Chapter 5: Simple problems in one dimension

5.1 The free particle

$$\hat{H} = \frac{\hat{P}^2}{2m} \qquad i\hbar\,|\dot{\psi}\rangle = \hat{H}|\psi\rangle = \frac{\hat{P}^2}{2m}|\psi\rangle$$

The stationary states are $|E(t)\rangle = |E\rangle e^{-iEt/\hbar}$

where $|E\rangle$ are the eigenstates of $\hat{H}$:

$$\hat{H}|E\rangle = \frac{\hat{P}^2}{2m}|E\rangle = E|E\rangle$$

Since eigenstates of $\hat{P}$ are also eigenstates of $\hat{P}^2$, we know that

$$\frac{\hat{P}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle$$

These $|p\rangle$-eigenstates solve the eigenvalue problem for $\hat{H}$

if $\left(\frac{\hat{P}^2}{2m} - E\right)|p\rangle = \left(\frac{p^2}{2m} - E\right)|p\rangle = 0 \Rightarrow \boxed{E = \frac{p^2}{2m}} \geq 0$

continuous spectrum!

$\rightarrow p = \pm\sqrt{2mE} \Rightarrow$ 2 solutions for each E:

$|E,+\rangle = |p = \sqrt{2mE}\rangle$ (right- and

$|E,-\rangle = |p = -\sqrt{2mE}\rangle$ left-moving particles)

$\Rightarrow$ each eigenvalue E is two-fold degenerate;

$$\langle E,+|E,-\rangle = \langle p = +\sqrt{\ }\,|\,p = -\sqrt{\ }\rangle = 0$$

$\Rightarrow \boxed{|E\rangle = \beta\,|p = +\sqrt{2mE}\rangle + \gamma\,|p = -\sqrt{2mE}\rangle}$ is also an eigenstate with eigenvalue E

It represents a state in which the particle can be caught either rightmoving or leftmoving with momentum $|p| = \sqrt{2mE}$. $\left(P(\text{right}) = \frac{|\beta|^2}{|\beta|^2 + |\gamma|^2}.\right)$

Due to the degeneracy of each eigenvalue E,

$$\int_0^\infty dE \, |E\rangle\langle E|$$ is not a complete decomposition of the

identity operator. To completely span the Hilbert space, need two orthogonal basis states $|p=+\sqrt{2mE}\rangle$ and $|p=-\sqrt{2mE}\rangle$ for each E. Hence

$$\hat{I} = \int_{-\infty}^{\infty} dp \, |p\rangle\langle p|$$

The states $|p\rangle$ and $|-p\rangle$ have the same energy $E = \frac{p^2}{2m}$, so negative p and positive complement each other to fully span the Hilbert space.

Propagator:

$$\hat{U}(t) = \int_{-\infty}^{\infty} |p\rangle\langle p| \, e^{-iE(p)t/\hbar} = \hat{U}(t,0)$$

[Note: the totally free particle discussed here presents a different problem from a free particle confined inside a box! Different eigenvalues E, different eigenstates $|E\rangle$!]

In the x-basis:

$$\langle x|\hat{U}(t)|x'\rangle = U(x,t;x',0) = \int_{-\infty}^{\infty} dp \, \langle x|p\rangle\langle p|x'\rangle e^{-i\frac{p^2}{2m}t/\hbar}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp \, e^{ip(x-x')/\hbar} \, e^{-ip^2t/2m\hbar}$$

$$= \sqrt{\frac{m}{2\pi i\hbar t}} \, e^{im(x-x')^2/2\hbar t}$$

$$\Rightarrow \quad \psi(x,t) \equiv \langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dx' \langle x|\hat{U}(t)|x'\rangle\langle x'|\psi(0)\rangle$$

$$= \int_{-\infty}^{\infty} dx'\, U(x,t;x',0)\,\psi(x',0)$$

For other initial time t':

$$\boxed{\psi(x,t) = \int_{-\infty}^{\infty} dx'\, U(x,t;x',t')\,\psi(x',t')} \qquad (*)$$

If $\psi(x',t') = \delta(x'-x_0')$, then

$$\psi(x,t) = U(x,t;x_0',t')$$

$\Rightarrow$ $U(x,t;x_0',t')$ is the wave function of a particle at time t that started out perfectly localized at x_0' at earlier time t'.

Equation $(*)$ then states that if you know how an initial δ-function evolves ($U(x,t;x',t')$), then you can figure out how any $\psi(x',t')$ evolves, by weighting $U(x,t;x',t')$ with $\psi(x',t')$ and summing over all x'.

Time evolution of a Gaussian wave packet

Consider $\psi(x',t=0) = e^{ip_0x'/\hbar}\,\dfrac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}}$

This wave function describes a particle in a state with mean position $\langle\hat{X}\rangle = 0$, position uncertainty $\Delta X = \frac{\Delta}{\sqrt{2}}$, mean momentum $\langle\hat{P}\rangle = p_0$ and momentum uncertainty $\Delta P = \frac{\hbar}{\Delta\sqrt{2}}$.

Using Eq. (*) together with the expression on p. 110 for the propagator,

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \sqrt{\frac{m}{2\pi i\hbar t}}\, e^{\frac{im(x-x')^2}{2\hbar t}} \cdot e^{ip_0x'/\hbar} \frac{e^{-\frac{x'^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}},$$

completing the square in x' in the exponent and doing the Gaussian integral gives

$$\psi(x,t) = \frac{1}{\left(\pi\left(\Delta + \frac{i\hbar t}{m\Delta}\right)^2\right)^{1/4}}\, e^{ip_0\left(x-\frac{1}{2}\frac{p_0}{m}t\right)/\hbar}\, e^{-\frac{\left(x-\frac{p_0}{m}t\right)^2}{2\Delta^2\left(1+\frac{i\hbar}{m\Delta^2}t\right)}}.$$

This looks pretty awful, but let's look at the probability density for the particle, $\frac{dP}{dx}(x,t) = |\psi(x,t)|^2$:

$$\frac{dP}{dx}(x,t) = \frac{1}{\sqrt{\pi\left(\Delta^2 + \frac{\hbar^2t^2}{m^2\Delta^2}\right)}}\, e^{-\frac{\left(x-\frac{p_0}{m}t\right)^2}{\Delta^2+\frac{\hbar^2t^2}{m^2\Delta^2}}}$$

The main features of this result are

(i) mean position of particle $\langle\hat{X}\rangle = \int_{-\infty}^{\infty} x\frac{dP}{dx}dx = \frac{p_0}{m}t = vt$

where the particle's velocity is $\boxed{v = \frac{p_0}{m} = \frac{\langle\hat{P}\rangle}{m}}$

$$\Rightarrow \boxed{\langle\hat{X}\rangle = \frac{\langle\hat{P}\rangle}{m}t}$$ classical EOM for the mean values!

"Ehrenfest theorem"

(ii) width of Gaussian packet increases with time:

$$\Delta X(t) = \frac{\Delta(t)}{\sqrt{2}} = \frac{\Delta}{\sqrt{2}}\sqrt{1+\frac{\hbar^2t^2}{m^2\Delta^4}} = \Delta X(0)\sqrt{1+\frac{\hbar^2t^2}{m\Delta^4}}$$

reflect uncertainty in the initial momentum (velocity)

Since $\Delta v(0) = \frac{\Delta P(0)}{m} = \frac{\hbar}{\sqrt{2}m\Delta}$, $\Delta X(t)$ grows for large t like $\boxed{\Delta X(t) \approx t\cdot\Delta v(0)}$

Note: The existence of an unavoidable non-zero uncertainty $\Delta v(0)$ of the initial velocity is a purely quantum mechanical feature; its effect on the position uncertainty at large times can be understood classically.

For a macroscopic particle of mass, say, $m = 1g$, with an initial uncertainty of the position of its center of mass of order 10^{-13} cm (i.e. the size of a proton – the atomic nucleus of hydrogen) we find for the initial uncertainty of the velocity

$$\Delta v(0) \simeq \frac{\hbar}{\sqrt{2}\, m \Delta} \approx 10^{-16} \frac{m}{s}$$

For the position uncertainty to grow to 1 micron (still pretty small and only visible under a microscope) it would take 300 years! This is one of the reasons why Newtonian physics worked so well for almost 3 centuries, and why quantum mechanics was not discovered earlier.

Particle in a potential $V(x)$

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{X})$$

$$\hat{H}|E\rangle = E|E\rangle \longrightarrow \int_{-\infty}^{\infty} \langle x| \frac{\hat{P}^2}{2m} + V(\hat{X}) |x'\rangle \langle x'|E\rangle = E\langle x|E\rangle$$

$$\Longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\psi_E(x) = E\psi_E(x)$$

$$\Rightarrow \boxed{\psi_E'' = -\frac{2m(E - V(x))}{\hbar^2}\psi_E}$$