

Heisenberg's uncertainty principle

Probably one of the most famous (and infamous, and abused) results from quantum mechanics is Heisenberg's Uncertainty Principle. When viewed mathematically, it's much more prosaic than its interpretations in philosophy and literature.

Some background: If a particle is constrained to be on the x -axis, then its *state function* $\varphi(x, t)$ (which satisfies the Schrödinger equation) is a complex-valued function of the real variables x and t . It tells us the probability distribution of the position x of the particle as follows

$$P_\varphi(a < x < b) = \int_a^b |\varphi(x, t)|^2 dx$$

is the probability that the position of the particle is between $x = a$ and $x = b$. The probability distribution of the momentum of the particle is given by the Fourier transform (in x) of the state function (divided by 2π), so the probability that the momentum is between $\omega = c$ and $\omega = d$ is

$$P_\varphi(c < \omega < d) = \int_c^d |\widehat{\varphi}(\omega, t)|^2 \frac{d\omega}{2\pi}.$$

We're going to look at this at a specific moment in time, so we'll drop the t and think of φ and $\widehat{\varphi}$ as functions of x and ω , respectively. Since we need $|\varphi|$ to be a probability density function, we must assume that

$$\int_{-\infty}^{\infty} |\varphi(x)|^2 dx = 1$$

We don't have to assume the same about $\widehat{\varphi}$, since Parseval's equality tells us that

$$\int_{-\infty}^{\infty} |\widehat{\varphi}(\omega)|^2 \frac{d\omega}{2\pi} = \int_{-\infty}^{\infty} |\varphi(x)|^2 dx = 1.$$

From probability, we know that the expected value $E_\varphi[x]$ of the position of the particle and the expected value $E_\varphi[\omega]$ of the momentum of the particle are given by

$$E_\varphi[x] = \int_{-\infty}^{\infty} x |\varphi(x)|^2 dx \quad \text{and} \quad E_\varphi[\omega] = \int_{-\infty}^{\infty} \omega |\widehat{\varphi}(\omega)|^2 \frac{d\omega}{2\pi}.$$

Likewise, the variances $V_\varphi[x]$ and $V_\varphi[\omega]$ are given by

$$V_\varphi[x] = E_\varphi[(x - E_\varphi[x])^2] = \int_{-\infty}^{\infty} (x - E_\varphi[x])^2 |\varphi(x)|^2 dx \quad \text{and} \quad V_\varphi[\omega] = \int_{-\infty}^{\infty} (\omega - E_\varphi[\omega])^2 |\widehat{\varphi}(\omega)|^2 \frac{d\omega}{2\pi}$$

The Heisenberg principle says that it's impossible for both $V_\varphi[x]$ and $V_\varphi[\omega]$ to be simultaneously very small, so there is a tradeoff between the accuracy of our knowledge of the position of the particle and our knowledge of its momentum, in particular

$$\boxed{\text{Heisenberg's inequality: } V_\varphi[x] V_\varphi[\omega] \geq \frac{1}{4}}$$

To simplify the proof, we're going to assume that $E_\varphi[x]$ and $E_\varphi[\omega]$ are both zero. That this is actually no restriction or loss of generality is assured by the following fact:

Lemma: Let $\varphi(x)$ be a state function with $E_\varphi[x] = a$ and $E_\varphi[\omega] = \beta$. Then

$$\psi(x) = e^{-i\beta x} \varphi(x + a)$$

is a state function with $E_\psi[x] = 0$ and $E_\psi[\omega] = 0$, and with the same variances as φ : $V_\psi[x] = V_\varphi[x]$ and $V_\psi[\omega] = V_\varphi[\omega]$.

Proof. Since $|e^{i\beta x}| = 1$, it's easy to show that ψ is also a state function, using the change of variables $y = x + a$:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} |e^{-i\beta x} \varphi(x + a)|^2 dx = \int_{-\infty}^{\infty} |\varphi(y)|^2 dy = 1.$$

Then we compute:

$$E_\psi[x] = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \int_{-\infty}^{\infty} x |e^{-i\beta x} \varphi(x + a)|^2 dx = \int_{-\infty}^{\infty} (y - a) |\varphi(y)|^2 dy = E_\varphi[x] - a = 0$$

Next, we have

$$\begin{aligned} \widehat{\psi}(\omega) &= \int_{-\infty}^{\infty} \psi(x) e^{-i\omega x} dx = \int_{-\infty}^{\infty} e^{-i\beta x} \varphi(x + a) e^{-i\omega x} dx \\ &= \int_{-\infty}^{\infty} \varphi(y) e^{-i(\omega + \beta)(y - a)} dy = e^{ia(\omega + \beta)} \int_{-\infty}^{\infty} \varphi(y) e^{-i(\omega + \beta)y} dy \\ &= e^{ia(\omega + \beta)} \widehat{\varphi}(\omega + \beta) \end{aligned}$$

Therefore (via the change of variables $\sigma = \omega + \beta$)

$$E_\psi[\omega] = \int_{-\infty}^{\infty} \omega |\widehat{\psi}(\omega)|^2 d\omega = \int_{-\infty}^{\infty} \omega |e^{ia(\omega + \beta)} \widehat{\varphi}(\omega + \beta)|^2 d\omega = \int_{-\infty}^{\infty} (\sigma - \beta) |\widehat{\varphi}(\sigma)|^2 d\sigma = E_\varphi[\omega] - \beta = 0$$

Next, we'll calculate the variances:

$$V_\psi[x] = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \int_{-\infty}^{\infty} x^2 |\varphi(x + a)|^2 dx = \int_{-\infty}^{\infty} (y - a)^2 |\varphi(y)|^2 dy = V_\varphi[x]$$

(where $y = x + a$) and (where $\sigma = \omega + \beta$)

$$V_\psi[\omega] = \int_{-\infty}^{\infty} \omega^2 |\widehat{\psi}(\omega)|^2 d\omega = \int_{-\infty}^{\infty} \omega^2 |\widehat{\varphi}(\omega + \beta)|^2 d\omega = \int_{-\infty}^{\infty} (\sigma - \beta)^2 |\widehat{\varphi}(\sigma)|^2 d\sigma = V_\varphi[\omega]$$

Next, it would be good to “review” a few things about inner products in complex vector spaces. First, we recall that for any complex number z , we have $|z|^2 = z\bar{z}$, and for any *real* number x it is the case that $|e^{ix}| = |\cos x + i \sin x| = 1$. Recall that the “standard” inner product of two complex-valued functions $f(x)$ and $g(x)$ is defined by

$$\langle f, g \rangle = \int_{-\infty}^{\infty} f(x) \overline{g(x)} dx$$

so that

$$\langle cf, g \rangle = c \langle f, g \rangle \quad \langle f, cg \rangle = \bar{c} \langle f, g \rangle \quad \langle f, g \rangle = \overline{\langle g, f \rangle}$$

so that $\|cf\| = |c| \|f\|$ for all functions f and $c \in \mathbb{C}$.

Lemma. For any (complex-valued) functions f and g ,

$$\|f + g\|^2 = \|f\|^2 + 2 \operatorname{Re} \langle f, g \rangle + \|g\|^2$$

and

$$\text{(Cauchy-Schwarz inequality:)} \quad |\langle f, g \rangle| \leq \|f\| \|g\|.$$

Proof: The first equation follows simply by expanding out the norm:

$$\begin{aligned} \|f + g\|^2 &= \langle f + g, f + g \rangle = \langle f, f \rangle + \langle f, g \rangle + \langle g, f \rangle + \langle g, g \rangle \\ &= \|f\|^2 + \langle f, g \rangle + \overline{\langle f, g \rangle} + \|g\|^2 = \|f\|^2 + 2 \operatorname{Re} \langle f, g \rangle + \|g\|^2 \end{aligned}$$

For the Cauchy-Schwarz inequality, we first observe that if either f or g is the zero function, then the inequality is trivially true, so we assume that neither f nor g is zero, and observe that neither $|\langle f, g \rangle|$ nor $\|f\|$ is affected if we replace $f(x)$ by $e^{i\theta} f(x)$ for a (real) constant θ , so we choose θ so that $\langle e^{i\theta} f, g \rangle$ is real. So we can assume that $\langle f, g \rangle$ is real and note that for any real number t , we have

$$0 \leq \|f + tg\|^2 = \|f\|^2 + 2t \langle f, g \rangle + t^2 \|g\|^2$$

so the discriminant of this quadratic polynomial in t must be non-positive, i.e.,

$$4 \langle f, g \rangle^2 - 4 \|f\|^2 \|g\|^2 \leq 0$$

which is equivalent to the Cauchy-Schwarz inequality.

Now we're ready to prove

Theorem (Heisenberg's inequality): For "any" state function φ ,

$$V_\varphi[x] V_\varphi[\omega] \geq \frac{1}{4}.$$

Proof: The quotation marks around "any" indicate that you have to be a bit careful about assumptions: saying that φ is a state function means that $\|\varphi\| < \infty$. But we're going to assume that $\|x\varphi\|$ and $\|\varphi'\|$ are finite as well (if they're not, then the Heisenberg inequality is trivially true, since the left side will be infinite, but we're going to omit the proof of this). We can also assume without loss of generality that $E_\varphi[x]$ and $E_\varphi[\omega]$ are both zero, thanks to the first lemma above. Assuming all these things, then, we have (integrating by parts) that

$$\int_{-\infty}^{\infty} x \overline{\varphi(x)} \varphi'(x) dx = x |\varphi(x)|^2 \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} |\varphi(x)|^2 + x \varphi(x) \overline{\varphi'(x)} dx$$

Now the assumption that $\|x\varphi\|$ is finite implies that the first term on the right is zero, and then we can rearrange this as

$$\int_{-\infty}^{\infty} |\varphi(x)|^2 dx = -2 \operatorname{Re} \int_{-\infty}^{\infty} \overline{x\varphi(x)} \varphi'(x) dx$$

Since

$$\left| -2 \operatorname{Re} \int_{-\infty}^{\infty} \overline{x\varphi(x)} \varphi'(x) dx \right| \leq 2 \left| \int_{-\infty}^{\infty} \overline{x\varphi(x)} \varphi'(x) dx \right|$$

and, from the Cauchy-Schwarz inequality,

$$\left| \int_{-\infty}^{\infty} \overline{x\varphi(x)} \varphi'(x) dx \right|^2 \leq \left(\int_{-\infty}^{\infty} x^2 |\varphi(x)|^2 dx \right) \left(\int_{-\infty}^{\infty} |\varphi'(x)|^2 dx \right)$$

we have that

$$\left(\int_{-\infty}^{\infty} |\varphi(x)|^2 dx \right)^2 \leq 4 \left(\int_{-\infty}^{\infty} x^2 |\varphi(x)|^2 dx \right) \left(\int_{-\infty}^{\infty} |\varphi'(x)|^2 dx \right)$$

Almost there! Since φ is a state function with $E_\varphi[x] = 0$, the left side of the last inequality is 1 and the first factor (after the 4) on the right is $V_\varphi[x]$. As for the last factor on the right, using the Parseval equality,

$$\int_{-\infty}^{\infty} |\varphi'(x)|^2 dx = \int_{-\infty}^{\infty} |\omega \widehat{\varphi}(\omega)|^2 \frac{d\omega}{2\pi} = \int_{-\infty}^{\infty} \omega^2 |\widehat{\varphi}(\omega)|^2 \frac{d\omega}{2\pi} = V_\varphi[\omega]$$

since $E_\varphi[\omega] = 0$. Heisenberg's inequality follows immediately from this.

Third time's the charm!!