Free Particle in Quantum Mechanics

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A video recording of this lecture is available in Part 1 and Part 2.

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• Consider a particle free to move in one dimension on the real line. No forces act on the particle and so the potential is $V = 0$. The hamiltonian is the kinetic energy $H = p^2/2m$. The time-independent Schrödinger equation for the wave function $\psi(x)$ is

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi''(x) &= E\psi(x) \quad \text{or} \\ \psi''(x) &= -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x). \end{aligned} \tag{1}$$

Here $k = \sqrt{2mE/\hbar^2} \geq 0$ is the positive square root.

• This equation is a eigenvalue problem for the Hamiltonian operator $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ and the eigenvalue E is the energy corresponding to the eigenfunction ψ.

• $\psi(x)$ is called the probability amplitude and according to Born's interpretation, $|\psi(x)|^2 dx$ is the probability for the particle to be within dx of the location x.

• There are two linearly independent solutions e^{ikx} and e^{-ikx} for any $k > 0$. So we have two linearly independent energy eigenstates for each energy eigenvalue $E = \hbar^2 k^2/2m > 0$. We say that the degeneracy of these energy levels is two.

• The energy eigenvalue E must be ≥ 0. If $E < 0$ the solutions to $-(\hbar^2/2m)\psi'' = E\psi$ are real exponentials $e^{\pm\kappa x}$ or $\cosh \kappa x$ and $\sinh \kappa x$ where $\kappa = \sqrt{-2mE/\hbar^2}$.

• In these states, the particle has an ever-growing amplitude of being found at larger and larger values of $|x|$. This is physically unacceptable to describe one or even a stream of particles.

• The ground state is the limiting case $E = 0$ where $k = 0$. The ground state is nondegenerate and corresponds to the constant eigenfunction $\psi(x) = 1$.

• The linear solution $\psi(x) = Ax + B$ with $A \neq 0$ for $E = 0$ is disallowed as the probability density grows without bound as $x \to \pm\infty$.

• However, even in the energy eigenstates $Ae^{\pm ikx}$, the position-space probability distribution ($|Ae^{\pm ikx}|^2 = |A|^2$) is constant and spread out uniformly over all of x-space. None of these eigenfunctions (nor any linear combination $ae^{ikx}+$

be^{-ikx}) is square integrable:

$$\int_{-\infty}^{\infty} |Ae^{ikx}|^2 dx = \int_{-\infty}^{\infty} |A|^2 dx = \infty. \tag{2}$$

The energy eigenstates do not represent localized particles.

• The time dependence of any state is determined by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi. \tag{3}$$

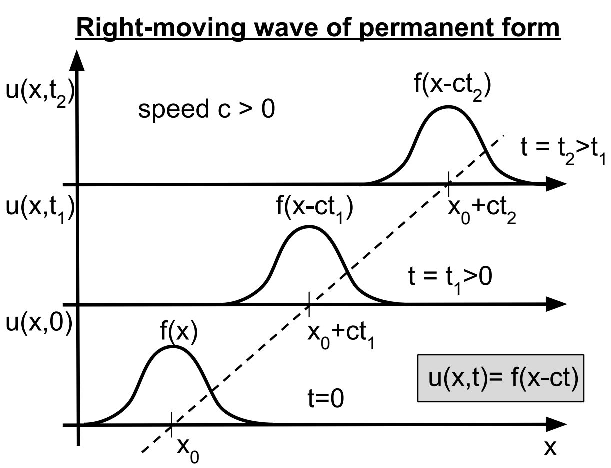
If ψ is an energy eigenstate with $H\psi = E\psi$ then

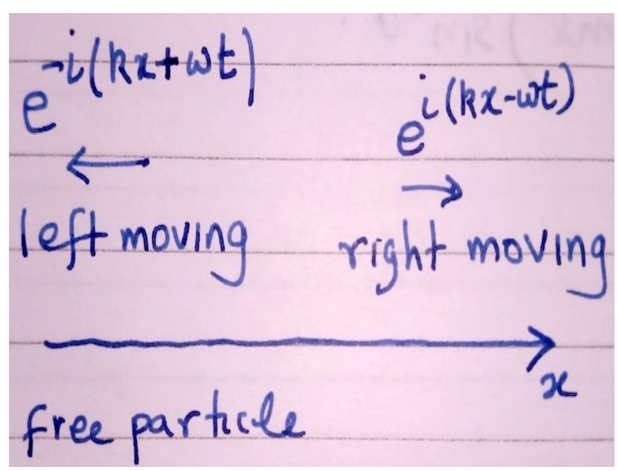
$$\partial_t \psi = -(iE/\hbar)\psi \quad \text{so} \quad \psi(x,t) = \psi(x,0)e^{-iEt/\hbar}. \tag{4}$$

• Thus, the time-dependence of any free particle energy eigenstate with energy $E = \hbar^2 k^2/2m = \hbar\omega$ is

$$(Ae^{ikx} + Be^{-ikx})e^{-iEt/\hbar} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}. \tag{5}$$

This is a linear combination of two traveling waves, a right-moving one and a left-moving one. Let us see why.





• In general, $f(x-ct)$ is a right-moving wave for $c>0$ and a left moving one for $c<0$. Each preserves its shape as it moves.

• The time-dependence $Ae^{i(kx-\omega t)}+Be^{-i(kx+\omega t)}$ can also be written as

$$e^{i(k'x-\omega t)}(A\theta(k'\geq 0)+B\theta(k'\leq 0)) \tag{6}$$

where θ is the Heaviside step function: $\theta(k'\geq 0)$ is 1 for $k'>0$, zero for $k'<0$ and half for $k'=0$. We introduced a new wave number k' which can take both positive and negative values. $k'=k>0$ for right-moving waves and $k'=-k<0$ for left-moving waves.

• To summarize, the energy eigenstates are the plane waves $e^{ik'x}$ for all $k'\in\mathbb{R}$. The eigenstates labeled by k' and $-k'$ are degenerate in energy. To keep notation simple, henceforth we will use k in place of k' and allow it to be both positive and negative.

• The energy eigenstates are called *plane waves* since the wave function $e^{i(kx-\omega t)}$ is constant on the y-z plane which is perpendicular to the direction of propagation. The direction of propagation is $k\hat{x}$, rightward or leftward depending on the sign of k. The wave fronts are planes orthogonal to the wave vector $k\hat{x}$.

• The energy eigenstates are also eigenstates of momentum $\hat{p}=-i\hbar\frac{\partial}{\partial x}$ with eigenvalue $\hbar k$:

$$-i\hbar\partial_x e^{ikx}=\hbar k e^{ikx}. \tag{7}$$

States with momentum eigenvalue $\hbar k > 0$ move to the right and those with momentum $\hbar k < 0$ move to the left.

• The Hamiltonian $\hat{H}$ and momentum $\hat{p}$ have common eigenstates as they commute

$$[H, p] = [p^2/2m, p] = 0. \tag{8}$$

They are simultaneously diagonalizable. Both are diagonal in the plane wave basis e^{ikx} where k ranges over all real numbers.

• Let us now restate our results using Dirac notation. $|k\rangle$ is a momentum eigenstate with eigenvalue $\hbar k$. It is also an energy eigenstate with eigenvalue $\hbar^2 k^2/2m$. The corresponding position-space wave function is

$$\psi_k(x) = \langle x|k\rangle = e^{ikx}. \tag{9}$$

Recall that $\langle k|x\rangle$ is the complex conjugate

$$\langle k|x\rangle = \langle x|k\rangle^* = e^{-ikx}. \tag{10}$$

• The time-dependence of an energy-momentum eigenstate is given by

$$|k, t\rangle = e^{-iEt/\hbar}|k, 0\rangle = e^{-i\omega t}|k\rangle. \tag{11}$$

• Energy eigenstates are also called stationary states. This is because the expectation value of any observable A in an energy eigenstate $\psi_k(x)e^{-i\omega t}$ is independent of time:

$$\langle k, t|A|k, t\rangle = \langle k|e^{i\omega t} A e^{-i\omega t}|k\rangle = \langle k|A|k\rangle. \tag{12}$$

• We have seen that energy/momentum eigenstates $|k\rangle$ are not localized in position.

$$|\psi_k(x)|^2 = |\langle x|k\rangle|^2 = |e^{ikx}|^2 = 1. \tag{13}$$

So a system in a momentum eigenstate is equally likely to be at all locations!

• This is consistent with Heisenberg's uncertainty principle. In a momentum eigenstate, the momentum is known precisely $\Delta p = 0$. Therefore, Δx must be infinite in order not to violate the inequality $\Delta x \Delta p \geq \hbar/2$.

• Energy eigenstates $|k\rangle$ do not represent particles. $|k\rangle$ do not have finite norm either:

$$\langle k|k\rangle = \int_{-\infty}^{\infty} |e^{ikx}|^2 dx = \infty. \tag{14}$$

However, they are orthogonal. To show this, we use the completeness relation

$$\int |x\rangle\langle x| dx = I \tag{15}$$

to evaluate the inner product

$$\begin{aligned} \langle k'|k\rangle &= \int \langle k'|x\rangle\langle x|k\rangle\, dx = \int e^{-ik'x} e^{ikx} dx \\ &= \int e^{i(k-k')x} dx = 2\pi\delta(k-k'). \end{aligned} \tag{16}$$

• So strictly speaking, energy eigenfunctions e^{ikx} do not have a probability interpretation.

• Though the total probability to be between $\pm\infty$ is infinite, we can still speak of relative probabilities. For example, in the state Ae^{ikx} with $k > 0$, the relative probability that a particle coming in from $-\infty$ scatters out to $+\infty$ is $\frac{|A|^2}{|A|^2} = 1$ while the relative probability for it to go back to $-\infty$ is $\frac{0}{|A|^2} = 0$.

• Such non-normalizable wave functions with oscillatory $e^{\pm ikx}$ behavior as $|x| \to \infty$ are called *scattering states*. They correspond to particle trajectories that escape to infinity in classical mechanics.

• On the other hand, *bound states* are represented by normalizable wave functions that decay as $|x| \to \pm\infty$. Bound states correspond to classical particle trajectories that do not escape to infinity. All the eigenstates of the free particle hamiltonian are scattering states.

• We may also draw an analogy with a fluid by computing the probability current density

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^*\psi' - \psi^{*\prime}\psi\right) \tag{17}$$

for the stationary state $\psi(x,t) = Ae^{i(kx-\omega(k)t)}$. We get

$$j(x,t) = |A|^2\frac{\hbar k}{m} = |A|^2 v \tag{18}$$

where $v = p/m$ is the corresponding classical velocity and

$$P(x,t) = |\psi(x,t)|^2 = |A|^2 \tag{19}$$

is the ‘probability’ density. This is similar to ρv for the mass current density in a fluid flow or the electric current density.

• So energy eigenstates can be loosely interpreted as an always-present constant stream of free particles ($|A|^2 dx$ particles in the interval dx). For $k > 0$, they enter from $x = -\infty$ and exit at $x = \infty$.

• Now we would like to describe the evolution of an initial state that represents a particle, i.e., a localized wave packet $\psi(x)$ with finite norm. It cannot be an energy eigenstate, but may be expressed as a linear combination of energy eigenstates (same as momentum eigenstates) which evolve via $e^{-i\omega t}$

$$\psi(x,t) = \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} \, \frac{dk}{2\pi}. \qquad (20)$$

• A particularly useful wave packet is the gaussian one corresponding to the initial state

$$\psi(x) \;=\; A e^{-\frac{x^2}{4a^2}}, \qquad A = \frac{1}{\sqrt{a}(2\pi)^{1/4}} \quad \text{gives}$$

$$||\psi|| \;=\; 1 \quad \text{and} \quad |\psi(x)|^2 = \frac{1}{a\sqrt{2\pi}} e^{-x^2/2a^2}. \qquad (21)$$

Here a is a constant with dimensions of length. The gaussian is an even function of x.

• The expectation value of x in this state is

$$\langle x \rangle_\psi = \frac{\langle \psi | x | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx}{\langle \psi | \psi \rangle} = 0, \qquad (22)$$

since $x|\psi(x)|^2$ is an odd function. So this packet is localized around $x = 0$.

• Similarly, $\psi(x) = Ae^{-(x-x_0)^2/4a^2}$ is localized around $\langle x \rangle = x_0$.

• The width of the packet is $\Delta x = \sqrt{\langle x^2 \rangle} = a$.

• This is a state of zero mean momentum $\langle p \rangle_\psi$ as the integrand $\psi^*(x)(-i\hbar\partial_x)\psi(x)$ in calculating the expectation value of momentum is odd.

• To find the time evolution of this Gaussian wave packet, we write it in the energy-momentum basis, which involves evaluating the Fourier transform:

$$\begin{aligned}
\tilde{\psi}(k) &= \langle k|\psi\rangle = \int dx \langle k|x\rangle\langle x|\psi\rangle \quad \text{or} \\
\tilde{\psi}(k) &= \int dx\, \psi(x) e^{-ikx} = \int A\, e^{-\left(\frac{x^2}{4a^2}+ikx\right)} dx \\
&= 2aA\sqrt{\pi} e^{-a^2k^2} = 2\sqrt{a}\left(\frac{\pi}{2}\right)^{1/4} e^{-a^2k^2}. \qquad (23)
\end{aligned}$$

The integral is done by *completing the square*, the change of variable

$$y = \frac{x}{2a} + ika \quad \text{and} \quad \text{using} \quad \int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}. \qquad (24)$$

The Fourier transform of the gaussian is again a gaussian.

• The width in momentum space is $\Delta p = \sqrt{\langle p^2 \rangle} = \frac{\hbar}{2a}$. We see that the gaussian wave function minimizes the uncertainty product $\Delta x \Delta p = a\frac{\hbar}{2a} = \frac{\hbar}{2}$.

• Time evolution is simple in the energy basis

$$\begin{aligned}\psi(x,t) &= \int [dk]\tilde{\psi}(k) e^{-iEt/\hbar} e^{ikx} \\ &= 2aA\sqrt{\pi} \int [dk] e^{-\left[k^2\left(a^2+\frac{i\hbar t}{2m}\right)-ikx\right]}. \end{aligned} \tag{25}$$

This is again a Gaussian integral done by completing the square $l = k\sqrt{a^2+\frac{i\hbar t}{2m}} - \frac{1}{2}\frac{ikx}{k\sqrt{a^2+\frac{i\hbar t}{2m}}}$. We get

$$\psi(x,t) = \frac{1}{(2\pi)^{1/4}\sqrt{a+\frac{i\hbar t}{2ma}}} \exp\left\{-\frac{x^2}{4\left(a^2+\frac{i\hbar t}{2m}\right)}\right\} \tag{26}$$

The probability density at time t is

$$\begin{aligned}|\psi(x,t)|^2 &= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{a^2+\frac{\hbar^2 t^2}{4m^2a^2}}} \exp\left\{\frac{-x^2}{2\left(a^2+\frac{\hbar^2t^2}{4m^2a^2}\right)}\right\} \\ &= \frac{1}{a(t)\sqrt{2\pi}} e^{-x^2/2a(t)^2}. \end{aligned} \tag{27}$$

Here $a(t) \equiv \sqrt{a^2+\frac{\hbar^2t^2}{4m^2a^2}}$.

• We see that a gaussian wave packet remains a gaussian wave packet under free particle Schrödinger time-evolution. However, the width of the Gaussian $\sqrt{\langle x^2\rangle} = a(t)$ grows with time. It remains centered at $\langle x\rangle = 0$.

• This is an indication of the dispersive behavior of de Broglie matter waves, the wave packet spreads out as its component plane waves travel at different phase speeds $c(k) = \omega/k = E/\hbar k = \hbar k/2m$. Higher wave number plane waves travel faster.

• The propagation of light in vacuum is nondispersive since all wave numbers (colors) of light travel at the same speed (the speed of light in vacuum, $c_{\rm light}$). The dispersion relation is $\omega = c_{\rm light} k$). By contrast, in a dispersive optical medium, where the angular frequency ω is a nonlinear function of wave number k, plane waves with different wave numbers travel at distinct speeds. This leads to the broadening of a pulse of light and the separation of various component colors of white light propagating through such a medium.

• Note that the group speed $\frac{\partial \omega}{\partial k}$ evaluated at the peak $k = 0$, gives the speed at which the wave packet as a whole moves. Here it is zero, the gaussian wave packet does not move.

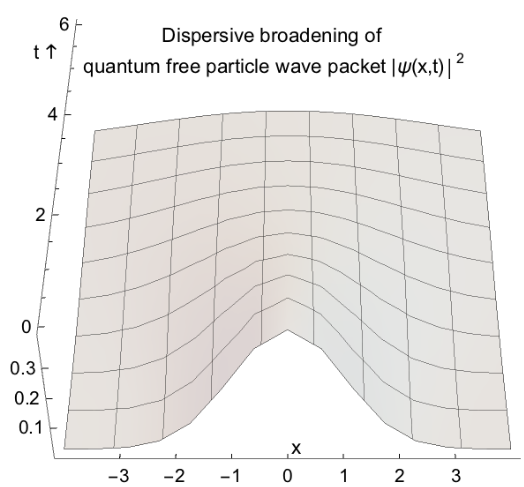


Figure 1: Dispersive broadening of a free particle Gaussian wave packet in 1d quantum mechanics. The probability density $|\psi(x,t)|^2 = e^{-x^2/2a(t)^2}/\sqrt{2\pi}a(t)$ where $a(t) = (a^2 + \hbar^2 t^2/4a^2 m^2)^{\frac{1}{2}}$ is plotted over the x-t plane in units where the initial width $a = 1$ and the particle mass and Planck's constant $m = \hbar = 1$. In these units $\tau = 2$.

• How fast does the wave packet disperse? We can write the width as

$$a(t) = a\sqrt{1+\frac{\hbar^2 t^2}{4m^2a^4}} = a\sqrt{1+\frac{t^2}{\tau^2}}, \quad \tau = \frac{2ma^2}{\hbar}. \quad (28)$$

τ has dimensions of time and gives the characteristic broadening time. For $t \ll \tau$ there is not much broadening. For example, if we make a measurement of position with accuracy a, the wave function 'collapses' roughly to a packet of width a.

• A subsequent measurement of position (after time t) will yield roughly the same position as long as $t \ll \tau$. If we wait a long time $t \gg \tau$ to make the next measurement, the wave packet broadens significantly: by a factor of $\sqrt{1+t^2/\tau^2}$. After such a time, we are no longer guaranteed to get roughly the same position.

• For example, suppose we know the position of the center of a tennis ball of mass 60g to within an accuracy of $a \sim 1$mm. If we model the center of the tennis ball as a wave packet with a width equal to the above accuracy, then $\tau = 1.8 \times 10^{26} s$. So it takes a very long time for the quantum mechanical broadening of the tennis ball wave packet to become significant. In other words, we will get the same position even if we wait several centuries between successive measurements of the position of a tennis ball (that was initially at rest and was acted upon by no forces).

• By contrast, τ is substantially shorter for an electron whose location is initially known to a precision comparable to the size of an atom. This is because the mass of an electron (9.1×10^{-31} kg) is so much smaller than that of a tennis ball.

• Interestingly, the uncertainty product $\Delta x \Delta p$ remains equal to $\hbar/2$ at all times, since all that changes is the width $a(t)$, and $\Delta x \Delta p = \hbar/2$ was independent of the width a.

• The expectation value of energy of the gaussian wave packet at $t = 0$ is

$$\langle H \rangle_{t=0} = \frac{\langle p^2 \rangle}{2m} = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{8ma^2}. \tag{29}$$

As we would expect from Ehrenfest's theorem on the evolution of expectation values, $\langle H \rangle$ is constant in time. This can be explicitly checked most easily in momentum space, where $\tilde{\psi}(k,t) = 2aA\sqrt{\pi} e^{-k^2(a^2 + \frac{i\hbar t}{2m})}$

$$\begin{aligned} \langle H \rangle_t &= \int [dk] \, |\tilde{\psi}(k,t)|^2 \, \frac{\hbar^2 k^2}{2m} \\ &= \frac{\hbar^2 a^2 A^2}{m} \int dk \, k^2 e^{-2a^2k^2} = \frac{\hbar^2}{8ma^2}. \end{aligned} \tag{30}$$

• This is a general feature, the expectation value of energy in *any* state is constant under Schrödinger time evolution, provided the hamiltonian is hermitian and does not depend explicitly on time. To see this we note that $i\hbar\dot{\psi} = H\psi$ and $-i\hbar\dot{\psi}^* = (H\psi)^*$, so that

$$i\hbar\partial_t \int \psi^* H \psi \; = \; i\hbar \int \left(\dot{\psi}^* H \psi + \psi^* H \dot{\psi} \right) dx$$

$$\begin{aligned} &= \int \left(-(H\psi)^* H\psi + \psi^* H H\psi\right) dx \\ &= -\langle H\psi | H\psi\rangle + \langle \psi | HH\psi\rangle = 0 \end{aligned} \quad (31)$$

since $H^\dagger = H$ is hermitian.

• So far, our wave packet represented a particle that was on average at rest. To get a gaussian wave packet with non-zero mean momentum $\langle p\rangle = \hbar k_0$, we merely have to center the gaussian at k_0 in momentum space

$$\tilde{\psi}(k) = 2aA\sqrt{\pi} e^{-a^2(k-k_0)^2} \quad (32)$$

so that $\langle \hbar \hat{k}\rangle = \hbar k_0$. This corresponds to the wave packet

$$\begin{aligned} \psi(x) &= \int [dk] e^{ikx} 2Aa\sqrt{\pi} e^{-a^2(k-k_0)^2} \\ &= e^{ik_0 x} \int [dl] e^{ilx} 2aA\sqrt{\pi} e^{-a^2 l^2} \\ &= A e^{ik_0 x} e^{-x^2/4a^2}. \end{aligned} \quad (33)$$

Check directly that $\langle p\rangle = \hbar k_0$ by observing that $\psi^*\psi' = i\psi^* k_0 \psi_0 e^{ik_0 x} + \psi^* e^{ik_0 x}\psi_0'$, where $\psi = \psi_0 e^{ik_0 x}$. The second term does not contribute to $\langle \hat{p}\rangle$ as it is odd and the first gives $\langle p\rangle = \hbar k_0$.

• The gaussian wave packet with non-zero mean momentum also has minimal uncertainty product $\Delta x \Delta p = \hbar/2$. $\Delta x = a$ is unaffected by the phase $e^{ik_0 x}$. $\langle p\rangle = \hbar k_0$. $\langle p^2\rangle = \hbar^2 k_0^2 + \frac{\hbar^2}{4a^2}$ is most easily evaluated in k-space. Thus $\langle p^2\rangle - \langle p\rangle^2 = \frac{\hbar^2}{4a^2}$ is independent of k_0. So $\Delta p = \hbar/2a$ and $\Delta x \Delta p = \hbar/2$.