Physics 741 – Graduate Quantum Mechanics 1

Solutions to Chapter 7

6. [30] Consider the spherical harmonic oscillator, $H = \mathbf{P}^2/2m + \frac{1}{2}m\omega^2\mathbf{R}^2$. This potential is most easily solved by separation of variables, but it is very helpful to take advantage of the spherical symmetry to find solutions.

(a) [3] Factor eigenstates of this Hamiltonian into the form $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$. Find a differential equation satisfied by the radial wave function $R(r)$.

We are attempting to find eigenstates of the Hamiltonian, that is, solutions of $H\psi = E\psi$. Since we have spherical symmetry, we expect their angular dependence to take the form of spherical harmonics, so that $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$. Plugging into Schrödinger's equation, we see from the lecture notes (7.27) that we have

$$ER(r) = -\frac{\hbar^2}{2mr}\frac{d^2}{dr^2}\left[rR(r)\right] + \frac{l^2+l}{2mr^2}\hbar^2 R(r) + V(r)R(r),$$

$$\frac{2mE}{\hbar^2}R(r) = -\frac{1}{r}\frac{d^2}{dr^2}\left[rR(r)\right] + \frac{l^2+l}{r^2}R(r) + \frac{m^2\omega^2}{\hbar^2}r^2 R(r).$$

(b) [5] At large *r*, which term besides the derivative term dominates? Show that for large *r*, we can satisfy the differential equation if $R(r) \sim \exp\left(-\frac{1}{2}Ar^2\right)$, and determine the factor *A* that will make this work.

For Hydrogen, the potential term vanished at infinity, but in this case, the potential becomes large at infinity, and cannot be ignored. The leading terms will then be the derivative term acting both times on $R(r)$ and the potential term, so we are approximately trying to satisfy the equation

$$\frac{d^2}{dr^2}R(r) \sim \frac{m^2\omega^2}{\hbar^2}r^2 R(r).$$

Since two derivatives are supposed to bring down two factors of *r*, it makes sense to try wave functions along the lines of $R(r) \sim \exp\left(-\frac{1}{2}Ar^2\right)$. Plugging this in, we have

$$\frac{d^2}{dr^2}\exp\left(-\tfrac{1}{2}Ar^2\right) \sim \frac{m^2\omega^2}{\hbar^2}r^2\exp\left(-\tfrac{1}{2}Ar^2\right),$$

$$\left(A^2r^2 - A\right)\exp\left(-\tfrac{1}{2}Ar^2\right) \sim \frac{m^2\omega^2}{\hbar^2}r^2\exp\left(-\tfrac{1}{2}Ar^2\right).$$

At large *r*, we can ignore the second term on the left compared to the first, so we see this will work if $A = m\omega/\hbar$. It would also work if $A = -m\omega/\hbar$, but this would be an exponentially growing wave function, not a damped wave function.

(c) [5] Write the radial wave function in the form $R(r)=f(r)\exp\left(-\tfrac{1}{2}Ar^2\right)$, and show that *f* must satisfy

$$\frac{2mE}{\hbar^2}f=-\frac{1}{r}\frac{d^2}{dr^2}(fr)+2A\frac{d}{dr}(fr)+Af+\frac{l^2+l}{r^2}f.$$

Plugging this into the differential equation we have, we need to simplify

$$\begin{aligned}\frac{2mE}{\hbar^2}f\exp\left(-\tfrac{1}{2}Ar^2\right)&=-\frac{1}{r}\frac{d^2}{dr^2}\left[rf\exp\left(-\tfrac{1}{2}Ar^2\right)\right]+\left(\frac{l^2+l}{r^2}+\frac{m^2\omega^2}{\hbar^2}r^2\right)f\exp\left(-\tfrac{1}{2}Ar^2\right)\\&=-\frac{1}{r}\frac{d^2}{dr^2}(fr)\exp\left(-\tfrac{1}{2}Ar^2\right)+\frac{2}{r}\frac{d}{dr}(fr)Ar\exp\left(-\tfrac{1}{2}Ar^2\right)\\&\quad-f\left((Ar)^2-A\right)\exp\left(-\tfrac{1}{2}Ar^2\right)+\left(\frac{l^2+l}{r^2}+A^2r^2\right)f\exp\left(-\tfrac{1}{2}Ar^2\right),\\\frac{2mE}{\hbar^2}f&=-\frac{1}{r}\frac{d^2}{dr^2}(fr)+2A\frac{d}{dr}(fr)+Af+\frac{l^2+l}{r^2}f.\end{aligned}$$

(d) [4] Assume that at small *r*, the wave func tion goes like $f(r)\sim r^k$. What value of *k* will make this equation work?

We simply plug this into our differential equation and keep only the lowest power of *r*. We have

$$\frac{2mE}{\hbar^2}r^k=-\left(k^2+k\right)r^{k-2}+2A(k+1)r^k+Ar^k+\left(l^2+l\right)r^{k-2}.$$

Keeping only the terms that go as r^{k-2}, we see that we must have $l^2+l=k^2+k$. This has two solutions, $k=l$ and $k=-l-1$, but the latter is unacceptable since it would lead to a function that blows up at the origin.

(e) [6] Assume that the radial wave function can be written as a power series, similar to what we did in class, $f(r)=\sum_{i=k}^{n}f_ir^i$. Substitute this into the differential equation for *f*, and thereby discover a recursion relation on the f_i's. Unlike the recursion relationship we found, you will get a recursion relationship relating f_i to f_{i+2}. Hence the series actually requires only odd power of *r* or even powers of *r*, not both.

If we substitute this into our equation, keeping in mind that $k=l$, we have

$$\frac{2mE}{\hbar^2}\sum_{i=l}^{\infty}f_ir^i=-\sum_{i=l}^{\infty}\left(i^2+i\right)f_ir^{i-2}+2\sum_{i=l}^{\infty}(i+1)f_ir^iA+A\sum_{i=l}^{\infty}f_ir^i+\left(l^2+l\right)\sum_{i=l}^{\infty}f_ir^{i-2}.$$

We now gather all the terms together based on their powers of *r*, so we have

$$\sum_{i=l}^{\infty} f_i r^i \left(\frac{2mE}{\hbar^2} - 2iA - 3A \right) = \sum_{i=l}^{\infty} f_i r^{i-2} \left(l^2 + l - i^2 - i \right).$$

Now we shift the sum on the right, by replacing the dummy index i by i+2 everywhere. This leads to

$$\sum_{i=l}^{\infty} f_i r^i \left(\frac{2mE}{\hbar^2} - 2A - 2iA \right) = \sum_{i=l-2}^{\infty} f_{i+2} r^i \left(l^2 + l - i^2 - 4i - 4 - i - 2 \right).$$

The only way these two sides can be equal is if the coefficients all match. We therefore have

$$f_{i+2} = \frac{2mE/\hbar^2 - 3A - 2iA}{l^2 + l - i^2 - 5i - 6} f_i$$

There are some details that need to be considered. The sum on the right seems to contain two terms that do not appear on the left. However, the $i = l - 2$ term has a coefficient that vanishes on the right. But the $i = l - 1$ term does not. The only way this can be made to work is if we assume that f_{l+1} vanishes, so that there are no terms on the right that do not appear on the left. Hence when calculating the f_i's, we will find that every other one vanishes, and only $i = l$, l+2, l+4 etc. can actually exist.

(f) [4] Assume, as in class, that the series terminates, so that f_n is the last term, and hence that f_{n+2} vanishes. Find a condition for the energy E in terms of n.

If the series does not terminate, we can show that for large i, the terms are growing by a factor of $2iA$ for each increase by *two* for i. With some work, this can be shown to lead to an exponentially growing radial function, not damped, so this is unacceptable. Therefore, we need to terminate the series. Specifically, we must make sure that for $i = n$, the expression just attained vanishes, so we have

$$0 = f_{n+2} = \frac{2mE/\hbar^2 - 3A - 2nA}{l^2 + l - n^2 - 5n - 6} f_n ,$$

$$\frac{2mE}{\hbar^2} = 3A + 2nA = \frac{m\omega}{\hbar}\left(2n+3\right),$$

$$E = \hbar\omega\left(n + \tfrac{3}{2}\right).$$

(g) [3] Given n, which describes the energy of the atom, what restrictions are there on l, the total angular momentum quantum number?

If we want the series to be non-trivial, we must have $n \geq l$. However, also recall that our series $f(r)$ contains only every other power of r, starting at r^l and terminating at r^n. Therefore, $n - l$ must be an even number.