東北大天文学専攻H20年、物理問題[4]

update: 2017 Aug. 11, author: Sho K. NAKAMURA

[1] 角運動量演算子の z 成分

$$L_z = xp_y - yp_x = i\hbar x\frac{\partial}{\partial y} - i\hbar y\frac{\partial}{\partial x} \tag{1}$$

を極座標で表現する。

$$r^2 = x^2 + y^2 + z^2 \implies \frac{\partial r}{\partial x} = \frac{x}{r},\ \frac{\partial r}{\partial y} = \frac{y}{r} \tag{2}$$

$$\tan^2\theta = \frac{x^2+y^2}{z^2} \implies \frac{\partial \theta}{\partial x} = \frac{\cos^3\theta}{\sin\theta}\frac{x}{z^2},\ \frac{\partial \theta}{\partial y} = \frac{\cos^3\theta}{\sin\theta}\frac{y}{z^2} \tag{3}$$

$$\tan\varphi = \frac{x}{y} \implies \frac{\partial \varphi}{\partial x} = -\frac{y}{x^2}\cos^2\varphi,\ \frac{\partial \varphi}{\partial y} = \frac{1}{x}\cos^2\varphi \tag{4}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x}\frac{\partial}{\partial \varphi} = \frac{x}{r}\frac{\partial}{\partial r} + \frac{\cos^3\theta}{\sin\theta}\frac{x}{z^2}\frac{\partial}{\partial \theta} - \frac{y}{x^2}\cos^2\varphi\frac{\partial}{\partial \varphi} \tag{5}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial y}\frac{\partial}{\partial \varphi} = \frac{y}{r}\frac{\partial}{\partial r} + \frac{\cos^3\theta}{\sin\theta}\frac{y}{z^2}\frac{\partial}{\partial \theta} + \frac{1}{x}\cos^2\varphi\frac{\partial}{\partial \varphi} \tag{6}$$

$$\therefore (1),(5),(6) \implies L_z = i\hbar\cos^2\varphi\frac{\partial}{\partial \varphi} + i\hbar\frac{y^2}{x^2}\cos^2\varphi\frac{\partial}{\partial \varphi} = i\hbar\frac{\partial}{\partial \varphi} \tag{7}$$

[2] $\hat{H}$, $\hat{\mathbf{L}}^2$, $\hat{L}_z$ の交換関係

$$[\hat{H},\hat{\mathbf{L}}^2] = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right),\hat{\mathbf{L}}^2\right] + \frac{1}{2m}\left[\frac{\hat{\mathbf{L}}^2}{r^2},\hat{\mathbf{L}}^2\right] + \left[V(r),\hat{\mathbf{L}}^2\right] = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right),\hat{\mathbf{L}}^2\right] + \left[V(r),\hat{\mathbf{L}}^2\right] \tag{8}$$

$\hat{\mathbf{L}}^2$ は θ,φ に関する微分演算子より

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right),\hat{\mathbf{L}}^2\right] = 0,\ \left[V(r),\hat{\mathbf{L}}^2\right] = 0 \tag{9}$$

$$\therefore [\hat{H},\hat{\mathbf{L}}^2] = 0 \tag{10}$$

$$[\hat{\mathbf{L}}^2,\hat{L}_z] = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right),-i\hbar\frac{\partial}{\partial\varphi}\right] - \hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2},-i\hbar\frac{\partial}{\partial\varphi}\right] = 0 \tag{11}$$

$$[\hat{H},\hat{L}_z] = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right),\hat{L}_z\right] + \frac{1}{2m}\underbrace{\left[\frac{\hat{\mathbf{L}}^2}{r^2},\hat{L}_z\right]}_{(11)} + [V(r),L_z] = 0 \tag{12}$$

これらの交換関係より $\hat{\mathbf{L}}^2, \hat{L}_z$ は観測量である。かつ (11) より同時観測が可能な量である。

[3] 動径方向のシュレディンガー方程式

$\hat{\mathbf{L}}^2 Y_{\ell m}(\theta,\varphi) = \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\varphi)$ のとき、$\Psi = R_\ell(r) Y_{\ell m}(\theta,\varphi)$ と書くと

$$\begin{aligned} H\Psi &= -\frac{\hbar^2}{2m} Y_{\ell m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_\ell}{dr}\right) + \frac{R_\ell}{2mr^2}\hat{\mathbf{L}}^2 Y_{\ell m} + V(r)R_\ell Y_{\ell m} \\ &= -\frac{\hbar^2}{2m} Y_{\ell m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_\ell}{dr}\right) + \frac{R_\ell}{2mr^2}\hbar^2\ell(\ell+1)Y_{\ell m} + V(r)R_\ell Y_{\ell m} = ER_\ell Y_{\ell m} \end{aligned} \tag{13}$$

両辺を $-\hbar^2/2mY_{\ell m}$ で割ると

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_\ell}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R_\ell + \frac{2m}{\hbar^2}(E-V(r))R_\ell = 0 \tag{14}$$

[4] 動径成分の直交性

$$\begin{aligned} &\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{E\ell}}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R_{E\ell} + \frac{2m}{\hbar^2}(E-V(r))R_{E\ell} = 0 \\ &\Longrightarrow\ R_{E'\ell}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{E\ell}}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R_{E'\ell}R_{E\ell} + \frac{2m}{\hbar^2}(E-V(r))R_{E'\ell}R_{E\ell} = 0 \end{aligned} \tag{15}$$

$$\begin{aligned} &\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{E'\ell}}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R_{E'\ell} + \frac{2m}{\hbar^2}(E'-V(r))R_{E'\ell} = 0 \\ &\Longrightarrow R_{E\ell}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{E'\ell}}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R_{E\ell}R_{E'\ell} + \frac{2m}{\hbar^2}(E'-V(r))R_{E\ell}R_{E'\ell} = 0 \end{aligned} \tag{16}$$

$r^2\{(15)-(16)\}$ より

$$R_{E'\ell}\frac{d}{dr}\left(r^2\frac{dR_{E\ell}}{dr}\right) - R_{E\ell}\frac{d}{dr}\left(r^2\frac{dR_{E'\ell}}{dr}\right) + \frac{2m}{\hbar^2}(E-E')r^2R_{E\ell}R_{E'\ell} = 0 \tag{17}$$

両辺を r, 区間 $[0,\infty]$ で積分することを考える。条件より

$$\int_0^\infty R_{E'\ell}\frac{d}{dr}\left(r^2\frac{dR_{E\ell}}{dr}\right)dr = \left[r^2R_{E'\ell}\frac{dR_{E\ell}}{dr}\right]_0^\infty - \int_0^\infty r^2\frac{dR_{E'\ell}}{dr}\frac{dR_{E\ell}}{dr}dr = -\int_0^\infty r^2\frac{dR_{E'\ell}}{dr}\frac{dR_{E\ell}}{dr}dr \tag{18}$$

$$\int_0^\infty R_{E\ell}\frac{d}{dr}\left(r^2\frac{dR_{E'\ell}}{dr}\right)dr = \left[r^2R_{E\ell}\frac{dR_{E'\ell}}{dr}\right]_0^\infty - \int_0^\infty r^2\frac{dR_{E\ell}}{dr}\frac{dR_{E'\ell}}{dr}dr = -\int_0^\infty r^2\frac{dR_{E\ell}}{dr}\frac{dR_{E'\ell}}{dr}dr \tag{19}$$

より

$$\frac{2m}{\hbar^2}(E-E')\int_0^\infty r^2 R_{E\ell}R_{E'\ell}dr = 0 \implies \therefore \int_0^\infty r^2 R_{E\ell}R_{E'\ell}dr = 0 \ (E \neq E') \tag{20}$$

が成立する。

[5] シュレディンガー方程式の動径成分の性質