2.6 Reality check...

The next few sections take a bodyswerve into more formal language. But they make some very important points, so its worth while to do them!
One thing that might worry us is whether our expectation values are real!! Our fundamental operator for p is $-i\hbar\partial/\partial x$ and thats got complex numbers in it, and we know that wavefunctions themselves can be complex. but anything we can measure has to be real - $< p >, < H >$ etc....
We can take the time derivative of the normalisation constraint

$$\frac{d}{dt}[\int \Psi^*(x,t)\Psi(x,t)dx] = \frac{d}{dt}[1] = 0$$

take the differential inside the integral (so its now a partial derivative not a total derivative)

$$\int \frac{\partial}{\partial t}[\Psi^*(x,t)\Psi(x,t)]dx = 0$$

$$\int \frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t} = 0$$

But our Schroedinger equation says

$$i\hbar\frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = H\Psi(x,t)$$

So substitute $\partial\Psi(x,t)/\partial t = \frac{1}{i\hbar}H\Psi = \frac{-i}{\hbar}H\Psi$ hence $\partial\Psi^*(x,t)/\partial t = \frac{i}{\hbar}H^*\Psi^* = \frac{i}{\hbar}(H\Psi)^*$. Then conservation of probability implies

$$\int \left[\frac{i}{\hbar}(H\Psi)^*\Psi - \frac{i}{\hbar}\Psi^*(H\Psi)\right]dx = 0$$

$$\int (H\Psi)^*\Psi dx - \int \Psi^*(H\Psi)dx = 0$$

$$\int \Psi(H\Psi)^* dx = \int \Psi^*(H\Psi)dx$$

$$< H >^* = < H >$$

any quantity which is equal to its own complex conjugate MUST be real. which is what we require for any physical quantity! And this is good because

$$< H > = \int \Psi^*\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\Big)\Psi dx = \int \Psi^* i\hbar\frac{\partial}{\partial t}\Psi dx = < E >$$

and energy had better be real!!
you can do a similar proof and show that $< p >=< p >^*$ so momentum is also real!!
any dynamical quantity $A(x, p, t)$ can be associated with an operator $\hat{A}(x, -i\hbar\partial/\partial x, t)$. The expectation value $< A >= \int \Psi^*(A\Psi)dx$ is guaranted to be real if (and only if) $\int \Psi^*(A\Psi) = \int \Psi(A\Psi)^* dx$ i.e $\hat{A}$ is Hermitian

2.7 Non-Hermitian operators and commutators

The wavefunction contains not just information on the probablity density, but also the expectation value of all physical quantities. in fact it contains all in information which we can learn about the associated particle subject to the uncertainty principle. We cannot know position and momentum to arbitrary accuracy . And so when we look at operators which constrain BOTH position and momentum then they are not necessarily hermitian. for example:

$$< xp >= \int \Psi^* x. - i\hbar\frac{\partial}{\partial x}\Psi dx$$

integrate by parts and get

$$= -i\hbar\Big([\Psi^* x.\Psi]_{-\infty}^{+\infty} - \int \Psi\frac{\partial}{\partial x}[x\Psi^*]\Big)dx$$

the wavefunction must be zero at $\pm\infty$ as there is no possibility of finding the particle at these points. hence

$$= i\hbar\int \Psi.\frac{\partial}{\partial x}[x\Psi^*]dx =< px >^*$$

i.e. it works so long as $xp = px$!! which is fine isn't it?? algebra is commutative, surely???? NO, actually its not when you are playing with operators.

$$xp\Psi = -i\hbar x\frac{\partial\Psi}{\partial x}$$

and

$$px\Psi = -i\hbar\frac{\partial(x\Psi)}{\partial x} = -i\hbar\Big(\Psi + x\frac{\partial\Psi}{\partial x}\Big) = -i\hbar\Psi - i\hbar x\frac{\partial\Psi}{\partial x} = -i\hbar\Psi + xp\Psi$$

so $(px - xp)\Psi = -i\hbar\Psi$. turn this around $(xp - px)\Psi = [x, p]\Psi = i\hbar\Psi$ where we define the square bracket as the commutator of two operators so $[x, p] = xp - px = i\hbar$. This is called the fundamental commutator.
if you are ever calculating a commutator explicitly, then its always MUCH safer to put the wavefunction in as in our calculation above for $[x, p]\Psi = xp\Psi - px\Psi = i\hbar\Psi$
we had $< xp >=< px >^*$. But we now know that $px = -i\hbar + xp$ so $< xp >=< -i\hbar + xp >^* =< xp >^* + i\hbar$. in other words so its not real so it can't be measured (which is what hermitian means)!

2.8 example using $\Psi(x, t = 0) = (\frac{a}{\pi})^{1/4} \exp(-ax^2/2)$

$$
\begin{aligned}
< xp >= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{+\infty} e^{-ax^2} x. - i\hbar \frac{\partial}{\partial x} e^{-ax^2/2} dx \\
= \sqrt{\frac{a}{\pi}}. - i\hbar \int_{-\infty}^{+\infty} e^{-ax^2} x[\frac{-a}{2}.2xe^{-ax^2/2} dx \\
= \sqrt{\frac{a}{\pi}}.ai\hbar \int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx \\
= \sqrt{\frac{a}{\pi}}.ai\hbar \frac{1}{2} \sqrt{\frac{\pi}{a^3}} \\
= \frac{i\hbar}{2}
\end{aligned}
$$

you can do $< px >= -\frac{i\hbar}{2}$, and hence show that $< xp > - < px >= i\hbar$
But this is quite unexpected - we know for this system that $< x >= 0$ and $< p >= 0$ so the only 'physical' answer to this should be zero!!! - and the way to actually form an operator for incompatible operators is to average them i.e. $\frac{1}{2}(xp + px) = 0$ as it should in our example above.

2.9 Commutators

We can define a general commutator of two operators $\hat{A}$ and $\hat{B}$ as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ again, its always MUCH safer to put the wavefunction in explicitally eg $\hat{A}\hat{B}\Psi - \hat{B}\hat{A}\Psi$ as otherwise its very easy to drop terms.
When this is NOT zero, the two operators do not commute and their product operators $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ are not hermitian - their expectation values are not real.

physically, it means we have somehow hit the heisenburg uncertainty principle. eg for x and p we can see this directly! if we try to measure xp or px we are trying to measure position and momentum together: and we can't so $[x,p] = i\hbar$. Any operators which don't commute are somehow hitting this physical limit on knowledge - these are incompatible observables.

2.10 Commutators and the Uncertainty principle

We can make the link with the uncertainty principle explicit, but its very formal (see griffiths section 3.5). I'll just quote it here

$$\sigma_A^2 \sigma_B^2 \geq \Big(\frac{1}{2i} < [\hat{A}, \hat{B}] > \Big)^2 = \Big(\frac{1}{2i}(< AB > - < BA >)\Big)^2$$

for x and p we know $< xp > - < px >= i\hbar$ so

$$\sigma_x^2 \sigma_p^2 \geq \Big(\frac{i\hbar}{2i}\Big)^2$$

so $\sigma_x \sigma_p = \Delta x \Delta p \geq \hbar/2$
The dispersion in any quantity, y from $N \to \infty$ measurements is

$$\sigma_y^2 = \frac{1}{N}\sum_{n=1}^{N}(y_n - < y >)^2$$

where $< y >= \frac{1}{N}\sum_{n=1}^{N} y_n$ expand this out and we get

$$\sigma_y^2 = \frac{1}{N}\sum_{n=1}^{N}(y_n^2 - 2y_n < y > + < y >^2)$$

$$= \frac{1}{N}\sum_{n=1}^{N} y_n^2 - 2 < y > \frac{1}{N}\sum_{n=1}^{N} y_n + < y >^2 \frac{1}{N}\sum_{n=1}^{N}$$

but $< y^2 >= \frac{1}{N}\sum_{n=1}^{N} y_n^2$ so we can write this as

$$=< y^2 > -2 < y >^2 + < y >^2 =< y^2 > - < y >^2$$

so $\sigma_y^2 = (\Delta y)^2 =< y^2 > - < y >^2$.
This means we can calculate $\Delta x = \sigma_x$ and $\Delta p = \sigma_p$. we have almost everything we need for our standard test wavefunction. we know $< p >= 0$ and $< p^2 >= a\hbar^2/2$ so $(\Delta p)^2 = a\hbar^2/2 - 0 = a\hbar^2/2$. Hence $\Delta p = \hbar\sqrt{\frac{a}{2}}$.

for position, we have $< x >= 0$ but we need $< x^2 >$ so

$$< x^2 >= \int_{-\infty}^{+\infty} N^* e^{-ax^2/2} x^2 N e^{-ax^2/2} dx$$

$$= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx$$

$$= \sqrt{\frac{a}{\pi}} \frac{1}{2} \sqrt{\frac{\pi}{a^3}}$$

$$= \frac{1}{2a}$$

hence $(\Delta x)^2 = \frac{1}{2a} - 0$ so $\Delta x = \sqrt{\frac{1}{2a}}$

$$\Delta x \Delta p = \sqrt{\frac{1}{2a}} \hbar \sqrt{\frac{a}{2}} = \hbar/2$$

this is the minimum possible according to heisenburg!!