Heisenberg's Uncertainty Principle

$$\Delta x \Delta p \geq \frac{1}{2}\hbar$$

In other words, we have a *limit* upon how precisely we can measure **position** and **momentum** of a particle.

Werner Heisenberg
1901 – 1976

$$\Delta E \Delta t \geq \frac{1}{2}\hbar$$

A similar relationship exists between **energy** and **time.**

Not this one!

Dr Andy French. June 2021

Schrödinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=E\psi$$

Erwin Schrödinger
1887 – 1961

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\psi}{\partial t}$$

Born interpretation

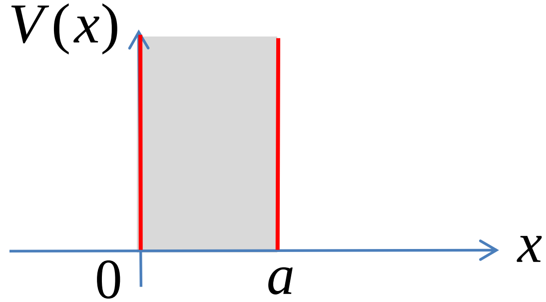
Max Born
1882 – 1970

$$\left|\psi\left(x,t\right)\right|^2 dx$$

is the *probability* of
a particle being at location
between x and $x + dx$

Particle in a box

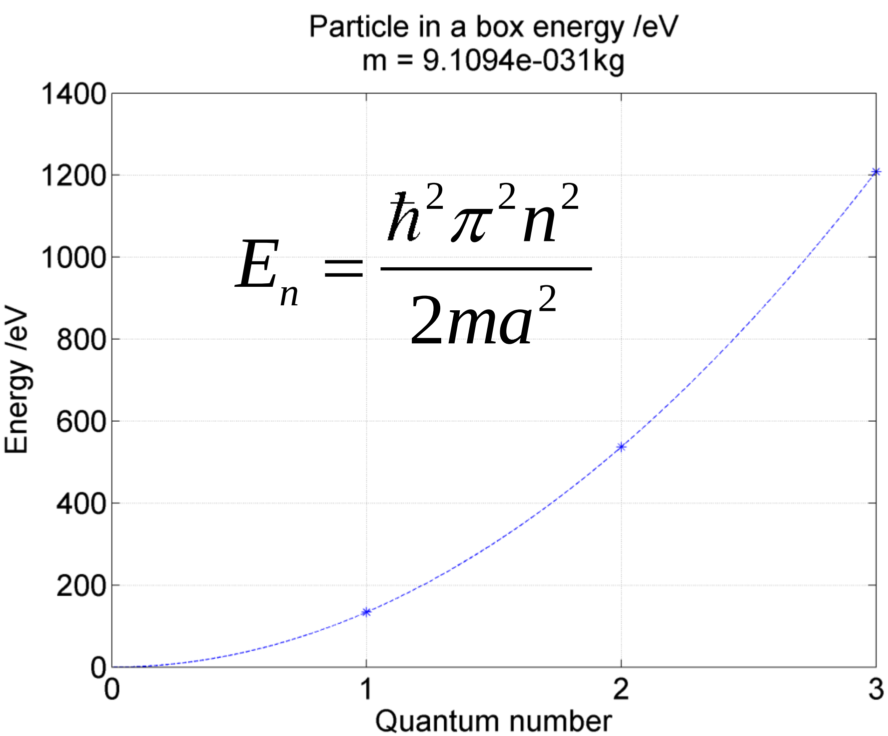
$$V(x)=\begin{cases}\infty & x\le 0,\ x\ge a\\ 0 & 0<x<a\end{cases}$$



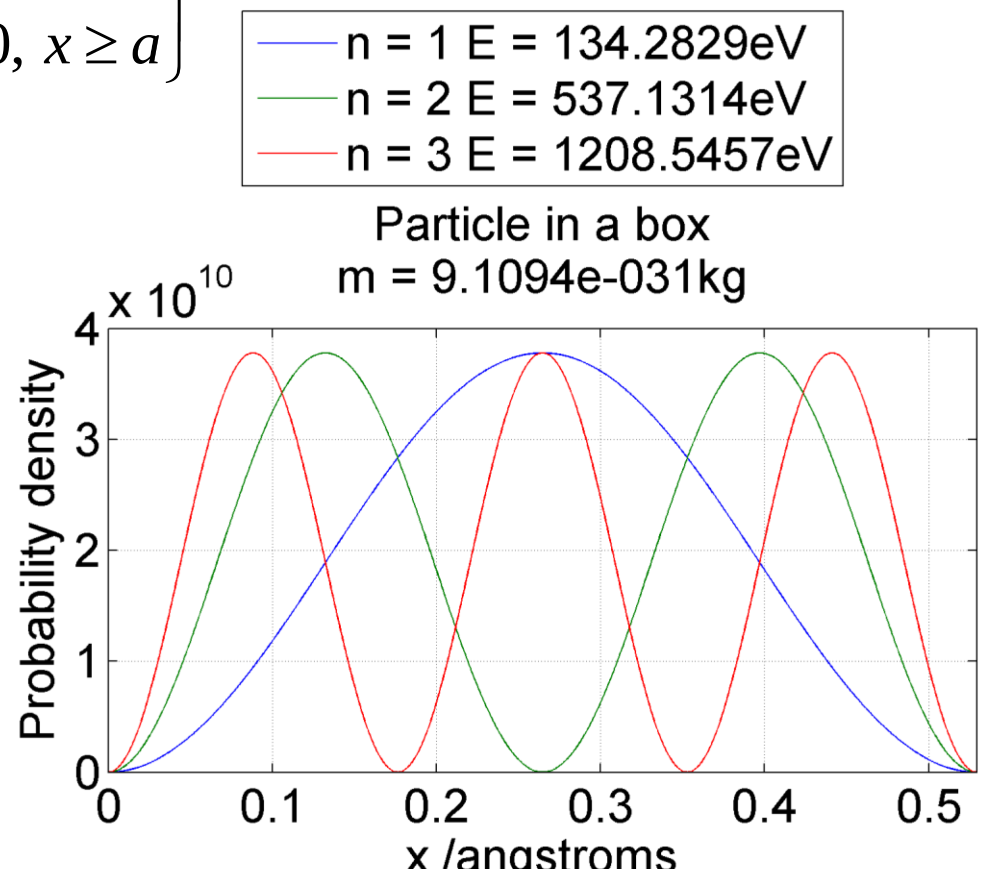
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\psi}{\partial t}$$

Schrödinger Equation

$$\psi_n(x,t)=\begin{cases}\sqrt{\frac{2}{a}}e^{-\frac{iEt}{\hbar}}\sin\left(\frac{n\pi x}{a}\right) & 0<x<a\\ 0 & x\le 0,\ x\ge a\end{cases}$$



$$E_n=\frac{\hbar^2\pi^2n^2}{2ma^2}$$



$$\psi(x,t) = \sqrt{\frac{2}{a}} e^{-\frac{iE_n t}{\hbar}} \sin\left(\frac{n\pi x}{a}\right)$$

Wavefunction

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

Quantized energy levels

Standard deviation in position *x*

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

Using $\psi(x,t) = \sqrt{\frac{2}{a}} e^{-\frac{iE_n t}{\hbar}} \sin\left(\frac{n\pi x}{a}\right)$

$$\begin{aligned}\langle x \rangle &= \int_0^a x \left|\psi(x,t)\right|^2 dx \\ &= \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx \\ &= \frac{1}{2} a\end{aligned}$$

To evalcuate the final step I have used the standard integral:

$$\int x \sin^2 \alpha x dx = \tfrac{1}{4}x^2 - \tfrac{1}{4\alpha} x \sin(2\alpha x) - \tfrac{1}{8\alpha^2} \cos(2\alpha x) + c$$

An example non-normal distribution: a "parabolic distribution"

$$p(x) = \begin{cases} \frac{3}{2}(x-1)^2 & 0 \le x \le 2 \\ 0 & \text{otherwise} \end{cases} \qquad F(x) = \begin{cases} 0 & x < 0 \\ \frac{1}{2}\left((x-1)^3 + 1\right) & 0 \le x \le 2 \\ 1 & x \ge 2 \end{cases}$$

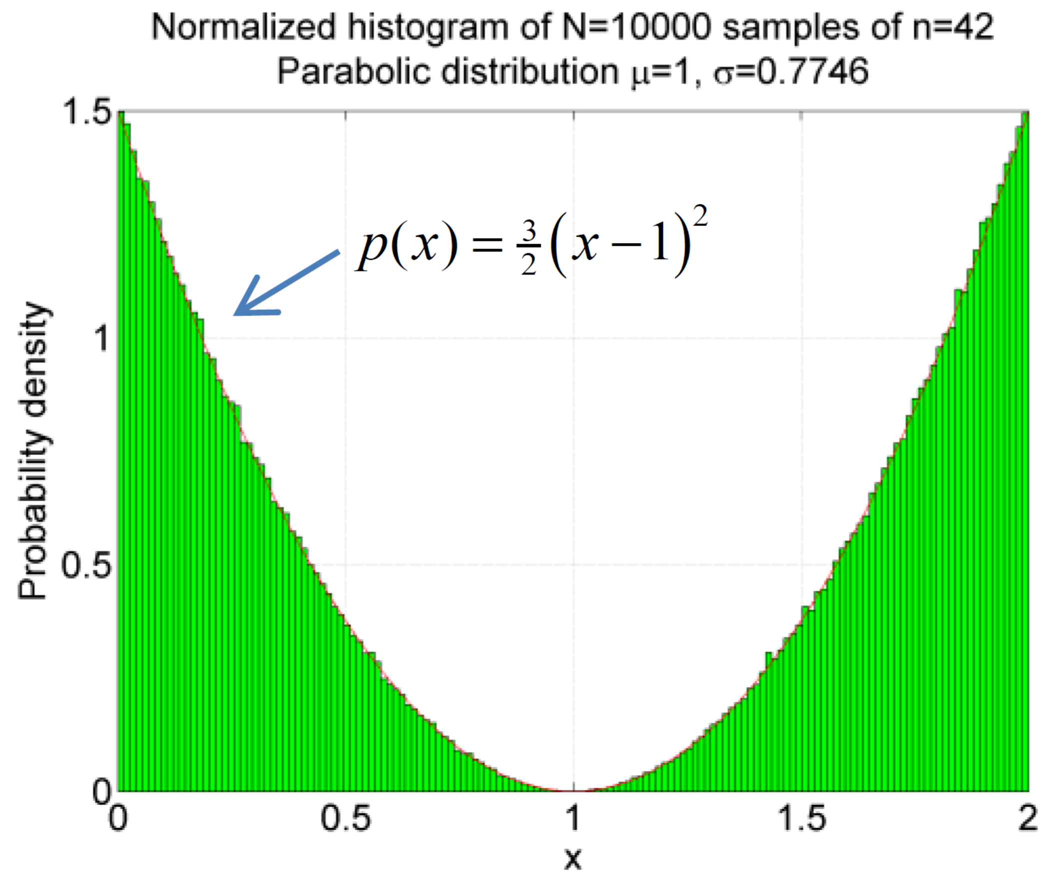
$$F^{-1}(x) = \sqrt[3]{2x-1} + 1 \qquad \mu = 1 \qquad \sigma^2 = \tfrac{3}{5}$$

$$\int_0^2 p(x)dx = 1$$

$$\langle x \rangle = \int_0^2 xp(x)dx = 1$$

$$\langle x^2 \rangle = \int_0^2 x^2 p(x)dx$$

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \tfrac{3}{5}$$



Eclecticon Maths link

The mean of the x^2 values can be found in a similar fashion:

$$\begin{aligned}\langle x^2 \rangle &= \int_0^a x^2 \left|\psi(x,t)\right|^2 dx \\ &= \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx \\ &= \boxed{\tfrac{1}{3}a^2\left(1 - \frac{3}{2n^2\pi^2}\right)}\end{aligned}$$

To evalcuate the final step I have used the standard integral:

$$\int x^2 \sin^2 \alpha x dx = \tfrac{1}{6}x^3 - \tfrac{1}{4\alpha^2}\cos(2\alpha x) - \tfrac{1}{8\alpha^3}\left(2\alpha^2 x^2 - 1\right)\sin(2\alpha x) + c$$

Putting this together:

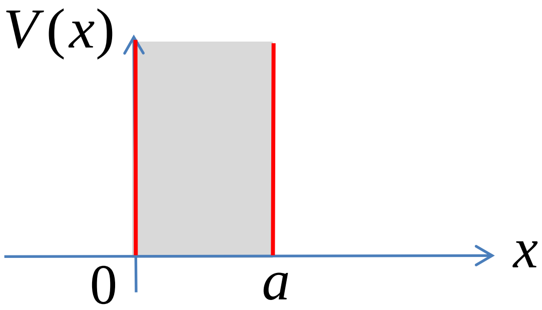
$$\begin{aligned}\langle x^2\rangle - \langle x\rangle^2 &= \tfrac{1}{3}a^2\left(1 - \frac{3}{2n^2\pi^2}\right) - \tfrac{1}{4}a^2\\ &= \tfrac{1}{12}a^2\left(1 - \frac{6}{n^2\pi^2}\right)\end{aligned}$$

So the positional uncertainty is:

$$\boxed{\Delta x = \tfrac{a}{\sqrt{12}}\left(1 - \frac{6}{n^2\pi^2}\right)^{\frac{1}{2}}}$$

The symmetry of the box about $x = \frac{1}{2}a$ implies left and right propagation directions for waves are equally likely. Therefore we expect the mean value of particle momentum to be zero.

$$\langle p \rangle = 0$$



Since $V = 0$ within the box, energy $E_n = \frac{p^2}{2m} + V$, and we have shown that $E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2$:

$$p^2 = \frac{\hbar^2\pi^2}{a^2}n^2$$

i.e. p^2 is independent of position x and time t. Therefore:

$$\langle p^2 \rangle = \frac{\hbar^2\pi^2}{a^2}n^2$$

and therefore since $\langle p \rangle = 0$

$$\boxed{\Delta p = \frac{\hbar\pi}{a}n}$$

Heisenberg's Uncertainty Principle (which we shall prove in general shortly) states that:

$$\Delta p \Delta x \geq \tfrac{1}{2}\hbar$$

This is profoundly important, as it means there is a fundamental limit on how precise we can know, simulteanously, the position and momentum of a particle. For the Particle in a Box

$$\Delta p \Delta x = \frac{\hbar\pi}{a} n \frac{a}{\sqrt{12}} \left(1 - \frac{6}{n^2\pi^2}\right)^{\frac{1}{2}}$$

$$= \tfrac{1}{2}\hbar\sqrt{\tfrac{1}{3}\pi^2 n^2 - 2}$$

The smallest value of $\sqrt{\frac{1}{3}\pi^2 n^2 - 2}$ is when $n = 1$ i.e.$\sqrt{\frac{1}{3}\pi^2 - 2} \approx 1.136$. i.e. 'Particle in a Box' satisfies $\Delta p \Delta x \geq \frac{1}{2}\hbar$. Note there is also an Uncertainty Principle connecting the energy of a particle E and the time t at which the measurement was made.

$$\Delta E \Delta t \geq \tfrac{1}{2}\hbar$$

A general derivation of the Uncertainty Principle

Heisenberg's Uncertainty Principle $\Delta p \Delta x \geq \frac{1}{2}\hbar$ can be derived in very general terms. I will summarize the argument in Haken & Wolf [3] pp466-468.

Firstly define an integral expression:

$$J(\xi) = \int_{-\infty}^{\infty} \left| \xi x \psi + \frac{\partial \psi}{\partial x} \right|^2 dx = \int_{-\infty}^{\infty} \left(\xi x \psi + \frac{\partial \psi}{\partial x} \right) \left(\xi x \psi^* + \frac{\partial \psi^*}{\partial x} \right) dx$$

Expanding the integrand, and noting $|\psi|^2 = \psi^* \psi$:

$$J(\xi) = \xi^2 \int_{-\infty}^{\infty} x^2 |\psi|^2 dx + \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx + \xi \int_{-\infty}^{\infty} x \left(\frac{\partial \psi^*}{\partial x} \psi + \psi^* \frac{\partial \psi}{\partial x} \right) \quad (6.276)$$

$$J(\xi) = \xi^2 \int_{-\infty}^{\infty} x^2 |\psi|^2 dx + \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx + \xi \int_{-\infty}^{\infty} x \frac{d}{dx} (\psi^* \psi) \, dx \quad (6.277)$$

Now if we set a coordinate system where $x = 0$ corresponds to the mean value of x, this implies $\langle x \rangle = 0$ by definition. Therefore since $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ and $\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi|^2 dx$:

$$J(\xi) = \xi^2 (\Delta x)^2 + \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx + \xi \int_{-\infty}^{\infty} x \frac{d}{dx} (\psi^* \psi) \, dx \quad (6.278)$$

$$J(\xi) = \xi^2 (\Delta x)^2 + \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx + \xi \int_{-\infty}^{\infty} x \frac{d}{dx} (\psi^* \psi)\, dx$$

Integrating the last term by parts, and again noting $|\psi|^2 = \psi^* \psi$:

$$\int_{-\infty}^{\infty} x \frac{d}{dx} (\psi^* \psi)\, dx = \left[x |\psi|^2 \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} |\psi|^2\, dx$$

$|\psi(\pm\infty)|^2 = 0$ and $\int_{-\infty}^{\infty} |\psi|^2\, dx = 1$, hence:

$$J(\xi) = \xi^2 (\Delta x)^2 + \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx - \xi$$

If we consider a plane wave of the form $\psi(x,t) = \psi_0 e^{i(kx - \omega t)}$:

$$\frac{\partial \psi}{\partial x} = ik\psi$$

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$$\frac{\partial \psi}{\partial x} = ik\psi$$

From de Broglie's relation between momentum and wavenumber $p = \hbar k$, therefore we can write:[7]

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar}\psi \tag{6.282}$$

Which means:

$$\int_{-\infty}^{\infty} \left|\frac{\partial \psi}{\partial x}\right|^2 dx = \int_{-\infty}^{\infty} \left|\frac{ip}{\hbar}\psi\right|^2 dx = \frac{1}{\hbar^2}\int_{-\infty}^{\infty} p^2 \left|\psi\right|^2 dx = \frac{\langle p^2 \rangle}{\hbar^2} \tag{6.283}$$

If left & right particle motion symmetry can be assumed, then expect $\langle p \rangle = 0$ as in the Particle in a Box model. Hence:

$$\int_{-\infty}^{\infty} \left|\frac{\partial \psi}{\partial x}\right|^2 dx = \frac{\langle p^2 \rangle}{\hbar^2} = \frac{(\Delta p)^2}{\hbar^2} \tag{6.284}$$

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[7] *Operator Methods* are employed in modern Quantum Mechanical theories, and the plane wave relation $\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar}\psi$ suggests the *momentum operator* $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.

and therefore:

$$J(\xi) = \xi^2 (\Delta x)^2 + \frac{(\Delta p)^2}{\hbar^2} - \xi \tag{6.285}$$

By definition, $J(\xi) = \int_{-\infty}^{\infty} \left| \xi x \psi + \frac{\partial \psi}{\partial x} \right|^2 dx$ must be a *positive* function of ξ. The minimum value is when $\frac{dJ}{d\xi} = 0$. i.e.

$$2\xi (\Delta x)^2 - 1 = 0 \tag{6.286}$$

Therefore the minimum of J is when:

$$\xi = \frac{1}{2(\Delta x)^2} \tag{6.287}$$

which means:

$$J_{\min} = \left(\frac{1}{2(\Delta x)^2} \right)^2 (\Delta x)^2 + \frac{(\Delta p)^2}{\hbar^2} - \frac{1}{2(\Delta x)^2} \tag{6.288}$$

$$= \frac{(\Delta p)^2}{\hbar^2} - \frac{1}{4(\Delta x)^2} \tag{6.289}$$

So if $J \geq 0$ for all values of ξ, and the minimum value of J is $J_{\min} = \frac{(\Delta p)^2}{\hbar^2} - \frac{1}{4(\Delta x)^2}$, this implies:

$$\frac{(\Delta p)^2}{\hbar^2} - \frac{1}{4(\Delta x)^2} \geq 0 \tag{6.290}$$

$$(\Delta p)^2 (\Delta x)^2 \geq \tfrac{1}{4}\hbar^2 \tag{6.291}$$

Since Δp and Δx are both positive quantities:

$$\Delta p \Delta x \geq \tfrac{1}{2}\hbar \tag{6.292}$$

which proves Heisenberg's Uncertainty Principle.
Recap of assumptions:

- Coordinate system set such that $\langle x \rangle = 0$.
- Assume mean momentum $\langle p \rangle = 0$. In practical terms, this means the centre of mass of the system is at rest (on average).

I am more uncertain now but that is *in ordnung*

$$\Delta x \Delta p \geq \frac{1}{2}\hbar$$