

L-Squared

1 Classical Identity

In these notes we discuss the computation of $\mathbf{L}^2 = (\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{r} \times \mathbf{p})$ and its quantum operator version. First we compute the classical version.

$$\begin{aligned} \mathbf{L}^2 &= (\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{r} \times \mathbf{p}) \\ &= \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) \\ &= \mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}). \end{aligned} \tag{1}$$

Note that

$$\begin{aligned} \mathbf{p} \times \mathbf{L} &= \mathbf{p} \times (\mathbf{r} \times \mathbf{p}) \\ &= \mathbf{r}(\mathbf{p} \cdot \mathbf{p}) - \mathbf{p}(\mathbf{p} \cdot \mathbf{r}). \end{aligned} \tag{2}$$

using the BAC-CAB rule,

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B}).$$

This gives the identity.

$$\mathbf{L}^2 = r^2 p^2 - (\mathbf{r} \cdot \mathbf{p})^2. \tag{3}$$

2 Quantum Operator Identity

Now we will turn to $\hat{\mathbf{L}}^2 = (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}})$. Here we need to be careful with the order of operators. Also, we will make use of the Levi-Civita permutation symbol. We first note that

$$\mathbf{r} \times \mathbf{p} = \sum_{i,j,k=1}^3 \epsilon_{ijk} x_j p_k \hat{\mathbf{e}}_i,$$

where

$$\epsilon_{ijk} = \begin{cases} 1, & ijk \text{ an even permutation of } 123, \\ -1, & ijk \text{ an odd permutation of } 123, \\ 0, & i = j, j = k, \text{ or } k = i. \end{cases}$$

Furthermore, we will need the identities

$$\sum_{k=1}^3 \delta_{kk} = 3, \tag{4}$$

$$\sum_{i=1}^3 \epsilon_{ijk} \epsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{lk}, \tag{5}$$

$$\hat{p}_k \hat{x}_j = \hat{x}_j \hat{p}_k - i\hbar \delta_{jk}. \quad (6)$$

Now we compute $\hat{\mathbf{L}}^2$:

$$\begin{aligned} \hat{\mathbf{L}}^2 &= (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \\ &= \sum_i (\hat{\mathbf{r}} \times \hat{\mathbf{p}})_i (\hat{\mathbf{r}} \times \hat{\mathbf{p}})_i \\ &= \sum_i \left(\sum_{j,k} \epsilon_{ijk} \hat{x}_j \hat{p}_k \right) \left(\sum_{\ell,m} \epsilon_{i\ell m} \hat{x}_\ell \hat{p}_m \right) \\ &= \sum_{j,k} \sum_{\ell,m} \sum_i \epsilon_{ijk} \epsilon_{i\ell m} \hat{x}_j \hat{p}_k \hat{x}_\ell \hat{p}_m \\ &= \sum_{j,k} \sum_{\ell,m} [\delta_{j\ell} \delta_{km} - \delta_{jm} \delta_{\ell k}] \hat{x}_j \hat{p}_k \hat{x}_\ell \hat{p}_m \\ &= \sum_{j,k} [\hat{x}_j \hat{p}_k \hat{x}_j \hat{p}_k - \hat{x}_j \hat{p}_k \hat{x}_k \hat{p}_j]. \end{aligned}$$

Looking at the last line, we see the possibility of some dot products, like $\sum_k A_k B_k = \mathbf{A} \cdot \mathbf{B}$. However, we need to be careful when switching the order of some operators. So, we need to insert expressions like (6).

$$\begin{aligned} \hat{\mathbf{L}}^2 &= \sum_{j,k} [\hat{x}_j \hat{p}_k \hat{x}_j \hat{p}_k - \hat{x}_j \hat{p}_k \hat{x}_k \hat{p}_j] \\ &= \sum_{j,k} [\hat{x}_j (\hat{x}_j \hat{p}_k - i\hbar \delta_{jk}) \hat{p}_k - \hat{x}_j \hat{p}_k (\hat{p}_j \hat{x}_k + i\hbar \delta_{jk})] \\ &= \sum_{j,k} [\hat{x}_j \hat{x}_j \hat{p}_k \hat{p}_k - i\hbar \delta_{jk} \hat{x}_j \hat{p}_k - \hat{x}_j \hat{p}_j \hat{p}_k \hat{x}_k - i\hbar \delta_{jk} \hat{x}_j \hat{p}_k] \\ &= \sum_{j,k} [\hat{x}_j \hat{x}_j \hat{p}_k \hat{p}_k - i\hbar \delta_{jk} \hat{x}_j \hat{p}_k - \hat{x}_j \hat{p}_j (\hat{x}_k \hat{p}_k - i\hbar \delta_{kk}) - i\hbar \delta_{jk} \hat{x}_j \hat{p}_k] \\ &= \sum_j [\hat{x}_j \hat{x}_j \hat{p}^2 - i\hbar \hat{x}_j \hat{p}_j - \hat{x}_j \hat{p}_j (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - 3i\hbar) - i\hbar \hat{x}_j \hat{p}_j] \\ &= \hat{r}^2 \hat{p}^2 - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + 3i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \\ &= \hat{r}^2 \hat{p}^2 - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}. \end{aligned} \quad (7)$$

3 Rewriting the Hamiltonian

We begin with the state $\hat{\mathbf{L}}^2|\psi\rangle$. Projecting onto the position basis,

$$\begin{aligned} \langle \mathbf{r} | \hat{\mathbf{L}}^2 | \psi \rangle &= \langle \mathbf{r} | [\hat{r}^2 \hat{p}^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2] | \psi \rangle \\ &= r^2 \langle \mathbf{r} | \hat{p}^2 | \psi \rangle + i\hbar \mathbf{r} \cdot \frac{\hbar}{i} \nabla \langle \mathbf{r} | \psi \rangle + \hbar^2 (\mathbf{r} \cdot \nabla)^2 \langle \mathbf{r} | \psi \rangle \\ r^2 \langle \mathbf{r} | \hat{p}^2 | \psi \rangle &= \langle \mathbf{r} | \hat{\mathbf{L}}^2 | \psi \rangle - \hbar^2 r \frac{\partial}{\partial r} \langle \mathbf{r} | \psi \rangle - \hbar^2 r \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) \langle \mathbf{r} | \psi \rangle \end{aligned}$$

$$\langle \mathbf{r} | \hat{H} | \psi \rangle = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \langle \mathbf{r} | \psi \rangle + \frac{\langle \mathbf{r} | \hat{\mathbf{L}}^2 | \psi \rangle}{2\mu r^2} + V(r) \langle \mathbf{r} | \psi \rangle = E \langle \mathbf{r} | \psi \rangle \quad (8)$$

Now, we make use of the eigenvalue problem for $\hat{\mathbf{L}}^2$. Namely,

$$\hat{\mathbf{L}}^2 |E, \ell, m\rangle = \ell(\ell + 1)\hbar^2 |E, \ell, m\rangle.$$

So, with $|\psi\rangle = |E, \ell, m\rangle$, we have

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2} + V(r) \right] \langle \mathbf{r} | E, \ell, m \rangle = E \langle \mathbf{r} | E, \ell, m \rangle$$

Letting $\langle \mathbf{r} | E, \ell, m \rangle = R(r)Y(\theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$,

$$\begin{aligned} -\frac{\hbar^2}{2\mu} \left(\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right) + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2} R + V(r)R &= ER, \\ \hat{\mathbf{L}}^2 Y &= \ell(\ell + 1)\hbar^2 Y \\ \hat{L}_z Y &= m\hbar Y. \end{aligned} \quad (9)$$