

Numerical Solutions to the Schrodinger Equation

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1 Project Proposal

The majority of problems in quantum mechanics can be linked to the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{x})_n + V(\vec{x})\Psi(\vec{x})_n = E_n\Psi(\vec{x})_n. \quad (1)$$

This equation describes the motion of particles defined by quantum mechanical properties as opposed to classical mechanics. Although, as the number of particles increases, the coulomb potential term becomes problematic and makes this differential an incredibly difficult one to solved analytically. To overcome this, there are quite a few algorithms that have allowed researchers to solve more difficult and more complex multi-body problems using numerical approximations. In this project, I will explore numerical approximations to some of the most commonly studied problems: particle in a box, particle in an infinite well, and the hydrogen atom model (harmonic oscillator). These three problems have been analytically solved, so I will be able to compare the approximation to the exact solution. These results allow me to explore convergence rates, order of accuracies, and explore interesting phenomenon such as quantum tunneling. Equation 1 shows the Schrodinger equation in multiple dimensions, but I will mainly be working with the 1D or 2D time independent Schrodinger equation. The 1D equation reduces equation 1 to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)_n}{dx^2} + V(x)\psi(x)_n = E_n\psi(x). \quad (2)$$