

TEACHING ONE DIMENSIONAL TIME INDEPENDENT SCHRÖDINGER EQUATION USING SPREADSHEET

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In this paper, we use the Numerov method to find the solutions of time independent Schrödinger equation for different cases and graphically plot and interpret wavefunctions or probability densities. Using Excel spreadsheet we have investigated three cases such as Infinite well with a cosine bump, step up and step down potential within an infinite well and sloping potential well. Using spreadsheets is more preferred rather than using advanced packages like Mathematica and Python as it is more commonly used and solving the Schrödinger equation does not require prior knowledge of a programming language. We believe working through these cases will enhance understanding of the shape of the wave function and probability density and improve students' qualitative understanding of Quantum Mechanics.

Introduction

In the traditional course of undergraduate quantum mechanics, students study the analytical solution of Schrödinger equation, which can be solved exactly only for a limited number of cases. A solution of the Schrödinger equation can be more conveniently obtained by using numerical techniques than using analytical techniques. In this paper, we solve the one dimension time independent Schrödinger equation for different potential wells and obtain a numerical solution using spreadsheets. Further, we graphically describe the wavefunction or probability density for each case. Different tools have been utilized to obtain the numerical solution to Schrödinger equation like Mathematica (Schmied, 2015) and Python (Srniec, Upadhyay, & Madura, 2017), but using the spreadsheet is preferred because it is widely used and also an approximate solution to the Schrödinger equation can be obtained without prior knowledge of programming. Although Microsoft excel spreadsheet has been utilized to find the solution to the Schrödinger equation for the Morse potential (Rioux, 1991) and Harmonic Oscillator (Levine, 2014), the cases we have included like the infinite potential well with a cosine bump and one dimensional step potential have not been addressed in these references. These spreadsheets can be used as part of laboratory experiments or assignments for the undergraduate course in quantum mechanics so that the students will develop further insight in the shape of the wavefunction and will develop a qualitative understanding of quantum theory. In the following sections, we describe the method and show how to obtain the numerical solution of the Schrödinger equation for Infinite Square well with a cosine bump, step-up and step down potential in an infinite well, infinite well with an internal sloping potential.