Specified Topic 2

Learning goals: implicit schemes, complex matrix manipulation, time-evolution visualization.

Time-dependent Schroedinger Equation

See distributed notes (tdse.pdf).

Helpful references are Giordano Ch 10, and the paper by Goldberg, Schey and Schwartz (Am. J. Phys. 35 (1967), 177).

For this topic use the following "minimum uncertainty wave-packet" initial wave-function with an appropriate normalization factor, C, where the average momentum of the wave-packet, $p_0 = \hbar k_0$.

$$\psi(x, 0) = C \exp\left[-(x - x_0)^2/(4\sigma^2)\right] \exp(ik_0 x)$$

where $x_0 = 0.4$, $k_0 = 500$, and $\sigma^2 = 0.001$.

Simulate the time-evolution of this wave-packet under the effect of various potentials. Restrict consideration to elapsed times where the only relevant range for the x-axis is the range [0,1.0].

For this choice of k_0, the average kinetic energy of the wave-packet, E_0, is $\hbar^2 k_0^2/(2m)$, namely 1.25×10^5 in units with $\hbar = 1$, $m = 1$. Potentials you should consider are:

1. Free particle ($V = 0$)
2. $V = 0$ except for a potential wall with $V = 8E_0$ for $x \geq 0.6$
3. $V = 0$ except for a potential well with $V = -8E_0$ for $x \geq 0.6$
4. $V = 0$ except for a potential barrier with $V = E_0$ for $0.6 \leq x \leq 0.65$
5. $V = 0$ except for a potential wall with $V = E_0$ for $x \geq 0.6$
6. $V = 0$ except for a potential barrier with $V = 0.5E_0$ for $0.6 \leq x \leq 0.65$

For 1, plot the evolution of the mean value of x and the width of the wave-packet vs time. For all six potentials display the time-evolution of the probability density function, and report the $< x >$ and $< x^2 >$ at $t = 5 \times 10^{-4}$.

Suitable ways of plotting the time evolution may be to make snap-shots of many time slices, stitching the various time slices into a movie, or may be done by filling for example a color enhanced plot in (x,t) with an intensity proportional to the probability.