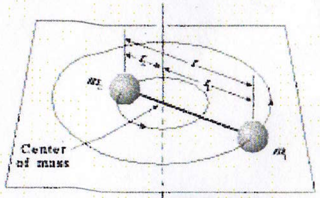
プリントNo.6

量子力学的剛体回転子



剛体回転子

角速度：$\varpi = 2\pi\nu = 2\pi / T$

速度：$v_1 = r_1\varpi, v_2 = r_2\varpi$

エネルギー：

$$K = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 = \frac{1}{2}\left(m_1 r_1^2 + m_2 r_2^2\right)\varpi^2 = \frac{1}{2}\mu r^2 \varpi^2$$

2体問題を1体問題として扱う
慣性モーメント：$\mu r^2 = m_1 r_1^2 + m_2 r_2^2$
(ただし$r = r_1 + r_2$)
角運動量：$l = \mu r^2 \varpi$

エネルギーを軌道角運動量で表す

$$K = \frac{l^2}{2\mu r^2}$$

$$\hat{l}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

ハミルトニアン：$\hat{H} = -\frac{\hbar^2}{2\mu r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$

固有値：$E_J = \frac{\hbar^2}{2\mu r^2}J(J+1)$

$$\hat{l}^2\phi = l(l+1)\hbar^2\phi$$

$r^2 = x^2 + y^2 + z^2$をx,y,zで偏微分すれば$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin\theta\cos\varphi, \frac{\partial r}{\partial y} = \frac{y}{r} = \sin\theta\sin\varphi, \frac{\partial r}{\partial z} = \frac{z}{r} = \cos\theta$

$\tan^2\theta = \frac{x^2+y^2}{z^2}$を$x,y,z$で偏微分すれば$\frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\varphi}{r}, \frac{\partial\theta}{\partial y} = \frac{\cos\theta\sin\varphi}{r}, \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}$

$\tan\varphi = \frac{y}{x}$を$x,y,z$で偏微分すれば$\frac{\partial\varphi}{\partial x} = -\frac{\sin\varphi}{r\sin\theta}, \frac{\partial\varphi}{\partial y} = \frac{\cos\varphi}{r\sin\theta}, \frac{\partial\varphi}{\partial z} = 0$

$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

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

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

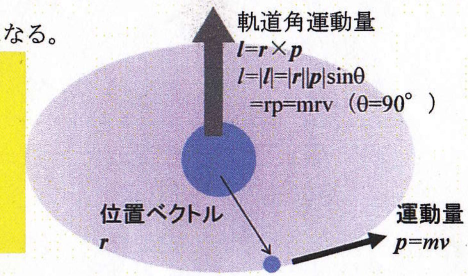
$$\hat{l}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{l}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{l}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi}$$

$$\hat{\mathbf{l}}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

角運動量$\mathbf{l} = \mathbf{r}\times\mathbf{p}$の演算子は以下のようになる。



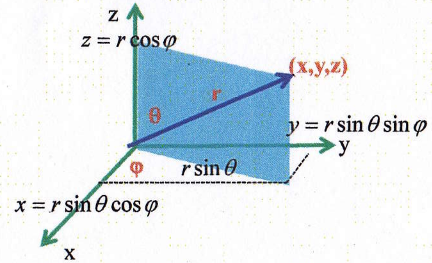
$$\hat{\mathbf{l}} = \hat{\mathbf{r}}\times\hat{\mathbf{p}}\begin{cases}\hat{l}_x = y\hat{p}_z - z\hat{p}_y = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\\ \hat{l}_y = z\hat{p}_x - x\hat{p}_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\\ \hat{l}_z = x\hat{p}_y - y\hat{p}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\end{cases}$$

この軌道角運動量を極座標表現する。

$x = r\sin\theta\cos\varphi$

$y = r\sin\theta\sin\varphi$

$z = r\cos\theta$



$r^2 = x^2 + y^2 + z^2, \tan^2\theta = \frac{x^2+y^2}{z^2}, \tan\varphi = \frac{y}{x}$

r,θ,φはx,y,zの関数なので

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

微分演算子の関係としては、

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}, \frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial y}\frac{\partial}{\partial\varphi}, \frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial z}\frac{\partial}{\partial\varphi}$$