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# Four Derivations of Schrödinger's Time Dependent Equation

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## Objectives

Obtain Schrödinger's time-dependent equation using four methods:

- Classical Simple Harmonic Motion (SHM)
- Classical electromagnetic wave equation
- Schrödinger's time independent equation
- Hamilton-Jacobi equation

Explain the applications of Schrödinger's equation, and failures of Newtonian physics where Quantum physics takes it's place.

## Introduction

Laws and theorems of classical physics apply nicely to macroscopic objects, but at the subatomic level they begin to break down, hence the advent of Quantum Mechanics. Just as Newton's laws describe large scale motion, the Schrödinger Equation attempts to describe the motion and properties of particles, such as electrons about a nucleus, and photons. It did not appear out of thin air, there a multiple ways to obtain the equation using classical starting points and a few logical assumptions.

## Prerequisite Knowledge

- Algebra - How to manipulate an equation for a specific variable or result
- Calculus I - Second order derivatives
- Physics:
  - Energy -  $\frac{1}{2}mv^2$  (Classical) and  $E = 2\pi\hbar\nu$
  - Frequency :  $\nu = \frac{v}{\lambda}$
  - Maxwell's equations of electrostatics
    - $\nabla \times E = -\partial B/\partial t$
    - $\nabla \times B = \frac{1}{c^2}\partial E/\partial t$
    - $\nabla \cdot E = 0$
    - $\nabla \cdot B = 0$
- Complex numbers:  $e^{-i\theta} = \cos(\theta) - i\sin(\theta)$
- Hamilton's equations for Canonical transformations
  - $dq_i/dt = \partial H/\partial p_i$
  - $dp_i/dt = -\partial H/\partial q_i$

## Method I: Simple Harmonic Motion

Begin with equation of a wave propagating through a medium:

$$x(t) = A \cdot [\cos(\omega t - \phi) - i\sin(\omega t - \phi)]$$

$$\Rightarrow \psi(t) = A \cdot e^{-i(\omega t - \phi)} \quad (1)$$

Take the spatial derivative of  $\psi$  twice and the time derivative once to find

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-p^2}{\hbar^2} \psi \quad (2)$$

$$\frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} E \psi \quad (3)$$

Apply eq. 2 and eq. 3 to classical total energy to obtain the TDSE.

## Method II: Time-Independent Schrödinger Equation

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad (4)$$

Assume a solution

$$\psi = A \cdot e^{-i\omega t} \quad (5)$$

Differentiate with respect to time, substitute, and manipulate eq. 4 to obtain the time-dependent equation.

The difference between the time-dependent and independent equations is analogous to Statics and Dynamics in Classical Physics.

## Method III: Classical Wave Equation

Begin with the wave equation for a particle in free space

$$\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0, \quad (7)$$

whose solution is

$$E(x, t) = E_0 e^{i(kx - \omega t)} \quad (8)$$

Assume non-zero rest mass, and approximate relativistic energy using  $\sqrt{a^2 + b^2} \approx \sqrt{a^2} + \frac{b^2}{2}$ . Discard the small (insignificant) terms. This method is along the lines of how Erwin Schrödinger originally developed his equations.

## Method IV: Hamilton-Jacobi Equation

Assume a solution of  $\psi(X, t) = e^{iS(X, t)}$  and solve for  $S(X, t)$ . Take the spatial and time derivatives of  $S$  and apply them to the Hamilton-Jacobi equation for a particle with mass  $m$  and potential  $V$ ,

$$\frac{1}{2} \left[ \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + \left( \frac{\partial S}{\partial z} \right)^2 \right] + V + \frac{\partial S}{\partial t} = 0 \quad (9)$$

This method makes the fewest assumptions and approximations.

## References

- John S. Townsend. *A Modern Approach to Quantum Mechanics*. University Science Books, 2nd edition, 2012.
- Jerry B. Marion and Stephen T. Thornton. *Classical Dynamics of Particles and Systems*. Cengage Learning, 5th edition, 2012.

## Schrödinger's Equation

$$-i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \psi - V \psi \quad (6)$$

The Heisenberg Uncertainty Principle states that the position and momentum of a particle cannot be known at the same time. The solution of the Schrödinger equation provides the probability of finding a particle at a point with certain properties.

## Why Do We Need To Know Quantum Physics?

There should be no limit for energy in the ultraviolet range, but that is impossible

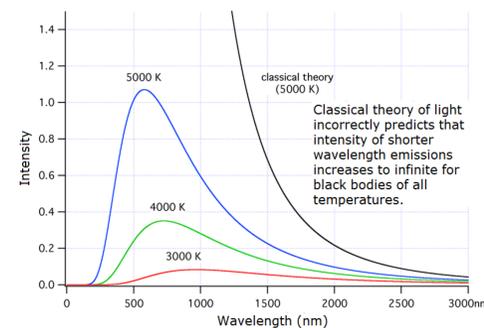


Figure 1: Ultraviolet Catastrophe

**Photoelectric Effect:** This explains why metals are shiny. If more or less intense light is shone upon a surface it should be shinier or dimmer, right? Wrong.

## Applications and Technology

**Research:** QM provides a means for understanding properties of electrons and then allows scientists to utilize those properties to understand the structures of materials, from the skeletons of rockets, to the solid state hard drive in your computer.

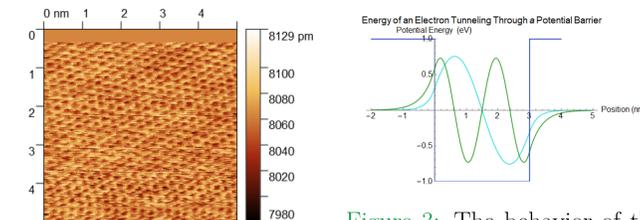


Figure 2: Topographical Image of Highly Oriented Pyrolytic Graphite

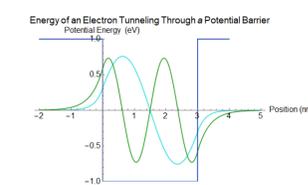


Figure 3: The behavior of the energy of two different electrons tunneling through a potential barrier

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