Term Project Outline

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Goals

- Solve the Time-Dependent Schrödinger Equation
  for an arbitrary time-independent potential
- Subgoals
  - Animation of Resulting Wavefunctions
  - Determine whether solution is Steady-State
  - Comparison solution to known analytic functions (using least-squares method)
  - Extensive, Structured help-commands

1 Synopsis of Project

The time-dependent Schrödinger equation:

$$i\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi$$

is a second-order partial differential equation. It is the governing equation in the non-Relativistic regime of Quantum Mechanics. Its solutions are called wavefunctions, ψ. The interpretation given to these functions is that:

$$\int_{x_0}^{x_1} \psi^*(x,t)\psi(x,t)dx$$

represents the probability of finding a system (or a particle) in a State $\psi(x,t)$ between x_0 and x_1 at time t. Once one finds the wavefunctions, all measurable quantities are available for analysis and calculation.

It is in general very difficult to solve this equation, even when it permits stationary-state solutions. Therefore a numerical analysis of this problem seems appropriate.

The problem will be attacked with a technique known as Cayley's method (a.k.a. Crank-Nicholson method). The method rests on appropriately approximating the differential equation as a finite-difference equation. This finite difference equation (which will turn out to be a diagonal system of linear equations) can then be plugged directly into a "blackbox" solver routine (such as LAPACK), and a solution will be returned.

One starts with the initial state $\psi(x, t = 0)$, and the boundary conditions that state, as x $\rightarrow\pm\infty$, $\psi \rightarrow 0$. Using these quantities one can derive a recurrence relation between the value of the function at a point x_i to the value of the function at its nearest neighbors (typically x_{i-1} and x_{i+1}).

Since we are concerned only with time-independent potentials, Schrödinger's equation can be separated into a spatial and temporal part:

$$i\frac{\psi_t(x,t)}{\psi(x,t)} = \frac{-\hbar^2}{2m}\frac{\psi_{xx}(x,t)}{\psi(x,t)} + V(x)$$

Note that the left-side of the equation depends only on t, and the right-side depends only on x. This is a classic seperable equation, therefore both sides equal a constant. The solution to this is, in general, a linear combination of stationary states. According to Numerical Recipes, the solution can be generalized to the form:

$$\psi(x,t) = e^{-iHt}\psi(x, t = 0)$$

where:

$$H \equiv \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)$$

The exponential can be expanded as a power series, and in Cayley's method is differenced as:

$$e^{iHt} \simeq \frac{1 - \frac{1}{2}iH\Delta t}{1 + \frac{1}{2}iH\Delta t}$$

This leads finally to the form:

$$(1 + \frac{1}{2}iH\Delta t)\psi_j^{n+1} = (1 - \frac{1}{2}iH\Delta t)\psi_j^n$$

Upon replacing H by its finite-difference approximation in x, a tridiagonal system unfolds. At which point we hand over our claims of knowledge to a mysterious black box known only as "tdgesv".

Once the solution is obtained for many times, it will be possible (so I'm told) to animate the time dependent wavefunctions, using software written by Dr. Matthew Choptuik. If the animation yields clues that perhaps the wavefunction is in a single stationary-state (i.e. time-independent), an option will be available to approximate the solution as an analytic function. he appropriate coefficients will be determined by a least-squares method. There will be an extensive help section (alluded to in the list of goals), which will be structured much like the help system available in "gnuplot". It will serve an obvious purpose.

It is the intent of this project to accomplish all of the goals set forward above. However, dependent on the difficulty of design and implementation of the problem, the above goals are simply to act as tenative guidlines. They are subject to change (either expand or deflate) according to time-constraints.