Equations and Derivations for Episode 3

Let's Talk QM Podcast

by

Dr. Dhokarh

Heisenberg's uncertainty principle

$$\Delta x \times \Delta p_x \geq \frac{\hbar}{2} \tag{1}$$

Some notation:

$$\begin{aligned}(\Delta x)^2 &\equiv \mathrm{Var}(x) = \langle (x - \langle x \rangle)^2 \rangle \\ (\Delta p_x)^2 &\equiv \mathrm{Var}(p_x) = \langle (p_x - \langle p_x \rangle)^2 \rangle\end{aligned} \tag{2}$$

We define two new operators α, β as,

$$\begin{aligned}&\alpha \equiv x - \langle x \rangle \\ &\beta \equiv p_x - \langle p_x \rangle = -i\hbar \left(\frac{\mathrm{d}}{\mathrm{d}x} - \langle \frac{\mathrm{d}}{\mathrm{d}x} \rangle \right)\end{aligned} \tag{3}$$

The variances are calculated as,

$$\begin{aligned}(\Delta x)^2 = \langle \alpha^2 \rangle = \int \mathrm{d}x\, \psi^*(x) \alpha^2 \psi(x) \\ (\Delta p_x)^2 = \langle \beta^2 \rangle = \int \mathrm{d}x\, \psi^*(x) \beta^2 \psi(x)\end{aligned} \tag{4}$$

From the definition,

$$\begin{aligned}\beta^* &= -\beta \\ \langle \alpha \rangle &= 0 \\ \langle \beta \rangle &= 0\end{aligned} \tag{5}$$

Cauchy-Schwarz inequality

$$\left|\sum_{k=1}^{n} a_k b_k^*\right|^2 \leq \sum_{k=1}^{n} |a_k|^2 \sum_{k=1}^{n} |b_k|^2 \tag{6}$$

For real vectors, a_k, b_k are real, so $b_k^* = b_k$ and absolute value sign is also redundant. The norm of $\boldsymbol{a}$ is,

$$\|\boldsymbol{a}\| = \left(\sum_{k=1}^{n} |a_k|^2\right)^{1/2} \tag{7}$$

The equality sign in (6) holds iff $b_k = \lambda a_k$. In the case of functions in a Hilbert space, this generalizes to

$$\left|\int \mathrm{d}x\, f^*(x) g(x)\right|^2 \leq \int \mathrm{d}x\, |f(x)|^2 \int \mathrm{d}x'\, |g(x')|^2 \tag{8}$$

The norm of f is

$$\|f\| = \left(\int \mathrm{d}x\, |f(x)|^2\right)^{1/2} \tag{9}$$

and the equality sign holds analogously iff

$$g = \lambda f \tag{10}$$

Here is how to derive this inequality,

$$0 \leq \int \mathrm{d}x \left| f - g \frac{\int \mathrm{d}y f g^*}{\int \mathrm{d}z |g|^2} \right|^2 = \int \mathrm{d}x \left(f - g \frac{\int \mathrm{d}y f g^*}{\int \mathrm{d}z |g|^2} \right) \left(f^* - g^* \frac{\int \mathrm{d}y' f^* g}{\int \mathrm{d}z |g|^2} \right) \tag{11}$$

Expanding the product of the terms in brackets,

$$\begin{aligned} 0 &\leq \int \mathrm{d}x |f|^2 - \frac{\int \mathrm{d}y f g^* \int \mathrm{d}y' f^* g}{\int \mathrm{d}z |g|^2} \\ \Rightarrow \left| \int \mathrm{d}y\, f^* g \right|^2 &\leq \int \mathrm{d}x\, |f|^2 \int \mathrm{d}z\, |g|^2 \end{aligned} \tag{12}$$

Deriving the uncertainty principle

Start with the product $(\Delta x)^2 \times (\Delta p_x)^2$ which using equation (4), is

$$\langle \alpha^2 \rangle \times \langle \beta^2 \rangle = \int \mathrm{d}x\, \psi^*(x)\alpha^2\psi(x) \int \mathrm{d}x'\, \psi^*(x')\beta^2\psi(x') \tag{13}$$

Identifying $f = \alpha\psi$ and since Cauchy-Schwarz inequality has the term, $\int |f|^2 = \int f^* f$, the first integral can be written as,

$$\int \mathrm{d}x\, \psi^*(x)\alpha^2\psi(x) = \int \mathrm{d}x\, \alpha^*\psi^*(x)\, \alpha\psi(x) \tag{14}$$

Note that $\alpha = \alpha^*$ and it is multiplicative. The integral involving β is more involved (here we identify, $g = \beta\psi$). We start with,

$$\int \mathrm{d}x'\, \beta(\psi^*\beta\psi) = \int \mathrm{d}x'\, p_x(\psi^*\beta\psi) - \langle p_x \rangle \int \mathrm{d}x'\, \psi^*\beta\psi \tag{15}$$

Recall equation (5),

$$\int \mathrm{d}x'\, \psi^*\beta\psi = \langle \beta \rangle = 0 \tag{16}$$

and therefore,

$$\int \mathrm{d}x'\, \beta(\psi^*\beta\psi) = \int \mathrm{d}x'\, p_x(\psi^*\beta\psi) = -i\hbar \int \mathrm{d}x' \frac{\mathrm{d}}{\mathrm{d}x'}(\psi^*\beta\psi) = 0 \tag{17}$$

So we have,

$$\begin{aligned} 0 = \int \mathrm{d}x'\, p_x(\psi^*\beta\psi) &= \int \mathrm{d}x'\, p_x(\psi^*)\beta\psi + \int \mathrm{d}x'\, \psi^* p_x(\beta\psi) \\ \Rightarrow \int \mathrm{d}x'\, \psi^* p_x(\beta\psi) &= -\int \mathrm{d}x'\, (p_x\psi^*)\beta\psi \\ \Rightarrow \int \mathrm{d}x'\, \psi^*\beta^2\psi &= -\int \mathrm{d}x'\, (\beta\psi^*)\beta\psi = \int \mathrm{d}x'\, (\beta^*\psi^*)\beta\psi \end{aligned} \tag{18}$$

Continuing with $f = \alpha\psi, g = \beta\psi$, we have now using the Cauchy-Schwarz inequality,

$$\begin{aligned} &\int \mathrm{d}x\, \alpha^*\psi^*(x)\, \alpha\psi(x) \int \mathrm{d}x'\, (\beta^*\psi^*)\beta\psi \geq \left| \int \mathrm{d}x\, \alpha^*\psi^*(x)\beta\psi(x) \right|^2 \\ &\Rightarrow (\Delta x)^2 \times (\Delta p_x)^2 \geq \left| \int \mathrm{d}x\, \psi^*(x)\alpha\beta\psi(x) \right|^2 \end{aligned} \tag{19}$$

as the integral on the RHS

$$\int \mathrm{d}x\, \alpha^* \psi^* \beta\psi = \int \mathrm{d}x\, \psi^* \alpha\beta\psi \tag{20}$$

Now we know that

$$\begin{aligned} |z|^2 &= (\mathrm{Re}(z))^2 + (\mathrm{Im}(z))^2 \text{ where} \\ \mathrm{Re}(z) &= \frac{z + z^*}{2} \\ \mathrm{Im}(z) &= \frac{z - z^*}{2i} \end{aligned} \tag{21}$$

Consider,

$$\begin{aligned} z &= \int \mathrm{d}x\, \psi^* \alpha\beta\psi \text{ so that,} \\ \mathrm{Re}(z) &= \frac{\int \mathrm{d}x\, (\psi^*\alpha\beta\psi + \psi\alpha\beta^*\psi^*)}{2} \\ \mathrm{Im}(z) &= \frac{\int \mathrm{d}x\, (\psi^*\alpha\beta\psi - \psi\alpha\beta^*\psi^*)}{2i} \end{aligned} \tag{22}$$

Now the second piece (using equation (5))

$$\int \mathrm{d}x\, \psi\alpha\beta^*\psi^* = -\int \mathrm{d}x\, (\beta\psi^*)\psi\alpha \tag{23}$$

As before (equations (17) and (18)),

$$\begin{aligned} 0 = \int \mathrm{d}x'\, \beta(\psi^*\alpha\psi) = \int \mathrm{d}x'\, p_x(\psi^*\alpha\psi) = \int \mathrm{d}x'\, (p_x\psi^*)\alpha\psi + \int \mathrm{d}x'\, \psi^* p_x(\alpha\psi) \\ \Rightarrow -\int \mathrm{d}x'\, (\beta\psi^*)\alpha\psi = \int \mathrm{d}x'\, \psi^*\beta(\alpha\psi) \end{aligned} \tag{24}$$

With this,

$$\begin{aligned} \mathrm{Re}(z) &= \frac{\int \mathrm{d}x\, \psi^*(\alpha\beta + \beta\alpha)\psi)}{2} \\ \mathrm{Im}(z) &= \frac{\int \mathrm{d}x\, \psi^*(\alpha\beta - \beta\alpha)\psi}{2i} \end{aligned} \tag{25}$$

In the $\mathrm{Im}(z)$ the commutator $[\alpha, \beta]$ shows up! Working this out,

$$\begin{aligned}[\alpha, \beta] = (x - \langle x \rangle)(p_x - \langle p_x \rangle) - (p_x - \langle p_x \rangle)(x - \langle x \rangle) = [x, p_x] = i\hbar \\ \Rightarrow \mathrm{Im}(z) = \frac{i\hbar}{2i} \int \mathrm{d}x \, \psi^* \psi = \frac{\hbar}{2}\end{aligned} \tag{26}$$

The RHS of equation (19) is,

$$\begin{aligned}&\left| \int \mathrm{d}x \, \psi^*(x) \alpha \beta \psi(x) \right|^2 = |z|^2 = \frac{(\int \mathrm{d}x \, \psi^* (\alpha\beta + \beta\alpha) \psi)^2}{4} + \frac{\hbar^2}{4} \\ &\text{which} \implies \\ &(\Delta x)^2 \times (\Delta p_x)^2 \geq \frac{\hbar^2}{4} + \frac{(\int \mathrm{d}x \, \psi^* (\alpha\beta + \beta\alpha) \psi)^2}{4} \\ &\Rightarrow (\Delta x)^2 \times (\Delta p_x)^2 \geq \frac{\hbar^2}{4}\end{aligned} \tag{27}$$

Taking positive square roots leads to,

$$\Delta x \times \Delta p_x \geq \frac{\hbar}{2} \tag{28}$$

which is the famous uncertainty principle.

Minimum uncertainty wave packet

Note that for equality, i.e.,

$$\Delta x \times \Delta p_x = \frac{\hbar}{2} \tag{29}$$

two conditions must hold, the condition in equation (10),

$$f = \lambda g, \text{where } \lambda \text{ is a complex constant;} \tag{30a}$$

$$\text{and from equation (27)} \int \mathrm{d}x \, \psi^* (\alpha\beta + \beta\alpha) \psi = 0 \tag{30b}$$

Working with the first condition,

$$\begin{aligned}\alpha\psi = \lambda\beta\psi \Rightarrow p_x \psi - \langle p_x \rangle \psi = \frac{x - \langle x \rangle}{\lambda} \\ \Rightarrow \frac{\mathrm{d}\psi(x)}{\mathrm{d}x} = \frac{i}{\lambda\hbar}(x - \langle x \rangle)\psi(x) + \frac{i \langle p_x \rangle}{\hbar} \psi(x)\end{aligned} \tag{31}$$

The solution to this ODE is,

$$\psi(x) = N \exp\left(\frac{i}{2\lambda\hbar}(x - \langle x\rangle)^2 + \frac{i\langle p_x\rangle}{\hbar}x\right) \tag{32}$$

N is determined using the normalization $\int |\psi|^2 = 1$. The second condition, equation (30b), is from equation (25), $\mathrm{Re}(z) = 0$, so that z is pure imaginary, i.e.,

$$z = \int \mathrm{d}x\, \psi^* \alpha\beta\psi = \frac{1}{\lambda}\int \mathrm{d}x\, \psi^* \alpha^2 \psi \tag{33}$$

is pure imaginary, where in the second equality, $\alpha\psi = \lambda\beta\psi$ is used. This means that λ is pure imaginary, i.e. $\lambda = i\kappa$ where κ is real. With this

$$\psi(x) = N \exp\left(\frac{(x - \langle x\rangle)^2}{2\kappa\hbar} + \frac{i\langle p_x\rangle}{\hbar}x\right) \tag{34}$$

Note that

$$\langle p_x\rangle = \frac{\hbar}{i}\int \mathrm{d}x\, \psi^* \frac{\mathrm{d}\psi}{\mathrm{d}x} \tag{35}$$

is real. How do we know this?
From Ehrenfest's theorem we have,

$$\frac{\langle \boldsymbol{p}\rangle}{m} = \frac{\mathrm{d}\langle \boldsymbol{r}\rangle}{\mathrm{d}t} \tag{36}$$

Another way is to look at this in momentum space (see equation (24) on page 4, from episode one)

$$\langle \boldsymbol{p}\rangle = \int \mathrm{d}^3p\, \boldsymbol{p}\, |\phi|^2 \tag{37}$$

There is yet another way, which involves the fact that $\boldsymbol{p}$ is a Hermitian operator.

With this we have,

$$\psi^*(x) = N^* \exp\left(\frac{(x - \langle x\rangle)^2}{2\kappa\hbar} - \frac{i\langle p_x\rangle}{\hbar}x\right) \tag{38}$$

so that, for the normalization condition

$$1 = \int_{-\infty}^{\infty} \mathrm{d}x\, |\psi(x)|^2 = \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(x)\psi(x) = |N|^2 \int_{-\infty}^{\infty} \mathrm{d}x\, \exp\left(\frac{(x - \langle x\rangle)^2}{\kappa\hbar}\right) \tag{39}$$

For this integral to converge, we require, $\kappa < 0$, so that $\kappa = -|\kappa|$ and the integral becomes,

$$|N|^2 \int_{-\infty}^{\infty} \mathrm{d}x \, \exp\left(-\frac{(x - \langle x \rangle)^2}{|\kappa|\hbar}\right) = 1 \tag{40}$$

Now,

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \exp(-ax^2) = \sqrt{\frac{\pi}{a}}, \text{ for } a > 0 \tag{41}$$

so that

$$|N|^2 \sqrt{\pi|\kappa|\hbar} = 1 \tag{42}$$

To determine $|\kappa|$ we can use

$$(\Delta x)^2 = \langle \alpha^2 \rangle = \int \mathrm{d}x \, \psi^*(x) \alpha^2 \psi(x) = \int \mathrm{d}x \, (x - \langle x \rangle)^2 |\psi(x)|^2 \tag{43}$$

It is also possible to use $\langle \beta^2 \rangle$. The above is,

$$|N|^2 \int_{-\infty}^{\infty} \mathrm{d}x \, (x - \langle x \rangle)^2 \exp\left(-\frac{(x - \langle x \rangle)^2}{|\kappa|\hbar}\right) = (\Delta x)^2 \tag{44}$$

Using the integral,

$$\int_{-\infty}^{\infty} \mathrm{d}x \, x^2 \exp(-ax^2) = \frac{1}{2}\sqrt{\frac{\pi}{a^3}} \tag{45}$$

the above is

$$\frac{|N|^2}{2} \sqrt{\pi(|\kappa|\hbar)^3} = (\Delta x)^2 \tag{46}$$

Together with equation (42) we have

$$\begin{aligned} \frac{|N|^2}{2} \sqrt{\pi(|\kappa|\hbar)^3} &= (\Delta x)^2 \\ |N|^2 \sqrt{\pi|\kappa|\hbar} &= 1 \end{aligned} \tag{47}$$

so dividing the two,

$$\hbar|\kappa| = 2(\Delta x)^2 \tag{48}$$

leading to,

$$N = \frac{1}{(2\pi(\Delta x)^2)^{1/4}} \tag{49}$$

With all this,

$$\psi(x) = \frac{1}{(2\pi(\Delta x)^2)^{1/4}} \exp\left(-\frac{(x - \langle x\rangle)^2}{4(\Delta x)^2} + \frac{i\langle p_x\rangle}{\hbar} x\right) \tag{50}$$

Time evolution of this wave packet $\psi(x)$ can be calculated by solving the time dependent Schrödinger equation

$$\begin{aligned} i\hbar\frac{\partial\psi(x,t)}{\partial t} &= H\psi(x,t), \\ \text{with } \psi(x,t_0) &= \psi(x) \end{aligned} \tag{51}$$

Typically, $t_0 = 0$. The Hamiltonian H is,

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x,t) \tag{52}$$

For a free particle, $V = 0$, and it is particularly simple to evaluate the time evolution.

End of Podcast Episode 3.