プリントNO.7

調和振動子の式の誘導

$$\frac{\partial^2\phi}{\partial x^2}+(\varepsilon-\beta^2x^2)\phi=0\left(\varepsilon=\frac{8\pi^2 mE}{h^2},\beta=\frac{2\pi m\omega}{h}\right)$$

$\varepsilon << \beta^2 x^2$

$$\frac{\partial^2\phi}{\partial x^2}=\beta^2x^2\phi$$

xが非常に大きい時の近似解

$\phi''=\beta^2x^2\{c_1\exp(\beta x^2/2)+c_2\exp(-\beta x^2/2)\}+\beta\{c_1\exp(\beta x^2/2)-c_2\exp(-\beta x^2/2)\}$

なので$\beta^2x^2>>\beta$の時、$\frac{\partial^2\phi}{\partial x^2}=\beta^2x^2\phi$を満たす

$$\phi=c_1\exp(\beta x^2/2)+c_2\exp(-\beta x^2/2)$$

cを$f(x)$として最初の式の解の漸近関数として使う
$|x|\to\infty$において$\phi\to 0$

$$\phi=f(x)\exp(-\beta x^2/2)$$

$$\frac{\partial\phi}{\partial x}=-\beta x f(x)\exp(-\beta x^2/2)+f'(x)\exp(-\beta x^2/2)$$

$$\frac{\partial^2\phi}{\partial x^2}=\beta^2x^2f(x)\exp(-\beta x^2/2)-\beta f(x)\exp(-\beta x^2/2)-2\beta x f'(x)\exp(-\beta x^2/2)+f''(x)\exp(-\beta x^2/2)$$

$$\frac{\partial^2\phi}{\partial x^2}+(\varepsilon-\beta^2x^2)\phi=0$$

$$\beta^2x^2f(x)\exp(-\beta x^2/2)-\beta f(x)\exp(-\beta x^2/2)-2\beta x f'(x)\exp(-\beta x^2/2)$$
$$+f''(x)\exp(-\beta x^2/2)+(\varepsilon-\beta^2x^2)f(x)\exp(-\beta x^2/2)=0$$
$$f''(x)-2\beta x f'(x)+(\varepsilon-\beta)f(x)=0$$

$R(r)$の場合：$Laguerre$の陪方程式、陪多項式 → 資料

$$\frac{r^2}{R}\frac{\partial^2R}{\partial r^2}+\frac{2r}{R}\frac{\partial R}{\partial r}+\frac{2m}{\hbar^2}r^2\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)=\frac{l(l+1)}{\hbar^2}$$

$$\frac{\partial^2R}{\partial r^2}+\frac{2}{r}\frac{\partial R}{\partial r}+\left[\frac{2m}{\hbar^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)-\frac{l(l+1)}{r^2\hbar^2}\right]R=0$$

$$R_{nl}(\rho)=-\sqrt{\frac{4(n-l-1)!}{n^4[(n+l)!]^3}}\left(\frac{Z}{a_0}\right)^{3/2}\rho^l\exp(-\rho/2)L_{n+1}{}^{2l+1}(\rho),\rho\approx\frac{2Z}{na_0}r$$

水素類似原子

$$\left[-\frac{\hbar^2}{2m_e}\Delta-\frac{Ze^2}{4\pi\varepsilon_0 r}\right]\phi=E\phi$$

$$\frac{\partial}{\partial x}=\sin\theta\cos\varphi\frac{\partial}{\partial r}+\frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta}-\frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$
$$\frac{\partial}{\partial y}=\sin\theta\sin\varphi\frac{\partial}{\partial r}+\frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta}+\frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$
$$\frac{\partial}{\partial z}=\cos\theta\frac{\partial}{\partial r}-\frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$
$$\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)-\frac{\mathbf{l}^2}{\hbar^2r^2}$$

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\mathbf{l}^2}{2mr^2}-\frac{Ze^2}{4\pi\varepsilon_0 r}\right]\phi=E\phi$$

変数分離：$\phi(r,\theta,\varphi)=R(r)Y(\theta,\varphi)$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2R}{\partial r^2}+\frac{2}{r}\frac{\partial R}{\partial r}\right)Y+\frac{R\mathbf{l}^2Y}{2mr^2}-\frac{Ze^2}{4\pi\varepsilon_0 r}RY=ERY$$

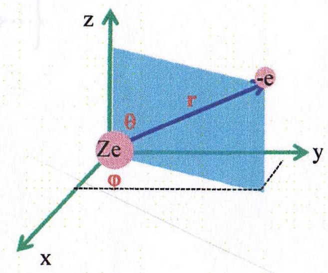
$$\frac{r^2}{R}\frac{\partial^2R}{\partial r^2}+\frac{2r}{R}\frac{\partial R}{\partial r}+\frac{2m}{\hbar^2}r^2\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)=\frac{\mathbf{l}^2Y}{\hbar^2Y}$$

$$\frac{r^2}{R}\frac{\partial^2R}{\partial r^2}+\frac{2r}{R}\frac{\partial R}{\partial r}+\frac{2m}{\hbar^2}r^2\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)=\alpha$$

rだけの関数

$$\frac{\mathbf{l}^2Y}{\hbar^2Y}=\alpha,\mathbf{l}^2Y=\hbar^2\alpha Y=l(l+1)Y$$

θ,φだけの関数



角運動量の２乗の固有状態

$$\mathbf{l}^2Y=\hbar^2\alpha Y$$

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

変数分離：$Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$

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

$$\frac{\hbar^2\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\hbar^2\alpha\sin^2\theta=-\frac{\hbar^2}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}$$

$$\frac{\hbar^2\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\hbar^2\alpha\sin^2\theta=m^2\hbar^2$$

θだけの関数

$$-\frac{\hbar^2}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=m^2\hbar^2$$

φだけの関数

$$\hbar^2\alpha=l(l+1)\hbar^2$$

*Legendre*の陪多項式 → 資料

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0$$

$$\Theta_{lm}(\theta)=\sqrt{\frac{21+1}{2}\frac{(l-|m|)!}{(l+|m|)!}}\sin^{|m|}\theta\frac{d^{|m|}}{(d\cos\theta)^{|m|}}\frac{1}{2^l l!}\frac{d^l}{(d\cos\theta)^l}(\cos^2\theta-1)^l$$

Φは誘導してみる

$$\frac{\partial^2\Phi}{\partial\varphi^2}=-m^2\Phi$$

$$\frac{\partial^2\Phi}{\partial\varphi^2}=-m^2\Phi$$

$\Phi=ce^{\alpha\varphi}$とおく

$$\frac{\partial^2 ce^{\alpha\varphi}}{\partial\varphi^2}=-m^2ce^{\alpha\varphi}$$

$$c\alpha^2e^{\alpha\varphi}=-m^2ce^{\alpha\varphi}$$

$$\alpha^2=-m^2,\alpha=im$$

$$\Phi=ce^{im\varphi}$$

$\Phi(\varphi)=\Phi(\varphi+2\pi)$の条件

$$cf(r,\theta)\exp(im\varphi)=cf(r,\theta)\exp(im(\varphi+2\pi))$$

$$\exp(im2\pi)=1, m=0,\pm1,\pm2,\cdots$$

規格化

$$\phi=R(r)\Theta(\theta)\Phi(\varphi)$$

$$\int_0^\infty\int_0^\pi\int_0^{2\pi}|\phi(r,\theta,\varphi)|^2r^2dr\sin\theta d\theta d\varphi=\int_0^\infty|R(r)|^2r^2dr\int_0^\pi|\Theta(\theta)|^2\sin\theta d\theta\int_0^{2\pi}|\Phi_m(\varphi)|^2d\varphi=1$$

$$\int_0^\infty|R(r)|^2r^2dr\int_0^\pi|\Theta(\theta)|^2\sin\theta d\theta=1$$

$$\int_0^{2\pi}|\Phi_m(\varphi)|^2d\varphi=c\int_0^{2\pi}|\exp(-im\varphi)\exp(im\varphi)|\,d\varphi=c^2\int_0^{2\pi}1d\varphi=2\pi c^2=1$$

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

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}\exp(im\varphi)$$

*Laguerre*の多項式

*Laguerre*の微分方程式：$x\frac{\partial^2y}{\partial x^2}-(1-x)\frac{\partial y}{\partial x}+\alpha y=0$

$$y=a_0\left\{1-\alpha x+\frac{\alpha(\alpha-1)}{(2!)^2}x^2-\cdots+(-1)^r\frac{\alpha(\alpha-1)\cdots(\alpha-r+1)}{(r!)^2}x^r+\cdots\right\}\to Laguerre\text{の多項式}$$

$\alpha=n$正整数（それ以外発散）、$r\geq n+1$で$0\to x^1\cdots x^n$までが残る

$$a_0=n!\text{とおく}\to L_n(x)=(-1)^n\left\{x^n-\frac{n^2}{1!}x^{n-1}+\frac{n^2(n-1)^2}{(2!)^2}x^{n-2}+\cdots+(-1)^n n!\right\}$$

$$y=x^\alpha\exp(-x)\to x\frac{\partial y}{\partial x}+(x-\alpha)y=0$$

$$q\text{回微分}\to x\frac{\partial^{q+1}y}{\partial x^{q+1}}+(x+q-\alpha)\frac{\partial^q y}{\partial x^q}+q\frac{\partial^{q-1}y}{\partial x^{q-1}}=0$$

$$q=\alpha+1\to x\frac{\partial^{\alpha+2}y}{\partial x^{\alpha+2}}+(x+1)\frac{\partial^{\alpha+1}y}{\partial x^{\alpha+1}}+(\alpha+1)\frac{\partial^\alpha y}{\partial x^\alpha}=0$$

*Laguerre*の多項式（つづき）

$$\frac{\partial^\alpha y}{\partial x^\alpha}=\frac{\partial^\alpha}{\partial x^\alpha}\{x^n\exp(-x)\}=\exp(-x)\cdot L_\alpha(x)\text{とおきかえ}$$

$$\frac{\partial^{\alpha+1}y}{\partial x^{\alpha+1}}=\exp(-x)\left(\frac{\partial L_\alpha}{\partial x}-L_\alpha\right)$$

$$\frac{\partial^{\alpha+2}y}{\partial x^{\alpha+2}}=\exp(-x)\left(\frac{\partial^2L_\alpha}{\partial x^2}-2\frac{\partial L_\alpha}{\partial x}+L_\alpha\right)$$

$$x\frac{\partial^2L_\alpha}{\partial x^2}-(1-x)\frac{\partial L_\alpha}{\partial x}+\alpha L_\alpha=0$$

$$x\frac{\partial^2y}{\partial x^2}-(\beta+1-x)\frac{\partial y}{\partial x}+(\alpha-\beta)y=0\to Laguerre\text{陪関数}$$

解：$y=\frac{\partial^2L_\alpha(x)}{\partial x^2}=L_\alpha{}^\beta(x)\to Laguerre$の陪多項式

*Legendre*の方程式

級数による解法：まともにぶつかって解けない

$y=\sum_{\lambda=0}^{\infty} a_\lambda x^{\kappa+\lambda}$という解が得られたとして

係数がどうなるか？級数が収束するか？を調べる。

$$(1-x^2)\frac{\partial^2 y}{\partial x^2}-2x\frac{\partial y}{\partial x}+l(l+1)y=0$$

$$y'=\sum_{\lambda=0}^{\infty} a_\lambda(\kappa+\lambda)x^{\kappa+\lambda-1}$$

$$y''=\sum_{\lambda=0}^{\infty} a_\lambda(\kappa+\lambda)(\kappa+\lambda-1)x^{\kappa+\lambda-2}$$

$$(1-x^2)\sum_\lambda a_\lambda(\kappa+\lambda)(\kappa+\lambda-1)x^{\kappa+\lambda-2}-2x\sum_\lambda a_\lambda(\kappa+\lambda)x^{\kappa+\lambda-1}+l(l+1)\sum_\lambda a_\lambda x^{\kappa+\lambda}=0$$

$$\sum_\lambda a_\lambda(\kappa+\lambda)(\kappa+\lambda-1)x^{\kappa+\lambda-2}-\sum_\lambda a_\lambda\{(\kappa+\lambda)(\kappa+\lambda-1)+2(\kappa+\lambda)-l(l+1)\}x^{\kappa+\lambda}=0$$

$\lambda=0, x^{\kappa-2}$の係数：$a_0\kappa(\kappa-1)=0$

第1項の係数$a_0\neq 0$なので、$\kappa=0 or 1$

$$\cdots a_{\lambda+2}(\kappa+\lambda+2)(\kappa+\lambda+2-1)x^{\kappa+\lambda+2-2}\cdots-\cdots a_\lambda\{(\kappa+\lambda)(\kappa+\lambda-1)+2(\kappa+\lambda)-l(l+1)\}x^{\kappa+\lambda}\cdots=0$$

$$a_{\lambda+2}(\kappa+\lambda+2)(\kappa+\lambda+1)=a_\lambda\{(\kappa+\lambda)(\kappa+\lambda-1)+2(\kappa+\lambda)-l(l+1)\}$$

$$a_{\lambda+2}=\frac{(\kappa+\lambda)(\kappa+\lambda+1)-l(l+1)}{(\kappa+\lambda+2)(\kappa+\lambda+1)}a_\lambda$$

*Legendre*の陪多項式

$$(1-x^2)\frac{\partial^2 y}{\partial x^2}-2x\frac{\partial y}{\partial x}+l(l+1)y=0$$

lが整数の場合、

$$y=c\frac{\partial^l}{\partial x^l}(1-x^2)^l$$

$(1-x^2)\frac{\partial y}{\partial x}+2lxy=0$の解：$y=c(1-x^2)^l$

$$\frac{\partial}{\partial x}\left((1-x^2)\frac{\partial y}{\partial x}+2lxy\right)=(1-x^2)\frac{\partial^2 y}{\partial x^2}+2(l-1)x\frac{\partial y}{\partial x}+2ly=0$$

$$\frac{\partial}{\partial x}\left((1-x^2)\frac{\partial^2 y}{\partial x^2}+2(l-1)x\frac{\partial y}{\partial x}+2ly\right)=(1-x^2)\frac{\partial^3 y}{\partial x^3}+2(l-2)x\frac{\partial^2 y}{\partial x^2}+2(2l-1)\frac{\partial y}{\partial x}=0$$

n回微分：$(1-x^2)\frac{\partial^{n+1} y}{\partial x^{n+1}}+2(l-n)x\frac{\partial^n y}{\partial x^n}+2(nl-\frac{n(n-1)}{2})\frac{\partial^{n-1} y}{\partial x^{n-1}}=0$

$n=l+1$

$$(1-x^2)\frac{\partial^{l+2} y}{\partial x^{l+2}}-2x\frac{\partial^{l+1} y}{\partial x^{l+1}}+l(l+1)\frac{\partial^l y}{\partial x^l}=0$$

$z=\frac{\partial^l y}{\partial x^l}=c\frac{\partial^l}{\partial x^l}(1-x^2)^l\rightarrow(1-x^2)\frac{\partial^2 z}{\partial x^2}-2x\frac{\partial z}{\partial x}+l(l+1)z=0\rightarrow$ *Legendre*の方程式

$z=\frac{1}{2^l\cdot l!}\frac{\partial^l}{\partial x^l}(x^2-1)^l=P_l(x)$：$l$次の*Legendre*の多項式

*Legendre*の方程式（つづき）

$$\kappa=0, a_{\lambda+2}=\frac{\lambda(\lambda+1)-l(l+1)}{(\lambda+2)(\lambda+1)}a_\lambda$$

$$y=a_0\left\{1-\frac{l(l+1)}{2}x^2-\frac{2\cdot3-l(l+1)}{3\cdot4}\cdot\frac{l(l+1)}{2}x^4-\frac{4\cdot5-l(l+1)}{5\cdot6}\cdot\frac{2\cdot3-l(l+1)}{3\cdot4}\cdot\frac{l(l+1)}{2}x^6-\cdots\right\}$$

$$+a_1\left\{x+\frac{1\cdot2-l(l+1)}{2\cdot3}x^3+\frac{3\cdot4-l(l+1)}{4\cdot5}\cdot\frac{1\cdot2-l(l+1)}{2\cdot3}x^5+\cdots\right\}$$

$$\kappa=1, a_{\lambda+2}=\frac{(\lambda+1)(\lambda+2)-l(l+1)}{(\lambda+2)(\lambda+3)}a_\lambda$$

$$y=a_0\left\{x+\frac{1\cdot2-l(l+1)}{2\cdot3}x^3+\frac{3\cdot4-l(l+1)}{4\cdot5}\cdot\frac{1\cdot2-l(l+1)}{2\cdot3}x^5+\cdots\right\}$$

$$+a_1\left\{x^2+\frac{2\cdot3-l(l+1)}{3\cdot4}x^4+\frac{4\cdot5-l(l+1)}{5\cdot6}\cdot\frac{2\cdot3-l(l+1)}{3\cdot4}x^6+\cdots\right\}$$

$\rightarrow$ *Legendre*の多項式

$\kappa=1$の解は、$\kappa=0$と同じ$\rightarrow\kappa=0$

$$y=\sum_{\lambda=0}^{\infty}a_\lambda x^\lambda$$

収束性：$\lim_{\lambda\to\infty}\frac{|a_{\lambda+2}|}{|a_\lambda|}=\lim_{\lambda\to\infty}\frac{|(\lambda-l)(\lambda+l+1)|}{|(\lambda+1)(\lambda+2)|}=1$

*Legendre*の陪多項式（つづき）

さらにm回微分

$$(1-x^2)\frac{\partial^{m+2} z}{\partial x^{m+2}}-2(m+1)x\frac{\partial^{m+1} z}{\partial x^{m+1}}+(m+l+1)(l-m)\frac{\partial^m z}{\partial x^m}=0$$

$\frac{\partial^m z}{\partial x^m}=(1-x^2)^{-m/2}u(x)$とおくと

$$\frac{\partial^{m+1} z}{\partial x^{m+1}}=(1-x^2)^{-m/2}\frac{\partial u}{\partial x}+mx(1-x^2)^{-m/2-1}u$$

$$\frac{\partial^{m+2} z}{\partial x^{m+2}}=(1-x^2)^{-m/2}\frac{\partial^2 u}{\partial x^2}+2mx(1-x^2)^{-m/2-1}\frac{\partial u}{\partial x}+m(1-x^2)^{-m/2-1}u+m(m+2)x^2(1-x^2)^{-m/2-2}u$$

$$(1-x^2)\frac{\partial^2 u}{\partial x^2}-2x\frac{\partial u}{\partial x}+\{l(l+1)-\frac{m^2}{1-x^2}\}u=0$$

$u=(1-x^2)^{m/2}\frac{\partial^m z}{\partial x^m}=(1-x^2)^{m/2}\frac{\partial^m}{\partial x^m}P_l(x)=P_l^m(x)\rightarrow$ *Legendre*の陪多項式

l：方位量子数、m：磁気量子数