

Interactions of Intense, Ultra-Short Lasers with Atoms

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The Schrodinger Equation: A Brief History

- In the 1920's, Austrian physicist Erwin Schrodinger used pre-existing concepts of Wave-Particle duality (de Broglie wavelength, photoelectric effect, etc...) to formulate his model for electron behavior, called a wavefunction, Ψ , which is used to represent all possible positions an electron can occupy.

Conditions of the Wavefunction

- ▶ Continuity- Ψ must be continuous everywhere
- ▶ Smoothness- the derivative of Ψ must also be continuous
- ▶ Square integrability and Unitarity-

$$\int_{-\infty}^{\infty} |\Psi|^2 dx \text{ must equal } 1$$

Operators in Quantum Mechanics

- ▶ $f(x)$: any function dependent on position operates as $f(x)$

- ▶ p_x : momentum in x operates as

$$-\iota \hbar \frac{\partial}{\partial x}$$

- ▶ T: kinetic energy operates as

$$\frac{p^2}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

- ▶ where \hbar is rationalized Planck's constant, and $\iota = \sqrt{-1}$

The Schrodinger Equation

- ▶ Time Dependent Schrodinger Equation (TDSE):

$$-i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}) \Psi(\vec{r}, t)$$

- ▶ Time Independent Schrodinger Equation

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}) + V(\vec{r}) \Psi(\vec{r}) = E \Psi(\vec{r})$$

Numerical Solutions of the TDSE

- ▶ Leap Frog Method

$$\frac{\partial^2 \Psi}{\partial x^2} \approx \frac{\Psi_{j-1} - 2\Psi_j + \Psi_{j+1}}{\Delta^2}$$

- ▶ By breaking our wavefunction into its real

and imaginary parts, $\Psi = \Psi_R + i\Psi_I$, we get a system of coupled Ordinary Differential Equations

The Principle of Superposition

- Ψ can be expressed as

$$|\Psi\rangle = \sum_{n=0}^N a_n |n\rangle$$

where $|n\rangle$ is the n th Eigenstate of the Wavefunction, and a_n^2 is the probability our wavefunction will be in that Eigenstate

Note that

$$\sum_{n=0}^N a_n^2 = 1$$

Propagation of Time-Independent Solutions

- We can see how the Time Independent solutions change over time by

$$\Psi(x, t) = \sum_{n=0}^N e^{-i \frac{E_n}{\hbar} t}$$

- E_n is the nth Eigenenergy of the particle

The Infinite Potential Well

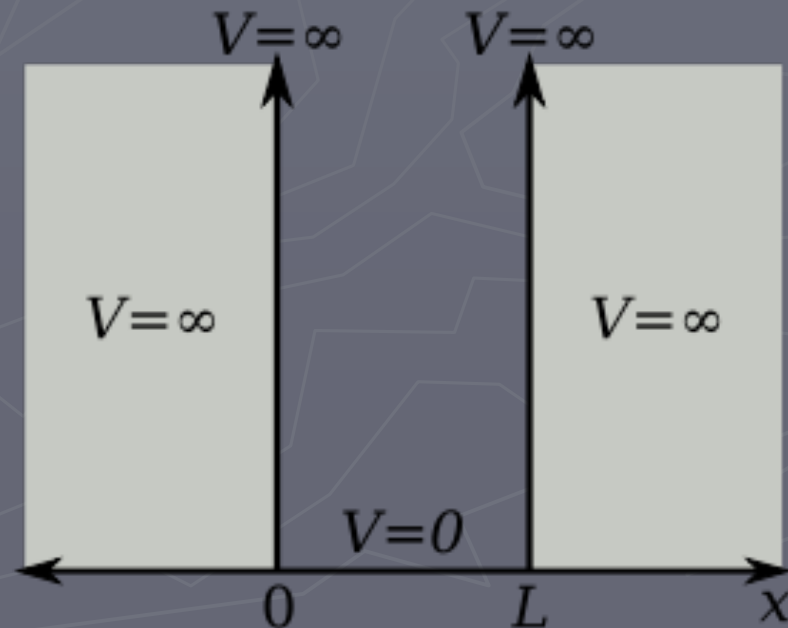
- ▶ The solutions in an infinite potential well of length L are $|n\rangle$

$$= A_n \sin\left(\frac{n\pi x}{L}\right)$$

where A is determined by normalization

- ▶ Eigenenergies are

$$\frac{(\hbar n\pi)^2}{2mL^2}$$



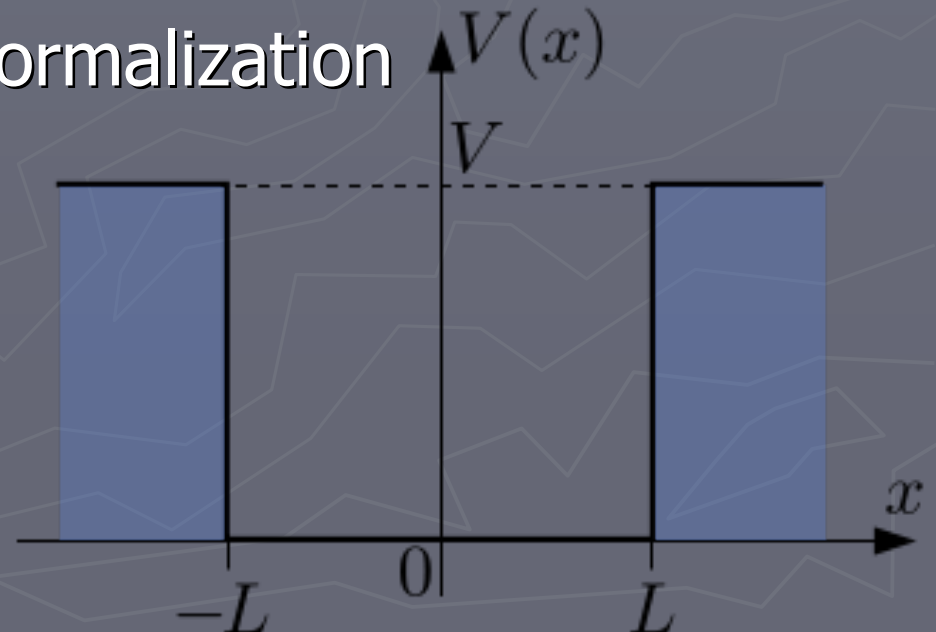
The Finite Potential Well

- ▶ Even solutions in the well are of the form $A\cos(qx)$ where

$$q = \frac{\sqrt{2mE}}{\hbar}$$

Odd solutions of the form $B\sin(qx)$

- ▶ A and B determined by normalization



Eigenenergies of the Finite Well

- ▶ The even and odd Eigenenergies are given by the transcendental equations

$$k = q \tan(q \cdot a) \text{ (Even)}$$

$$k = -q \cot(q \cdot a) \text{ (Odd)}$$

- ▶ where a is half of the well width, and

$$k = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

Future Work

- ▶ Investigate numerical solutions of the TDSE using various numerical methods
- ▶ Compare methods with various approximation methods, along with each other

References

- ▶ <http://user.mc.net/~buckeroo/BHSE.html>
- ▶ <http://hyperphysics.phy-astr.gsu.edu/Hbase/quantum/qmoper.html>