Understanding the Schrodinger Equation

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At the heart of quantum mechanics is the Schrodinger equation. We discuss the thought process behind its formulation. I am hesitant to refer to this as understanding the 'derivation' of the Schrodinger equation as many believe the Schrodinger equation to be a postulate itself.

1 The Classical Wave Equation

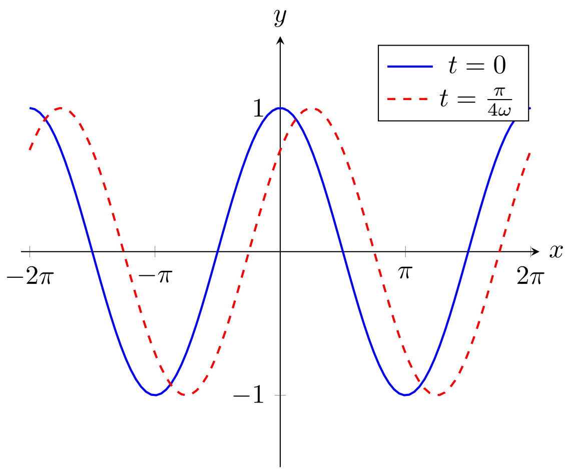
The classical wave equation is given by

$$\frac{\partial^2 u}{\partial t^2} - v^2 \nabla^2 u = 0 \tag{1}$$

In mechanics, the typical traveling wave solution to this equation is given by

$$y(x,t) = A\cos(kx - \omega t) \tag{2}$$

Where A represents the amplitude of the wave, $k = \frac{2\pi}{\lambda}$, and $\omega = 2\pi f$. λ is the wavelength of the wave and f is the frequency of oscillation.



To see why this form of a traveling wave satisfies the wave equation, we can plug it into (1)

$$-A\omega^2 \cos(kx - \omega t) + v^2 A k^2 \cos(kx - \omega t) = 0 \tag{3}$$

$$v^2 k^2 = \omega^2 \rightarrow vk = \omega \tag{4}$$

$$v = f\lambda \tag{5}$$

Which is the fundamental classical wave relation.

2 Demands of a Quantum Wave Equation

de Broglie theorized that all particles have fundamental wave-like properties. To formalize this, he connected the wave properties of frequency and wavelength to the particle properties of energy and momentum. Specifically, he stated

$$E = hf, \quad p = \frac{h}{\lambda} \tag{6}$$

Thus, our quantum wave equation must

- Satisfy the de Broglie relations.
- Satisfy the particle energy relation $E = T + V$.

Additionally, we demand the wave equation to be linear. Frankly, I don't have a super intuitive reason to require this. However, one rationale is due to the ability to use the superposition principle. This is important as it directly allows for the interference and constructive patterns observed with waves.

Finally, we note that if our potential function V is constant C, we have

$$F = -\nabla V = -\nabla C = 0 \rightarrow \frac{dp}{dt} = 0 \rightarrow p = C' \tag{7}$$

But if momentum is a constant, wavelength is a constant. And, if no force is acting on the system, energy is conserved, so frequency is constant. This implies a sinusoidal traveling wave. So we have two more conditions for the quantum wave equation. It must

- Be linear.
- Be satisfied by a sinusoidal traveling wave given a constant potential.

3 Cooking Up the Equation

We start with the particle energy relation

$$E = \frac{p^2}{2m} + V \tag{8}$$

$$hf = \frac{h^2}{2m\lambda^2} + V \tag{9}$$

We substitute $\lambda = \frac{2\pi}{k}$ and $f = \frac{\omega}{2\pi}$

$$\frac{h}{2\pi}\omega = \frac{h^2k^2}{2m \cdot (2\pi)^2} + V \tag{10}$$

$$\hbar\omega = \frac{\hbar^2k^2}{2m} + V \tag{11}$$

We note the factor of ω on the LHS and the factor of k^2 on the RHS. If we take a general wavefunction ansantz

$$\psi(x,t) = \cos(kx - \omega t) + \gamma \sin(kx - \omega t) \tag{12}$$

Then taking a first derivative with respect to t yields a factor of ω and a second derivative with respect to x yields a factor of k^2. We calculate both expressions explicitly

$$\frac{\partial \psi}{\partial t} = \omega \sin(kx - \omega t) - \gamma\omega \cos(kx - \omega t) \tag{13}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \cos(kx - \omega t) - \gamma k^2 \sin(kx - \omega t) \tag{14}$$

At this point, we take a step back to discuss how to proceed from here. If we multiply (11) by the wave function, the equality still holds. Then, we can replace the $\omega\psi$ and $k^2\psi$ terms with some constants times the partial derivatives we just calculated. This would give a wave equation for our general ansatz. And, by linearity, we can construct new solutions with the sum of existing ones. Since we're using sines and cosines, we hope that we might be able to deal with practically any wavefunction using some sort of Fourier analysis.

3.1 The Importance of Complex Numbers

So, we solve $\alpha \frac{\partial \psi}{\partial t} = \omega\psi$ for α. We write

$$\omega\alpha(\sin(kx - \omega t) - \gamma \cos(kx - \omega t) = \omega(\cos(kx - \omega t) + \gamma \sin(kx - \omega t)) \tag{15}$$

$$\alpha = \gamma, \quad -\alpha\gamma = 1 \to -\gamma^2 = 1 \to \gamma = \alpha = i \tag{16}$$

An extremely interesting result. To ensure consistency, we also solve $\beta \frac{\partial^2 \psi}{\partial x^2} = k^2\psi$ for β

$$-k^2\beta(\cos(kx - \omega t) + \gamma \sin(kx - \omega t)) = k^2(\cos(kx - \omega t) + \gamma \sin(kx - \omega t)) \tag{17}$$

$$\beta = -1 \tag{18}$$

So we have no conflicts in our choice of γ. Then, we have the equation

$$\hbar i \frac{\partial \psi}{\partial t} = V\psi - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x} \tag{19}$$

Or in several spacial dimensions

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla\psi + V\psi \tag{20}$$

3.2 Assumptions and Extensions to Non-Constant Potentials

Astute readers may have noticed a critical assumption in our outlined approach after equation (14)—namely, that this analysis strictly holds for a constant potential V. This is explicitly clear because:

$$V(q_0, \ldots, q_n, t) \neq \hbar\omega - \frac{\hbar^2 k^2}{2m} \tag{21}$$

where the right-hand side is a constant, conflicting with a spatially or temporally varying V. However, for non-constant potentials, the Schrödinger equation can still be addressed using superpositions of plane waves. For well-behaved potential functions, these solutions can be expressed as:

$$\psi(x,t) = \int A(k)e^{i(kx-\omega t)}dk, \tag{22}$$

This approach allows us to model more complex quantum systems and aligns with experimental observations of quantum phenomena such as scattering and interference.