

3.3 Orbital angular momentum
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1. Orbital angular momentum

We discuss the connection between the differential operator \mathbf{L}^2 ($\hat{\mathbf{L}}$ is the orbital angular momentum in quantum mechanics) and the angular part of the Laplacian in the spherical coordinates.

Here we use the identity (epsilon-delta relation)

$$\sum_k \varepsilon_{ijk} \varepsilon_{lmk} = \delta_{i,l} \delta_{j,m} - \delta_{i,m} \delta_{j,l}.$$

Together with the commutation relations of the position and momentum operators and expression for the orbital angular momentum operators to verify that $\hat{\mathbf{L}}^2$ operator is expressed by

$$\hat{\mathbf{L}}^2 = (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) = \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}.$$

((Proof))

The proof is straightforward. To this end, we use the epsilon-delta relation (the proof is given later). Thus, we get

$$\begin{aligned} \hat{\mathbf{L}}^2 &= (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \\ &= \sum_{i,j,k,l,m} \varepsilon_{ijk} \varepsilon_{lmk} \hat{x}_i \hat{p}_j \hat{x}_l \hat{p}_m \\ &= \sum_{i,j,l,m} (\delta_{i,l} \delta_{j,m} - \delta_{i,m} \delta_{j,l}) \hat{x}_i \hat{p}_j \hat{x}_l \hat{p}_m \\ &= \sum_{i,j,l,m} [\delta_{i,l} \delta_{j,m} \hat{x}_i \hat{p}_j \hat{x}_l \hat{p}_m - \delta_{i,m} \delta_{j,l} \hat{x}_i \hat{p}_j \hat{x}_l \hat{p}_m] \\ &= \sum_{i,j,l,m} [\delta_{i,l} \delta_{j,m} \hat{x}_i (\hat{x}_l \hat{p}_j - i\hbar \delta_{j,l}) \hat{p}_m - \delta_{i,m} \delta_{j,l} \hat{x}_i \hat{p}_j (\hat{p}_m \hat{x}_l + i\hbar \delta_{l,m})] \end{aligned}$$

or

$$\begin{aligned}
\hat{\mathbf{L}}^2 &= (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \\
&= \sum_{i,j,l,m} [\delta_{i,l} \delta_{j,m} \hat{x}_i (\hat{x}_l \hat{p}_j - i\hbar \delta_{j,l}) \hat{p}_m - \delta_{i,m} \delta_{j,l} (\hat{x}_i \hat{p}_m \hat{p}_j \hat{x}_l + i\hbar \delta_{l,m} \hat{x}_i \hat{p}_j)] \\
&= \sum_{i,j,l,m} [\delta_{i,l} \delta_{j,m} (\hat{x}_i \hat{x}_l \hat{p}_j \hat{p}_m - i\hbar \delta_{j,l} \hat{x}_i \hat{p}_m) - \delta_{i,m} \delta_{j,l} (\hat{x}_i \hat{p}_m \hat{p}_j \hat{x}_l + i\hbar \delta_{l,m} \hat{x}_i \hat{p}_j)] \\
&= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - \sum_{i,j,l,m} \delta_{i,m} \delta_{j,l} [\hat{x}_i \hat{p}_m (\hat{x}_l \hat{p}_j - i\hbar \delta_{l,j}) + i\hbar \delta_{l,m} \hat{x}_i \hat{p}_j] \\
&= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - \sum_{i,j,l,m} \delta_{i,m} \delta_{j,l} (\hat{x}_i \hat{p}_m \hat{x}_l \hat{p}_j - i\hbar \delta_{l,j} \hat{x}_i \hat{p}_m + i\hbar \delta_{l,m} \hat{x}_i \hat{p}_j) \\
&= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + 3i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \\
&= \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2
\end{aligned}$$

or

$$\hat{\mathbf{L}}^2 = (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) = \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2$$

Note that

$$\begin{aligned}
\sum_{i,j,l,m} \delta_{i,l} \delta_{j,m} \hat{x}_i \hat{x}_l \hat{p}_j \hat{p}_m &= \sum_{i,j} \hat{x}_i^2 \hat{x}_i \hat{p}_j^2 = \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2, \\
\sum_{i,j,l,m} \delta_{i,l} \delta_{j,m} \delta_{j,l} \hat{x}_i \hat{p}_m &= \sum_{i,j,l} \delta_{i,l} \delta_{j,l} \hat{x}_i \hat{p}_j = \sum_{i,l} \delta_{i,l} \hat{x}_i \hat{p}_l = \sum_i \hat{x}_i \hat{p}_i = \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \\
\sum_{i,j,l,m} \delta_{i,m} \delta_{j,l} \delta_{l,j} \hat{x}_i \hat{p}_m &= \left(\sum_{i,m} \delta_{i,m} \hat{x}_i \hat{p}_m \right) \sum_{j,l} \delta_{j,l} \delta_{l,j} = 3 \sum_i \hat{x}_i \hat{p}_i = 3(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}), \\
\sum_{j,l} \delta_{j,l} \delta_{l,j} &= \sum_{j,l} \langle j|l \rangle \langle l|j \rangle = \sum_j \langle j|j \rangle = 3
\end{aligned}$$

2. $\varepsilon - \delta$ relation

In the above proof we use the relation given by

$$\sum_k \varepsilon_{ijk} \varepsilon_{lmk} = \delta_{i,l} \delta_{j,m} - \delta_{i,m} \delta_{j,l}$$

((Proof))

We use the formula in vector analysis (Cartesian coordinates, 3D)

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

where

$$(\mathbf{A} \times \mathbf{B})_k = \sum_{i,j} \varepsilon_{ijk} A_i B_j,$$

$$(\mathbf{C} \times \mathbf{D})_k = \sum_{l,m} \varepsilon_{lmk} C_l D_m.$$

This we have

$$(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{C} \times \mathbf{D}) = \sum_{i,j,k,l,m} \varepsilon_{ijk} \varepsilon_{lmk} A_i B_j C_l D_m,$$

$$\begin{aligned} (\mathbf{A} \cdot \mathbf{C}) \cdot (\mathbf{B} \cdot \mathbf{D}) &= \sum_{i,l} \delta_{i,l} A_i C_l \sum_{j,m} \delta_{j,m} B_j D_m \\ &= \sum_{i,j,l,m} \delta_{i,l} \delta_{j,m} A_i B_j C_l D_m \end{aligned}$$

$$\begin{aligned} (\mathbf{A} \cdot \mathbf{D}) \cdot (\mathbf{B} \cdot \mathbf{C}) &= \sum_{i,m} \delta_{i,m} A_i D_m \sum_{j,l} \delta_{j,l} B_j C_l \\ &= \sum_{i,j,l,m} \delta_{i,m} \delta_{j,l} A_i B_j C_l D_m \end{aligned}$$

So that, we get the epsilon-delta relation

$$\sum_k \varepsilon_{ijk} \varepsilon_{lmk} = \delta_{i,l} \delta_{j,m} - \delta_{i,m} \delta_{j,l}.$$

3. The expression: $\mathbf{p}^2 = p_r^2 + \frac{\mathbf{L}^2}{r^2}$

We note that

$$\hat{\mathbf{L}}^2 = (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) = \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 + i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2$$

In the $|\mathbf{r}\rangle$ representation, we get the following expressions,

$$\langle \mathbf{r} | \hat{\mathbf{L}}^2 | \psi \rangle = \mathbf{L}^2 \langle \mathbf{r} | \psi \rangle = \mathbf{L}^2 \psi(\mathbf{r})$$

where \mathbf{L}^2 is the differential operator.

$$\begin{aligned}\langle \mathbf{r} | \hat{\mathbf{r}}^2 \hat{\mathbf{p}}^2 | \psi \rangle &= -\hbar^2 \mathbf{r}^2 \nabla^2 \langle \mathbf{r} | \psi \rangle \\ &= -\hbar^2 \mathbf{r}^2 \nabla^2 \psi(\mathbf{r})\end{aligned}$$

where $\mathbf{p} = \frac{\hbar}{i} \nabla$ is the differential operator of the momentum $\hat{\mathbf{p}}$ of quantum mechanics.

$$\begin{aligned}\langle \mathbf{r} | i\hbar \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} | \psi \rangle &= i\hbar \mathbf{r} \cdot \frac{\hbar}{i} \nabla \langle \mathbf{r} | \psi \rangle \\ &= \hbar^2 (\mathbf{r} \cdot \nabla) \langle \mathbf{r} | \psi \rangle \\ &= \hbar^2 r \frac{\partial}{\partial r} \psi(\mathbf{r})\end{aligned}$$

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

Thus, we have

$$\mathbf{L}^2 \psi(\mathbf{r}) = -\hbar^2 r^2 \nabla^2 \psi(\mathbf{r}) + \hbar^2 (r^2 \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r}) \psi(\mathbf{r})$$

or

$$\begin{aligned}\frac{\mathbf{p}^2}{2\mu} &= -\frac{\hbar^2}{2\mu} \nabla^2 \psi(\mathbf{r}) \\ &= -\frac{\hbar^2}{2\mu} (\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r}) \psi(\mathbf{r}) + \frac{1}{2\mu r^2} \mathbf{L}^2 \psi(\mathbf{r}) \\ &= \frac{1}{2\mu} (p_r^2 + \frac{1}{r^2} \mathbf{L}^2) \psi(\mathbf{r})\end{aligned}$$

where μ is the mass of particle and p_r is the radial linear momentum.

$$\begin{aligned}
p_r^2 \psi(\mathbf{r}) &= \frac{\hbar}{ir} \frac{\partial}{\partial r} \left(r \frac{\hbar}{ir} \frac{\partial}{\partial r} r \right) \psi(\mathbf{r}) \\
&= -\frac{\hbar^2}{r} \frac{\partial^2}{\partial r^2} [r \psi(\mathbf{r})] \\
&= -\frac{\hbar^2}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} \psi(\mathbf{r}) + \psi(\mathbf{r}) \right] \\
&= -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi(\mathbf{r})
\end{aligned}$$

4. Proof using the Mathematica

Using the Mathematica (the differential operator in the spherical coordinate) we show that

$$\mathbf{p}^2 = -\hbar^2 \nabla^2 = p_r^2 + \frac{1}{r^2} \mathbf{L}^2$$

or

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\mathbf{L}^2}{\hbar^2 r^2}$$

with $p_r = \frac{\hbar}{ir} \frac{\partial}{\partial r} r$

((Mathematica))

Orbital angular momentum in the spherical coordinates

```
Clear["Global`"];
ux = {Sin[θ] Cos[φ], Cos[θ] Cos[φ], -Sin[φ]};
uy = {Sin[θ] Sin[φ], Cos[θ] Sin[φ], Cos[φ]};
uz = {Cos[θ], -Sin[θ], 0};
ur = {1, 0, 0};
Lap := Laplacian[#, {r, θ, φ}, "Spherical"] &;
Gra := Grad[#, {r, θ, φ}, "Spherical"] &;
Diva := Div[#, {r, θ, φ}, "Spherical"] &;
Curla := Curl[#, {r, θ, φ}, "Spherical"] &;
L := (-i ħ (Cross[ur r, Gra[#]]) &) // Simplify;
Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
LP := (Lx[#] + i Ly[#]) & // Simplify;
LM = (Lx[#] - i Ly[#]) & // Simplify;
prq :=  $\left( \frac{-i \hbar}{2} \text{ur} \cdot \text{Gra}[\#] + \frac{-i \hbar}{2} \text{Diva}[\# \text{ur}] \right) \&;$ 
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$$\text{prq} := \left(\frac{-i \hbar}{2} \text{ur} \cdot \text{Gra}[\#] + \frac{-i \hbar}{2} \text{Diva}[\# \text{ur}] \right) \&;$$

eq1=prq²ψ(r,θ,φ); prq is the radial linear momentum

$$\text{eq1} = \text{Nest}[\text{prq}, \psi[r, \theta, \phi], 2] // \text{FullSimplify}$$

$$-\frac{\hbar^2 (2 \psi^{(1,\theta,\theta)}[r, \theta, \phi] + r \psi^{(2,\theta,\theta)}[r, \theta, \phi])}{r}$$

$$\text{eq2} = \frac{1}{r^2} L^2 \psi(r, \theta, \phi)$$

$$\text{eq2} =$$

$$\frac{1}{r^2} (\text{Nest}[\text{Lx}, \psi[r, \theta, \phi], 2] + \text{Nest}[\text{Ly}, \psi[r, \theta, \phi], 2] + \text{Nest}[\text{Lz}, \psi[r, \theta, \phi], 2]) // \text{Simplify}$$

$$-\frac{1}{r^2} \hbar^2 (\text{Csc}[\theta]^2 \psi^{(\theta,\theta,2)}[r, \theta, \phi] + \text{Cot}[\theta] \psi^{(\theta,1,\theta)}[r, \theta, \phi] + \psi^{(\theta,2,\theta)}[r, \theta, \phi])$$

$$\text{eq3} = -\hbar^2 \Delta \psi(r, \theta, \phi)$$

$$\text{eq3} = -\hbar^2 \text{Lap}[\psi[r, \theta, \phi]] // \text{Simplify}$$

$$-\frac{1}{r^2} \hbar^2 (\text{Csc}[\theta]^2 \psi^{(\theta,\theta,2)}[r, \theta, \phi] + \text{Cot}[\theta] \psi^{(\theta,1,\theta)}[r, \theta, \phi] + \psi^{(\theta,2,\theta)}[r, \theta, \phi] + 2 r \psi^{(1,\theta,\theta)}[r, \theta, \phi] + r^2 \psi^{(2,\theta,\theta)}[r, \theta, \phi])$$

$$\text{eq1} = \text{eq2} - \text{eq3} = 0; \text{ Proof of } p^2 = \text{prq}^2 + L^2/r^2$$

$$\text{eq1} + \text{eq2} - \text{eq3} // \text{FullSimplify}$$

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