Homework 6. ***Due Mon Nov 16 at the *start* of lecture, in lecture***
****Sets turned in 5 minutes or more after the start of lecture will be considered late****

Levine Problems: 6th Ed (5th Ed)

9.3 – Perturbation for anharmonic oscillator

8.9 (8.1) – Hydrogen variation. If you're clever you might not have to do any math, but must explain fully.

8.14 (8.12) – What went wrong?

8.49 (8.42) - Normalized eigenvalues and eigenvectors of a matrix

Additional Problems:

OPTIONAL-) Pick any one problem from Exam 1. Rework this problem and turn it in by ***Fri. Nov. 12****. If you get it perfect* (no partial credit) *you will get up to 50% of the points you missed back. (i.e. if you got a 5 out of 25 you could raise your score to a 15/25). Since the key is online you will be judged very closely on your explanations/understanding of the solution!*

Understanding Selection Rules

1) Derive the selection rules for the particle in a 1D box by finding when the transition dipole moment is nonzero. Create a Maple animation of the time evolution of the electron probability density of an equal superposition of two states between which transitions are allowed, and for two states between which transitions are forbidden. ***Interpret the resulting motion***. You may scale the equations to dimensionless quantities for the plots. (This will be a VERY fast problem if you've been thorough in your homework solutions up till now).

2) The particle-in-a-box wave functions form a complete set. Use an appropriate number of them to create a linear variation function for the potential given in Levine 8.2 (8.5 in 5th edition) and find upper limits for the ground and first 3 excited state energies, ensuring that your calculation of the ground state energy is accurate within 0.0013% (note: the true energies of the first 2 states are given in the Levine problems if you read them). Make sure you use assume(L>0) etc.

3) Suppose the Hamiltonian in some vector space is written in matrix form as:

$$H=\begin{pmatrix} 10 & 0 & 1 \\ 0 & 5 & 1 \\ 1 & 1 & 3 \end{pmatrix}$$

a) Find the energy eigenvalues for this Matrix/Hamiltonian (note that this is a symmetric real matrix, so it must be Hermitian, and accordingly the eigenvalues must be real!)

b) Find the eigenvectors associated with each of these eigenvalues

c) Verify that $H|n> = E_n|n>$ for the E_n=10.143895 eigenvalue

d) Verify that $<m|n>=0$ for any two eigenvectors

4) Use a Gaussian trial function $\exp(-\alpha r^2)$ for the ground state for the Hydrogen atom.

A) Compare your result to the exact ground state energy.

B) Draw plots on the same axis comparing your wavefunction.

C) See how close you can get to the 'best values' for the number of terms in your trial function. (Note that having alpha as a variable makes this a *nonlinear* variational function and is in general very difficult to minimize).

TABLE 7-1

The Ground-State Energy of a Hydrogen Atom Using a Trial Function of the Form

$$\phi = \sum_{j=1}^{N} c_j e^{-\alpha_j r^2}$$

where the c_j and the α_j Are Treated as Variational Parameters

N	$E_{min}/(\mu e^4/16\pi^2\varepsilon_0^2\hbar^2)$
1	−0.424413
2	−0.485813
3	−0.496967
4	−0.499276
5	−0.49976
6	−0.49988
8	−0.49992
16	−0.49998