Physics 214: Introduction to Quantum Mechanics
Spring 2015

Problem Set 10

Due: Fri 1 May 2015

Reminder: Exam 3 will be distributed on Friday 1 May. It is a closed book 2.5 hour take-home exam, but you may prepare one page of notes (front and back) to use during the exam. It is due by the end final exam period, Friday 17 May, at noon. The exam will cover the material since the last exam. In the homework this corresponds to Problem Sets 8–10, and in the textbook it corresponds to Townsend Secs. 4.2–4.7 (excluding Sec. 4.5), Secs. 5.3–5.4, and Sec. 6.2. From Sec. 4.3, you will only be responsible for the definition of the harmonic oscillator and the application of Heisenberg’s uncertainty principle to estimates of the ground state energy. Finally, you should be able to identify the states of hydrogen as in the “name that wavefunction” game. Additional suggestions for preparation will be provided via email.

Reading:

Mon 4/27: Lecture notes on the periodic table, Townsend Sec. 6.4.

Wed 4/29: Townsend Secs 6.4 and 6.5.

Problems (four pages total):

   Hint: Assume that $\langle |x| \rangle \sim \Delta x$ to rough approximation.
2. Angular wavefunctions.

(a) Using the handout on spherical harmonics, please verify that the angular wavefunctions

\[ d_{xy} = \frac{1}{2} \sqrt{\frac{15}{\pi}} \frac{xy}{r^2}, \]
\[ d_{xz} = \frac{1}{2} \sqrt{\frac{15}{\pi}} \frac{xz}{r^2}, \]
\[ d_{yz} = \frac{1}{2} \sqrt{\frac{15}{\pi}} \frac{yz}{r^2}, \]
\[ d_{x^2-y^2} = \frac{1}{4} \sqrt{\frac{15}{\pi}} \frac{(x^2-y^2)}{r^2}, \]
\[ d_{z^2} = \frac{1}{4} \sqrt{\frac{5}{\pi}} \left( \frac{3z^2}{r^2} - 1 \right), \]

(1)
can be written in terms of the spherical harmonics \( Y_{\ell}^{m}(\theta, \phi) \) as

\[ d_{xy}(\theta, \phi) = \frac{1}{i \sqrt{2}} (Y_2^{-2} - Y_2^{2}), \]
\[ d_{xz}(\theta, \phi) = \frac{1}{\sqrt{2}} (Y_2^{-1} - Y_2^{1}), \]
\[ d_{yz}(\theta, \phi) = \frac{i}{\sqrt{2}} (Y_2^{-1} + Y_2^{1}), \]
\[ d_{x^2-y^2}(\theta, \phi) = \frac{1}{\sqrt{2}} (Y_2^{2} + Y_2^{-2}), \]
\[ d_{z^2}(\theta, \phi) = Y_2^{0}, \]

(2)

(b) *Mathematica* knows about spherical harmonics. Using the file

http://www.brynmawr.edu/physics/courses/214/Mathematica/d_orbitals.nb
to help you get started, please plot \(|d_i(\theta, \phi)|^2\) for each of the functions in Eq. (2) and verify that it agrees with the corresponding \( d \) orbital in the handout “Fig. 3.1 Geometry of orbitals in the \( s, p \) and \( d \) subshells.”

(c) Using the attached copy of Townsend Fig. 6.3, please label: (i) all nodes at \( \theta \neq 0, \pi \), (ii) all nodes at \( \theta = 0, \pi \). Show that your results agree with the general rules

\[ \text{(i) Number of nodes away from the poles} = \ell - |m|. \]
\[ \text{(ii) Nodes at the poles exist for} \ m \neq 0, \ 	ext{but not} \ m = 0. \]

(3)

3. Radial wavefunctions. In class, we will define the radial effective potential to be

\[ V_{\text{eff}}(r) = V(r) + \frac{\ell(\ell + 1)\hbar^2}{2mr^2}, \]

(4)

and show that for each value of \( \ell \), the effective 1D Schrödinger equation for the radial function \( u(r) = rR(r) \) is

\[ \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right) u_{n\ell}(r) = E_{n\ell} u_{n\ell}(r). \]

(5)
Then, the full 3D time-independent wavefunction is $\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r)Y_{\ell}^{m}(\theta, \phi)$, where $R_{n\ell}(r) = u_{n\ell}(r)/r$.

(a) For a hydrogenlike atom, $V(r) = -Ze^2/(4\pi\epsilon_0 r)$. Sketch the effective potential for $\ell = 2$ and $\ell \gg 1$, indicating how the two qualitatively differ from one another.

(b) For each $\ell$, the Schrödinger equation (5) has a sequence of radial solutions $u(r)$ of increasing number of nodes $n' = 0, 1, 2, \ldots$ (not counting $r = 0, \infty$) and increasing energy. While it would be natural to label these solutions by $\ell$ and $n'$, it is customary to use the principle quantum number $n = n' + \ell + 1$ instead of $n'$. Please sketch $u_{n\ell}(r)$ and $|u_{n\ell}(r)|^2$ for $\ell = 2$ and $n = 3, 4, 5$. Make sure to line up your sketches of $u_{n\ell}(r)$ underneath the effective potential sketched in part (a) (as in our wavefunction sketches in class and in the solutions to Problem Set 8). Note that $u_{n\ell}(0) = 0$.

(c) The orthogonality condition on the normalized wavefunctions $\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r)Y_{\ell}^{m}(\theta, \phi)$ is

$$\int dV \psi_{n_1,\ell_1,m_1}^* \psi_{n_2,\ell_2,m_2} = \delta_{n_1,n_2}\delta_{\ell_1,\ell_2}\delta_{m_1,m_2} = \begin{cases} 1 & n_1,\ell_1,m_1 = n_2,\ell_2,m_2, \\ 0 & \text{otherwise,} \end{cases}$$

where $dV$ is the volume element. In spherical coordinates, we have

$$dV = r^2 \sin \theta dr d\theta d\phi.$$ Using the normalization condition on the $Y_{\ell}^{m}$,

$$\int_0^\pi \int_0^{2\pi} \sin \theta d\theta d\phi Y_{\ell_1}^{m_1}(\theta, \phi)^* Y_{\ell_2}^{m_2}(\theta, \phi) = \delta_{\ell_1,\ell_2}\delta_{m_1,m_2},$$

show that the orthogonality condition (6) becomes

$$\int_0^\infty dr u_{n_1\ell}^*(r)u_{n_2\ell}(r) = \delta_{n_1,n_2},$$

with no extra factors of $r$ inside the integral.

4. Feedback. By Thursday of each week, please send me an email message to provide feedback on the class and on your reading. (My email address is mbschulz at brynmawr.edu). For example: Which parts were easier or harder to understand? Do you have any questions that you would like to clarify or areas where you would like more practice in recitation section? Was there something that you found particularly interesting or uninteresting? Was the problem set of reasonable length and difficulty. If you have any thoughts on how to improve the textbook for future students using future editions, please let me know and I
will pass that information on to the author, John Townsend. The purpose of the feedback is to help you to reflect on your learning process and to provide me with brief but valuable information that will help to make this class the best possible experience for everyone.
Figure 6.3: Plots of $|Y_{l,m}(\theta, \phi)|^2$ for $l = 0, 1, 2, 3$. 