

## Problem Set 6

(due Wednesday, October 17, 5:00 p.m.)

- Qualitative wavefunction sketches: Please sketch the indicated wavefunctions on the accompanying worksheet.
- In this problem you will solve the Schrödinger equation numerically, for the potential energy function  $V(x) = \alpha|x|$ .
  - Before attempting to solve a complicated differential equation, it's always a good idea to rewrite it using dimensionless variables. To do this, show first that the quantity  $\ell \equiv (\hbar^2/2m\alpha)^{1/3}$  has units of length. Then define the dimensionless variable  $z \equiv x/\ell$  and the dimensionless energy parameter  $\eta \equiv 2m\ell^2 E/\hbar^2$ . Rewrite the Schrödinger equation in terms of  $z$  and  $\eta$ .
  - Use *Mathematica* to find the five lowest-energy definite-energy wavefunctions and the corresponding values of  $\eta$  (to four or five significant figures). Turn in a printout showing your work, including plots of the wavefunctions. (Hints: For the lowest-energy wavefunction, try a horizontal range of  $z$  values from  $-6$  to  $6$ . You'll have to increase this range for some of the higher excited states. Try an "initial" wavefunction value of some small number like .001, and an initial derivative of zero.)
  - Discuss the qualitative features of these wavefunctions, and their energies, in some detail.
  - Evaluate the five lowest allowed energies in electron-volts, assuming that the particle in question is an electron and that  $\alpha$  equals one electron-volt per Ångström (or  $10^{10}$  eV/m).
- Show that, when  $U(x) = \frac{1}{2}k_s x^2$ , the function  $e^{-ax^2}$  satisfies the Schrödinger equation, provided that the constant  $a$  is chosen appropriately. What is  $a$  in terms of  $m$  and  $k_s$ ? What is the energy corresponding to this wavefunction?
- A CO molecule can vibrate with a natural frequency of  $6.4 \times 10^{13} \text{ s}^{-1}$ .
  - What are the energies (in eV) of the five lowest vibrational states of a CO molecule?
  - If a CO molecule is initially in its ground state and you wish to excite it into its first vibrational level, what wavelength of light should you aim at it?
- In this problem you will analyze the spectrum of molecular nitrogen; please refer to Figure A.11 in the handout. You may assume that all of the transitions are correctly identified in the energy level diagram.
  - What is the approximate difference in energy between the upper and lower electronic states, neglecting any vibrational energy (aside from the zero-point energies  $\frac{1}{2}hf$ )?
  - Determine the approximate spacing in energy between the vibrational levels, for both the lower and upper electronic states.
  - Repeat part (b) using a different set of spectral lines, to verify that the diagram is consistent.
  - For the lower electronic state, what is the classical oscillation frequency  $f$  of the vibrational motion?