6. Angular Momentum
(Gasiorowicz, Chapter 7)
http://reynolds.ph.man.ac.uk/~pablo/QM/

6.1 Quantum Mechanics in 3D:
- The wave function depends on three spatial coordinates, $\psi(x,y,z,t)$.
- Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi+V(x,y,z)\psi$$

- Operators:

$$\hat{p}_x\psi=-i\hbar\frac{\partial\psi}{\partial x}$$

$$\hat{p}_y\psi=-i\hbar\frac{\partial\psi}{\partial y}$$

$$\hat{p}_z\psi=-i\hbar\frac{\partial\psi}{\partial z}$$

$$\underline{\hat{P}}=(\hat{p}_x,\hat{p}_y,\hat{p}_z)$$

$$\hat{X}\psi=x\psi$$

$$\hat{Y}\psi=y\psi$$

$$\hat{Z}\psi=z\psi$$

$$\underline{\hat{R}}=(\hat{x},\hat{y},\hat{z})$$

Commutation relations:

$$\left[\hat{X},\hat{p}_x\right]=ih$$

$$\left[\hat{X},\hat{Y}\right]=\left[\hat{X},\hat{Z}\right]=\left[\hat{Y},\hat{Z}\right]=0$$

$$\left[\hat{p}_x,\hat{p}_y\right]=\left[\hat{p}_x,\hat{p}_z\right]=\left[\hat{p}_y,\hat{p}_z\right]=0$$

$$\left[\hat{X},\hat{p}_y\right]=\left[\hat{p}_z,\hat{Y}\right]=...=0$$

$$\left[\hat{X},\hat{p}_x\right]=\left[\hat{Y},\hat{p}_y\right]=\left[\hat{Z},\hat{p}_z\right]=i\hbar$$

Bases:
If two operators commute we can use bases of their respective state spaces to build a basis for the enlarged state space.
Example:

$$|x\rangle=\delta(x-x')$$

$$|y\rangle=\delta(y-y')$$

$$|z\rangle=\delta(z-z')$$

The basis for the 3D space is:

$$|x,y,z\rangle=\delta(x-x')\delta(y-y')\delta(z-z')$$

$$\langle x|\psi\rangle=\psi(x)$$

$$\langle x,y,z|\psi\rangle=\psi(x,y,z)$$

$$|x\rangle=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}a(x,y,z)|x,y,z\rangle dxdydz$$

$$a(x,y,z)=\langle x,y,z|\psi\rangle$$

6.2 Angular Momentum

$\underline{\ell} = \underline{r} \times \underline{p}$

In analogy with classical mechanics, we define the angular momentum $\underline{\hat{L}}$:

$\underline{\hat{L}} = \underline{\hat{R}} \times \underline{\hat{P}}$

In components:

$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y$

$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z$

$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x$

$\hat{L}^2 = \left\langle \underline{\hat{L}}, \underline{\hat{L}} \right\rangle = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2$

$$\begin{aligned}\left[\hat{L}_x, \hat{L}_y\right] &= \left[\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z\right] \\ &= \left[\hat{Y}\hat{P}_z, \hat{Z}\hat{P}_x\right] - \left[\hat{Y}\hat{P}_z, \hat{X}\hat{P}_z\right] - \left[\hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x\right] + \left[\hat{Z}\hat{P}_y, \hat{X}\hat{P}_z\right] \\ &= -i\hbar\hat{Y}\hat{P}_x + i\hbar\hat{X}\hat{P}_y = i\hbar\hat{L}_z\end{aligned}$$

$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z$

$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$

$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$

$$\left[\hat{L}^2, \hat{L}_z\right] = \left[\hat{L}_x{}^2, \hat{L}_z\right] + \left[\hat{L}_y{}^2, \hat{L}_z\right] + \underbrace{\left[\hat{L}_z{}^2, \hat{L}_z\right]}_{0}$$

$\left[\hat{L}_x{}^2, \hat{L}_z\right] = -i\hbar\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right)$

$\left[\hat{L}_y{}^2, \hat{L}_z\right] = i\hbar\left(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\right)$

$\rightarrow \left[\hat{L}^2, \hat{L}_z\right] = 0$

$\left[\hat{L}^2, \hat{L}_x\right] = 0$

$\left[\hat{L}^2, \hat{L}_y\right] = 0$

6.3 General Definition of Angular Momentum

We call angular momentum $\underline{\hat{J}} = \left(\hat{J}_x, \hat{J}_y, \hat{J}_z\right)$

To any observables, $\hat{J}_x, \hat{J}_y, \hat{J}_z$ that satisfies three relasions:

$\left[\hat{J}_x, \hat{J}_y\right] = i\hbar\hat{J}_z$

$\left[\hat{J}_y, \hat{J}_z\right] = i\hbar\hat{J}_x$

$\left[\hat{J}_z, \hat{J}_x\right] = i\hbar\hat{J}_y$

Note: we've proved before $\hat{J}^2 = \hat{J}_x{}^2 + \hat{J}_y{}^2 + \hat{J}_z{}^2$, and $\left[\hat{J}^2, \hat{J}_x\right] = 0$ etc.)

6.4 The $\hat{J}_+$ and $\hat{J}_-$ Ladder Operators

$\hat{J}_+ = \hat{J}_x + i\hat{J}_y$

$\hat{J}_- = \hat{J}_x - i\hat{J}_y$

$\hat{J}_+^\dagger = \hat{J}_x^\dagger + \left(i\hat{J}_y\right)^\dagger = \hat{J}_x - i\hat{J}_y = \hat{J}_-$

So $\hat{J}_+^\dagger = \hat{J}_- = 0$, i.e. $\hat{J}_+^\dagger$ and $\hat{J}_-$ are not hermitian.

→ $\hat{J}_+$ and $\hat{J}_-$ cannot be observables.

Useful relations:

$\left[\hat{J}_z, \hat{J}_+\right] = \hbar\hat{J}_+$ (6-1)

$\left[\hat{J}_z, \hat{J}_-\right] = -\hbar\hat{J}_-$ (6-2)

$\left[\hat{J}_+, \hat{J}_-\right] = 2\hbar\hat{J}_z$ (6-3)

$\left[\hat{J}^2, \hat{J}_+\right] = \left[\hat{J}^2, \hat{J}_-\right] = \left[\hat{J}^2, \hat{J}_z\right] = 0$ (6-4)

$\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}_z^2 + \hbar\hat{J}_z$ (6-5)

$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_z^2 - \hbar\hat{J}_z$ (6-6)

$\hat{J}^2 = \frac{1}{2}\left(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+\right) + \hat{J}_z^2$ (6-7)

6.5 Eigenvalues and Eigenfunctions of $\hat{J}^2$ and $\hat{J}_z$

If $|\lambda\rangle$ is an eigenfunction of $\hat{J}^2$ with eigenvalue $\lambda\hbar^2$, then $\hat{J}^2|\lambda\rangle = \lambda\hbar^2|\lambda\rangle$

$\langle\lambda|\hat{J}^2|\lambda\rangle = \lambda\hbar^2\langle\lambda|\lambda\rangle = \lambda\hbar^2\left\||\lambda\rangle\right\|^2 \geq 0$

(expand out $\hat{J}^2$)

$\langle\lambda|\hat{J}^2|\lambda\rangle = \langle\lambda|\hat{J}_x^2|\lambda\rangle + \langle\lambda|\hat{J}_y^2|\lambda\rangle + \langle\lambda|\hat{J}_z^2|\lambda\rangle$

and now expand out $\hat{J}_x^2$ etc.

$$\langle\lambda|\hat{J}_x^2|\lambda\rangle = \underbrace{\langle\lambda|\hat{J}_x}_{\langle\phi|}\underbrace{\hat{J}_x|\lambda\rangle}_{|\phi\rangle} = \left\||\phi\rangle\right\|^2 = \left\|\hat{J}_x|\lambda\rangle\right\|^2$$

and back to the original:

$$\langle\lambda|\hat{J}^2|\lambda\rangle = \underbrace{\left\|\hat{J}_x|\lambda\rangle\right\|^2}_{\geq 0} + \underbrace{\left\|\hat{J}_y|\lambda\rangle\right\|^2}_{\geq 0} + \underbrace{\left\|\hat{J}_z|\lambda\rangle\right\|^2}_{\geq 0}$$

Therefore $\langle\lambda|\hat{J}^2|\lambda\rangle \geq 0 = \lambda\hbar^2\left\||\lambda\rangle\right\|^2 \geq 0$

For convenience, we write $\lambda = j(j+1)$ with $j \geq 0$

If $|m\rangle$ is the eigenfunction of $\hat{J}_z$,

$\hat{J}_z|m\rangle = m\hbar|m\rangle$

$\hat{J}^2$ and $\hat{J}_z$ commute and then they have a common set of eigenfunctions $|j,m\rangle$.

$\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$

$\hat{J}_z|j,m\rangle = m\hbar|j,m\rangle$

$\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle = \left\|\hat{J}_+|j,m\rangle\right\| \geq 0$

$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = \left\|\hat{J}_-|j,m\rangle\right\| \geq 0$

Using (6-5) and (6-6):

$\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle = \langle j,m|\hat{J}_-^2\hat{J}_z - \hbar\hat{J}_z|j,m\rangle = \left[j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2\right]\langle j,m|j,m\rangle$

(6-8)

$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$ (6-9)

From (6-8):

$j(j+1) - m(m+1) = (j-m)(j+m+1) \geq 0$ (6-10)

and from (6-9):

$j(j+1) - m(m-1) = (j-m+1)(j+1) \geq 0$ (6-11)

From 6-10:

$-j(j+1) \leq m \leq j$

and also (from (6-11)):

$-j \leq m \leq (j+1)$

6.6 Action of $\hat{J}_+$ and $\hat{J}_-$ on the $|j,m\rangle$

$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \geq 0$ (6-9)

For $j = -m$, $\langle j,-j|\hat{J}_+\hat{J}_-|j,-j\rangle = 0$.

$\langle j,-j|\hat{J}_+\hat{J}_-|j,-j\rangle = \left\|\hat{J}_-|j,-j\rangle\right\|^2 = 0$

For $m > -j$;

$\left[\hat{J}_Z,\hat{J}_-\right] = -\hbar\hat{J}_-$ (6-2)

$\hat{J}_z\hat{J}_-|j,m\rangle = \underbrace{\hat{J}_-\hat{J}_Z|j,m\rangle}_{\hbar m\hat{J}_-|j,m\rangle} - \hbar\hat{J}_-|j,m\rangle$

$= \hbar(m-1)J_-|j,m\rangle$

→ $\hat{J}_-|j,m\rangle$ is an eigenfunction of $\hat{J}_z$ with eigenvalue $\hbar(m-1)$.

$\left[\hat{J}^2,\hat{J}_-\right] = 0$ (6-4)

$\hat{J}^2\left[J_-|j,m\rangle\right] = \hat{J}_-\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)\left[\hat{J}_-|j,m\rangle\right]$

→ $\hat{J}_-|j,m\rangle$ is an eigenfunction of $\hat{J}^2$ with eigenvalue $j(j+1)\hbar^2$.

→ $\hat{J}_-|j,m\rangle = C|j,m-1\rangle$

$\left\|\hat{J}_-|j,m\rangle\right\|^2 = \langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = |C|^2\langle j,m-1|j,m-1\rangle = |C|^2$

From (6-9),

$\left\|\hat{J}_-|j,m\rangle\right\|^2 = \hbar^2 j(j+1) - m^2\hbar^2 + m\hbar^2$

→ $C = \hbar\sqrt{j(j+1) - m(m-1)}$

$\hat{J}_-|j,m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}|j,m-1\rangle$

$\hat{J}_+|j,m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|j,m+1\rangle$

$\hat{J}_-|j,-j\rangle = 0$, $\hat{J}_+|j,j\rangle = 0$ as $-j \le m \le j$

The action of $\hat{J}_+$ and $\hat{J}_-$ shows that the difference between j and m has to be integer.

$m = -j, -j+1, ..., j-1, j$

If we start with $m = j$,

$\hat{J}_-^{\,p}|j,j\rangle = A|j,m\rangle$

$m = j - p$ (6-12)

p is a positive integer $p \ge 0$.

In the same way,

$\hat{J}_+^{\,q}|j,-j\rangle = B|j,m\rangle$

$m = -j + q$ (6-13)

q is an integer, $q \ge 0$

From (6-12) and (6-13):

$zj = p + q$

→ j has to be an integer or half integer (depending on the system).

If j is integer then m is integer.

If j is half-integer, then m is half-integer.

6.7 Notation for orbital angular momentum

$\underline{\hat{L}} = \left(\hat{L}_x, \hat{L}_y, \hat{L}_z\right)$

$\hat{L}^2|\ell, m_\ell\rangle = \hbar^2 \ell(\ell+1)|\ell, m_\ell\rangle$

$\hat{L}_z|\ell, m_\ell\rangle = \hbar m_\ell|\ell, m_\ell\rangle$

$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$

$\hat{L}_- = \hat{L}_x - i\hat{L}_y$

$\hat{L}_+|\ell, m_\ell\rangle = \hbar\sqrt{\ell(\ell+1) - m_\ell(m_\ell+1)}|\ell, m_\ell+1\rangle$

$\hat{L}_-|\ell, m_\ell\rangle = \hbar\sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}|\ell, m_\ell-1\rangle$

$\langle x|\psi\rangle = \psi(x)$

$|x\rangle = \delta(x - x')$

Using spherical coordinates,

$\langle\theta,\varphi|\ell, m_\ell\rangle = Y_{\ell,m}(\theta,\varphi)$

$Y_{\ell,m}(\theta,\varphi)$ are spherical harmonics.