

# Schroedinger.m: A Mathematica Package for Solving the Time-Independent Schrödinger Equation

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Schroedinger.m is a package for use with the Mathematica software system (1). It defines commands to enable the user of Mathematica to define a potential and determine bound-state energy eigenvalues for a one-dimensional Hamiltonian. It is intended to be easy to use for students who are beginners to both quantum mechanics and Mathematica.

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## Hardware and Software Requirements

In addition to the hardware and software requirements for Series D (see Getting Started), Schroedinger.m requires a version of Mathematica with a notebook-type interface.

Although the package was developed on a Macintosh computer it is supplied here in Windows format. Mathematica is available for most commonly used platforms. Because the package is a source program, it should be usable with Mathematica on any computer system. All that is required is a version of the package Schroedinger.m saved in text-only format and translated to the particular text format used by the other system. Mathematica, running on the other system, should be capable of reading such a file and interpreting the program contained therein.

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## Features

Similar quantum mechanical computer applications have been published that make use of the Mathcad (2) and Theorist (3) software. The use of Mathematica for teaching quantum mechanics has also been discussed. (4, 5) The package discussed here extends this work by providing within Mathematica a general numerical method for solving the one-dimensional Schrödinger equation.

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### *Applicability and limitations*

The commands defined in this package allow one to set the potential, solve the Schrödinger equation obtaining both energies and wave functions, display the solutions graphically, and calculate certain integrals involving the wave func-

tions. It is limited to one-dimensional bound-state problems that have the boundary conditions  $Y(-\infty) = Y(\infty) = 0$ . It cannot be applied to other one-dimensional problems such as the hydrogen atom, the particle on the circle, or other problems with periodic boundary conditions. It is well suited to solving the one-dimensional R-dependent Schrödinger equation that describes most diatomic molecular potentials. In these cases, although the range of the variable R is actually  $[0, \infty]$  and not  $[-\infty, \infty]$ , it can ordinarily be treated as the latter because of the presence of a barrier, which assures that the wave function can be assumed to vanish at some  $R > 0$ . The method cannot be directly applied to the particle in a box or other problems with an infinite barrier. However, any such problem can be closely approximated by defining a very large (but not infinite) potential for the forbidden region.

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### *Method*

You do not need to know the details of how this package works to use it. However, it helps to be able to understand how the computer represents the solutions, particularly for the purpose of moving beyond the simplest applications or understanding the limitations of the package. The numerical method is described in detail in the Technical Information section of this Manual.

The wave function is represented by a set of its values on a discrete grid of points along the  $x$ -axis. The inherent limitations of a grid-based method are as follows. First, a grid must have a relatively small spacing between points to adequately represent a wave function. If the spacing is too large, then a particular wave function may change rapidly enough so that the grid misses important features. Second, the grid must extend far enough in the positive and negative directions in order to represent the entire wave function up to the points where it goes almost to 0. If either of these conditions is not met, the resulting wave functions and associated energies will be inaccurate.

You have direct control over parameters that define the extent of the grid, its spacing, and the range of solutions. In many cases, however, it is not necessary to worry about these numerical parameters at all. Simply using built-in defaults gives an adequate answer. However, if you are trying to apply the method to an unusual or complex problem, it may be necessary to carefully consider how to set these parameters. Fortunately, the methods for doing so are fairly straightforward.

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### **Curriculum Notes**

Schroedinger.m is intended to be easy to use for students who are beginners to both quantum mechanics and Mathematica. It can be used in a junior-level physical chemistry course to provide examples or to provide the means for students in such a course to carry out numerical experiments. The commands defined in the package are sufficiently self-contained so that the user does not need to know very much about Mathematica. However, the more of Mathematica that one knows, the further one will be able to go with the applications. Even knowing a very few basic Mathematica functions will enable a student to use solutions from this package to do some fairly sophisticated computations with one-dimensional wave functions.

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## Utilities Used

The package was developed using Mathematica 2.2.1 Enhanced for the Macintosh computer.

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## Citations

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