Quantum Mechanics - HW7

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4.1

a.

All of the position operators commute. They are all orthogonal states.

$$[x, y]\, f = xyf - yxf = 0$$

$$[r_i, r_j]\, f = r_i r_j f - r_j r_i f = 0$$

$$[x, p_x]\, f = x p_x f - p_x x f$$

Their corresponding momenta are also orthogonal and commute.

$$[p_y, p_x]\, f = p_y p_x f - p_x p_y f$$

$$[p_y, p_x]\, f = \left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) f - \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) f$$

$$[p_y, p_x]\, f = \hbar^2 \frac{\partial^2}{\partial y \partial x} f - \hbar^2 \frac{\partial^2}{\partial x \partial y} f$$

We assume the functions are continuous, and therefore the mixed partials are equivalent, so

$$[p_y, p_x] = 0$$

From these results,

$$[r_i, r_j] = [p_i, p_j] = 0$$

For any position operator and it's conjugate momentum,

$$[x, p_x] f = x\frac{\hbar}{i}\frac{\partial f}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(xf) = x\frac{\hbar}{i}\frac{\partial f}{\partial x} - \frac{\hbar}{i}\left(f\frac{\partial x}{\partial x} + x\frac{\partial f}{\partial x}\right)$$

$$[x, p_x] f = x\frac{\hbar}{i}\frac{\partial f}{\partial x} - \frac{\hbar}{i}f - \frac{\hbar}{i}x\frac{\partial f}{\partial x}$$

$$[x, p_x] f = -\frac{\hbar}{i}f = i\hbar f$$

$$[x, p_x] = i\hbar$$

$$[p_x, x] f = \frac{\hbar}{i}\frac{\partial}{\partial x}(xf) - x\frac{\hbar}{i}\frac{\partial f}{\partial x} = \frac{\hbar}{i}\left(f\frac{\partial x}{\partial x} + x\frac{\partial f}{\partial x}\right) - x\frac{\hbar}{i}\frac{\partial f}{\partial x}$$

$$[p_x, x] f = \frac{\hbar}{i}f\frac{\partial x}{\partial x} + x\frac{\hbar}{i}\frac{\partial f}{\partial x} - x\frac{\hbar}{i}\frac{\partial f}{\partial x} = \frac{\hbar}{i}f$$

$$[p_x, x] = \frac{\hbar}{i} = -i\hbar = -[x, p_x]$$

For any position operator and an operator which it is not conjugate to,

$$[x, p_y] f = x\frac{\hbar}{i}\frac{\partial f}{\partial y} - \frac{\hbar}{i}\frac{\partial}{\partial y}(xf) = x\frac{\hbar}{i}\frac{\partial f}{\partial y} - \frac{\hbar}{i}x\frac{\partial f}{\partial y} = 0$$

Combining these results,

$$[r_i, r_j] = -[r_j, r_i] = i\hbar\delta_{ij}$$

Problem

$$V(x, y, z) = \begin{cases} \frac{1}{2}m\omega^2 z^2 & 0 < x < a,\ 0 < y < b \\ \infty & \text{elsewhere} \end{cases}$$

a.

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + \frac{1}{2}m\omega^2 z^2\Psi$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2 z^2\psi = E\psi$$

$$\Psi = \sum c_n\psi_n e^{-iE_n t/\hbar}$$

$$\psi(x, y, z) = \begin{cases} ? & 0 < x < a,\ 0 < y < b \\ 0 & \text{elsewhere} \end{cases}$$

Within the potential's finite region,

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

Rearranging things by multiplying through by $-\frac{2m}{\hbar^2}$ and moving the potential term,

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=-\frac{2m}{\hbar^2}E\psi+\frac{m^2\omega^2z^2}{\hbar^2}\psi$$

Using separation of variables,

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

$$YZ\frac{\partial^2X}{\partial x^2}+XZ\frac{\partial^2Y}{\partial y^2}+XY\frac{\partial^2Z}{\partial z^2}=-\frac{2m}{\hbar^2}EXYZ+\frac{m^2\omega^2z^2}{\hbar^2}XYZ$$

Dividing through by XYZ,

$$\frac{1}{X}\frac{\partial^2X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2Z}{\partial z^2}=-\frac{2m}{\hbar^2}E+\frac{m^2\omega^2z^2}{\hbar^2}$$

This is split into a z dependent part, and a non-z dependent part.

$$\frac{1}{X}\frac{\partial^2X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2Y}{\partial y^2}=-\frac{2m}{\hbar^2}E=-\frac{2m}{\hbar^2}\left(E_x+E_y\right)$$

$$\frac{1}{Z}\frac{\partial^2Z}{\partial z^2}=\frac{m^2\omega^2z^2}{\hbar^2}+E_z$$

Solving each component,

$$X\left(x\right)=A_x\sin\left(\kappa_xx\right)+B_x\cos\left(\kappa_xx\right)\qquad\kappa_x=\frac{\sqrt{2mE_x}}{\hbar}$$

$$Y\left(y\right)=A_y\sin\left(\kappa_yy\right)+B_y\cos\left(\kappa_yy\right)\qquad\kappa_y=\frac{\sqrt{2mE_y}}{\hbar}$$

Applying boundary conditions

$$X(0) = 0 = A_x \sin(0) + B_x \cos(0) = 0 + B_x \Rightarrow B_x = 0$$

$$X(a) = A_x \sin(\kappa_x a) = 0 \Rightarrow \kappa_x a = n\pi$$

$$Y(0) = 0 \Rightarrow B_y = 0$$

$$Y(b) = 0 \Rightarrow \kappa_y b = l\pi$$

$$X(x) = A_x \sin(\kappa_x x) = A_x \sin\left(\frac{n\pi}{a} x\right)$$

$$Y(y) = A_y \sin(\kappa_y y) = A_y \sin\left(\frac{l\pi}{b} y\right)$$

Normalization yields $A_x = A_y = 1$.

$$E_x = \frac{\kappa_x^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \qquad E_y = \frac{\kappa_x^2 \hbar^2}{2m} = \frac{l^2 \pi^2 \hbar^2}{2mb^2}$$

By Mathematica, for the z dependent portion,

$$\text{DSolve}\left[\frac{1}{Z[z]} Z''[z] == E_Z + \frac{m^2 \omega^2 z^2}{\hbar^2}, Z, z\right]$$

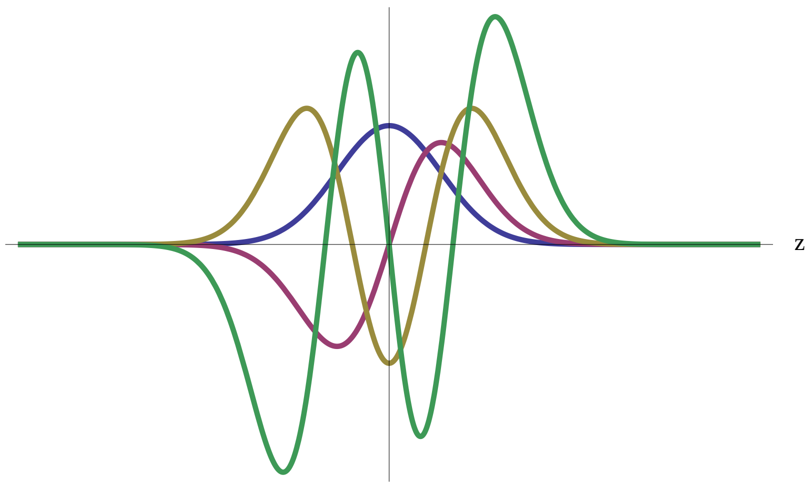
$$\kappa_z = \sqrt{\frac{2m\omega}{\hbar}}$$

$$n_{z1} = \frac{1}{2}\left(\frac{E_z \hbar}{m\omega} - 1\right) \qquad n_{z2} = -\frac{1}{2} + \frac{E_z \hbar}{2m\omega}$$

$$Z(z) = A_z \text{ParabolicCylinderD}\left(\frac{-m\omega - E_z \hbar}{2m\omega}, \kappa_z z\right) + B_z \text{ParabolicCylinderD}\left(\frac{-m\omega + E_z \hbar}{2m\omega}, i\kappa_z z\right)$$

I reject solutions where n_{z1} and n_{z2} are negative, because the function blows up for $z < 0$ and quickly drops to 0 for $z > 0$. Fractions for these also have a similarly unpleasant behaviour, so these should be ignored. The square when the complex also has horrible infinity approaching behaviour, so I set $B_z = 0$. Some of these functions look like

D_0,D_1,D_2,D_3



This looks somewhat reasonable. While not prevented from reaching infinity, the increasing potential as z^2 reduces the chance of the particle being found in the extremes either way. Since this is restricted now to positive integers, the parabolic cylinder function reduces to

$$D_n(x) = 2^{-\frac{n}{2}} e^{-\frac{x^2}{4}} \mathrm{H}_n\left(\frac{x}{\sqrt{2}}\right)$$

where $\mathrm{He}_n(x)$ is a Hermite polynomial. This is also similar to the spherical examples where the solutions also involved special polynomial functions.

$$Z(z) = A_z D_{n_z}(\kappa_z z) = A_z 2^{-\frac{n}{2}} e^{-\frac{x^2}{4}} \mathrm{H}_n\left(\frac{x}{\sqrt{2}}\right)$$

$$n_z = \frac{1}{2}\left(\frac{E_z \hbar}{m\omega} - 1\right)$$

$$E_z = \frac{(2n_z + 1)\, m\omega}{\hbar}$$

Trying to normalize, I find that only even n's give solutions for the normalization constant A_z. Finding solutions for A_{n_z} gives terms like

$$\left\{A_0 = \frac{1}{2\sqrt{\pi}}, A_2 = \frac{1}{6\sqrt{\pi}}, A_4 = \frac{1}{54\sqrt{\pi}}, A_6 = \frac{1}{810\sqrt{\pi}}, A_8 = \frac{1}{17010\sqrt{\pi}}, A_{10} = \frac{1}{459270\sqrt{\pi}}\right\}$$

This appears to be of the form $\frac{1}{2}\frac{1}{q(n)\sqrt{\pi}}$. The ratios between $q\left(n\right)$ in this sequence increase by factors of $3, 9, 15, 21, 27$ from the previous term. The factor increases by a $+2$ multiple of 3. This will look something like

$$q\left(n\right) = 3 \cdot \left(n+2\right) q\left(n-1\right)$$

although this isn't quite right.

Putting the pieces together,

$$\psi = A_{n_z} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{l\pi}{b}y\right) D_{n_z}\left(\kappa_z z\right)$$

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} + \frac{l^2\pi^2\hbar^2}{2mb^2} + \frac{\left(2n_z+1\right)m\omega}{\hbar}$$

This could be rewritten saying $j = 2n_z + 1$ for an odd integer.

b.

$$\hbar\omega > \frac{5\pi^2\hbar^2}{ma^2}$$

$$\frac{\omega}{\hbar} > \frac{5\pi^2}{ma^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} + \frac{l^2\pi^2\hbar^2}{2mb^2} + \left(2n_z+1\right)\frac{5\pi^2}{a^2}$$

There doesn't seem to be anything restricting the relation between indices. There doesn't seem to be a way for this to be degenerate except for the cases where the wavefunction is 0, at least without the possibility of $a = b$.

c.

$$\hat{H}_z = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{1}{2}m\omega^2 z^2 - q\epsilon z$$

Repeating the solving for the Z component from part a, this time with the added term from $q\epsilon z$,

$$n_z' = \frac{q^2\epsilon^2 - m\omega^3\hbar - E_z\omega^2\hbar^2}{2m\omega^3\hbar}$$

$$Z\left(z\right) = D_{n_z'}\left(-\sqrt{\frac{2}{m\hbar}}\frac{q\epsilon}{\omega^{3/2}} + \sqrt{\frac{2m\omega}{\hbar}}z\right)$$

$$E_z = -\frac{2m\omega^3\hbar n_z' + m\omega^3\hbar - q^2\epsilon^2}{\omega^2\hbar^2}$$

The x and y components aren't changed.