Quantum Mechanics 2 Homework #1

1) Use separation of variables in Cartesian coordinates to solve the infinite 3-dimensional well:

$$V(x,y,z) = \begin{cases} 0 & \text{if } x,\ y, \text{ and } z \text{ are all between 0 and a} \\ \infty & \text{otherwise} \end{cases}$$

(a) Find the eigenfunctions and eigenenergies

(b) Call the first six distinct energies E_1, E_2, ..., E_6. Determine the degeneracy of each of these energies (i.e., find the number of different states that share the same energy.)

2) How that any Hamiltonian of the form

$$H = \frac{p^2}{2m} + V(|r|),$$

where $|r|$ is the magnitude of the three-dimensional distance $\vec{r}$, commutes with all three components L_x, L_y, and L_z of the operator $\vec{L}$. Since we already know that L^2 and L_z commute, this result indicates that H, L_z, and L^2 are mutually compatible observables.

3) Formulate Heisenberg's Uncertainty Principle for three dimensions. Support your answer with commutators.

4) Show that

(a) $[x, f(p)] = i\hbar \dfrac{\partial f}{\partial p}$

(b) $[x, p^n] = i\hbar n p^{n-1}$

Answers to QM 2 Homework #1

(1) $$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi = E\Psi$$ inside the well.

Guess $\Psi = X_{(x)}\cdot Y_{(y)}\cdot Z_{(z)}$. Plug this in above, then divide by $X\cdot Y\cdot Z$:

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2} = \frac{-2mE}{\hbar^2}$$

$$\downarrow$$

$$\frac{1}{X}\frac{d^2X}{dx^2} = -\frac{2mE}{\hbar^2}-\frac{1}{Y}\frac{d^2Y}{dy^2}-\frac{1}{Z}\frac{d^2Z}{dz^2}$$

Both sides must = the same constant; call it $-k_x^2$

So $$\frac{d^2X}{dx^2} = -k_x^2X \rightarrow X = A_x\sin k_xx + B_x\cos k_xx$$

and $$\underbrace{-\frac{2mE}{\hbar^2}-\frac{1}{Y}\frac{d^2Y}{dy^2}-\frac{1}{Z}\frac{d^2Z}{dz^2} = -k_x^2}$$

Rewrite

$$\downarrow$$

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = k_x^2-\frac{2mE}{\hbar^2}-\frac{1}{Z}\frac{d^2Z}{dz^2}$$

Both sides must = the same constant; call it $-k_y^2$

So $$\frac{d^2Y}{dy^2} = -k_y^2Y \rightarrow Y = A_y\sin k_yy + B_y\cos k_yy$$

and $\underbrace{k_x^2 - \frac{2mE}{\hbar^2} - \frac{1}{Z}\frac{d^2Z}{dz^2} = -k_y^2}$

$\downarrow$ Rewrite

$$\frac{d^2Z}{dz^2} = \underbrace{\left[\frac{-2mE}{\hbar^2} + k_x^2 + k_y^2\right]}_{\text{call this } -k_z^2} Z$$

So $Z = A_z \sin k_z z + B_z \cos k_z z$

Apply boundary conditions:

$X(x=0) = 0 \longrightarrow B_x = 0$

$Y(x=0) = 0 \longrightarrow B_y = 0$

$Z(z=0) = 0 \longrightarrow B_z = 0$

$X(x=a) = 0 \longrightarrow \sin k_x a = 0 \rightarrow k_x = \frac{n_x \pi}{a}$, where $n_x = 1, 2, 3 \ldots$

$Y(y=a) = 0 \rightarrow \sin k_y a = 0 \rightarrow k_y = \frac{n_y \pi}{a}$, where $n_y = 1, 2, 3, \ldots$

$Z(z=a) = 0 \rightarrow \sin k_z a = 0 \rightarrow k_z = \frac{n_z \pi}{a}$, where $n_z = 1, 2, 3, \ldots$

Normalize to get $A_x = B_x = C_x = \sqrt{\frac{2}{a}}$

So the eigenfunctions are

$$\boxed{\psi = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right)}$$

The eigenenergies are $E = \left(k_x^2 + k_y^2 + k_z^2\right)\frac{\hbar^2}{2m}$

$$\boxed{= \frac{\left(n_x^2 + n_y^2 + n_z^2\right)\pi^2\hbar^2}{2ma^2}}$$

(b) The following combinations of n_x, n_y, n_z produce the first 4 energy levels

n_x	n_y	n_z	$(n_x^2+n_y^2+n_z^2)$	Level #	degeneracy
1	1	1	3	E_1	1
1	1	2			
1	2	1	6	E_2	3
2	1	1			
1	2	2			
2	1	2	9	E_3	3
2	2	1			
1	1	3			
1	3	1	11	E_4	3
3	1	1			
2	2	2	12	E_5	1
1	2	3			
1	3	2			
2	1	3	14	E_6	6
2	3	1			
3	1	2			
3	2	1			

③ $H = \frac{1}{2m} p^2 + V(\sqrt{r^2})$

$$[L_z, p^2] = [L_z, (p_x^2 + p_y^2 + p_z^2)]$$

$$= [L_z, p_x^2] + [L_z, p_y^2] + [L_z, p_z^2]$$

$$= p_x \underbrace{[L_z, p_x]} + [L_z, p_x] p_x + p_y [L_z, p_y] + \underbrace{[L_z, p_y]} p_y$$

$$+ p_z \underbrace{[L_z, p_z]}_{0} + \underbrace{[L_z, p_z]}_{0} p_z$$

$$[L_z, p_x] = [(x p_y - y p_x), p_x] =$$

exchange exchange

$$= x p_y p_x - p_x x p_y - y p_x p_x + p_x y p_x$$

$$= p_y \underbrace{[x, p_x]}_{i\hbar} - \cancel{y p_x p_x} + \cancel{y p_x p_x}$$

$$= i\hbar p_y$$

$$[L_z, p_y] = [(x p_y - y p_x), p_y]$$

exchange

$$= x p_y p_y - p_y x p_y - y p_x p_y + p_y y p_x$$

$$= \cancel{x p_y p_y} - \cancel{x p_y p_y} - p_x \underbrace{[y, p_y]}_{i\hbar}$$

$$= -i\hbar p_y$$

So $[L_z, p^2] = i\hbar p_y + i\hbar p_y - i\hbar p_y - i\hbar p_y + 0 + 0 = \boxed{0}$

$$[L_z, r^2] = [L_z, (x^2+y^2+z^2)]$$

$$= [L_z, x^2] + [L_z, y^2] + [L_z, z^2]$$

$$= x\underbrace{[L_z, x]}_{i\hbar y} + \underbrace{[L_z, x]}_{i\hbar y}x + y\underbrace{[L_z, y]}_{-i\hbar x} + \underbrace{[L_z, y]}_{-i\hbar x}y$$

$$+ z\underbrace{[L_z, z]}_{0} + \underbrace{[L_z, z]}_{0}$$

$$= i\hbar xy + i\hbar yx - i\hbar yx - i\hbar xy + 0 + 0 = \boxed{0}$$

Similarly for $[L_x, p^2]$, $[L_y, p^2]$, $[L_x, r^2]$, $[L_y, r^2]$

③ Let $x \equiv r_1$
$y = r_2$
$z = r_3$
$p_x = p_1$
$p_y = p_2$
$p_z = p_3$

$[x, y] = xy - yx = 0$, etc., so $[r_i, r_j] = 0$

$$[p_x, p_y]\psi = \left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d\psi}{dy}\right) - \left(-i\hbar\frac{d}{dy}\right)\left(-i\hbar\frac{d\psi}{dx}\right)$$

$$= -\hbar^2\left(\frac{d^2\psi}{dx\,dy} - \frac{d^2\psi}{dy\,dx}\right) = 0$$

So $[p_i, p_j] = 0$

$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$ from Physics 491

$$[y, p_x]\psi = -i\hbar\left(y\frac{d\psi}{dx} - \frac{d}{dx}(y\psi)\right)$$

$$= -i\hbar\left(y\frac{d\psi}{dx} - \psi\frac{dy}{dx} - y\frac{d\psi}{dx}\right) = 0$$

So $\underbrace{[r_i, p_j] = i\hbar\delta_{ij}}$

The General Uncertainty Relation

$$\Delta r_i \Delta p_j \geq \left|\frac{\langle [r_i, p_j]\rangle}{2i}\right| = \left|\frac{1}{2i} i\hbar\delta_{ij}\right| = \boxed{\frac{\hbar}{2}\delta_{ij}}$$

$$\Delta r_i \Delta r_j \geq \left|\frac{\langle [r_i, r_j]\rangle}{2i}\right| = \boxed{0}$$

$$\Delta p_i \Delta p_j \geq \left|\frac{\langle [p_i, p_j]\rangle}{2i}\right| = \boxed{0}$$

4 (b) Recall $[x,p] = i\hbar$

Notice that in general $[A,BC] = ABC - BCA$

Insert $0 = -BAC + BAC$

$$= ABC - BAC + BAC - BCA$$

$$= [A,B]C + B[A,C]$$

Plug in $A = x$
$B = p$
$C = p$

Then

$$[x,p^2] = [x,p]p + p[x,p] = 2i\hbar p$$

Then by induction

$$\boxed{[x,p^n] = n i\hbar p^{n-1}}$$

(a) Consider a function $f(p) = \sum_n a_n p^n$

Then $[x,f(p)] = \sum_n a_n [x,p^n] = \sum_n a_n n i\hbar p^{n-1}$ (from part b)

$$= i\hbar \sum_n a_n n p^{n-1} = \boxed{i\hbar \frac{df}{dp}}$$