

Chem 21a: Assignment #3  
Assigned: October 17, 2006  
Due: October 24, 2007 @ 1pm

### **Free Particle, Particle in a Box, and Particle in an Harmonic Potential**

1. *Molecular Quantum Mechanics*, page 41 problem 2.12
2. *Molecular Quantum Mechanics*, page 41 problem 2.29
3. *Molecular Quantum Mechanics*, page 41 problem 2.32
4. A particle in a one dimensional box can be used as a simple model for approximating the  $\pi$  bond orbitals in a molecule like butadiene ( $C_4H_6$ ). Given that the length of the molecule is 424 pm, calculate the first three energy levels of butadiene. Calculate the energy of the electrons in the  $\pi$  system (assume that the potential in the box is zero), remembering that two electrons occupy each energy level. What wavelength of light is required to excite an electron from the ground to the first excited state?
5. Go to the chapter 2 interactive mathematical functions for the textbook's companion website: (<http://www.oup.com/uk/orc/bin/9780199274987/01student/functions/ch02/>, if this link does not work for you go to <http://www.oup.com/uk/booksites/chemistry> select the "Atkins and Friedman," click on "Interactive Mathematical Functions" under "Student Resources," and go to "Chapter 02") select and download the spreadsheet for equation 2.22. This is the equation for the transmission probability of a particle tunneling through a barrier.  
The second sheet of spreadsheet (look for the "Tunneling Probability" tab on the bottom of the sheet) allows you to manipulate the mass of the particle ( $m$  in units of  $m_e$ ), the length of the barrier ( $L$  in Bohr radii,  $a_0$ ) and the potential energy of the barrier ( $V$  in hartrees,  $E_h$ ), and see the resulting tunneling probability.  
Use the spreadsheet along with the equation 2.22 to answer the following questions (remembering to make the appropriate unit conversions):
  - A. What is the approximate probability that electrons are able to tunnel across a 1.2 nm barrier with a potential of  $4.36 \times 10^{-19}$  J ( $1\frac{1}{2}$  times their energy)?
  - B. Now look at the same electron tunneling across a barrier with the same potential but half the width, and then a fifth and tenth the width. What are the tunneling probabilities?
  - C. STM uses the current generated by electron tunneling between the surface and the tip to regulate the distance between them and thus map the surface. If current is proportional to tunneling probability, what is the relative change in current for the electrons in part A between 0.11 and 0.10 nm. How about between 0.10 nm and 0.09 nm? What does this say about the sensitivity of STM?
  - D. Replace the electrons in question C with protons. Given that STM works well for electrons, is using protons a feasible alternative? Explain?

**Please write how much time you spent on this assignment at the top of your paper. This will help us keep the length of the assignments reasonable.**