**PHYS 661 Homework Set 4 Due Thursday, February 13, 2025**

Reading assignment: sections 16.4, 17.1, and 17.2 of the notes.

Problem 1. [This problem may look long and intimidating, but that is partly because there will be lots of hints and milestones along the way, to help make sure you stay on the right path. General hints: in the following, each constant $N_i$ is a positive integer that you should determine. If you find otherwise, that means something has gone wrong, and you should talk to me or send me email showing what you did, and we will get you on the right path again. You do *not* want to use the explicit forms of the spherical harmonics; instead you should make use of equation (8.6.31) which will enable you to evaluate the $(\theta, \phi)$ integrals in a very simple way.]

Consider a particle of mass $\mu$ moving in the 3-dimensional isotropic linear potential

$$V(R) \;=\; \lambda R,$$

where $R$ is the radial coordinate operator, and $\lambda$ is a constant. Since this is not easy to solve exactly, and there is no obvious way to apply perturbation theory, we will try the variational principle. Consider trial wavefunctions in spherical coordinates:

$$\psi_{l,m}(n,k) \;=\; r^n e^{-kr/2}\, Y_l^m(\theta,\phi).$$

Here, $l, m$ are fixed angular momentum quantum numbers associated with the operators $L^2$ and $L_z$, respectively. The quantities $n$ and $k$ are variational parameters. We could take $n$ to vary continuously, but we will allow it to only take on integer values in this problem.

(a) Find $\langle\psi|\psi\rangle$ for the trial wavefunction above labeled by $l, m$. Hint: You should get the answer $(2n+N_1)!/k^{2n+3}$, where $N_1$ is a positive integer that you will find. Note that this result does not depend on $l$ or $m$ at all.

(b) Compute $\langle\psi|V|\psi\rangle$, for which you should get the result $\lambda(2n+N_2)!/k^{2n+4}$, where $N_2$ is a positive integer that you will find. Note that this result again does not depend on $l$ or $m$ at all.

(c) Compute $\langle\psi|P^2|\psi\rangle/2\mu$ in a similar way. [Hints: you should make use of equation (8.6.12) in the text in order to evaluate $P^2$ acting on the wavefunction in position space. The book-keeping of the radial integrals involved in this part might be the hardest part of this whole problem. Your result should depend on $l$, but not on the magnetic angular momentum quantum number $m$, and you can check your answer from the form of the result for $A$ in the next part...]

(d) Use the previous results to find the energy function $E(n, k) = \langle\psi|H|\psi\rangle \,/\, \langle\psi|\psi\rangle$. Hint: to simplify the results, factor out a common factor of $(2n)!$ from each of the terms in parts (a), (b), and (c). You should write your answer in the form $E(n, k) = Ak^2 + B/k$, where $A$ and $B$ should be put in simplest form:

$$\begin{aligned} A &= \left[\frac{2l(l+1) + n + N_3}{4(2n+1)(2n+2)}\right] \frac{\hbar^2}{\mu}, \\ B &= (2n + N_4)\lambda, \end{aligned}$$

where $N_3$ and $N_4$ are certain positive integers that you will discover.

(e) Minimize the result $E(n, k)$ with respect to $k$. To do this, it is easiest to first find the answer in terms of $A$ and $B$; you should find an answer of the form

$$E(n, k_{\text{min}}) = N_5 \left(\frac{AB^2}{4}\right)^{1/3},$$

where you will determine the value of the integer $N_5$. Then, plug in the results you found for $A$ and $B$. Your answer for $E(n, k_{\text{min}})$ should depend only on $\hbar$, $\lambda$, $\mu$, $l$, and $n$.

(f) Estimate the ground state energy for $l = 0$, in terms of $\hbar$, $\lambda$, and $\mu$, by finding out which integer $n$ does the best job. (Plug in $n = 0, 1, 2, 3, 4, 5, 6$, and evaluate numerically, to find out.)

(g) Estimate the energy of the lowest state with $l = 1$, by finding out which integer $n$ does the best job. (Plug in $n = 0, 1, 2, 3, 4, 5, 6$, and evaluate numerically, to find out.)

(h) Estimate the energy of the lowest state with $l = 2$, by finding out which integer $n$ does the best job. (Plug in $n = 0, 1, 2, 3, 4, 5, 6$, and evaluate numerically, to find out.)

Problem 2. This problem is about the effect of the Darwin term on the hydrogen atom energy eigenvalues. For an electron in the presence of an electric field $\vec{E}$, the Darwin term is given in general by: $H_D = \frac{e\hbar^2}{8m_e^2c^2}\vec{\nabla} \cdot \vec{E}$. For a point source charge $+e$, like the idealized proton in the hydrogen atom, one has $\vec{\nabla} \cdot \vec{E} = 4\pi e\delta^{(3)}(\vec{r})$, so

$$H_D = \frac{\pi e^2\hbar^2}{2m_e^2c^2}\,\delta^{(3)}(\vec{r})$$

in the position space representation.

(a) Consider the hydrogen atom wavefunction $\psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r)Y_l^m(\theta, \phi)$, evaluated at the origin ($r = 0$). It is given in terms of associated Laguerre polynomials and spherical harmonics by eqs. (11.1.31), (11.1.32), and (11.1.34). For non-zero orbital angular momentum, $l \neq 0$, then $\psi_{n,l,m} = 0$ at $r = 0$. Why? (This should be a one-sentence answer; you are just supposed to point out the one key feature of $R_{n,l}(r)$ that makes it true.)

(b) Consider the associated Laguerre polynomials, as defined by eq. (10.5.36) in the text. Evaluate the special case $L^1_{n-1}(0)$ in simplest form, by plugging in $N = n-1$ and $\alpha = 1$ and taking the limit $z \to 0$ in that formula. [Hint: in general, if you are not sure how to proceed, a good problem-solving strategy is to start with simple special cases. So, try it with $n = 1, 2, 3, 4, \ldots$ and see if you can spot the pattern. Note that $z$ in eq. (10.5.36) is not the rectangular coordinate, it is just a generic variable.]

(c) Using the results above, compute the probability density for the electron to be at the origin, $|\psi_{n,l,m}(0)|^2$, for general $n, l, m$. Your answer should involve Kronecker deltas.

(d) Use your answer to part (c) to find (showing your work) that the resulting energy shifts, from first-order perturbation theory, for the $|n, l, m\rangle$ states can be written as

$$\Delta E_D \;=\; \delta_{l,0} \frac{\alpha^2}{n^3} \left( \frac{e^2}{2a_0} \right).$$

Hint: integrating delta functions is easy.

(e) How big are the resulting Darwin term energy shifts, numerically in eV, for the $n = 1$ ground state and the $n = 2$ first excited state and the $n = 3$ second excited state of the hydrogen atom?

Problem 3. It can be shown, but you don't need to do it, that the expectation values of powers of the radial coordinate, $\langle R^q \rangle$, in the hydrogen atom stationary states $|n, l, m\rangle$ obey the recursion relation:

$$\frac{q+1}{n^2} \langle R^q \rangle - (2q+1) a_0 \langle R^{q-1} \rangle + \frac{q}{4} \left[ (2l+1)^2 - q^2 \right] a_0^2 \langle R^{q-2} \rangle \;=\; 0,$$

where $a_0$ is the Bohr radius, $n$ is the principal quantum number, and $l$ is the orbital angular momentum quantum number. (This is called the Kramers–Pasternack formula, and the proof is not trivial but is outlined in the text.) Use this formula to compute and tabulate the expectation values, $\langle n, l, m | R^q | n, l, m \rangle$, for all integers $-3 \leq q \leq 3$. As seeds, you may use the obvious result $\langle 1 \rangle = 1$ and also $\langle 1/R^2 \rangle = 2/(a_0^2 n^3 (2l+1))$, which is derived in the text in section 15.6. For which case or cases does the answer diverge? [Hint: some of the results can be found in the text, but don't just quote them, show your work.]