MOMENTO ANGULAR ORBITAL EM COORDENADAS ESFÉRICAS

Notas de aula de Mecânica Quântica I

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A transformação de coordenadas cartezianas para esféricas é dada por

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned} \tag{1}$$

e a transformação inversa é

$$\begin{aligned} r &= \sqrt{x^2 + y^2 + z^2} \\ \tan\theta &= \sqrt{x^2 + y^2}/z \\ \tan\phi &= y/x. \end{aligned} \tag{2}$$

Em coordenadas cartezianas os operadores de momento angular são dados por:

$$\begin{aligned} L_x &= -i\hbar(y\partial/\partial z - z\partial/\partial y) \\ L_y &= -i\hbar(z\partial/\partial x - x\partial/\partial z) \\ L_z &= -i\hbar(x\partial/\partial y - y\partial/\partial x). \end{aligned} \tag{3}$$

Para ilustrar o cálculo desses operadores em coordenadas esféricas faremos o caso L_z. As derivadas $\partial/\partial x$ e $\partial/\partial y$ são escritas como:

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}$$

e

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}.$$

As derivadas das coordenadas esféricas em relação às cartezianas podem ser obtidas derivando implicitamente ambos os lados das equações 2 em relação a x, y ou z:

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin\theta\cos\phi$$

$$\frac{1}{\cos^2\theta}\frac{\partial \theta}{\partial x} = \frac{x}{\sqrt{x^2+y^2}z} = \frac{\cos\phi}{r\cos\theta} \qquad ou \qquad \frac{\partial \theta}{\partial x} = \frac{\cos\theta\cos\phi}{r}$$

$$\frac{1}{\cos^2\phi}\frac{\partial\phi}{\partial x} = -\frac{y}{x^2} = -\frac{\sin\phi}{r\sin\theta\cos^2\phi} \qquad ou \qquad \frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}.$$

Fazendo o mesmo processo com as derivadas em relação a y obtemos

$$\frac{\partial r}{\partial y} = \sin\theta\sin\phi$$

$$\frac{\partial\theta}{\partial y} = \frac{\cos\theta\sin\phi}{r}$$

$$\frac{\partial\phi}{\partial y} = \frac{\cos\phi}{r\sin\theta}.$$

Voltando à equação (3) para L_z temos:

$$x\frac{\partial}{\partial y} = r\sin\theta\cos\phi\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \tag{4}$$

e

$$y\frac{\partial}{\partial x} = r\sin\theta\sin\phi\left(\sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right). \tag{5}$$

Subtraindo (5) de (4) e multiplicando por $-i\hbar$ obtemos L_z. Os dois primeiros termos de cada equação se cancelam e os últimos termos se somam:

$$L_z = -i\hbar(\cos^2\phi\frac{\partial}{\partial\phi} + \sin^2\phi\frac{\partial}{\partial\phi}) = -i\hbar\frac{\partial}{\partial\phi}. \tag{6}$$

O cálculo de L_x e L_y é completamente análogo e resulta em

$$L_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}) \tag{7}$$

e

$$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}). \tag{8}$$

Os operadores L_+ e L_- também podem ser calculados:

$$L_+ = \hbar e^{i\phi}(\frac{\partial}{\partial\theta} + \frac{i}{\tan\theta}\frac{\partial}{\partial\phi}) \tag{9}$$

$$L_- = (L_+)^\dagger = \hbar e^{-i\phi}(-\frac{\partial}{\partial\theta} + \frac{i}{\tan\theta}\frac{\partial}{\partial\phi}). \tag{10}$$

Fica como exercício provar essas equações, principalmente a última relação para L_-.

Finalmente calculamos L^2. Começamos com L_x^2:

$$
\begin{aligned}
L_x^2 &= -\hbar^2(\sin\phi\frac{\partial}{\partial\theta}+\frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi})(\sin\phi\frac{\partial}{\partial\theta}+\frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi})\\
&= -\hbar^2\left(\sin^2\phi\frac{\partial^2}{\partial\theta^2}-\frac{\sin\phi\cos\phi}{\tan^2\theta\cos^2\theta}\frac{\partial}{\partial\phi}+2\frac{\sin\phi\cos\phi}{\tan\theta}\frac{\partial^2}{\partial\phi\partial\theta}+\frac{\cos^2\phi}{\tan\theta}\frac{\partial}{\partial\theta}-\right.\\
&\left.\frac{\sin\phi\cos\phi}{\tan^2\theta}\frac{\partial}{\partial\phi}+\frac{\cos^2\phi}{\tan^2\theta}\frac{\partial^2}{\partial\phi^2}\right).
\end{aligned}
$$

Da mesma forma obtemos:

$$
\begin{aligned}
L_y^2 &= -\hbar^2(-\cos\phi\frac{\partial}{\partial\theta}+\frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi})(-\cos\phi\frac{\partial}{\partial\theta}+\frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi})\\
&= -\hbar^2\left(\cos^2\phi\frac{\partial^2}{\partial\theta^2}+\frac{\sin\phi\cos\phi}{\tan^2\theta\cos^2\theta}\frac{\partial}{\partial\phi}-2\frac{\sin\phi\cos\phi}{\tan\theta}\frac{\partial^2}{\partial\phi\partial\theta}+\frac{\sin^2\phi}{\tan\theta}\frac{\partial}{\partial\theta}+\right.\\
&\left.\frac{\sin\phi\cos\phi}{\tan^2\theta}\frac{\partial}{\partial\phi}+\frac{\sin^2\phi}{\tan^2\theta}\frac{\partial^2}{\partial\phi^2}\right)
\end{aligned}
$$

e

$$L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2}.$$

Somando tudo obtemos finalmente

$$L^2 = -\hbar^2\left(-\frac{\partial^2}{\partial\theta^2}+\frac{1}{\tan\theta}\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$