極座標表示の角運動量演算子とラプラシアン

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カーテシアン座標と極座標表示の間には以下の関係が成り立つ.

$$\begin{pmatrix} x & y & z \end{pmatrix} = \begin{pmatrix} rsin\theta cos\phi & rsin\theta sin\phi & rcos\theta \end{pmatrix} \tag{1}$$

$$\begin{pmatrix} dx & dy & dz \end{pmatrix} = \begin{pmatrix} dr & d\theta & d\phi \end{pmatrix} \begin{pmatrix} sin\theta cos\phi & sin\theta sin\phi & cos\theta \\ rcos\theta cos\phi & rcos\theta sin\phi & -rsin\theta \\ -rsin\theta sin\phi & rsin\theta cos\phi & 0 \end{pmatrix} \tag{2}$$

$$\begin{aligned} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} &= \begin{pmatrix} sin\theta cos\phi & sin\theta sin\phi & cos\theta \\ rcos\theta cos\phi & rcos\theta sin\phi & -rsin\theta \\ -rsin\theta sin\phi & rsin\theta cos\phi & 0 \end{pmatrix}^{-1} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \\ &= \begin{pmatrix} sin\theta cos\phi & \frac{cos\theta cos\phi}{r} & -\frac{sin\phi}{rsin\theta} \\ sin\theta sin\phi & \frac{cos\theta sin\phi}{r} & \frac{cos\phi}{rsin\theta} \\ cos\theta & \frac{-sin\theta}{r} & 0 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \end{aligned} \tag{3}$$

以上から、角運動量演算子は,

$$\begin{aligned} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} &= -i\hbar \begin{pmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{pmatrix} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} \\ &= -i\hbar \begin{pmatrix} 0 & -rcos\theta & rsin\theta sin\phi \\ rcos\theta & 0 & -rsin\theta cos\phi \\ -rsin\theta sin\phi & rsin\theta cos\phi & 0 \end{pmatrix} \begin{pmatrix} sin\theta cos\phi & \frac{cos\theta cos\phi}{r} & -\frac{sin\phi}{rsin\theta} \\ sin\theta sin\phi & \frac{cos\theta sin\phi}{r} & \frac{cos\phi}{rsin\theta} \\ cos\theta & \frac{-sin\theta}{r} & 0 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \\ &= -i\hbar \begin{pmatrix} 0 & -sin\phi & -\frac{cos\phi}{tan\theta} \\ 0 & cos\phi & -\frac{sin\phi}{tan\theta} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix}. \end{aligned} \tag{4}$$

昇降演算子は,

$$\begin{aligned} \begin{pmatrix} L_+ \\ L_- \end{pmatrix} &= \begin{pmatrix} 1 & i & 0 \\ 1 & -i & 0 \end{pmatrix} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} \\ &= \hbar \begin{pmatrix} -i & 1 & 0 \\ -i & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -sin\phi & -\frac{cos\phi}{tan\theta} \\ 0 & cos\phi & -\frac{sin\phi}{tan\theta} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \\ &= \hbar \begin{pmatrix} 0 & e^{i\phi} & \frac{ie^{i\phi}}{tan\theta} \\ 0 & -e^{-i\phi} & \frac{ie^{-i\phi}}{tan\theta} \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix}. \end{aligned} \tag{5}$$

したがって角運動量演算子の自乗は, $\partial_\theta = \frac{\partial(cos\theta)}{\partial\theta}\frac{\partial}{\partial(cos\theta)} = -sin\theta\frac{\partial}{\partial(cos\theta)}$ に注意すると,

$$L^2 = -\hbar^2 \begin{pmatrix} L_x & L_y & L_z \end{pmatrix} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix}$$

$$
\begin{aligned}
&= -\hbar^2 \begin{pmatrix} -sin\phi\partial_\theta - \frac{cos\phi}{tan\theta}\partial_\phi, & cos\phi\partial_\theta - \frac{sin\phi}{tan\theta}\partial_\phi, & \partial_\phi \end{pmatrix} \begin{pmatrix} 0 & -sin\phi & -\frac{cos\phi}{tan\theta} \\ 0 & cos\phi & -\frac{sin\phi}{tan\theta} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \\
&= -\hbar^2[\partial_\theta^2 + \frac{1}{tan^2\theta}\partial_\phi^2 + \partial_\phi^2] - \hbar^2 \begin{pmatrix} 0 & \frac{1}{tan\theta} & 0 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} \\
&= -\hbar^2[\frac{1}{sin\theta}\partial_\theta(sin\theta\partial_\theta) + \frac{1}{sin^2\theta}\partial_\phi^2] \\
&= -\hbar^2[\frac{\partial}{\partial(cos\theta)}\frac{1}{1-cos^2\theta}\frac{\partial}{\partial(cos\theta)} + \frac{1}{1-cos^2\theta}\partial_\phi^2]. \qquad (6)
\end{aligned}
$$

ここで関係 $\nabla^2 = -p_r^2 - \frac{L^2}{\hbar^2 r^2}$ を思い出すと (ノート: 水素原子の Schrodinger 方程式を参照), ラプラシアンは極座標表示で

$$
\nabla^2 = (\frac{1}{r}\partial_r r)^2 + \frac{1}{r^2}[\frac{1}{sin\theta}\partial_\theta(sin\theta\partial_\theta) + \frac{1}{sin^2\theta}\partial_\phi^2] \qquad (7)
$$