C455A - Homework 3
Due Tues Oct. 17 at **5PM**
Circle your answers. Submit your problems in order. Staple your work together.

1) P2.12 - more eigenfunctions practice
2) P4.4 - superposition of momentum eigenfunctions
3) P4.21 - degeneracies for 2D and 3D boxes
5) P4.25 - averages and superpositions (again? do you think this might be important!?)
6) Q4.7 – qualitative question on zero point energies
7) Q5.3 – qualitative question on tunneling
8) P6.10 – Variance of an operator—Hint: this problem is more than just a plug and chug math problem in that you should get to steps where you *recognize* that certain integrals have particular values. It also has the added benefit of allowing you to *understand* the uncertainty principle *quantitatively.*
9) P6.12 – position/momentum uncertainty for an electron in a TV
10) P6.15 – the Heisenberg uncertainty principle and the particle in a box
11) Using your qualitative understanding of the solutions for the finite square well, explain the distinction between “valence” and “core” electrons in chemistry. In other words, why is it only the electrons with the highest principle quantum numbers that form bonds between atoms?
12) *Nonstationary states*
Consider a particle in an infinite square well (box) of width L. Initially, (at t=0) the system is described by a wavefunction that is equal parts a superposition of the ground and first excited states:

$$\Psi(x,0) = C[\psi_1(x) + \psi_2(x)]$$

a) Find C so that the wavefunction is normalized
b) Find the wave function $\Psi(x,t)$ at any later time t. (For extra credit, use your favorite computer package to create an animation of the probability density as a function of time.)
c) Compute $\Psi^*(x,t)\Psi(x,t)$ to show that this superposition is *not* a stationary state.
d) If many systems are prepared in this state and their energies are measured, what will the result be? Discuss both the average of these measurements, and discuss the statistics of the specific results of a series of individual measurements.
13) Aside from its great technological importance in Scanning Tunneling Microscopy (STM) (and in some electronic devices) tunneling is also important to many chemical reactions. For instance, electrons tunnel during redox reactions and proton tunneling is important in many proton transfer reactions (and the rapid “umbrella inversion” of ammonia is due to tunneling). How important do you think carbon atom tunneling is to organic reactions in general? *First, give a qualitative justification of your answer in writing*. *Next, justify your answer quantitatively by comparing the relative tunneling rates for electrons, protons and carbon atoms across a potential barrier 1 Angstrom wide, and height of 1 eV assuming that the kinetic energy of each particle is 0.5 eV.* Ultimately the relative importance of tunneling depends on the rate of competing processes and it is true that for some reactions (the automerization of 1,3-cyclobutadiene and ring expansion of 1-methylcyclobutylefluorcarbene, an example in your text) carbon tunneling plays a central role.