How does Quantum Mechanics turn into Classical Mechanics?
The Motion of Wavepackets in a Box

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"Correspondence"

First Problem: What corresponds with what? —

Classical Mechanics $x(t) \iff \Psi(x,t)$ Quantum Mechanics??

The connection is through the expectation values:

$$\langle x(t)\rangle = \int \Psi^\star(x,t)\,\hat{x}\,\Psi(x,t)\,dx \qquad \text{and} \qquad \langle p(t)\rangle = \int \Psi^\star(x,t)\,\hat{p}\,\Psi(x,t)\,dx$$

We immediately see that if Ψ is a single eigenstate:

$$u_n(x)e^{iE_nt/\hbar} \qquad \text{where for the box} \qquad u_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

then both these expectation values are time-independent, as the only t-dependence cancels.

This is not the only problem with eigenstates: the waves always fill the box. (Examples.)

Eigenstates are always maximally de-localised and stationary - not very classical?

'Classical' states must be superposition states with a localised, moving, wavefunction — a *wavepacket* — with a macroscopically small dispersion in x and p.

But of course these are constrained by the uncertainty principle

$$\Delta x\,\Delta p \geq \frac{\hbar}{2}.$$

Ehrenfest's Theorem . . .

tells us that if we can make such a state then the wavepacket will obey classical mechanics: Consider the rate of change of an expectation value $\langle Q\rangle$:

$$\frac{d\langle Q\rangle}{dt} = \int \Psi^\star \hat{Q}\frac{\partial\Psi}{\partial t}\,dx + \int \frac{\partial\Psi^\star}{\partial t}\hat{Q}\Psi\,dx.$$

We can substitute from the Schrodinger equation for the Ψ-derivatives —
$\dfrac{\partial\Psi}{\partial t} = \dfrac{1}{i\hbar}H\Psi$, $\dfrac{\partial\Psi^\star}{\partial t} = \dfrac{-1}{i\hbar}(H\Psi)^\star$ — and then use the Hermitian property of H:

$$\boxed{\frac{d\langle Q\rangle}{dt} = \frac{1}{i\hbar}\int \Psi^\star[\hat{Q},H]\Psi\,dx.}$$

If H is the usual one-particle Hamiltonian $H = p^2/2m + V(x)$ then we find that

$$[x,H] = \frac{1}{2m}[x,p^2] = i\hbar\frac{p}{m} \quad\rightarrow\quad \frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$$

whereas

$$[p,H] = [p,V(x)] = -i\hbar\frac{\partial V}{\partial x} \quad\rightarrow\quad \frac{d\langle p\rangle}{dt} = \langle -\frac{\partial V}{\partial x}\rangle$$

Simple Superposition

We start with the simplest possible superposition state — just two states, equally mixed:

$$\Psi(x,t) = c_n u_n e^{-i\omega_n t} + c_{n+1}u_{n+1}e^{-i\omega_{n+1}t} \quad\text{with}\quad |c_n| = |c_{n+1}| = \frac{1}{\sqrt{2}}, \quad \hbar\omega_n = E_n.$$

This is normalised:

$$\int_0^a |\Psi(x,t)|^2\,dx = \int_0^a \frac{1}{2}\left(u_n(x)^2 + u_{n+1}(x)^2\right) + u_n(x)u_{n+1}(x)\left(c_n^\star c_{n+1}e^{-i\Delta\omega\,t} + \text{c.c.}\right)\,dx$$

so the only choices are the phases of the two c coeffs.
But since the two states evolve at different frequencies, all relative phases occur at some time!
So just add them for example: $c_n = c_{n+1} = 1/\sqrt{2}$. (Example.) Then for $\langle x\rangle$ we get:

$$\begin{aligned}\langle x(t)\rangle &= \int_0^a \frac{1}{2}x\Big(u_n(x)^2 + u_{n+1}(x)^2\Big)\,dx + \frac{1}{2}\left(e^{i\Delta\omega\,t} + e^{-i\Delta\omega\,t}\right)\int_0^a x u_n u_{n+1}\,dx \\ &= \frac{a}{2} + I\cos\Delta\omega\,t \qquad\text{where}\qquad I = \int_0^a x u_n u_{n+1}\,dx\end{aligned}$$

So although Ψ looks messy the expectation value just oscillates sinusoidally at the difference frequency $\Delta\nu = \Delta E/h$ (or angular frequency $\Delta\omega = \Delta E/\hbar$).

Can we understand this in wavefunction terms?

$t = 0$: We are just adding the u, which are in phase at $x = 0$ and out of phase at $x = a$.

$t = 1/2\Delta\nu$: They now add at $x = a$.

At intermediate times it helps to decompose the sin function into forwards and backwards travelling waves:

$$\Psi(x,t) = \frac{1}{2i}\left[e^{i(n\pi x/a-\omega_n\, t)} + e^{i((n+1)\pi x/a-\omega_{n+1}\, t)} - e^{-i(n\pi x/a+\omega_n\, t)} - e^{-i((n+1)\pi x/a+\omega_{n+1}\, t)}\right]$$

We can factor out the mean forward or backwards wave phase from each term:

$$\begin{aligned}\Psi(x,t) =& \frac{1}{2i}e^{i(\bar{k}x-\bar{\omega}t)}\left[e^{i(-\pi x/a+\Delta\omega\, t)/2} + e^{i(\pi x/a-\Delta\omega\, t)/2}\right] \\ & - \frac{1}{2i}e^{-i(\bar{k}x+\bar{\omega}t)}\left[e^{i(\pi x/a+\Delta\omega\, t)/2} + e^{-i(\pi x/a+\Delta\omega\, t)/2}\right] \\ =& -i\left[e^{i(\bar{k}x-\bar{\omega}t)}\cos\frac{\pi x/a-\Delta\omega\, t}{2} - e^{-i(\bar{k}x+\bar{\omega}t)}\cos\frac{\pi x/a+\Delta\omega\, t}{2}\right]\end{aligned}$$

The two forward (or two backward) waves interfere with each other to produce beats.

The wavefunction consists of one whole beat pattern folded back on itself, with a π phase shift at each reflection.

In other words, there's just one place where either the + or − waves interfere in phase, and one place where they interfere destructively.

Then the forward and backward waves interfere to produce the short-wavelength standing wave.

This whole explanation is completely generic for all one-dimensional systems.

This is because in all sets of eigenfunctions each successive function has one more oscillation per round trip. The only aspect particular to the box is the linear increase of phase with x, which follows from the constant velocity between reflections.

A Large Superposition

A macroscopic object moving with a perceptible speed in a visible box has a quantum number $n \sim 10^{30}$ or more, and the range of possible quantum numbers consistent with observation could easily be 10^{20}

So we are dealing with a very large superposition:

$$\Psi(x,t) = \sum_n c_n u_n(x) e^{-iE_n t/\hbar}$$

which generates an expectation value

$$\langle x(t) \rangle = \frac{a}{2} + \sum_{n \neq m} c_n^\star c_m e^{i(E_n - E_m)t/\hbar} I_{nm} \quad \text{where} \quad I_{nm} = \int_0^a x\, u_n(x) u_m(x)\, dx$$

Even though the number of states in the superposition is so large, they vary over a tiny fraction of their value. So the frequencies that appear are all multiples of the adjacent state difference frequency.

So we generate the classical $x(t)$ as its Fourier series.

Correspondence Re-visited

For this to work the quantum and classical frequencies have to be the same:

$$\text{Classical: } \nu = \frac{\sqrt{2E/m}}{2a} \qquad \text{Quantum: } \nu = \frac{1}{2\pi\hbar}\frac{dE}{dn} = \frac{\hbar\pi n}{2ma^2}$$

Furthermore, the amplitudes of the Fourier components have to match:

$$\text{Classical: } x(t) = \frac{a}{2} - \sum_{k=\text{odd}} \frac{2a}{k^2\pi^2} \cos k\omega t \qquad \text{Quantum: } I_{nm} = -\frac{2a}{\pi^2}\left[\frac{1}{(n-m)^2} - \frac{1}{(n+m)^2}\right]$$

So finally the prescription for a wavepacket is:

a large number of states

phases of c_n increase in equal steps.

This leaves unattempted many important questions . . . !