vectors k with a suitable amount or amplitude



Mathematical expression of this is

$$\varphi_{WP}(x) = \sum_k a_k e^{ikx} \mapsto \frac{1}{\sqrt{2\pi}} \int a(k) e^{ikx} dk \qquad (14)$$

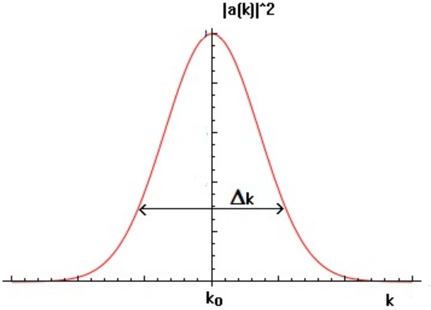
(From Fourier summation to Fourier integral.)

A normalized Gaussian wave packet is constructed from a normalized Gaussian distribution function of the plane wave amplitude

$$a(k) = \frac{1}{\sqrt{\sigma_k\sqrt{\pi}}} e^{-(k-k_0)^2/2\sigma_k^2} \tag{15}$$

$$\mapsto \int |a(k)|^2 dk = \frac{1}{\sigma_k\sqrt{\pi}} \int e^{-(k-k_0)^2/\sigma_k^2} dk = 1 \tag{16}$$

where $\sigma_k = \sqrt{2}\Delta k$ is the (1/e)-width of Gaussian peak of $|a(k)|^2$



Let us determine from (14)

$$\begin{aligned}
\varphi_{WP}(x) &= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma_k\sqrt{\pi}}}e^{ik_0x}\ldots \\
&\quad \ldots\int e^{-(k-k_0)^2/2\sigma_k^2+i(k-k_0)x}dk \\
&= \sqrt{\frac{\sigma_k}{\sqrt{\pi}}}e^{-x^2\sigma_k^2/2+ik_0x} && (17)\\
&= \frac{1}{\sqrt{\sigma_x\sqrt{\pi}}}e^{-x^2/2\sigma_x^2+ik_0x},\ \sigma_x=\frac{1}{\sigma_k} && (18)\\
\mapsto &\quad \int|\varphi_{WP}(x)|^2dx=1 && (19)
\end{aligned}$$

where $\sigma_x=\sqrt{2}\Delta x$, the (1/e)-width of the wave packet.
From (18) we have

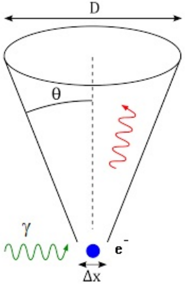
$$\Delta x\Delta k=\frac{1}{2}\mapsto\Delta x\Delta p=\frac{\hbar}{2} \tag{20}$$

It is called *Heisenberg's uncertainty relation*.

For non-Gaussian distribution of the wave packet, the uncertainty relation extended into the form

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Its meaning is that *we cannot have the simultaneous precision of the position and momentum measurements, in the regime of Schrodinger wave mechanics.* The best we can have appear in (20), but it's always greater in generic case. It was first explained by Heisenberg using gamma ray microscope hypothesis



In the energy-time domain, we also have Heisenberg's uncertainty relations between the precision of time and energy measurements in the same form as

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

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Applications of Heisenberg's uncertainty relations

- estimate energy of quantum particle, for example of an electron in hydrogen atom of diameter of $d = 1^0 A$ will have maximum kinetic energy about

$$\Delta x = d, \Delta p = p - 0 \mapsto p = \frac{\hbar}{2d}$$

$$K = \frac{p^2}{2m_e} = \frac{\hbar^2}{8m_e d^2} = \frac{(\hbar c)^2}{8m_e c^2 d^2}$$

$$\hbar c = \frac{12.4 \times 10^{-7} eV \cdot m}{2\pi} = 1.97 \times 10^{-7} eV \cdot m$$

$$\mapsto K = \frac{(1.97 \times 10^{-7} eV \cdot m)^2}{8(0.512 \times 10^6 eV)(10^{-10} m)^2} = 0.95 eV \qquad (21)$$

Let estimate the maximum kinetic energy of a proton inside an atomic nucleus of diameter about $d = 2.4 fm$

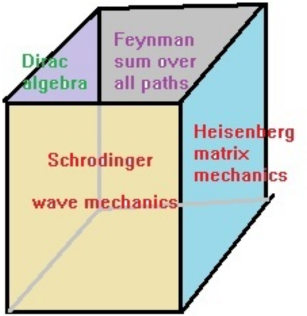
- estimate the life time $\Delta t = \tau$ of unstable particle live with uncertainty of energy ΔE, or vice versa, for example of neutral Pion π_0, has its life time of $\tau = 8.5 \times 10^{-17} s$. We can estimate the uncertainty in mass of the rest pion to be

$$\Delta E = \Delta m_\pi c^2 = \frac{\hbar}{2\tau} = \frac{6.58 \times 10^{-16} eV \cdot s}{2 \times 8.5 \times 10^{-17} s} = 3.87 eV$$
$$\mapsto \Delta m_\pi = 3.87 eV/c^2$$

It is so small when compared to its rest mass of $m_\pi = 134.9 MeV$

Many Faces of Quantum Physics

There appears many faces of quantum physics, i.e, Schrodinger's wave mechanics, Heisenberg's matrix mechanics, Dirac algebraic of kets and bras, and Feynman sum over all paths



We just enter the field through Schrodinger's glasses.