Rotations and Angular Momentum

In three dimensions, the position and momentum eigenvalue problems read

$$\widehat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle = \boldsymbol{r}\,|\boldsymbol{r}\rangle \quad \text{and} \quad \widehat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle, \tag{1}$$

with

$$|\boldsymbol{r}\rangle = |x_1, x_2, x_3\rangle,\ \boldsymbol{r} = \sum_{i=1}^{3} x_i\,\boldsymbol{e}_i$$
$$|\boldsymbol{p}\rangle = |p_1, p_2, p_3\rangle,\ \boldsymbol{p} = \sum_{i=1}^{3} p_i\,\boldsymbol{e}_i$$

1 Rotation operators

Rotations of a vector about the x_i ($i = 1, 2, 3 = x, y, z...$) axes by a finite angle are represented by the rotation matrices

$$\widehat{\mathbb{R}}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad \widehat{\mathbb{R}}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad \widehat{\mathbb{R}}_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

Here, I used the same angle θ for the three rotations for simplicity; in general, the angles should be different to cover all possibilities.

The generator of infinitesimal rotations

Consider rotations by an infinitesimal angle $\delta\theta$. Using Taylor expansions to the lowest order in $\delta\theta$ i.e. $\cos\delta\theta \approx 1 - \frac{1}{2}\delta\theta^2$, $\sin\delta\theta \approx \delta\theta$, the rotation operators become

$$\widehat{\mathbb{R}}_x(\delta\theta) \approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{1}{2}\delta\theta^2 & -\delta\theta \\ 0 & \delta\theta & 1-\frac{1}{2}\delta\theta^2 \end{pmatrix}, \tag{3}$$

$$\widehat{\mathbb{R}}_y(\delta\theta) \approx \begin{pmatrix} 1-\frac{1}{2}\delta\theta^2 & 0 & \delta\theta \\ 0 & 1 & 0 \\ -\delta\theta & 0 & 1-\frac{1}{2}\delta\theta^2 \end{pmatrix}, \tag{4}$$

$$\widehat{\mathbb{R}}_z(\delta\theta) \approx \begin{pmatrix} 1-\frac{1}{2}\delta\theta^2 & -\delta\theta & 0 \\ \delta\theta & 1-\frac{1}{2}\delta\theta^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

Expressing the non-commutativity of successive rotations,

$$[\widehat{\mathbb{R}}_x(\delta\theta), \widehat{\mathbb{R}}_y(\delta\theta)] = \begin{pmatrix} 0 & -\delta\theta^2 & 0 \\ \delta\theta^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \widehat{\mathbb{R}}_z(\delta\theta) - \widehat{\mathbb{I}} \overset{!}{=} -i\,\frac{\delta\theta}{\hbar}\widehat{G}. \tag{6}$$

The last line of Eq. 6 introduces $\widehat{G}$, the generator of infinitesimal rotations about the z axis, through

$$\widehat{\mathbb{R}}_z(\delta\theta) = \widehat{\mathbb{I}} - i\,\frac{\delta\theta}{\hbar}\widehat{G}.$$

The nature of $\widehat{G}$

Let's assume a quantum system (e.g. a molecule) is in state $|\psi\rangle$, and focus on rigid-body rotations about the z axis, given by $\widehat{\mathbb{R}}_z(\theta)$. Any three-dimensional vector operator $\widehat{\boldsymbol{V}}$ is transformed into $\widehat{\boldsymbol{V}}' = \widehat{\mathbb{R}}_z(\theta)\widehat{\boldsymbol{V}}$. As a consequence, its expectation value in the given state $|\psi\rangle$ is transformed via $\langle \boldsymbol{V}' \rangle = \widehat{\mathbb{R}}_z(\theta)\langle \boldsymbol{V} \rangle$, where $\langle \boldsymbol{V}' \rangle = \langle\psi|\widehat{\boldsymbol{V}}'|\psi\rangle$ and $\langle \boldsymbol{V} \rangle = \langle\psi|\widehat{\boldsymbol{V}}|\psi\rangle$. In particular, for the position vector operator $|\boldsymbol{r}\rangle$ one has

$$|\boldsymbol{r}\rangle' = \widehat{\mathbb{R}}_z(\theta)\widehat{\boldsymbol{r}}.$$

We then impose—postulate—forward (positive) and reverse (negative) rotations about the z axis as

$$|\boldsymbol{r}_+\rangle' \equiv \widehat{\mathbb{R}}_z(\theta)\widehat{\boldsymbol{r}} \overset{!}{=} |x\cos\theta - y\sin\theta,\; x\sin\theta + y\cos\theta,\; z\rangle, \tag{7}$$

$$|\boldsymbol{r}_-\rangle' \equiv \widehat{\mathbb{R}}_z^\dagger(\theta)\widehat{\boldsymbol{r}} \overset{!}{=} |x\cos\theta + y\sin\theta,\; -x\sin\theta + y\cos\theta,\; z\rangle = \widehat{\mathbb{R}}_z(-\theta). \tag{8}$$

Now, we can construct $\widehat{G}$ from infinitesimal rotations. First, define the corresponding forward and reverse rotations by keeping up to $\mathcal{O}(\delta\theta)$:

$$\widehat{\mathbb{R}}_z(\delta\theta)|\boldsymbol{r}\rangle \stackrel{!}{=} |x - y\delta\theta,\, x\delta\theta + y,\, z\rangle, \tag{9}$$

$$\widehat{\mathbb{R}}_z^\dagger(\delta\theta)|\boldsymbol{r}\rangle \stackrel{!}{=} |x + y\delta\theta,\, -x\delta\theta + y,\, z\rangle = \widehat{\mathbb{R}}_z(-\delta\theta). \tag{10}$$

Next, consider the effect of rotations on a wavefunction, through $\psi(\boldsymbol{r}) \to \psi'(\boldsymbol{r}) = \langle \boldsymbol{r}|\widehat{\mathbb{R}}_z(\delta\theta)|\psi\rangle$.

$$\langle \boldsymbol{r}|\widehat{\mathbb{R}}_z(\delta\theta)|\psi\rangle = \langle x + y\delta\theta,\, -x\delta\theta + y,\, z|\psi\rangle = \psi(x + y\delta\theta,\, -x\delta\theta + y,\, z) \tag{11}$$

which becomes

$$\langle \boldsymbol{r}|\widehat{\mathbb{I}} - i\,\frac{\delta\theta}{\hbar}\widehat{G}|\psi\rangle = \psi(\boldsymbol{r}) + \left(\frac{\partial\psi}{\partial x}\right)y\delta\theta - \left(\frac{\partial\psi}{\partial y}\right)x\delta\theta + \mathcal{O}(\delta\theta^2)$$

$$\cancel{\psi(\boldsymbol{r})} - i\frac{\delta\theta}{\hbar}\langle \boldsymbol{r}|\widehat{G}|\psi\rangle = \cancel{\psi(\boldsymbol{r})} + \big[x(-i\hbar\partial_y) + y(i\hbar\partial_x)\big]\psi(\boldsymbol{r}).$$

The net result is

$$\langle \boldsymbol{r}|\widehat{G}|\psi\rangle = \langle \boldsymbol{r}|\,\widehat{x}\,\widehat{p}_y - \widehat{y}\,\widehat{p}_x\,|\psi\rangle \equiv \langle \boldsymbol{r}|\widehat{L}_z|\psi\rangle. \tag{12}$$

Eq.12 concludes that the generator of rotations about the z axis is the z-component of the orbital angular momentum i.e. $\widehat{G} = \widehat{L}_z$; this translates to

$$\widehat{\mathbb{R}}_z(\delta\theta) = \widehat{\mathbb{I}} - i\,\frac{\delta\theta}{\hbar}\widehat{L}_z. \tag{13}$$

Finite-angle rotations

A rotation by a finite angle θ is obtained as an infinite sequence of successive infinitesimal rotations by angle $\delta\theta = \lim_{N\to\infty}(\theta/N)$. Using Eq.13,

$$\widehat{\mathbb{R}}_z(\theta) = \lim_{N\to\infty}\left[\widehat{\mathbb{R}}_z(\delta\theta)\right]^N = \lim_{N\to\infty}\left[\widehat{\mathbb{I}} - i\left(\frac{\theta}{N}\right)\frac{\widehat{L}_z}{\hbar}\right]^N = \exp\left(-i\frac{\theta}{\hbar}\widehat{L}_z\right). \tag{14}$$

The negative-angle action imposed on a position eigenket through Eqs. 8 and 10 ensures that the rotation operator $\widehat{\mathbb{R}}_z$ is unitary i.e. $\widehat{\mathbb{R}}_z^\dagger\widehat{\mathbb{R}}_z = \widehat{\mathbb{I}} = \widehat{\mathbb{R}}_z\widehat{\mathbb{R}}_z^\dagger$. This, in turn, makes the generator, $\widehat{L}_z$, Hermitian. Equations 13 and 14 apply equally to rotations about the x and y axes; the corresponding generators are the respective operators $\widehat{L}_x$ and $\widehat{L}_y$, also Hermitian. The three components of the vector angular momentum operator $\widehat{\boldsymbol{L}}$ can be expressed in condensed form using the Levi-Civita tensor,

$$\widehat{L}_k = \sum_{i,j=1}^{3}\epsilon_{ijk}\widehat{x}_i\widehat{p}_j.$$

2 Important commutators

$$[\widehat{x}_i, \widehat{p}_j] = i\hbar\delta_{ij}, \qquad [\widehat{x}_i, \widehat{x}_j] = 0 = [\widehat{p}_i, \widehat{p}_j], \tag{15}$$

$$[\widehat{L}_i, \widehat{L}_j] = i\hbar \sum_{i=1}^{3} \epsilon_{ijk} \widehat{L}_k. \tag{16}$$