

## 5 Exact and Approximate Solutions to the Schrödinger Equation

- 11/3:
1. In the book *Flatland*, Edwin Abbott explores the amazement of the inhabitants of a two-dimensional world when they are visited by a three-dimensional sphere. In class, we developed the Schrödinger equation for an atom in three dimensions. Consider how a two-dimensional atom would differ from a three-dimensional atom.
    - (a) Express the Schrödinger equation in the Cartesian coordinates  $x$  and  $y$ .
    - (b) Re-express the Schrödinger equation in the polar coordinates  $r$  and  $\phi$ .
    - (c) Factoring the wave function  $\psi(r, \phi)$  as  $R(r)Q(\phi)$ , separate the Schrödinger equation into a Schrödinger equation for  $R(r)$  with quantum numbers  $n$  and  $m$  and a Schrödinger equation for  $Q(\phi)$  with quantum number  $m$ .
    - (d) Solve the Schrödinger equation for  $Q(\phi)$  and explain its connection with the two-dimensional rigid rotor.
    - (e) For *only*  $n = 1$  and  $m = 0$ , solve the Schrödinger equation for the ground-state energy and wave function.
    - (f) What is the ratio of the ground-state energy of the two-dimensional hydrogen atom to the ground-state energy of the three-dimensional hydrogen atom?
    - (g) On the same figure, draw (or graph electronically) as a function of  $r$  the probability for finding the electron in the ground state of the 3D hydrogen atom as well as the probability for finding the electron in the ground state of the 2D hydrogen atom. Briefly compare and contrast these two probability distributions.
  2. Using your lecture notes and Problem 7-1 as a guide, give a proof of the variational theorem, i.e., that...
    - (a) The energy from a trial wave function will always be greater than or equal to the exact ground-state energy.
    - (b) The energy from a trial wave function, constrained to be orthogonal to the exact ground-state wave function, will always be greater than or equal to the exact energy of the first excited state.
  3. Consider a particle in a box in the interval  $[-a, a]$ .
    - (a) Use the trial wave function
$$\psi_t = x(a^2 - x^2)$$
to obtain an approximate energy for the first excited state of the box as a function of  $a$ .
    - (b) Why does this function give an approximation to the first excited state rather than the ground state?
    - (c) Use the more accurate trial wave function
$$\psi_t = c_1x(a^2 - x^2) + c_2x^3(a^2 - x^2)$$
to obtain an approximate energy for the first excited state of the box as a function of  $a$ .
    - (d) Compare the approximate energies with the exact energy (including their dependence on  $a$ ) and the approximate wave functions with the exact wave functions. (Hint: In comparing the wave functions, you may want to select  $a = 1$ .)
  4. Use the Quantum Chemistry Toolbox in Maple to answer the lettered questions in the worksheet "Variational Methods" on Canvas.