EMA 601/NE 602
Problem set #3
Due 12/4 at 11:59 pm on Canvas, in pdf format
Total points: 35 (plus 15 extra credit points)

Guidelines:

- Typed solutions are preferred, but you may scan your handwritten solutions as long as the writing is legible.
- Please compile your responses into a single pdf document.
- You are welcome to work together on the problems, but you must write your own responses and code.
- Please show your derivations or describe how you arrived at your responses.

1. (15 points) **Numerical solution of the Schrodinger equation** In this problem, you will go through a method of finding the wave functions and their energies for a potential using the central-field approximation.

   (a) (3 points) Show that you can write the radial wave equation (shown on Slide 8 of Lecture 11, and you may assume that $\mu \approx m_e$) as the following:
   $$\frac{d^2R}{dx^2} + \frac{2}{x}\frac{dR}{dx} + \left(\tilde{E} - \tilde{V}(x)\right)R = 0,$$
   where $R = R(x)$; the position and energy variables are dimensionless with $x = r/a_0$ and $\tilde{E}$ is scaled by $\frac{e^2}{8\pi\epsilon_0 a_0} = 13.6\ eV$. Show that the effective potential is
   $$\tilde{V}(x) = \frac{l(l+1)}{x^2} - \frac{2}{x},$$
   where l is the orbital angular momentum number.

   (b) (2 points) The first- and second-order derivatives of a function $f(x)$ can be approximated by
   $$\frac{df}{dx} = \frac{f\left(x + \frac{\delta_x}{2}\right) - f\left(x - \frac{\delta_x}{2}\right)}{\delta_x}$$
   $$\frac{d^2f}{dx^2} = \frac{f(x+\delta_x) + f(x-\delta_x) - 2f(x)}{\delta_x^2}$$
   where δ_x is a small step size. Show that by applying these approximations on the radial wave equation, we arrive at the recurring expression for R at $x + \delta_x$ based on its value at the two previous points:
   $$R(x+\delta_x) = \frac{\left\{2R(x) + \left(\tilde{V}(x) - \tilde{E}\right)R(x)\delta_x^2 - \left(1 - \frac{\delta_x}{x}\right)R(x-\delta_x)\right\}}{1 + \frac{\delta_x}{x}}$$

   (c) (6 points) Develop a method that allows you to find the eigenenergies $\tilde{E}$, for a given l, using the recurring expression for R. Compute the eigenenergies and the effective quantum numbers using $n^* = 1/\sqrt{\tilde{E}}$, for $l = 0, 1, 2$.

   Hints: The calculated function will not be normalized and the starting values, *e.g.*, $R(\delta_x)$, can be arbitrary. For your numerical implementation here, you should start the calculation at $x = \delta_x$ and set $R(\delta_x) = 1$ as the initial condition. Finally, we are searching for bound state solutions, where $R(\infty) \to 0$.

(d) (4 points) Plot R and rR based on your numerical results for the solutions associated with the lowest energies corresponding to $l = 0, 1, 2$. Compare your results (general shapes of the curves, eigenenergies, and effective quantum numbers) with the known results of the hydrogen atom.

2. **(15 points – Extra credit) Quantum defects in alkali atoms** The effective quantum number n^* is equal to $n - \delta_{nl}$, where δ_{nl} is the quantum defect. Using the numerical method you implemented in Problem 1, you will now calculate the quantum defects in sodium.
   (a) (1 points) The potential of an alkali atom can be approximated by the Coulomb potential with central charge $+Ze$ for $r < r_c$, where r_c is the mean radius of the highest closed electron shell, and the Coulomb potential with charge $+e$ for $r > r_c$. An offset constant is added to the potential inside r_c to ensure continuity of the potential. Justify why the aforementioned approximation is valid for alkali atoms.
   (b) (3 points) Write down the expressions for $V(r)$ and $\tilde{V}(x)$, based on the radial equation on Slide 4, Lecture 15. Show that

$$\tilde{V}(x) = \begin{cases} -\dfrac{2Z}{x} + \dfrac{l(l+1)}{x^2} + \dfrac{(Z-1)2a_0}{r_c} & \text{for } r \le r_c \\ -\dfrac{2}{x} + \dfrac{l(l+1)}{x^2} & \text{for } r > r_c \end{cases}$$

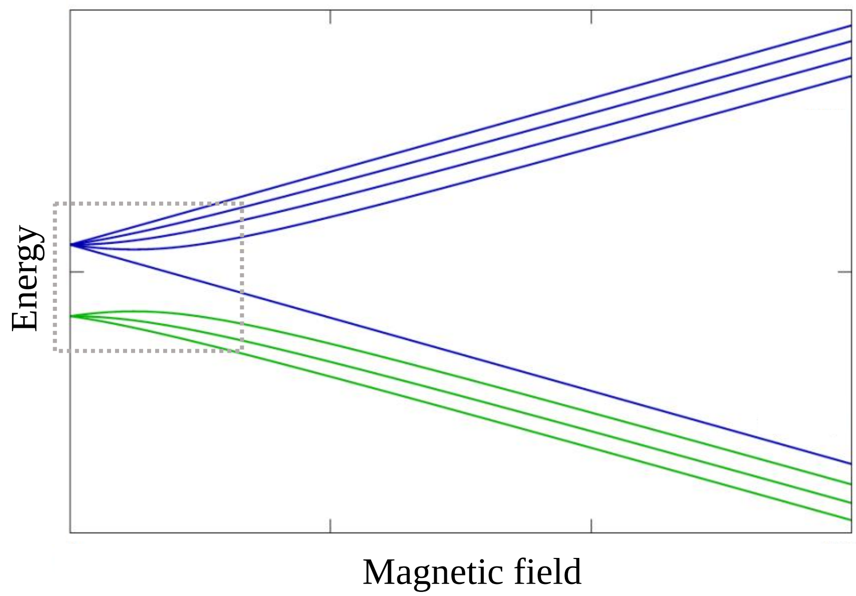
   (c) (5 points) Plot $V(r)$ and $\tilde{V}(x)$ for $l = 0, 1, 2$.
   (d) (5 points) Implement your numerical method to calculate the energies, effective quantum numbers, and quantum defects for the first two principal energy levels of sodium ($n = 3, n = 4$). You can estimate r_c using the plot provided on Slide 23 in Lecture 14.
   (e) (1 point) Compare your results with the table on Slide 3 in Lecture 15 and evaluate the accuracy of your method.

3. (20 points) **Effect of magnetic field on hyperfine levels** In class, we discussed the energy shifts experienced by the hyperfine levels under weak and strong magnetic fields. For intermediate fields, a general form of the hyperfine energy levels is known as the Breit-Rabi formula:

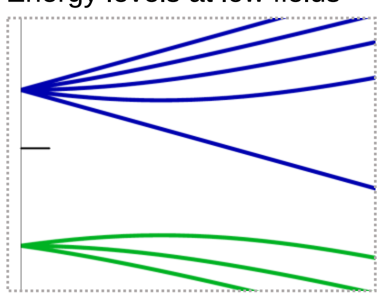
$$E^{\pm}_{m_F} = -\frac{\mathrm{A}\left(I+\frac{1}{2}\right)}{2(2I+1)} + g_I \mu_B m_F B \pm \frac{\mathrm{A}\left(I+\frac{1}{2}\right)}{2}\left(1 + \frac{4m_F x}{2I+1} + x^2\right)^{\frac{1}{2}},$$

where $x = \frac{(g_j - g_I)\mu_B B}{\mathrm{A}(I+\frac{1}{2})}$; g_I is the nuclear g-factor; g_j is the Lande g-factor; B is the projection of magnetic field along the z axis; I is the nuclear spin; $m_F = m_I \pm m_j$; A is the magnetic dipole constant that is unique for each total angular momentum value.

The Breit-Rabi formula leads to the following plot which shows the hyperfine structure of the lowest energy levels of the valence electron in rubidium-87 as a function of applied external magnetic field. Here, $\frac{A}{h} = 3.417$ GHz; $g_j = 2.002$; $g_I = -0.000995$.



Energy levels at low fields



(a) (2 points) Write the ground-state of the valence electron in Rubidium-87 in spectroscopic notation.

(b) (3 points) Based on the above plot, deduce the nuclear spin of Rubidium-87.

(c) (5 points) Label the appropriate quantum numbers for the weak and strong field limits for each state in the figure. Indicate the allowed transitions (based on $\Delta m_F = 0, \pm 1$) on the figure.

(d) (5 points) Identify a transition that is generally first-order insensitive to magnetic fields <u>at low fields</u>. What is the frequency associated with this "clock" transition? Using the Breit-Rabi formula, obtain an expression for the second-order dependence of this transition to external magnetic fields (*Hint*: assume low fields).

(e) (3 points) Due to the crossover between the weak and strong field limits, there are some values of magnetic field in which an allowed transition is first-order independent of the magnetic field. Identify those transitions.

(f) (2 points) Give an approximate value for the cross-over magnetic field between the weak and strong limits, recalling that the weak-field limit is one in which $A \ll \mu_B B$.