Assignment # 4

We will consider the 3-dimensional harmonic oscillator.

$$H = \frac{\mathbf{p^2}}{2M} + \frac{1}{2}Kr^2 \tag{1}$$

with K the spring constant.

1. Warm-up. Starting from the equation

$$H\psi = E\psi \tag{2}$$

and the rule $p_x \to -i\hbar\frac{\partial}{\partial x}$, Show that the Schrödinger Equation can be written

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}Kr^2\right]\Psi = E\Psi \tag{3}$$

2. Dimension-less variables. The dimension-full constants in this equation are

$$\hbar, M, K \tag{4}$$

- Only one combination of these parameters has dimension of length. Determine this combination. Answer:

$$R_o = \left(\frac{\hbar^2}{M\,K}\right)^{1/4} \tag{5}$$

- Only one combination of these has units of frequency. Determine this combination Answer:

$$\omega_o = \sqrt{\frac{K}{M}} \tag{6}$$

- The only combination of parameters with dimension of energy is

$$\hbar\omega_o \tag{7}$$

Express this amount energy in terms of K and R_o. Express this amount of energy $\hbar, M, R_o$.

- Introduce a bunch of dimensionless variables. For example

$$\bar{r} = r/R_o \tag{8}$$

$$\bar{E} = E/(\hbar\omega_o) \tag{9}$$

$$\bar{\psi}(\bar{r}) = R_o^{3/2}\psi(r) \tag{10}$$

$$\bar{\nabla}^2 = \frac{\partial^2}{\partial\bar{x}^2} + \frac{\partial^2}{\partial\bar{y}^2} + \frac{\partial^2}{\partial\bar{z}^2} \tag{11}$$

  Show that

$$\int d^3\bar{r}\,|\psi(\bar{r})|^2 = 1 \tag{12}$$

- With this set of units show that the Schrödinger equation can be written

$$\left[-\frac{1}{2}\bar{\nabla}^2 + \frac{1}{2}\bar{r}^2\right]\psi = \bar{E}\bar{\psi} \tag{13}$$

- After going through this excercise a bunch of times one realizes is that this is the same as saying

$$\hbar = K = M = 1 \tag{14}$$

- The condition that the particle be considered non-relativistic is

$$\left(\frac{v}{c}\right)^2 \ll 1 \tag{15}$$

  Show that this condition can be written as a constraint that the oscillator energy $\hbar\omega_o$ be much less than the rest mass energy mc^2. (Hint what are the units of velocity.)

3. Angular momentum is

$$L_z = x\,p_y - y\,p_x \tag{16}$$

Work in polar coordinates to show that

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{17}$$

Using the relations $x = r\,\cos(\phi)$ and $y = r\sin(\phi)$, show that

$$\frac{\partial}{\partial x} = \cos(\phi)\frac{\partial}{\partial r} - \frac{\sin(\phi)}{r}\frac{\partial}{\partial\phi} \tag{18}$$

$$\frac{\partial}{\partial y} = \sin(\phi)\frac{\partial}{\partial r} + \frac{\cos(\phi)}{r}\frac{\partial}{\partial\phi} \tag{19}$$

Then use the fact that

$$p_x = -i\hbar \frac{\partial}{\partial x} \tag{20}$$

$$p_y = -i\hbar \frac{\partial}{\partial y} \tag{21}$$

To deduce $L_z/\hbar$. In a similar way it may be shown that be shown that

$$-\frac{L^2}{\hbar^2} = \frac{1}{\sin(\theta)} \frac{\partial}{\partial\theta} \sin(\theta) \frac{\partial}{\partial\theta} + \frac{1}{\sin(\theta)} \frac{\partial^2}{\partial\phi^2} \tag{22}$$

4. Looking up ∇^2 in spherical coordinates show that

$$\frac{-\hbar^2}{2M}\nabla^2 = \underbrace{\frac{-\hbar^2}{2M} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}}_{\text{radial KE}} + \underbrace{\frac{L^2}{2Mr^2}}_{\text{angular KE}} \tag{23}$$

5. Use classical physics to show that the kinetic energy of a particle moving around in a circle is

$$KE = \frac{L_{\rm cl}^2}{2Mr^2} \tag{24}$$

where $L_{\rm cl} = mvr$

6. Show that the three spherical harmonics for $\ell = 1$, $Y_{lm}(\theta, \phi)$

$$\begin{aligned} Y_{10} &= \sqrt{\frac{3}{4\pi}} \cos(\theta) && (25) \\ Y_{1\pm1} &= \mp\sqrt{\frac{3}{8\pi}} \sin(\theta)\, e^{\pm i\phi} && (26) \end{aligned}$$

Have definite definite total angular momentum and have definite angular momentum around the z axis, i.e. show by straight forward differentiation that

$$\begin{aligned} L^2\, Y_{lm} &= \ell(\ell+1)\hbar^2\, Y_{lm} && (27) \\ L_z\, Y_{lm} &= m\hbar\, Y_{lm} && (28) \end{aligned}$$

7. For the Schrödinger equation in Eq. **??**, first rewrite the Laplace operator as in Eq. **??**. Show that if one substitutes

$$\psi(r,\theta,\phi) = \frac{u_\ell(r)}{r}\, Y_{lm}(\theta,\phi) \tag{29}$$

One obtains an equation for $u(r)$

$$\left[\frac{-\hbar^2}{2M}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} + \frac{1}{2}Kr^2\right] u(r) = Eu(r) \tag{30}$$

8. Show that the norm condition

$$\int d^3r\, |\psi|^2 = 1 \tag{31}$$

Becomes a condition on $u(r)$

$$\int_0^\infty dr\, |u(r)|^2 = 1 \tag{32}$$

Use the fact that

$$\int_0^\pi d\theta \int_0^{2\pi} d\phi\, \sin(\theta)\, |Y_{lm}|^2 = 1 \tag{33}$$

9. Show that in terms of "barred" variables this radial Schrödinger equation becomes

$$\left[\frac{-1}{2}\frac{d^2}{d\bar{r}^2} + \frac{\ell(\ell+1)}{2\bar{r}^2} + \frac{1}{2}\bar{r}^2\right] u(\bar{r}) = \bar{E}u(\bar{r}) \tag{34}$$

with

$$\bar{u}_\ell(\bar{r}) = R_o^{1/2}\, u(r) \tag{35}$$

10. This equation always has solutions. Only for particular values of the energy does this solution decay to zero for $r \to \infty$. We label these energies as E_n $n = 0, 1, 2....$ The radial wave functions $u(r)$ depend on what is $\bar{E}_n$ and ℓ we therefore denote these as

$$\bar{u}_{n,\ell}(\bar{r}) \tag{36}$$

- For every n the energies are

$$\bar{E}_n = \frac{E_n}{\hbar\omega_o} = n + \frac{3}{2} \tag{37}$$

The $\frac{3}{2}\,\hbar\omega_o$ is the zero point energy
For every n, ℓ takes on the values

$$\ell = n, n-2, \ldots 1 \text{ or } 0 \tag{38}$$

The lowest energy eigen-functions and there (dimensonless) eigen-values are

$$u_{n,\ell} = C\,\bar{r}^{\ell+1} e^{-\frac{\bar{r}^2}{2}} P_{n,\ell}(\bar{r}) \tag{39}$$

where $P_{n,\ell}(r)$ is a polynomial

$$\begin{aligned} P_{0,0}(r) &= 1 && (40)\\ P_{1,1}(r) &= 1 && (41)\\ P_{2,2}(r) &= 1 && (42)\\ P_{2,0}(r) &= \frac{3}{2} - r^2 && (43)\\ P_{3,3}(r) &= 1 && (44)\\ P_{3,1}(r) &= \frac{5}{2} - r^2 && (45) \end{aligned}$$

- Verify that $n = 1$, $\bar{u}_{1,1}$ is in fact a solution to the dimensionless Schrödinger equation Eq. 34 with the correct eigen-energy $\bar{E}_n$. Without using dimensionless variables this excercise would quickly degenerate into a morass of symbols.

11. The wave function is actually a doublet

$$\Psi = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} \tag{46}$$

Everything that we did in the previous section applies for ψ_+ and ψ_- separately.

$$|\psi_+|^2 = \text{the probability to have spin up} \tag{47}$$

The spin operators act in this 2×2 doublet space

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{48}$$

12. Show that

$$\Psi = \psi(r, \theta, \phi) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{49}$$

has spin $\hbar/2$ in the z direction.

13. Determine the spin wave function

$$\Psi = \psi(r, \theta, \phi) \begin{pmatrix} a \\ b \end{pmatrix} \tag{50}$$

which has definite spin of $+\hbar/2$ in the y direction. That is: (1) determine the eigen-values and and eigen-vectors of S_y (2) One of the eigen-values is $+\hbar/2$ determine the corresponding eigen vector.

14. For definiteness consider $\ell = 1$, the six states

$$f(r) \begin{pmatrix} Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix} \qquad f(r) \begin{pmatrix} 0 \\ Y_{lm}(\theta, \phi) \end{pmatrix} \tag{51}$$

with $m = -1, 0, 1$ are spin $\frac{1}{2}$. Show this by showing that showing that they are eigensates of

$$S^2 = S_x^2 + S_y^2 + S_z^2 \tag{52}$$

with eigenvalue

$$s(s+1)\hbar^2 = \frac{3}{4}\hbar^2 \tag{53}$$

Similarly, they have orbital angular momentum 1 by since

$$L^2 \left[f(r) \begin{pmatrix} Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix} \right] = f(r) \begin{pmatrix} L^2 Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix} \tag{54}$$

$$= f(r) \begin{pmatrix} \ell(\ell+1)\hbar^2 Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix} \tag{55}$$

$$= \ell(\ell+1)\hbar^2 \left[f(r) \begin{pmatrix} Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix} \right] \tag{56}$$

15. These six states recombine to become eigenstates of definite total angular momentum squared, J^2 and J_z. The total angular momentum is

$$\mathbf{J} = \mathbf{L} + \mathbf{S}\,. \tag{57}$$

For instance show that by mixing together two of these state

$$\Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} = \sqrt{\frac{2}{3}} \begin{pmatrix} Y_{10} \\ 0 \end{pmatrix} + \sqrt{\frac{1}{3}} \begin{pmatrix} 0 \\ Y_{11} \end{pmatrix} \tag{58}$$

One obtains a state with definite value of J_z, i.e. show that

$$(L_z + S_z)\Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} = +\frac{\hbar}{2}\Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} \tag{59}$$

The fractors $\sqrt{2/3}$ and $\sqrt{1/3}$ are known as Clebsch-Gordan coefficients.

16. Show that $\Psi_{J=\frac{3}{2},M_J=\frac{1}{2}}$ has definite value of total angular momentum $j = 3/2$, i.e. that

$$J^2\Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} = \left[L^2 + S^2 + 2L_xS_x + 2L_yS_y + 2L_zS_z\right] \Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} \tag{60}$$

$$= \frac{3}{2}\left(\frac{3}{2}+1\right)\hbar^2\, \Psi_{J=\frac{3}{2},M_J=\frac{1}{2}} \tag{61}$$

- You may find that the following relations are helpful

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos(\phi)}{\tan(\theta)}\frac{\partial}{\partial\phi}\right) \tag{62}$$

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin(\phi)}{\tan(\theta)}\frac{\partial}{\partial\phi}\right) \tag{63}$$

- Or just use the fact that

$$L_xY_{lm} = \frac{1}{2}\sqrt{\ell(\ell+1) - m(m+1)}Y_{lm+1} \tag{64}$$

$$+\frac{1}{2}\sqrt{\ell(\ell+1) - m(m-1)}Y_{lm-1} \tag{65}$$

$$L_yY_{lm} = \frac{-i}{2}\sqrt{\ell(\ell+1) - m(m+1)}Y_{lm+1} \tag{66}$$

$$+\frac{i}{2}\sqrt{\ell(\ell+1) - m(m-1)}Y_{lm-1} \tag{67}$$

17. In class we have discussed how we can combine $\ell = 1$ and $s = \frac{1}{2}$ to make states of definite J^2 and J_z, thus the six states combine together to make

$$j = \ell + s, \ell + s - 1, \ldots, |\ell - s| \tag{68}$$

$$= \underbrace{\frac{3}{2}}_{4 \text{ states}}, \underbrace{\frac{1}{2}}_{2 \text{ states}} \tag{69}$$

Hopefully the previous excercise have made this procedure more than numerology.