

付録 A - 2

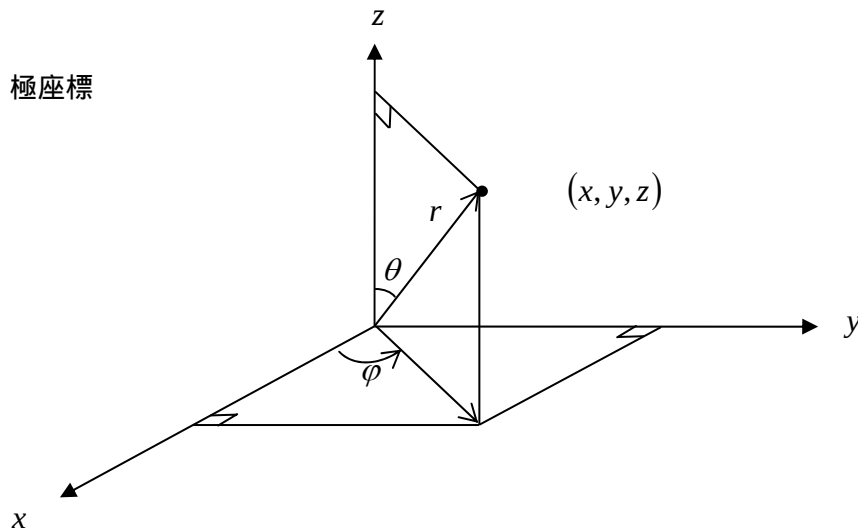
水素原子の波動関数を求める。

質量 m の粒子がポテンシャル $V(r)$ の力場内にあるとき，Schrodinger 方程式は

$$-\frac{\hbar^2}{2m} \nabla^2 u + V(r)u = Eu \quad \text{である。ここで，}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{は Laplacian を表わす。}$$

まず，ラプラシアンを極座標で表示する。極座標は，



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

$$\begin{aligned} r &= (x^2 + y^2 + z^2)^{1/2} \\ \theta &= \tan^{-1} \frac{\sqrt{x^2 + y^2}}{z} \\ \varphi &= \tan^{-1} \frac{y}{x} \end{aligned}$$

ここで， $f(r, \theta, \varphi)$ という関数を考える。

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

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

同様に

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

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

となる。この時,

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

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

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

また, $y = \tan^{-1} x$, $x = \tan y = \frac{\sin y}{\cos y}$ であるから

$$\frac{dx}{dy} = \frac{\cos^2 y + \sin^2 y}{\cos^2 y} = \frac{1}{\cos^2 y}$$

$$\frac{dy}{dx} = \cos^2 y$$

$$\frac{d \tan \theta}{d \theta} = \frac{d}{d \theta} \cdot \frac{\sin \theta}{\cos \theta} = \frac{\cos^2 \theta + \sin^2 \theta}{\cos^2 \theta} = \frac{1}{\cos^2 \theta}$$

$$\frac{\sqrt{x^2 + y^2}}{z} = \frac{\sin \theta}{\cos \theta}$$

$$\frac{\sin^2 \theta}{\cos^2 \theta} = \frac{x^2 + y^2}{z^2} = \frac{1 - \cos^2 \theta}{\cos^2 \theta}$$

$$\cos^2 \theta (x^2 + y^2) = z^2 (1 - \cos^2 \theta)$$

$$\therefore \cos^2 \theta = \frac{z^2}{x^2 + y^2 + z^2}$$

$$\theta = \tan^{-1} \frac{\sqrt{x^2 + y^2}}{z} \quad \left(\frac{\sqrt{x^2 + y^2}}{z} = \tan \theta \right) \quad \text{よ り,}$$

$$\frac{\partial \theta}{\partial x} = \frac{\partial \theta}{\partial (\tan \theta)} \cdot \frac{\partial (\tan \theta)}{\partial x} = \cos^2 \theta \cdot \frac{\frac{\partial \sqrt{x^2 + y^2}}{z}}{\partial (x^2 + y^2)} \cdot \frac{\partial (x^2 + y^2)}{\partial x}$$

$$\begin{aligned}
&= \cos^2 \theta \cdot \frac{1}{z} \cdot \frac{1}{2\sqrt{x^2 + y^2}} \cdot 2x \\
&= \frac{z^2}{x^2 + y^2 + z^2} \cdot \frac{1}{z} \cdot \frac{x}{\sqrt{x^2 + y^2}} \\
&= \frac{1}{r^2} \cdot \frac{x}{\sqrt{x^2 + y^2}} \cdot z = \frac{x}{r} \cdot \frac{1}{r} \cdot \frac{z}{\sqrt{x^2 + y^2}} \\
&= \frac{1}{r} \sin \theta \cos \varphi \frac{1}{\tan \theta} = \frac{1}{r} \cos \theta \cos \varphi
\end{aligned}$$

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

$$= \frac{1}{r} \sin \theta \cdot \sin \varphi \cdot \frac{1}{\tan \theta} = \frac{1}{r} \cos \theta \sin \varphi$$

$$\begin{aligned}
\frac{\partial \theta}{\partial z} &= \cos^2 \theta \cdot \frac{\partial}{\partial z} \cdot \left(\frac{\sqrt{x^2 + y^2}}{z} \right) = \frac{z^2}{x^2 + y^2 + z^2} \cdot \sqrt{x^2 + y^2} \cdot \left(-\frac{1}{z^2} \right) \\
&= -\frac{\sqrt{x^2 + y^2}}{x^2 + y^2 + z^2} = -\frac{z}{r^2} \cdot \frac{\sqrt{x^2 + y^2}}{z} = -\frac{1}{r} \cos \theta \cdot \tan \theta = -\frac{1}{r} \sin \theta
\end{aligned}$$

となる。一方，

$$\varphi = \tan^{-1} \frac{y}{x}$$

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial \tan \varphi} \cdot \frac{\partial \tan \varphi}{\partial x} = \cos^2 \varphi \cdot \left(-\frac{y}{x^2} \right)$$

$$= -\cos^2 \varphi \cdot \frac{y}{x} \cdot \frac{1}{x} = -\cos^2 \varphi \cdot \tan \varphi \cdot \frac{1}{r \sin \theta \cos \varphi}$$

$$= -\cos^2 \varphi \cdot \frac{\sin \varphi}{\cos \varphi} \cdot \frac{1}{r \sin \theta \cos \varphi} = -\frac{\sin \varphi}{r \sin \theta}$$

$$\frac{\partial \varphi}{\partial y} = \frac{\partial \varphi}{\partial \tan \varphi} \cdot \frac{\partial \tan \varphi}{\partial y} = \cos^2 \varphi \cdot \frac{1}{x}$$

$$= \cos^2 \varphi \cdot \frac{1}{r \sin \theta \cdot \cos \varphi} = \frac{\cos \varphi}{r \sin \theta}$$

$$\frac{\partial \varphi}{\partial z} = \frac{\partial \varphi}{\partial \tan \varphi} \cdot \frac{\partial \tan \varphi}{\partial z} = 0$$

$$\left(\frac{\partial}{\partial \theta} \left(\frac{1}{\sin \theta} \right) = -\frac{\cos \theta}{\sin^2 \theta} \right)$$

よって ,

$$\frac{\partial}{\partial x} = \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi}$$

$$\frac{\partial}{\partial y} = \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi}$$

$$\frac{\partial}{\partial z} = \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta}$$

次に

$$\begin{aligned} \frac{\partial^2}{\partial x^2} &= \sin \theta \cos \varphi \frac{\partial}{\partial r} \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\ &\quad + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\ &\quad - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \end{aligned}$$

$$\begin{aligned} &= \sin^2 \theta \cos^2 \varphi \frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \sin \theta \cos \theta \cos^2 \varphi \frac{\partial}{\partial \theta} \\ &\quad + \frac{1}{r} \sin \theta \cos \theta \cos^2 \varphi \frac{\partial}{\partial r} \frac{\partial}{\partial \theta} + \frac{\cos \varphi \sin \varphi}{r^2} \frac{\partial}{\partial \varphi} \\ &\quad - \frac{\sin \varphi \cos \varphi}{r} \frac{\partial}{\partial r} \frac{\partial}{\partial \varphi} + \frac{1}{r} \cos^2 \theta \cos^2 \varphi \frac{\partial}{\partial r} \\ &\quad + \frac{1}{r} \sin \theta \cos \theta \cos^2 \varphi \frac{\partial}{\partial \theta} \frac{\partial}{\partial r} - \frac{1}{r^2} \sin \theta \cos \theta \cos^2 \varphi \frac{\partial}{\partial \theta} \\ &\quad + \frac{1}{r^2} \cos^2 \theta \cos^2 \varphi \frac{\partial^2}{\partial \theta^2} + \frac{\cos^2 \sin \varphi \cos \varphi}{r^2 \sin^2 \theta} \frac{\partial}{\partial \varphi} \\ &\quad - \frac{\cos \theta \sin \varphi \cos \varphi}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \frac{\partial}{\partial \varphi} + \frac{\sin \theta \sin^2 \varphi}{r \sin \theta} \frac{\partial}{\partial r} \\ &\quad - \frac{\sin \varphi \cos \varphi}{r} \frac{\partial}{\partial \varphi} \frac{\partial}{\partial r} + \frac{\cos \theta \sin^2 \varphi}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \\ &\quad - \frac{\cos \theta \sin \varphi \cos \varphi}{r^2 \sin \theta} \frac{\partial}{\partial \varphi} \frac{\partial}{\partial \theta} + \frac{\sin \varphi \cos \varphi}{r^2 \sin^2 \theta} \frac{\partial}{\partial \varphi} + \frac{\sin^2 \varphi}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \end{aligned}$$

$$\frac{\partial^2}{\partial y^2} = \sin \theta \sin \varphi \frac{\partial}{\partial r} \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right)$$

$$\begin{aligned}
& + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\
& + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\
& = \sin^2 \theta \sin^2 \varphi \frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \sin \theta \cos \theta \sin^2 \varphi \frac{\partial}{\partial \theta} \\
& + \frac{1}{r} \sin \theta \cos \theta \sin^2 \varphi \frac{\partial}{\partial r} \frac{\partial}{\partial \theta} - \frac{1}{r^2} \frac{\sin \theta \sin \varphi \cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \\
& + \frac{\sin \theta \sin \varphi \cos \varphi}{r \sin \theta} \frac{\partial}{\partial r} \frac{\partial}{\partial \varphi} + \frac{1}{r} \cos^2 \theta \sin^2 \varphi \frac{\partial}{\partial r} \\
& + \frac{1}{r} \sin \theta \cos \theta \sin^2 \varphi \frac{\partial}{\partial \theta} \frac{\partial}{\partial r} - \frac{1}{r^2} \sin \theta \cos \theta \sin^2 \varphi \frac{\partial}{\partial \theta} \\
& + \frac{1}{r^2} \cos^2 \theta \sin^2 \varphi \frac{\partial^2}{\partial \theta^2} - \frac{1}{r^2} \frac{\cos^2 \theta \sin \varphi \cos \varphi}{\sin^2 \theta} \frac{\partial}{\partial \varphi} \\
& + \frac{1}{r^2} \frac{\cos \theta \sin \varphi \cos \varphi}{\sin \theta} \frac{\partial}{\partial \theta} \frac{\partial}{\partial \varphi} + \frac{\sin \theta}{r \sin \theta} \cos^2 \varphi \frac{\partial}{\partial r} \\
& + \frac{\sin \theta}{r \sin \theta} \sin \varphi \cos \varphi \frac{\partial}{\partial \varphi} \frac{\partial}{\partial r} + \frac{\cos \theta \cos^2 \varphi}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \\
& + \frac{\cos \theta \sin \varphi \cos \varphi}{r^2 \sin \theta} \frac{\partial}{\partial \varphi} \frac{\partial}{\partial \theta} - \frac{\sin \varphi \cos \varphi}{r^2 \sin^2 \theta} \frac{\partial}{\partial \varphi} \\
& + \frac{\cos^2 \varphi}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial^2}{\partial z^2} &= \cos \theta \frac{\partial}{\partial r} \left(\cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(\cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) \\
&= \cos^2 \theta \frac{\partial^2}{\partial r^2} + \frac{\sin \theta \cos \theta}{r^2} \frac{\partial}{\partial \theta} - \frac{\sin \theta \cos \theta}{r} \frac{\partial}{\partial r} \frac{\partial}{\partial \theta} \\
&+ \frac{\sin^2 \theta}{r} \frac{\partial}{\partial r} - \frac{\sin \theta \cos \theta}{r} \frac{\partial}{\partial \theta} \frac{\partial}{\partial r} \\
&+ \frac{\sin \theta \cos \theta}{r^2} \frac{\partial}{\partial \theta} + \frac{\sin^2 \theta}{r^2} \frac{\partial^2}{\partial \theta^2}
\end{aligned}$$

以上の項をまとめると

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\begin{aligned}
&= \sin^2 \theta \frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{r} \sin \theta \cos \theta \frac{\partial}{\partial r} \frac{\partial}{\partial \theta} \\
&+ \frac{1}{r} \cos^2 \theta \frac{\partial}{\partial r} + \frac{1}{r} \sin \theta \cos \theta \frac{\partial}{\partial \theta} \frac{\partial}{\partial r} - \frac{1}{r^2} \sin \theta \cos \theta \frac{\partial}{\partial \theta} \\
&+ \frac{1}{r^2} \cos^2 \theta \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \frac{\partial}{\partial r} \\
&+ \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\
&+ \cos^2 \theta \frac{\partial^2}{\partial r^2} + \frac{\sin \theta \cos \theta}{r^2} \frac{\partial}{\partial \theta} - \frac{\sin \theta \cos \theta}{r} \frac{\partial}{\partial r} \frac{\partial}{\partial \theta} \\
&+ \frac{\sin^2 \theta}{r} \frac{\partial}{\partial r} - \frac{\sin \theta \cos \theta}{r} \frac{\partial}{\partial \theta} \frac{\partial}{\partial r} \\
&+ \frac{\sin \theta \cos \theta}{r^2} \frac{\partial}{\partial \theta} + \frac{\sin^2 \theta}{r^2} \frac{\partial^2}{\partial \theta^2} \\
&= \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\
&= \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\cos \theta}{r^2 \sin \theta} \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}
\end{aligned}$$

これで，ラプラシアンを極座標に変換出来た事になる。

従って，Schrodinger方程式は

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial u}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2} + \frac{2mr^2}{\hbar^2} [E - V(r)]u = 0$$

となる。

この方程式を解くためにまず，変数分離を行う。

$u(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$ とおく。

$$\frac{\partial}{\partial r} \left(r^2 Y \frac{dR}{dr} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(R \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} R \frac{\partial^2 Y}{\partial \varphi^2} + \frac{2mr^2}{\hbar^2} [E - V(r)]RY = 0$$

RY で割ると,

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} \right]$$

左右両辺は定数でなければならない。この定数を λ で表わせば,

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2m}{\hbar^2} [E - V(r)] - \frac{\lambda}{r^2} \right] R = 0$$

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} + \lambda Y = 0$$

更に, $Y(\theta, \varphi) = \Theta(\theta)\Phi(\varphi)$ とする

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \cdot \Phi \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \Theta \frac{\partial^2 \Phi}{\partial \varphi^2} + \lambda \Theta \Phi = 0$$

$$\frac{1}{\Theta} \frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi} \frac{1}{\sin^2 \theta} \frac{d^2 \Phi}{d\varphi^2} + \lambda = 0$$

$$\frac{1}{\Theta} \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \sin^2 \theta \cdot \lambda = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\varphi^2} = \nu$$

とすると

$$\frac{d^2 \Phi}{d\varphi^2} + \nu \Phi = 0,$$

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \left(\lambda - \frac{\nu}{\sin^2 \theta} \right) \Theta = 0$$

まず, 関数 $\Phi(\alpha)$ を考えよう。

$$\frac{d^2 \Phi}{d\varphi^2} + \nu \Phi = 0 \quad \text{ここで, } \sqrt{\nu} = m \quad \text{とおく。}$$

この一般解は,

$$\Phi = Ae^{im\varphi} + Be^{-im\varphi}; \nu \neq 0$$

$$\Phi = A + B\varphi; \nu = 0$$

$\varphi = \phi$ と $\varphi = 2\pi$ で波は連続していなければならない。

$$A + B = Ae^{im2\pi} + Be^{-im2\pi} \quad \text{—————}$$

又 $\varphi = 0$ と $\varphi = 2\pi$ 波動関数になめらかにつながらなければならない(微分係数が等しい。)という条件から,

$$imA(e^0) - imB(e^0) = imAe^{im \cdot 2\pi} - imBe^{-im2\pi}$$

$$A - B = Ae^{im2\pi} - Be^{-im2\pi} \quad \text{—————}$$

$$+ \quad A = Ae^{i2m\pi}$$

$$\therefore e^{im2\pi} = 1$$

$$m = \dots, -3, -2, -1, 0, 1, 2, 3, \dots \quad \text{整数}$$

A と B をひとつにまとめると

$$\Phi = Ae^{im\varphi} \quad (m = 0, \pm 1, \pm 2, \pm 3, \dots)$$

次に規格化を行う。

確率密度関数 $\Phi^* \Phi$ を 0 から 2π まで積分した値が 1 でなくてはならない。

$$\int_0^{2\pi} A^* e^{-im\varphi} \cdot Ae^{im\varphi} d\varphi = 1$$

$$\int_0^{2\pi} A^* A d\varphi = 1$$

$$A^* A [\varphi]_0^{2\pi} = 1$$

$$A^2 \cdot 2\pi = 1$$

A を正の実数とすると

(波動関数に $e^{i\theta}$ をかけた ψ は常に同じ解)

$$A = \frac{1}{\sqrt{2\pi}}$$

$$\therefore \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \quad m = 0, \pm 1, \pm 2, \dots$$

ここで, m を磁気量子数という。

次に, $\Theta(\theta), R(r)$ に関しては, それぞれ, 球面調和関数及びLaguerreの陪関数という特殊関数で表わされることが分かっている。

$$u_{n,l,m}(r, \theta, \varphi) = \left[\left(\frac{2Z\mu}{na_0m_e} \right)^{2l+3} \frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!} \frac{(n-l-1)!}{2n[(n+l)!]^3} \right]^{1/2} \times r^l e^{-\frac{Z\mu}{na_0m_e}r} L_{n+l}^{2l+1} \left(\frac{2Z\mu}{na_0m_e}r \right) P_l^{|m|}(\cos\theta) e^{im\varphi}$$

n : 量子数 (principal quantum number)	$n = 1, 2, 3, \dots$
l : 方位量子数 (azimuthal quantum number)	$0 \leq l \leq n-1$
m : 磁気量子数 (magnetic quantum number)	$-l \leq m \leq l$

$u_{n,l,m}(r, \theta, \varphi)$ は Hamiltonian $\hat{H}$, 角運動量の 2 乗 $\hat{l}^2$, 角運動量の z 成分 $\hat{l}_z$ の同時の固有関数で

$$\hat{H}u_{n,l,m}(r, \theta, \varphi) = E_n u_{n,l,m}(r, \theta, \varphi),$$

$$\hat{l}^2 u_{n,l,m}(r, \theta, \varphi) = l(l+1)\hbar^2 u_{n,l,m}(r, \theta, \varphi),$$

$$\hat{l}_z u_{n,l,m}(r, \theta, \varphi) = m\hbar u_{n,l,m}(r, \theta, \varphi).$$

詳細については , 下記の書物を参照。

原島 鮮著 . 初等量子力学 裳華房 S.47 年 .