HOMEWORK 2

1. (a) For the Time-Independent Schrödinger Equation in 3-D, we have:

$$-\frac{\hbar}{2\mu}\nabla^2 + U(x,y,z)\,\psi(x,y,z) = E\psi(x,y,z)$$

Plugging in the potential $U(x,y,z) = \frac{1}{2}\mu\omega^2\left(x^2+y^2+z^2\right)$, we have:

$$-\frac{\hbar}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega^2\left(x^2+y^2+z^2\right)\psi(x,y,z) = E\psi(x,y,z)$$

For using the separation of variables method, we must split the Schrödinger equation into parts which depend only on x, y, and z.

First, we expand the "del" operator into its separate terms:

$$-\frac{\hbar}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}\mu\omega^2\left(x^2+y^2+z^2\right)\psi(x,y,z) = E\psi(x,y,z)$$

Now, consider the separable wave function:

$$\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$$

Now rewrite the schrödinger equation:

$$-\frac{\hbar}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}\mu\omega^2\left(x^2+y^2+z^2\right)XYZ = E\,XYZ$$

And divide both sides by $\psi = XYZ$:

$$-\frac{\hbar}{2\mu}\left(\frac{1}{X}\frac{\partial^2}{\partial x^2}+\frac{1}{Y}\frac{\partial^2}{\partial y^2}+\frac{1}{Z}\frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}\mu\omega^2\left(x^2+y^2+z^2\right) = E$$

Expanding terms, we get:

$$\left[-\frac{\hbar}{2\mu}\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{2}\mu\omega^2x^2\right] + \left[-\frac{\hbar}{2\mu}\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{2}\mu\omega^2y^2\right] + \left[-\frac{\hbar}{2\mu}\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{1}{2}\mu\omega^2z^2\right] = E$$

Hence, we have shown that the Time-Independent Schrödinger can be rewritten using separation of variables, each separation in terms of only x, y, and z respectively.

Now, we will show that each separation can be solved by treating it as a 1-D QHO which we solved in class.

Consider the component which is only a function of x:

$$-\frac{\hbar}{2\mu}\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{2}\mu\omega^2x^2 = E_x$$

Now multiply both sides by X:

$$-\frac{\hbar}{2\mu}\frac{d^2X}{dx^2}+\frac{1}{2}\mu\omega^2x^2X = E_x$$

The equation now matches the 1-D QHO from class. From the lecture notes, we have:

$$\frac{1}{2}m\omega x_0^2 = E_0$$

Thus,

$$x_0^2 = \frac{\hbar}{\mu\omega}$$

And

$$x_0 = \sqrt{\frac{\hbar}{\mu\omega}} = \ell_{zp}$$

Thus, we can take the wave function from class, and substitute $x_0 = \ell_{zp}$, getting

$$X_p\left(x\right) = A_x H_p\left(\frac{x}{\ell_{zp}}\right) e^{\frac{-x^2}{2\ell_{zp}^2}}$$

For the eigenenergy, we have:

$$E_x = \left(p + \frac{1}{2}\right)\hbar\omega$$

Repeating the same steps for y and z and multiplying the separated wavefunctions together to get the complete wavefunction, we get:

$$\psi_{pqs}\left(x, y, z\right) = A_{pqs}H_p\left(x/\ell_{zp}\right)H_q\left(y/\ell_{zp}\right)H_s\left(z/\ell_{zp}\right)e^{-(x^2+y^2+z^2)/2\ell_{zp}}$$

With $E_n = E_p + E_q + E_s$, we get:

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega$$

(b) Using the notation (p, q, s):

- $n = 0$: we have 1 degenerate state:

$$(0, 0, 0)$$

- $n = 1$: we have 3 degenerate states:

$$(1, 0, 0)$$
$$(0, 1, 0)$$
$$(0, 0, 1)$$

- $n = 2$: we have 6 degenerate states:

$$(1,1,0)$$
$$(1,0,1)$$
$$(0,1,1)$$
$$(2,0,0)$$
$$(0,2,0)$$
$$(0,0,2)$$

2. (a) We guess that a superposition of Ψ_{100} and Ψ_{010} will yield a stationary state.

$$\Psi_{100} = A_{100} 2x e^{-(x^2+y^2+z^2)/2\ell_{zp}^2} e^{iEt/\hbar}$$

$$\Psi_{010} = A_{010} 2y e^{-(x^2+y^2+z^2)/2\ell_{zp}^2} e^{iEt/\hbar}$$

Now, starting with the time-dependent SE:

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi + U\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$
$$-\frac{\hbar^2}{2\mu}\nabla^2\left(\psi_{100}+\psi_{010}\right)e^{-iEt/\hbar} + U\left(\psi_{100}+\psi_{010}\right)e^{-iEt/\hbar} = Ee^{-Et/\hbar}\left(\psi_{100}+\psi_{010}\right)$$

Since these are two degenerate eigenstates, they have the same Energy, E, and thus we can divide both sides by $e^{-iEt/\hbar}$

$$-\frac{\hbar}{2\mu}\nabla^2\left(\psi_{100}+\psi_{010}\right) + U\left(\psi_{100}+\psi_{010}\right) = E\left(\psi_{100}+\psi_{010}\right)$$

Since there is no time dependence, this superposition state is a stationary state. Also, we know that it is (one of) the superposition state(s) with the lowest possible energy, because $n = 1$ yields the smallest eigenenergy which has degeneracies.

(b) We guess the superposition of Ψ_{000} and Ψ_{100} will yield the lowest possible energy that is not a stationary state.

$$\Psi_{000} = A_{000} e^{-(x^2+y^2+z^2)/2\ell_{zp}^2} e^{iE_0t/\hbar} = \psi_{000}e^{iE_0t/\hbar}$$
$$\Psi_{100} = A_{100} 2x e^{-(x^2+y^2+z^2)/2\ell_{zp}^2} e^{iE_1t/\hbar} = \psi_{100}e^{iE_1t/\hbar}$$

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi + U\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$
$$-\frac{\hbar^2}{2\mu}\nabla^2\left(\psi_{000}e^{iE_0t/\hbar}+\psi_{100}e^{iE_1t/\hbar}\right) + U\left(\psi_{000}e^{iE_0t/\hbar}+\psi_{100}e^{iE_1t/\hbar}\right) = i\hbar\frac{\partial}{\partial t}\left(\psi_{000}e^{iE_0t/\hbar}+\psi_{100}e^{iE_1t/\hbar}\right)$$

We note that, unlike the last problem, we cannot cancel out the time-dependent terms in this equation, and thus this superposition is not a stationary state. Furthermore, it must be the superposition state with the lowest possible energy since it is a superposition of the two lowest eigenenergies.

(c) Adding back the normalization constants to the corresponding eigenstates, we have:

$$\Psi = A_{100}\psi_{100}e^{-iE_1 t/\hbar} + A_{010}\psi_{010}e^{-iE_1 t/\hbar}$$

In dirac notation, we have:

$$\begin{aligned}\langle\Psi|\Psi\rangle &= A_{100}^2\langle\psi_{100}|\psi_{100}\rangle + A_{010}^2\langle\psi_{010}|\psi_{010}\rangle + A_{100}A_{010}\left(\langle\psi_{100}|\psi_{010}\rangle + \langle\psi_{010}|\psi_{100}\rangle\right)e^{-2iE_1 t/\hbar}\\ &= A_{100}^2 + A_{010}^2 = 1\end{aligned}$$

Since $A_{100} = A_{010}$, we get

$$A_{100} = A_{010} = \frac{1}{\sqrt{2}}$$

$$\begin{aligned}\langle E\rangle &= \langle\Psi|\hat{H}\Psi\rangle\\ &= E_1\langle\Psi|\Psi\rangle\\ &= E_1\left[A_{100}^2\langle\psi_{100}|\psi_{100}\rangle + A_{010}^2\langle\psi_{010}|\psi_{010}\rangle + A_{100}A_{010}\left(\langle\psi_{100}|\psi_{010}\rangle + \langle\psi_{010}|\psi_{100}\rangle\right)e^{-2iE_1 t/\hbar}\right]\\ &= E_1\left[A_{100}^2 + A_{010}^2\right]\\ &= E_1\end{aligned}$$

We see that the expectation value, $\langle E\rangle$, is independent of time.

3. We start with the Hamiltonian:

$$\hat{H} = -\frac{\hbar}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2} + U(r)$$

Propose the separable form for the wave function $\psi(r,\theta,\varphi)$:

$$\psi(r,\theta,\phi) = R(r)\,Y(\theta,\varphi)$$

See that $R(r)$ is only in terms of radial component, r and $Y(\theta,\varphi)$ is only in terms of the angular components θ,φ.

Substituting the new wave separated wave function with the Hamiltonian, the equation $\hat{H}\psi = E\psi$ becomes:

$$\left[-\frac{\hbar}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2} + U(r)\right]R(r)\,Y(\theta,\varphi) = ER(r)\,Y(\theta,\varphi)$$

Now dividing both sides by $Y(\theta,\varphi)$:

$$-\frac{\hbar}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2} + U(r)\,R(r) = ER(r)$$

4. (a) The function $\Phi(\varphi) = \cos(m\varphi)$ is not an eigenfunction for the $\hat{L}_z$ operator. I will prove this by showing that there is no constant eigenvalue:

$$\begin{aligned}\hat{L}_z \Phi(\varphi) &= \frac{\hbar}{i}\frac{\partial}{\partial\varphi}\cos(m\varphi) \\ &= -\frac{m\hbar}{i}\sin(m\varphi)\end{aligned}$$

Now we see that there is no λ for which $\hat{L}_z\Phi = \lambda\Phi$.

(b) I will show that a wave function with $\Phi(\varphi)\cos(m\varphi)$ as the φ dependence can be a stationary state. First, we use the identity from last homework to rewrite:

$$\cos(m\varphi) = e^{im\varphi}/2 + e^{-im\varphi}/2$$

Now, consider the two separate Hamiltionians associated with each term:
First, for $e^{im\varphi}/2$:

$$\hat{H}\Phi(\varphi) = E\Phi(\varphi)$$

Becomes...

$$\begin{aligned}-\frac{\hbar}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}F(r,\theta)\,e^{im\varphi}/2\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}F(r,\theta)\,e^{im\varphi}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}F(r,\theta)\,e^{im\varphi}\right] &= EF(r,\theta)\,e^{im\varphi} \\ e^{im\varphi} - \frac{\hbar}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}F(r,\theta)\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}F(r,\theta)\right) + \frac{1}{\sin^2\theta}F(r,\theta)\left(-m^2\right)\right] &= EF(r,\theta)\,e^{im\varphi} \\ -\frac{\hbar}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}F(r,\theta)\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}F(r,\theta)\right) + \frac{1}{\sin^2\theta}F(r,\theta)\left(-m^2\right)\right] &= EF(r,\theta)\end{aligned}$$

Since $\frac{d}{d\varphi}\left[e^{-im\varphi}\right] = -m^2$ also, we get the same result for $e^{-im\varphi}$. Therefore, since we have a superposition of states with identical eigenenergies, and we know that the superposition of two stationary eigenstates with the same eigenenergy also yields a stationary state, we have that this superposition is also a stationary state. Hence, we have shown that a wave function with $\Phi(\varphi) = \cos(m\varphi)$ as its φ dependence can be a stationary state.

5.

$$\begin{aligned}\hat{L}^2 Y_1^{-1}(\theta,\varphi) &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\varphi}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\varphi}\right] \\ &= -\hbar^2\frac{1}{2}\sqrt{\frac{3}{2\pi}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\cos\theta e^{-i\varphi} - \frac{1}{\sin^2\theta}\sin\theta e^{-i\varphi}\right] \\ &= -\hbar^2\frac{1}{2}\sqrt{\frac{3}{2\pi}}\left[\frac{\cos^2\theta - \sin^2\theta}{\sin\theta}e^{-i\varphi} - \frac{1}{\sin\theta}e^{-i\varphi}\right] \\ &= -\hbar^2\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\varphi}\left[\frac{1-2\sin^2\theta}{\sin\theta} - \frac{1}{\sin\theta}\right] \\ &= \hbar^2\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\varphi}2\sin\theta \\ &= 2\hbar^2\ Y_1^{-1}(\theta,\varphi)\end{aligned}$$

Thus, $2\hbar^2$ is the eigenvalue.

$$\begin{aligned}\hat{L}_z Y_1^{-1}(\theta,\varphi) &= \frac{\hbar}{i}\frac{\partial}{\partial\varphi}\left[\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\varphi}\right]\\ &= -i\frac{\hbar}{i}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\varphi}\\ &= -\hbar\ Y_1^{-1}(\theta,\varphi)\end{aligned}$$

Thus, $-\hbar$ is the eigenvalue.

$$\begin{aligned}\hat{L}^2 Y_2^2(\theta,\varphi) &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\varphi}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\varphi}\right]\\ &= -\hbar^2\frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{2i\varphi}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}2\sin^2\theta\cos\theta-\frac{4\sin^2\theta}{\sin^2\theta}\right]\\ &= -\hbar^2\frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{2i\varphi}\left[\frac{1}{\sin\theta}\left(4\cos^2\theta\sin\theta-2\sin^3\theta\right)-4\right]\\ &= -\hbar^2\frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{2i\varphi}\left[4\cos^2\theta-2\sin^2\theta-4\right]\\ &= -\hbar^2\frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{2i\varphi}\left[4-4\sin^2\theta-2\sin^2\theta-4\right]\\ &= 6\hbar^2\ Y_2^2(\theta,\varphi)\end{aligned}$$

Thus, the eigenvalue is $6\hbar^2$.

$$\begin{aligned}\hat{L}_z Y_2^2(\theta,\varphi) &= \frac{\hbar}{i}\frac{\partial}{\partial\varphi}\left[\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\varphi}\right]\\ &= 2\hbar\ \hat{L}_z Y_2^2(\theta,\varphi)\end{aligned}$$

Thus, the eigenvalue is $2\hbar$.