Physics of Atoms and Molecules
Physics 2202S
University of Toronto
Problem Set #1

September 25, 2015 due: October 9, 2015 *(revised)*

Reading Assignment: Backgrounds vary among students, in graduate courses. Use your favorite quantum mechanics texts to brush up on the following topics we'll need and use in this course:

• General properties of solutions of the 1D Schrodinger equation, including orthogonality, boundary conditions and the oscillation theorem (N.B. we will be interested in functions defined over the positive real numbers).

• Perturbation theory, including the degenerate case.

• Clebsch-Gordan coefficients and the addition of two angular momenta.

Problem: *The spherical well.*
This is a multi-part question intended to exercise your understanding of the above topics. You should use a combination of analytic techniques, computer-based symbolic manipulation and numerical methods to solve it (just as you would in a real research problem). While you may discuss ideas with others, **the work you turn in must be your own, you must be able to reproduce it independently**. You should append print-outs of code (which should be properly commented; if you used subroutines you did not write, you must cite their source); I do not care what programs or languages you use, but if it looks questionable to me I may require you to demonstrate it running. Also, pay special attention to *presenting your results clearly and logically*: if I cannot figure out what you have done, your mark may reflect only the value I can find.

1. Suppose a spinless particle of mass M is confined by a finite-range potential $V(\mathbf{r})$, for which $\lim_{|\mathbf{r}|\to\infty} V(\mathbf{r}) = 0$. The coordinate representation of the energy eigenfunctions is $\langle \boldsymbol{r}|\psi_{\boldsymbol{E}} = \psi_E(\boldsymbol{r})\rangle$, where E is the energy. Show that, for bound energy eigenstates (i.e. states for which $\lim_{|\mathbf{r}|\to\infty} r^2|\psi_E(\mathbf{r})|^2 = 0$), E must be negative.

2. Now consider a spherically symmetric potential, for which $V(\mathbf{r}) = V(r)$, where r = $|\mathbf{r}|$. Writing $\psi_E(\mathbf{r})$ in terms of spherical Harmonics, i.e.,

$$\psi_E(\mathbf{r}) = \sum_{lm_l} a_{m_l} Y_{l,m_l}(\theta,\phi) u_{E,l}(r) ,$$

find an equation for the radial wavefunction $\mu_{E,l}(r)$. Why is it correct not to include the subscript m_ℓ in the function $\mu_{E,\ell}(r)$? If V (r) is a mathematically regular function close to and at the origin, what is the form of the leading term of $\mu_{E,\ell}(r)$ in this region? Use the oscillation theorem and your knowledge of the form of the radial wave function for small and large values of r to sketch the generic form of the lowest three p-state energy eigenfunctions.

3. Now consider the special case of a spherically symmetric square well potential of radius R, i.e.

$$V(r) = \begin{cases} -V_0, & if\ 0 \leq r \leq R \\ 0, & if\ r > R \end{cases}$$

Find an expression for the bound-state eigenfunctions $\mu_{E,}(r)$ in terms of *spherical Bessel functions.*

4. What are the boundary conditions at $r = R$? Substitute your solution for the p-wave case into these boundary condition at $r = R$ to find a formula that determines the energy eigenvalues. Determine the numerical energy eigenvalues (expressed in terms of V_0) for the case that $\sqrt{2MV_0R^2/\hbar^2}$ = 20. Plot the correctly normalized radial wave functions for the lowest three eigenvalues.

5. How would the formulation and solution of the problem differ if the trapped particle was an electron of spin 1/2? For the p-state electrons, write down the generic form of a function which is an eigenfunction of $E, \hat{L}^2, \hat{S}^2, \hat{J}^2$ and $\hat{J}_z$. Using the Clebsch-Gordan coefficients, construct the eigenstate with quantum numbers $\ell = 1$, s =1/2, j = 3/2, m_j = 1/2, expressing your answers in terms of the radial wavefunction $\mu_{E,1}(r)$ the spherical harmonics $Y_{1}, m\ (\theta, \emptyset)$ the electron spinors $v_\uparrow$ and $v_\downarrow$.

6. Now suppose some a spin-orbit interaction is magically "turned on", transforming the Hamiltonian to the following form:

$$\hat{H} = \frac{1}{2M}\,\hat{p}^2 + V(\hat{r}) + \xi\frac{R^2}{\hbar^2}\left(\frac{1}{\hat{r}}\frac{dV(\hat{r})}{d\hat{r}}\right)\hat{\mathbf{L}} \bullet \hat{\mathbf{S}}$$

where $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$ are the orbital and spin angular momenta, $\xi << 1$ is a dimensionless parameter, and the potential $V(\hat{r})$ is that given in (3) above. Use perturbation theory to find the splitting between the j = 3/2 and the j = 1/2 levels of the lowest energy p-state for a trapped electron, with $\sqrt{2MV_0R^2/\hbar^2}$ = 20 (as before). Express your answer as a numerical factor multiplying the constant ξV_0.