Computational Physics Project 6—Time Dependent Schrödinger Equation

In this project, you will develop a program to simulate the Time Dependent Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}+V\Psi=i\frac{\partial\Psi}{\partial t},$$

here quoted in units where $\hbar=1$ and $m=1$. *[What units of length does this imply?]* It must plot the real and imaginary parts of the wavefunction,

Begin by implementing the obvious finite difference scheme

$$\left[\frac{\Psi_{j+1}^{n+1}-2\Psi_j^{n+1}+\Psi_{j-1}^{n+1}}{(\Delta x)^2}\right]+V_j\Psi_j^{n+1}=i\left[\frac{\Psi_j^{n+1}-\Psi_j^n}{\Delta t}\right].$$

Numerical Recipes contains a helpful suggestion for a better algorithm in section 20.2.1 (eq. 20.2.36)—An implementation of this other algorithm may be found as a *Mathematica* notebook on my website. `http://sites.tufts.edu/softmattertheory/2012/12/21/visualizing-quantum-mechanics-with-mathematica/` As part of the project, I want you to compare the two algorithms for their fidelity on some simple potentials.

1. Begin by testing a free wavepacket, i.e. with $V(x)=0$. Does it do what you expect physically? What happens with periodic boundary conditions versus zero boundary conditions (i.e. setting $\Psi=0$ at the edge). Check on the discrepancy between the two algorithms.
2. Look as some simple potentials for which you know the solution, e.g. the infinite square well; the harmonic oscillator, the triangle well. Can you find the eigenstates? What do they look like? Are the energy levels correct?
3. Look at a potential barrier. Determine the fraction of the wavefunction that's reflected and transmitted and cross check this with analytical calculations *[see Griffiths]*.
4. Look at a potential barrier with the incident energy set to equal the barrier height. *[This is truly remarkable!]*
5. Look at a periodic array of potential wells, i.e. a Kronig-Penney crystal; send in wavepackets with narrow δk and hence identify bands.
6. Remarkably, the potential

$$V(x)=\begin{cases} ix & -L<x<L \\ \infty & x\le -L,\ x\ge L \end{cases}$$

yields a Hamiltonian that possess real eigenvalues despite being non-Hermitian. Check this analytically if you like *[hard!]* Use your program to establish what the eigenstates look like. Does the potential

$$V(x)=\begin{cases} x+ix & -L<x<L \\ \infty & x\le -L,\ x\ge L \end{cases}$$

possess eigenstates?