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Proof If $\hat{x}\psi = ia\hat{p}\psi$ then we have

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Proof If $\hat{x}\psi = ia\hat{p}\psi$ then we have

$$(\psi, \{\hat{x}, \hat{p}\}\psi) \quad = \quad (\psi, \hat{x}\hat{p}\psi) + (\psi, \hat{p}\hat{x}\psi)$$

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&= (ia\hat{p}\psi, \hat{p}\psi) + (\hat{p}\psi, ia\hat{p}\psi) \\
&= (-ia + ia)(\hat{p}\psi, \hat{p}\psi) = 0\,,
\end{aligned}$$

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This is the condition for the first term on the RHS of (6.26) to vanish.

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This is the condition for the first term on the RHS of (6.26) to vanish. We also have that $\langle\hat{x}\rangle_\psi = ia\langle\hat{p}\rangle_\psi$

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This is the condition for the first term on the RHS of (6.26) to vanish. We also have that $\langle\hat{x}\rangle_\psi = ia\langle\hat{p}\rangle_\psi$and, since both expectations are real, this implies that $\langle\hat{x}\rangle_\psi = \langle\hat{p}\rangle_\psi = 0$.

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$$(\hat{x} - \langle\hat{x}\rangle_\psi)\psi = ia(\hat{p} - \langle\hat{p}\rangle_\psi)\psi\,,$$ from (6-29), ⊛

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$A = \hat{x}$
$B = \hat{p}$

$(A'\psi, A'\psi)(B'\psi, B'\psi)$
"
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$(A\psi, A\psi) = (ia\hat{p}\psi, ia\hat{p}\psi)$
$(B\psi, B\psi) = (\hat{p}\psi, \hat{p}\psi)$
product $= |a|^2 |(\hat{p}\psi, \hat{p}\psi)|^2$
$= |a|^2 |(\psi, (\hat{p}^2\psi)|^2$

Here

$A' = x - \langle x \rangle_\psi$
$B' = p - \langle p \rangle_\psi$

This is the condition for the first term on the RHS of (6.26) to vanish. We also have that $\langle\hat{x}\rangle_\psi = ia\langle\hat{p}\rangle_\psi$ and, since both expectations are real, this implies that $\langle\hat{x}\rangle_\psi = \langle\hat{p}\rangle_\psi = 0$. Hence

$\hat{p}$ hermitian

$$(\hat{x} - \langle\hat{x}\rangle_\psi)\psi = ia(\hat{p} - \langle\hat{p}\rangle_\psi)\psi\,,$$

$A'\psi = aB'\psi$

and we have equality in (6.24) and hence (6.28). ■

Heisenberg's uncertainty principle

$$\hat{x}\psi = ia\hat{p}\psi \tag{6.29}$$

Lemma

The condition (6.29) holds if and only if $\psi(x) = C\exp(-bx^2)$ *for some positive constants* b, C.

Correction: the condition (6.29) holds for any function of this form, regardless of whether b and C are positive.
However, it only defines a normalisable wavefunction for positive b and nonzero C.

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$\Rightarrow$ minimum uncertainty.

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Conversely, any wavefunction of the form $\psi(x) = C\exp(-bx^2)$ satisfies $\hat{x}\psi = ia\hat{p}\psi$ for some real a. ■

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Gaussian wavepackets are the minimum uncertainty states with <x>=<p>=0. With a bit more algebra one can generalise this to nonzero expectation values.

Note: not every Gaussian wave packet at every time has minimum uncertainty.

What does the uncertainty principle tell us?

The uncertainty principle is a mathematical statement relating the uncertainties of x and p which are quantities defined for a given state ψ.

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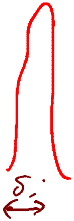
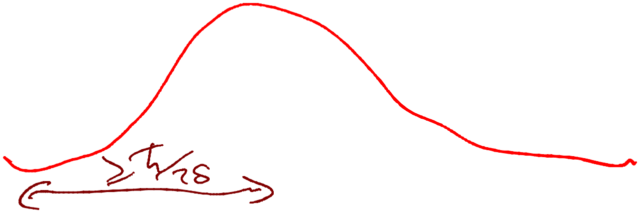


position space wave
function narrowly peaked



Fourier expansion in
momentum widely spread

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Problems with the naive interpretation of the uncertainty principle:

- There is generally no definite fixed pre-measurement value of either A or B.

Not the case that (e.g.) an electron had definite momentum before we measured its position (nor afterwards).

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- There is generally no definite fixed pre-measurement value of either A or B.
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Problems with the naive interpretation of the uncertainty principle:

- There is generally no definite fixed pre-measurement value of either A or B.
- The mathematical derivation of the uncertainty principle does not require us to consider measurements of A or B actually taking place.The quantity $\Delta_{\psi}A$ is mathematically defined whether or not we choose to carry out a measurement of A.

Ehrenfest's theorem

Theorem

The expectation value $\langle A \rangle_\psi$ *of an operator* A *in the state* ψ *evolves by*

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$$\frac{d}{dt}\langle A\rangle_\psi$$

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Theorem

The expectation value $\langle A \rangle_\psi$ *of an operator* A *in the state* ψ *evolves by*

$$\frac{d}{dt}\langle A \rangle_\psi = \frac{i}{\hbar}\langle [\hat{H}, A] \rangle_\psi + \langle \frac{\partial A}{\partial t} \rangle_\psi \, . \tag{6.30}$$

Ehrenfest's theorem

Proof.

We have

definition of expectation value $\langle A \rangle_\psi$

$$\frac{d\langle A\rangle_\psi}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} \psi^* A \psi dx$$

Ehrenfest's theorem

Proof.

We have

$$\frac{d\langle A\rangle_\psi}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty}\psi^* A\psi dx$$

product rule

$$\overset{\text{product rule}}{=} \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}A\psi + \psi^*\frac{\partial A}{\partial t}\psi + \psi^* A\frac{\partial\psi}{\partial t}\right)dx$$

Ehrenfest's theorem

Proof.

We have

$$\frac{d\langle A\rangle_\psi}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty}\psi^* A\psi dx$$

$$= \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}A\psi + \boxed{\psi^*\frac{\partial A}{\partial t}\psi} + \psi^* A\frac{\partial\psi}{\partial t}\right)dx$$

$$= \langle\frac{\partial A}{\partial t}\rangle_\psi + \frac{i}{\hbar}\int_{-\infty}^{\infty}((\hat{H}\psi)^* A\psi - \psi^* A(\hat{H}\psi))dx$$

$$\int_{-\infty}^{\infty}\psi^*(x)\,\frac{\partial A}{\partial t}\,\psi(x)\,dx$$

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\hat{H}\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t}$$

Ehrenfest's theorem

Proof.

We have

$$\begin{aligned}
\frac{d\langle A\rangle_\psi}{dt} &= \frac{d}{dt}\int_{-\infty}^{\infty}\psi^* A\psi dx \\
&= \int_{-\infty}^{\infty}(\frac{\partial\psi^*}{\partial t}A\psi + \psi^*\frac{\partial A}{\partial t}\psi + \psi^* A\frac{\partial\psi}{\partial t})dx \\
&= \langle\frac{\partial A}{\partial t}\rangle_\psi + \frac{i}{\hbar}\int_{-\infty}^{\infty}((\hat{H}\psi)^* A\psi - \psi^* A(\hat{H}\psi))dx \\
&= \langle\frac{\partial A}{\partial t}\rangle_\psi + \frac{i}{\hbar}\int_{-\infty}^{\infty}(\psi^*\hat{H}A\psi - \psi^* A(\hat{H}\psi))dx
\end{aligned}$$

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Proof.

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&= \langle\frac{\partial A}{\partial t}\rangle_\psi + \frac{i}{\hbar}\int_{-\infty}^{\infty}(\psi^*\hat{H}A\psi - \psi^* A(\hat{H}\psi))dx \\
&= \frac{i}{\hbar}\langle[\hat{H}, A]\rangle_\psi + \langle\frac{\partial A}{\partial t}\rangle_\psi\,. \qquad (6.31)
\end{aligned}$$

■

Applications of Ehrenfest's theorem

For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

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For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

$$[\hat{H}, \hat{p}] = [V(x), \hat{p}]$$

$$\parallel$$

$$\left[\frac{1}{2m}\hat{p}^2 + V(x), \hat{p} \right]$$

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For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

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For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

$$\begin{aligned}[\hat{H}, \hat{p}] &= [V(x), \hat{p}] \\ &= [V(x), -i\hbar\frac{\partial}{\partial x}] \\ &= i\hbar\frac{dV}{dx} \qquad (6.32)\end{aligned}$$

$$V(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi - \left(-i\hbar\frac{\partial}{\partial x}\right)\left(V(x)\psi\right)$$

$$= \cancel{V(x)\left(-i\hbar\frac{\partial\psi}{\partial x}\right)} - \cancel{V(x)\left(-i\hbar\frac{\partial\psi}{\partial x}\right)} + i\hbar\frac{dV}{dx}\psi(x)$$

Applications of Ehrenfest's theorem

$$V(x)\,\hat{x}\,\psi - \hat{x}\,V(x)\,\psi$$

$$= V(x)\,x\,\psi - x\,V(x)\,\psi$$

$$= 0.$$

For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

$$\begin{aligned}
[\hat{H}, \hat{p}] &= [V(x), \hat{p}] \\
&= [V(x), -i\hbar\frac{\partial}{\partial x}] \\
&= i\hbar\frac{dV}{dx} \qquad\qquad (6.32) \\
[\hat{H}, \hat{x}] &= [\frac{\hat{p}^2}{2m}, \hat{x}]
\end{aligned}$$

$$[AB, C] = A[B, C] + [A, C]B$$

$$\underset{\hat{p}}{\shortparallel}\ \ \underset{\hat{p}}{\shortparallel}\ \ \underset{\hat{x}}{\shortparallel} \quad = \hat{p}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{p}$$

Applications of Ehrenfest's theorem

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$$
\begin{aligned}
[\hat{H}, \hat{p}] &= [V(x), \hat{p}] \\
&= [V(x), -i\hbar\frac{\partial}{\partial x}] \\
&= i\hbar\frac{dV}{dx} && (6.32) \\
[\hat{H}, \hat{x}] &= [\frac{\hat{p}^2}{2m}, \hat{x}] \\
&\xleftarrow{\text{Check this step}} \frac{1}{2m}2[\hat{p}, \hat{x}]\hat{p} = \frac{-i\hbar}{m}\hat{p} && (6.33)
\end{aligned}
$$

Check this step
(see last slide)

Applications of Ehrenfest's theorem

For $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have

apply to $\hat{p}$

$$\begin{aligned}
[\hat{H}, \hat{p}] &= [V(x), \hat{p}] \\
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$\hat{x}$

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\end{aligned}$$

$\hat{H}$

$$[\hat{H}, \hat{H}] = 0\,. \qquad (6.34)$$

Applications of Ehrenfest's theorem

Since none of these operators is explicitly time-dependent, we have that $\frac{\partial \hat{H}}{\partial t} = \frac{\partial \hat{x}}{\partial t} = \frac{\partial \hat{p}}{\partial t} = 0$

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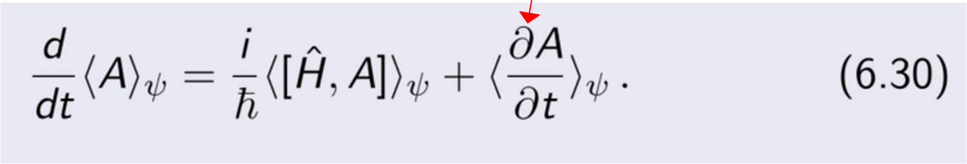

$$\frac{d}{dt}\langle A\rangle_\psi = \frac{i}{\hbar}\langle[\hat{H}, A]\rangle_\psi + \langle\frac{\partial A}{\partial t}\rangle_\psi \, . \qquad (6.30)$$

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$$\frac{d}{dt} \langle \hat{p} \rangle_\psi \quad = \quad -\langle \frac{dV}{dx} \rangle_\psi \, ,$$

Applications of Ehrenfest's theorem

Since none of these operators is explicitly time-dependent, we have that $\frac{\partial \hat{H}}{\partial t} = \frac{\partial \hat{x}}{\partial t} = \frac{\partial \hat{p}}{\partial t} = 0$ and so the $\langle \frac{\partial A}{\partial t} \rangle_\psi$ term on the RHS of (6.30) vanishes in each case, giving

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So the average behaviour predicted by quantum mechanics is consistent with classical mechanics for macroscopic systems. If that were not true, we should be able to detect discrepancies with classical mechanics, even for large objects, without doing complicated interference experiments.

For example, if the average energy for some quantum system was not conserved, we should be able to build an energy source or sink by making lots of copies of that system and letting it evolve.

(not a proof)

Consistency check for classical mechanics emerging as a limit from quantum mechanics.

$$
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Note that Ehrenfest's theorem shows that expectation values follow equations analogous to classical laws, but does not describe the behaviour of uncertainties, which have no real classical analogue.
For example, the uncertainty in position typically increases with time:

$$
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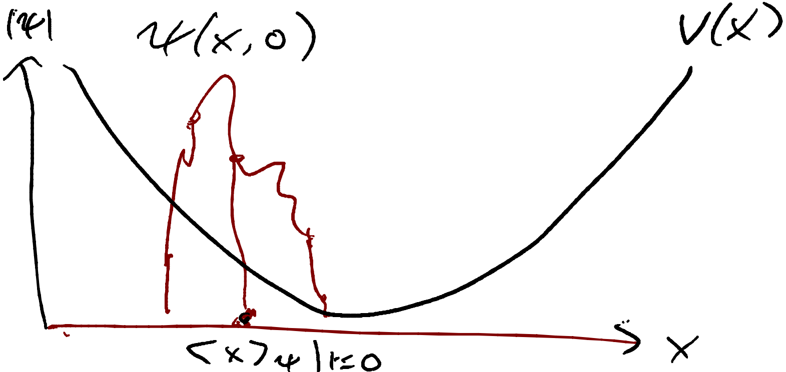
Consider the quantum harmonic oscillator: $V(x) = \frac{1}{2} m \omega^2 x^2$

$$\frac{d}{dt}\langle \hat{x} \rangle_\psi = \frac{1}{m}\langle \hat{p} \rangle_\psi$$

$$\frac{d}{dt}\langle \hat{p} \rangle_\psi = -\langle \frac{dV}{dx} \rangle_\psi = -m\omega^2 \langle \hat{x} \rangle_\psi$$



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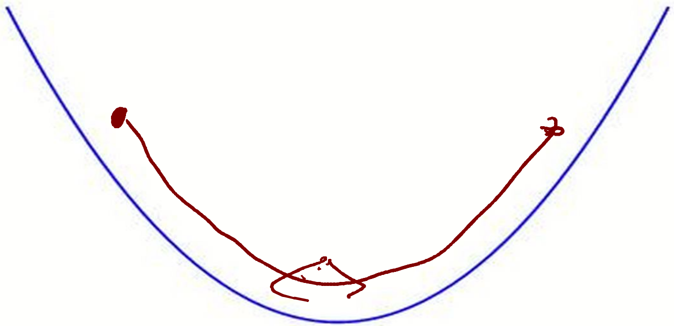
$$= -m\omega^2 \langle \hat{x} \rangle_\psi$$

$$\therefore \frac{d^2}{dt^2}\langle \hat{x} \rangle_\psi = -\omega^2 \langle \hat{x} \rangle_\psi$$

$$\boxed{\begin{aligned} \langle \hat{x} \rangle_\psi &= A\cos\omega t + B\sin\omega t \\ \langle \hat{p} \rangle_\psi &= -Am\omega \sin\omega t + Bm\omega\cos\omega t . \end{aligned}}$$

We get the same equations as those for x,p for the classical harmonic oscillator.

(Particular fact about the harmonic oscillator: not true for general potentials.)



https://www.youtube.com/watch?v=1fMi1nriS8Q

For another interesting example where Ehrenfest's theorem leads to simple equations of motion for the expectation values, consider a linear potential V(x) = Ax

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$$\begin{aligned}\hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \\ &= \frac{1}{2m}(\hat{p} + im\omega\hat{x})(\hat{p} - im\omega\hat{x}) + \frac{i\omega}{2}[\hat{p}, \hat{x}]\end{aligned}$$

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$$\hat{H} = a^\dagger a + \frac{1}{2}\hbar\omega\,. \qquad (6.37)$$

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We have the following commutation relations:

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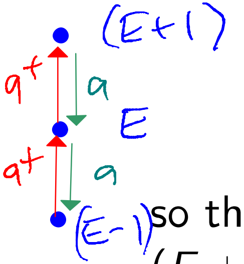

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so that $a\psi$ and $a^\dagger\psi$ are eigenfunctions of energy $(E - \hbar\omega)$ and $(E + \hbar\omega)$.

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We can use this to prove by induction that $a^n \psi$ and $(a^\dagger)^n \psi$ are eigenfunctions of energy $(E - n\hbar\omega)$ and $(E + n\hbar\omega)$.

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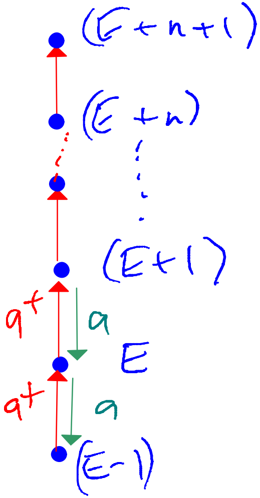

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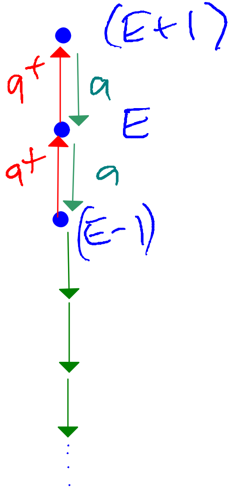

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However, given any physical wavefunction ψ, we have that

$$\langle\hat{H}\rangle_\psi = \int_{-\infty}^{\infty}\psi^*(\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi)dx$$

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In particular, if it were true that $a^n\psi \neq 0$ for all n, there would be eigenfunctions of arbitrarily low energy, and so there would be no ground state.

However, given any physical wavefunction ψ, we have that

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positive constants

$$\int_{-\infty}^{\infty}\left(C\left|\frac{d\psi}{dx}\right|^2 + C'|\psi|^2\right)dx. \quad = \int_{-\infty}^{\infty}\frac{\hbar^2}{2m}\frac{d\psi}{dx}\frac{d\psi^*}{dx} + \frac{1}{2}m\omega^2x^2\psi^*(x)\psi(x)$$

*The harmonic oscillator revisited

We can use this to prove by induction that $a^n\psi$ and $(a^\dagger)^n\psi$ are eigenfunctions of energy $(E - n\hbar\omega)$ and $(E + n\hbar\omega)$. For example,

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and we see immediately that their energies are $(n + \frac{1}{2})\hbar\omega$.

Note: we can also see that there cannot be eigenfunctions with energies other than these values. If there were, we could apply (a)^n to them for arbitrarily large n, without obtaining the zero function, and so there would be negative energy eigenstates.

With a little more thought we can also show that the eigenspaces must be nondegenerate.