Numerical Integration of the Time-Independent Schrodinger Equation:
Possible Potentials

One-Dimensional Potentials

Linear half-potential:
Let $V(x) = \alpha x$, for $x > 0$, and infinity elsewhere, with $\alpha = 1$ eV/angstrom.
Find the energies of the four lowest levels. ($E_3 \sim 8.6217$ eV)

Quadratic half-potential (half-harmonic-oscillator):
Let $V(x) = \alpha x^2$, for $x > 0$, and infinity elsewhere, with $\alpha = 3$ eV/angstrom.
Find the energies of the four lowest levels, and determine the expected energies from α and the exact solutions for the harmonic oscillator.

Cubic half-potential:
Let $V(x) = \alpha x^3$ for $x > 0$, and infinity elsewhere, with $\alpha = 5$ eV/angstrom^3.
Find the energies of the four lowest levels. ($E_2 \sim 40.443$ eV)

Quartic half-potential:
Let $V(x) = \alpha x^4$ for $x > 0$, and infinity elsewhere, with $\alpha = 5$ eV/angstrom^3.
Find the energies of the four lowest levels. (Exact values unknown.)

Four more possible potentials:
For each of the above potentials there is a corresponding symmetric potential – $\alpha|x|$, αx^2, $\alpha|x^3|$, αx^4 – that could be analyzed, using the α's given above.

NOTE: Since each half-potential has an infinite wall at $x = 0$, the wavefunction must go to zero at this point. This means that the wavefunctions of these half-potentials look exactly like those for the full corresponding symmetric potentials in the region $x > 0$, for the eigenstates with a node at $x = 0$. Think about what this implies for the energy levels of these two cases.

3D: Radial Equation for Central Potentials

$$\frac{d^2R}{dr^2} = l(l+1)\frac{R}{r^2} - \frac{2dR}{rdr} - \beta[E - V(r)]R$$

To do any of the following potentials you would need to create a new version of your program since the 1D Schrodinger equation does not have the first two terms on the right-hand side. Nevertheless, you would still be calculating curvature, slope, and value in the same order. Since the angular momentum quantum number l is in this equation, it will appear as a given in these 3D problems.

Linear radial potential:
Let $V(r) = kr$, with k = 1 eV/angstrom. Find the three lowest energy levels for $l = 0$. ($E_2 \sim 6.38$ eV)

Exponential radial potential:
Let $V(r) = Ae^{kr}$, with A = 5 eV and k = 0.2 angstroms. Find the three lowest energy levels for $l = 0$ and $l = 1$. ($l = 0$: $E_2 \sim 13.635$; $l = 1$: $E_1 \sim 11.646$)

Wood-Saxon potential:
This potential is used to model energy levels of protons and neutrons inside a nucleus: $V(r) = -\frac{A}{1+e^{(r-b)/d}}$. Take A = 100 eV, b = 2 angstroms, and d = 0.03 angstroms. Find the three lowest energy levels for $l = 0$ and $l = 1$. ($l = 0$: $E_2 \sim -51.192$ eV; $l = 1$: $E_1 \sim -65.991$ eV)