Duane's Science Enrichment Series

Why the Classical Hamiltonian Doesn't Work for Quantum Mechanics

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Target: Mechanics, Quantum Mechanics, Physical Chemistry

Let's consider the Hamiltonian as formulated for a classical harmonic oscillator:

$$H = \frac{1}{2} m\dot{\mathbf{x}}^2 + \frac{1}{2} k\mathbf{x}^2 \quad \text{(I)}$$

This is a perfectly good Hamiltonian for a classical system, but it fails in the quantum mechanical case. To see why, it might be helpful to put it into the canonical $\mathbf{x},\mathbf{p}$ form:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} k\mathbf{x}^2 \quad \text{(II)}$$

You should see it now. This expression specifies both position and momentum to arbitrary precision, which we know from quantum mechanical principles is impossible. We can assume that given the Heisenberg relation for the two conjugate operators, $[\hat{\mathbf{x}},\hat{\mathbf{p}}] = i\hbar$, that an i and an $\hbar$ have to go in there somehow. Let's persue how that happens.

The solution to Schrödinger's equation in one dimension yields:

$$\Psi = e^{ikx - i\omega t} \quad \text{(III)}$$

Since our atribute conjugation is between momentum and position, we take the first partial derivative with respect to x :

$$\frac{\partial \Psi}{\partial x} = ike^{ikx - i\omega t} = ik\Psi \quad \text{(IV)}$$

Now we add the quantum mechanics. The De Broglie is almost always taught in relation to time frequency, but it is equally valid with space frequency by the relation $p = \hbar k$. Substituting into the above equation yields:

$$\frac{\partial \Psi}{\partial x} = i\frac{p}{\hbar}\Psi \quad \text{(V)}$$

Dropping the Ψ's and rearranging gives the operator equivalent with which we are all familiar:

$$\hat{\mathbf{p}} = -i\hbar\frac{\partial}{\partial x} \quad \text{(VI)}$$

Substituting this definition back into (II) gives a Hamiltonian that is compatible with quantum mechanics, and results in the proper one for a quantum harmonic oscillator:

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}k\hat{x}^2 \qquad \text{(VII)}$$