Homework 6. ***Due Mon Nov 6 at 5pm*** in Prof. Ginger's mailbox.
CIRCLE YOUR ANSWERS AND KEY INTERMEDIATE RESULTS
USE MAPLE WHENEVER POSSIBLE
STAPLE YOUR PAPERS TOGETHER
INCLUDE ALL COMPUTER PRINTOUTS (with commentary)

Levine Problems

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

8.12– What went wrong?

8.42-Normalized eigenvalues and eigenvectors of a matrix

Additional Problems:

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) Complete the missing steps from lecture in the calculation of the radiative lifetime of the $2p_0$ state of a hydrogen atom.

2a) Calculate the transition dipole moment for $2p_0$ to 1s.

2b) Calculate the Einstein A coefficient for this transition and the lifetime of the state.

2c) Check your answer in 2b) against the experimental values from the NIST reference tables online at http://physics.nist.gov/PhysRefData/ASD/lines_form.html

3) 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 8.5 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 Levine 8.5 and 8.15). Make sure you use assume(L>0) etc.

4) 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 Hamiltonian (note that this is a symmetric real matrix, so it must be Hermitian, so the eigenvals must be real)

b) Find the eigenvectors associated with each of these eigenvalues

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

d) Verify that $\langle m|n\rangle=0$ for two eigenvectors

5) 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 with 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