全角運動量演算子 L^2

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1. 概要

全角運動量演算子 L^2 をシュッと表す。

2. 計算

$$L^2\psi = \left(x\frac{\hbar}{i}\partial_y - y\frac{\hbar}{i}\partial_x\right)\left(x\frac{\hbar}{i}\partial_y - y\frac{\hbar}{i}\partial_x\right)\psi + \dots$$

$$= x\frac{\hbar}{i}\partial_y x\frac{\hbar}{i}\partial_y\psi - x\frac{\hbar}{i}\partial_y y\frac{\hbar}{i}\partial_x\psi - y\frac{\hbar}{i}\partial_x x\frac{\hbar}{i}\partial_y\psi + y\frac{\hbar}{i}\partial_x y\frac{\hbar}{i}\partial_x\psi + \dots$$

$$= -\hbar^2\left(x\partial_y x\partial_y\psi - x\partial_y y\partial_x\psi - y\partial_x x\partial_y\psi + y\partial_x y\partial_x\psi + \dots\right)$$

$$= -\hbar^2\left(x^2\partial_y^2\psi + y^2\partial_x^2\psi - x\partial_y\left(y\partial_x\psi\right) - y\partial_x\left(x\partial_y\psi\right) + \dots\right)$$

これの前半 2 項 ×3 は

$$-\hbar^2\left(x^2\partial_y^2\psi + y^2\partial_x^2\psi + y^2\partial_z^2\psi + z^2\partial_y^2\psi + z^2\partial_x^2\psi + x^2\partial_z^2\psi\right)$$

$$= \hbar^2\left(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\right) - \hbar^2\left(x^2 + y^2 + z^2\right)\left(\partial_x^2\psi + \partial_y^2\psi + \partial_z^2\psi\right)$$

$$= \hbar^2\left(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\right) - \hbar^2 \mid \vec{x} \mid^2 \nabla^2\psi$$

であり、これの後半 2 項は

$$\hbar^2\left(x\partial_y\left(y\partial_x\psi\right) + y\partial_x\left(x\partial_y\psi\right) + \dots\right) = \hbar^2\left(x\partial_x\psi + xy\partial_y\partial_x\psi + y\partial_y\psi + yx\partial_x\partial_y\psi + \dots\right)$$

$$= \hbar^2\Big(x\,\partial_x\psi + y\partial_y\psi + 2xy\partial_y\partial_x\psi + \dots\Big)$$

$$= \hbar^2\Big(2x\,\partial_x\psi + 2y\partial_y\psi + 2z\partial_z\psi + 2xy\,\partial_x\partial_y\psi + 2yz\,\partial_y\partial_z\psi + 2zx\,\partial_z\partial_x\psi\Big)$$

$$= 2\hbar^2\Big(x\,\partial_x\psi + y\partial_y\psi + z\,\partial_z\psi\Big) - \hbar^2\Big(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\Big)$$

$$+\,\hbar^2\Big(2xy\,\partial_x\partial_y\psi + 2yz\,\partial_y\partial_z\psi + 2zx\,\partial_z\partial_x\psi + x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\Big)$$

$$= 2\hbar^2\vec{x}\cdot\nabla\psi - \hbar^2\Big(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\Big)$$

$$+\,\hbar^2x\Big(x\,\partial_x + y\partial_y + z\,\partial_z\Big)\partial_x\psi + \hbar^2y\Big(x\,\partial_x + y\partial_y + z\,\partial_z\Big)\partial_y\psi + \hbar^2z\Big(x\,\partial_x + y\partial_y + z\,\partial_z\Big)\partial_z\psi$$

$$= 2\hbar^2\vec{x}\cdot\nabla\psi - \hbar^2\Big(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\Big) + \hbar^2x(\vec{x}\cdot\nabla)\partial_x\psi + \hbar^2y(\vec{x}\cdot\nabla)\partial_y\psi + \hbar^2z(\vec{x}\cdot\nabla)\partial_z\psi$$

$$= 2\hbar^2\vec{x}\cdot\nabla\psi - \hbar^2\Big(x^2\partial_x^2\psi + y^2\partial_y^2\psi + z^2\partial_z^2\psi\Big) + \hbar^2\vec{x}\cdot\Big((\vec{x}\cdot\nabla)\nabla\psi\Big)$$

したがって

$$L^2\psi = -\hbar^2\,|\,\vec{x}\,|^2\,\nabla^2\psi + 2\hbar^2\vec{x}\cdot\nabla\psi + \hbar^2\vec{x}\cdot\Big((\vec{x}\cdot\nabla)\nabla\psi\Big)$$

3. 極座標

$$L^2\psi = -\hbar^2\,|\,\vec{x}\,|^2\,\nabla^2\psi + 2\hbar^2\vec{x}\cdot\nabla\psi + \hbar^2\vec{x}\cdot\Big((\vec{x}\cdot\nabla)\nabla\psi\Big)$$

に

$$\vec{x} = r\vec{e}_r$$

$$r^2\nabla^2\psi = \partial_r\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\partial_\varphi^2\psi$$

$$\nabla\psi = \vec{e}_r\frac{\partial\psi}{\partial r} + \frac{1}{r}\vec{e}_\theta\frac{\partial\psi}{\partial\theta} + \frac{1}{r\sin\theta}\vec{e}_\varphi\frac{\partial\psi}{\partial\varphi}$$

$$\vec{x}\cdot\nabla = r\,\partial_r$$

を代入すると

$$L^2\psi = -\hbar^2\left(\partial_r\left(r^2\partial_r\psi\right) + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\psi\right) + \frac{1}{\sin^2\theta}\partial_\varphi^2\psi\right)$$

$$+\, 2\hbar^2 r\,\partial_r\psi + \hbar^2\vec{x}\cdot\left(r\,\partial_r\right)\left(\vec{e}_r\frac{\partial\psi}{\partial r} + \frac{1}{r}\vec{e}_\theta\frac{\partial\psi}{\partial\theta} + \frac{1}{r\sin\theta}\vec{e}_\varphi\frac{\partial\psi}{\partial\varphi}\right)$$

$$= -\hbar^2\left(\partial_r\left(r^2\partial_r\psi\right) + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\psi\right) + \frac{1}{\sin^2\theta}\partial_\varphi^2\psi\right) + 2\hbar^2 r\,\partial_r\psi + \hbar^2 r\left(r\,\partial_r\right)\frac{\partial\psi}{\partial r}$$

$$= -\hbar^2\left(\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\psi\right) + \frac{1}{\sin^2\theta}\partial_\varphi^2\psi\right) - \hbar^2\partial_r\left(r^2\partial_r\psi\right) + 2\hbar^2 r\,\partial_r\psi + \hbar^2 r^2\frac{\partial^2\psi}{\partial r^2}$$

$$= -\hbar^2\left(\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\psi\right) + \frac{1}{\sin^2\theta}\partial_\varphi^2\psi\right)$$

となって、ラプラシアンの θ・ φ 絡みだけを残したやつが全角運動量演算子になることにもそこそこ納得がいきそうな気がしそうである。