Orbital Angular Momentum in Spherical Coordinates

A change $d\vec{r}$ in the position is

$$d\vec{r} = \hat{x}\,dx + \hat{y}\,dy + \hat{z}\,dz$$

$$= \hat{r}\,dr + r\hat{\theta}\,d\theta + r\sin\theta\,\hat{\phi}\,d\phi \qquad (1)$$

in euclidean and spherical coordinates.

In terms of $\hat{x}$, $\hat{y}$, & $\hat{z}$, the vectors $\hat{r}$, $\hat{\theta}$, & $\hat{\phi}$ are

$$\hat{r} = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$$

$$\hat{\theta} = \hat{x}\cos\theta\cos\phi + \hat{y}\cos\theta\sin\phi - \hat{z}\sin\theta$$

$$\hat{\phi} = -\hat{x}\sin\phi + \hat{y}\cos\phi. \qquad (2)$$

The inverse relations are

$$\hat{x} = \hat{x}\cdot\hat{r}\,\hat{r} + \hat{x}\cdot\hat{\theta}\,\hat{\theta} + \hat{x}\cdot\hat{\phi}\,\hat{\phi}$$

$$\hat{x} = \sin\theta\cos\phi\,\hat{r} + \cos\theta\cos\phi\,\hat{\theta} - \sin\phi\,\hat{\phi}$$

$$\hat{y} = \sin\theta\sin\phi\,\hat{r} + \cos\theta\sin\phi\,\hat{\theta} + \cos\phi\,\hat{\phi}$$

$$\hat{z} = \cos\theta\,\hat{r} - \sin\theta\,\hat{\theta}, \qquad (3)$$

The gradient $\vec{\nabla} f$ is defined by

$$df = \vec{dr} \cdot \vec{\nabla} f = dr \frac{\partial f}{\partial r} + d\theta \frac{\partial f}{\partial \theta} + d\phi \frac{\partial f}{\partial \phi} \quad (4)$$

and is in view of (1)

$$\vec{\nabla} f = \hat{r} \frac{\partial f}{\partial r} + \frac{\hat{\theta}}{r} \frac{\partial f}{\partial \theta} + \frac{\hat{\phi}}{r \sin\theta} \frac{\partial f}{\partial \phi} . \quad (5)$$

So

$$\vec{\nabla} = \hat{r}\, \partial_r + \frac{\hat{\theta}}{r} \partial_\theta + \frac{\hat{\phi}}{r \sin\theta} \partial_\phi \quad (6)$$

and the orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} \quad (7)$$

is represented as

$$\langle \vec{r} \,|\, \vec{L} \,|\, \psi \rangle = \vec{r} \times \frac{\hbar}{i} \vec{\nabla} \langle \vec{r} \,|\, \psi \rangle \quad (8)$$

$$= \frac{\hbar r}{i} \hat{r} \times \left(\hat{r}\, \partial_r + \frac{\hat{\theta}}{r} \partial_\theta + \frac{\hat{\phi}}{r \sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

$$= \frac{\hbar}{i} \left(\hat{\phi}\, \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle . \quad (9)$$

The rectangular components of $\vec{L}$ are represented by

$$\langle \vec{r} \,|\, L_z \,|\, \psi \rangle = \langle \vec{r} \,|\, \hat{z} \cdot L \,|\, \psi \rangle$$

$$= \hat{z} \cdot \frac{\hbar}{i} \left(\hat{\phi} \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

$$= \frac{\hbar}{i} \partial_\phi \langle \vec{r} \,|\, \psi \rangle \qquad (10)$$

and, less simply, by

$$\langle \vec{r} \,|\, L_x \,|\, \psi \rangle = \langle \vec{r} \,|\, \hat{x} \cdot \vec{L} \,|\, \psi \rangle$$

$$= \hat{x} \cdot \frac{\hbar}{i} \left(\hat{\phi} \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

$$= \frac{\hbar}{i} \left(\cos\theta \cos\phi \, \hat{\theta} - \sin\phi \, \hat{\phi} \right) \cdot \left(\hat{\phi} \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

$$= \frac{\hbar}{i} \left(-\sin\phi \, \partial_\theta - \cot\theta \cos\phi \, \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle \qquad (11)$$

and

$$\langle \vec{r} \,|\, L_y \,|\, \psi \rangle = \langle \vec{r} \,|\, \hat{y} \cdot \vec{L} \,|\, \psi \rangle = \hat{y} \cdot \frac{\hbar}{i} \left(\hat{\phi} \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

$$= \frac{\hbar}{i} \left(\cos\theta \sin\phi \, \hat{\theta} + \cos\phi \, \hat{\phi} \right) \cdot \left(\hat{\phi} \partial_\theta - \frac{\hat{\theta}}{\sin\theta} \partial_\phi \right) \langle \vec{r} \,|\, \psi \rangle$$

that is,

$$\langle \vec{r} | L_y | \psi \rangle = \frac{\hbar}{i}\left(\cos\phi \, \partial_\theta - \cot\theta \sin\phi \, \partial_\phi\right)\langle \vec{r} | \psi \rangle . \quad (12)$$

It follows from (11) & (12) that the raising and lowering operators $L_\pm$ are

$$\langle \vec{r} | L_\pm | \psi \rangle = \langle \vec{r} | L_x \pm i L_y | \psi \rangle$$

$$= \frac{\hbar}{i}\Big[(-\sin\phi \pm i \cos\phi)\partial_\theta - \cot\theta\,(\cos\phi \pm i \sin\phi)\partial_\phi \Big]\langle \vec{r} | \psi \rangle$$

$$= \frac{\hbar}{i} e^{\pm i\phi}\left(\pm i \, \partial_\theta - \cot\theta \, \partial_\phi\right)\langle \vec{r} | \psi \rangle . \quad (13)$$

Since
$$\vec{L}^2 = L_z^2 + \tfrac{1}{2}\left(L_+ L_- + L_- L_+\right) \quad (14)$$
one can show that

$$\langle \vec{r} | \vec{L}^2 | \psi \rangle = -\hbar^2 \left[\frac{1}{\sin^2\theta}\partial_\phi^2 + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta \, \partial_\theta\right)\right]\langle \vec{r} | \psi \rangle \quad (15)$$

by using (10) and (13).

In spherical coordinates, the laplacian

$$\Delta = \vec{\nabla} \cdot \vec{\nabla} = \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} \tag{16}$$

is

$$\Delta = \frac{1}{r^2}\left[\partial_r(r^2\partial_r) + \frac{\partial_\theta(\sin\theta\,\partial_\theta)}{\sin\theta} + \frac{\partial_\phi^2}{\sin^2\theta}\right]. \tag{17}$$

Thus

$$\langle \vec{r}\,|\,\vec{p}^{\,2}|\psi\rangle = -\hbar^2\,\nabla\cdot\nabla\langle\vec{r}|\psi\rangle = -\hbar^2\Delta\langle\vec{r}|\psi\rangle$$

$$= -\frac{\hbar^2}{r^2}\left[\partial_r(r^2\partial_r) + \frac{\partial_\theta(\sin\theta\,\partial_\theta)}{\sin\theta} + \frac{\partial_\phi^2}{\sin^2\theta}\right]\langle\vec{r}|\psi\rangle$$

$$= -\frac{\hbar^2}{r^2}\partial_r(r^2\partial_r)\langle\vec{r}|\psi\rangle + \frac{1}{r^2}\langle\vec{r}\,|\vec{L}^2|\psi\rangle. \tag{18}$$

If $|\psi\rangle$ is an e.vec of $\vec{L}^2$ with e-val $\hbar^2 l(l+1)$ (and of L_z with e-val $m\hbar$), then

$$\vec{L}^2|\psi\rangle = \hbar^2 l(l+1)|\psi\rangle \text{ and } L_z|\psi\rangle = m\hbar|\psi\rangle \tag{19}$$

and

$$\langle\vec{r}\,|\vec{p}^{\,2}|\psi\rangle = -\frac{\hbar^2}{r^2}\partial_r(r^2\partial_r)\langle\vec{r}|\psi\rangle + \frac{\hbar^2}{r^2}l(l+1)\langle\vec{r}|\psi\rangle. \tag{20}$$

This is the starting point for a discussion of central potentials $V = V(r)$.