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Schrödinger Equation with Finite Difference Method

1 Motivation

In high school, we learned about the Schrödinger equation in physics or chemistry class, for example, particle in a box, tunnel effect, and orbital of electrons. However, we learned just simple cases. In this project, I will try to solve more complicated cases about the equation using finite-difference schemes.

2 What to do

Solve the linear time-dependent Schrödinger equation $i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x},t)\right]\Psi(\mathbf{x},t)$ in several conditions.

1. A free particle in the 1d, 2d - box or in the ring
2. Harmonic Oscillator in the 1d, 2d - plane
3. Schrödinger equation for hydrogen atoms in spherical coordinates with Columb Potential

Where the harmonic oscillator is $V(\mathbf{x},t) = \sum_{i=1}^{1,2}\frac{1}{2}m\omega^2 x_i^2$

Challenge

If I can handle all topics above, I will try to solve the 2d - non-linear Schrödinger equation

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + \kappa\|\psi\|^2\psi$$

Or trying to show the tunnel effect which the 1d - domain has geometry.

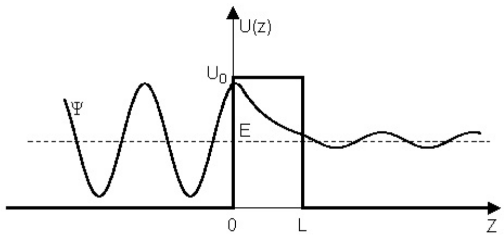

Figure 1: Tunnel Effect

3 How to

I will refer to the article, Becerril et al. 2008 for the first and second cases. The third one uses Spherical Harmonics to show the quantum numbers and orbital. Image

References

Becerril, R., Guzmán, F., Rendón-Romero, A., and Valdez, S. (2008). Solving the time-dependent schrödinger equation using finite difference methods. *Revista mexicana de física E*, 54:120–132.

https://physicsopenlab.org/author/physics7/#author (2017). Tunnel Effect.