No.

Date ・5 ・29

201810876 野村由仁香

1. Γ関数とB関数

- $\Gamma(z) = \int_0^\infty dt\, e^{-t} t^{z-1}$ $\quad (\mathrm{Re}z > 0)$

  $\Gamma(z+1) = z\Gamma(z)$

  $\Gamma(1) = 1$

  $\Gamma(\tfrac{1}{2}) = \pi^{\frac{1}{2}}$

  $\Gamma(n) = (n-1)!$ $\quad n = 1, 2, 3, \dots$

- $B(x, y) = \int_0^1 dt\, t^{x-1}(1-t)^{y-1}$ $\quad (\mathrm{Re}x > 0, \mathrm{Re}y > 0)$

  $= B(y, x)$

  変数変換

  $= 2\int_0^{\frac{\pi}{2}} d\theta \sin^{2x-1}\theta \cos^{2y-1}\theta = \int_0^\infty du \frac{u^{x-1}}{(1+u)^{x+y}}$

$B(x, y) = \dfrac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$, $\Gamma(z)\Gamma(1-z) = \dfrac{\pi}{\sin\pi z}$ $\quad (0 < z < 1)$

など…

2. 球面調和関数の導出

◦ Y_{ll} の決定

$L_+[e^{im\phi}f(\theta)] = e^{im\phi}\hbar e^{i\phi}\left[\frac{df}{d\theta} - mf\cot\theta\right]$

$Y_{lm}(\Omega) = \Theta_{lm}(\theta)\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}\Theta_{lm}(\theta)$

$L_+ Y_{ll} = 0$ から Θ_{ll} が満たす方程式を書けば、

$$\frac{\partial\Theta_{ll}}{\partial\theta} - l\cot\theta\,\Theta_{ll} = 0$$

この解は $\Theta_{ll} = C_l \sin^l\theta$ とかける。 ∵ $\frac{d}{d\theta}\sin^l\theta = l\sin^{l-1}\theta\cos\theta = l\sin^l\theta\cot\theta$

規格化条件

$$\int_0^\pi d\theta \sin\theta |\Theta_{ll}(\theta)|^2 = 1$$ より 定数 C_l を決定する

$\to C_l = (-1)^l \sqrt{\dfrac{(2l+1)!}{2}} \dfrac{1}{2^l l!}$ 　ただし、$(-1)^l \times$ (正の部分) となるように符号を選んだ

$$\to Y_{ll}(\Omega) = (-1)^l \frac{1}{\sqrt{2\pi}}\sqrt{\frac{(2l+1)!}{2}} \cdot \frac{1}{2^l l!} e^{il\phi}\sin^l\theta$$

$\boxed{\text{規格化条件}}$ $\int_0^\pi d\theta \sin\theta |\Theta_{ll}(\theta)|^2 = C_l^2 \int_0^\pi \sin^{2l+1}\theta\, d\theta = C_l^2 \int_0^1 d(-\cos\theta)(1-\cos^2\theta)^l$

$(-\cos\theta = t) \to$ $\quad = 2C_l^2 \int_0^1 dt (1-t^2)^l$

$t = s^{\frac{1}{2}} \to$ $\quad = C_l^2 \int_0^1 ds\, s^{-\frac{1}{2}}(1-s)^l = C_l^2 B(\tfrac{1}{2}, l+1)$

$$= C_l^2 \frac{\Gamma(\frac{1}{2})\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} = C_l^2 \frac{\Gamma(\frac{1}{2})\, l!}{(l+\frac{1}{2})\cdots(\frac{1}{2})\Gamma(\frac{1}{2})} = C_l^2 \frac{2^{l+1} l!}{1\cdot 3 \cdots (2l+1)}$$

$$= C_l^2 \frac{2^{l+1} l! (2^l l!)}{(2l+1)!} = C_l^2 \frac{(2^l l!)^2}{(2l+1)!} \cdot 2$$

Date

。Y_{l0}の決定

$$|jm-k\rangle = \hbar^{-k}\left[\frac{(j+m-k)!}{(j+m)!}\frac{(j-m)!}{(j-(m-k))!}\right]^{\frac{1}{2}}(J_-)^k|jm\rangle$$ の $j=m=k=l$ を考える。

$$\to |l0\rangle = \hbar^{-l}\left[\frac{l!}{(2l)!}\frac{1!}{l!}\right]^{\frac{1}{2}}(L_-)^l|ll\rangle$$

$$L_-^k[e^{im\phi}f(\theta)] = \hbar^k e^{i(m-k)\phi}\sin^{-(m-k)}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^m\theta f(\theta)]$$

$$\to L_-^l[e^{il\phi}\sin^l\theta] = \hbar^l\left(\frac{d}{d\cos\theta}\right)^l\sin^{2l}\theta$$

$$\Rightarrow Y_{l0} = \hbar^{-l}\sqrt{\frac{l!}{(2l)!}\frac{1}{l!}}L_-^l Y_{ll} = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$$

$\downarrow$

l次のルジャンドル多項式 $P_l(t) = \frac{1}{2^l l!}\frac{d^l}{dt^l}(t^2-1)^l$ ロドリグスの公式

。Y_{lm}の決定 $(m\geq 0)$

$$|jm+k\rangle = \hbar^{-k}\left[\frac{(j+m)!}{(j+m+k)!}\frac{(j-(m+k))!}{(j-m)!}\right]^{\frac{1}{2}}(J_+)^k|jm\rangle$$ 、$j=l$、$m=0$、$k=m$を考える

$$\to |lm\rangle = \hbar^{-m}\left[\frac{l!}{(l+m)!}\cdot\frac{(l-m)!}{l!}\right]^{\frac{1}{2}}L_+^m|l0\rangle$$

$$L_+^k[e^{im\phi}f(\theta)] = (-\hbar)^k e^{i(m+k)\phi}\sin^{m+k}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^{-m}\theta f(\theta)]$$

$$\to L_+^m[P_l] = (-\hbar)^m e^{im\phi}\sin^m\theta\left(\frac{d}{d\cos\theta}\right)^m P_l$$

$m>0$に対して Y_{lm}を求めれば、$Y_{lm} = \hbar^{-m}\left[\frac{l!}{(l+m)!}\frac{(l-m)!}{l!}\right]^{\frac{1}{2}}L_+^m Y_{l0}$ より、

$$Y_{lm}(\Omega) = (-)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\sin^m\theta\left[\frac{d}{d\cos\theta}\right]^m P_l(\cos\theta)e^{im\phi}$$

No.

Date

○ $Y_{lm'}$ の決定 $(m' = -m,\ m \geq 0)$

$$|jm-k\rangle = \hbar^{-k}\left[\frac{(j+m-k)!}{(j+m)!}\frac{(j-m)!}{(j-(m-k))!}\right]^{\frac{1}{2}}(J_-)^k|jm\rangle \qquad j=l,\ m=0,\ k=m \text{ を考える}$$

$$\rightarrow |l-m\rangle = \hbar^{-m}\left[\frac{(l-m)!}{l!}\frac{l!}{(l+m)!}\right]^{\frac{1}{2}} L_-^m|l0\rangle$$

$$L_-^k[e^{im\phi}f(\theta)] = \hbar^k e^{i(m-k)\phi}\sin^{-(m-k)}\theta\left[\frac{d}{d\cos\theta}\right]^k[\sin^m\theta f(\theta)]$$

$$\rightarrow L_-^m[P_l] = \hbar^m e^{-im\phi}\sin^m\theta\left(\frac{d}{d\cos\theta}\right)^m P_l$$

$m' = -m,\ m \geq 0$ に対して $Y_{lm'} = Y_{l-m}$ を求めれば、$Y_{l-m} = \hbar^{-m}\sqrt{\frac{(l-m)!}{l!}\frac{l!}{(l+m)!}}\,L_-^m Y_{l0}$ より

$$Y_{lm'}(\Omega) = Y_{l-m}(\Omega) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\sin^m\theta\left[\frac{d}{d\cos\theta}\right]^m P_l(\cos\theta)\,e^{-im\phi}$$

$$\rightarrow Y_{lm}^* = (-)^m Y_{l-m}$$

3. まとめ

軌道角運動量 $\mathbb{L} = \mathbb{r}\times\mathbb{p} = -i\hbar\left(e_\phi\partial_\theta - e_\theta\frac{1}{\sin\theta}\partial_\phi\right)$

→ 球面調和関数

$$\mathbb{L}^2 Y_{lm} = \hbar l(l+1)Y_{lm}$$
$$L_z Y_{lm} = \hbar m Y_{lm}$$
$$L_+ Y_{lm} = L_- Y_{l-l} = 0$$

$$Y_{lm} = (-)^{\frac{1}{2}(m+|m|)}\sqrt{\frac{2l+1}{4\pi}\frac{l-|m|}{l+|m|}}\sin^{|m|}\theta\left[\frac{d}{d\cos\theta}\right]^{|m|}P_l(\cos\theta)\,e^{im\phi}$$

$$= (-)^{\frac{1}{2}(m+|m|)}\sqrt{\frac{2l+1}{4\pi}\frac{l-|m|}{l+|m|}}P_l^{|m|}(\cos\theta)\,e^{im\phi}$$

$$\frac{1}{2}(m+|m|) = \begin{cases} m & (m \geq 0) \\ 0 & (m<0)\end{cases}$$

Legendre 多項式

$$P_l(t) = \frac{1}{2^l l!}\frac{d^l}{dt^l}(t^2-1)^l$$

Legendre の陪関数

$$P_l^{|m|}(t) = (1-t^2)^{\frac{|m|}{2}}\frac{d^{|m|}}{dt^{|m|}}P_l(t)$$

Date

4. 全角運動量演算子とルジャンドル陪関数

全角運動量 $\mathbb{L}^2$ について考える。

$\mathbb{L} = -i\hbar(\mathbf{e}_\phi \partial_\theta - \mathbf{e}_\theta \frac{1}{\sin\theta}\partial_\phi)$

$\mathbf{e}_\theta = \begin{pmatrix} \cos\phi\cos\theta \\ \sin\phi\cos\theta \\ -\sin\theta \end{pmatrix}$ $\mathbf{e}_\phi = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}$

$\partial_\theta \mathbf{e}_\theta = \begin{pmatrix} -\cos\phi\sin\theta \\ -\sin\phi\sin\theta \\ -\cos\theta \end{pmatrix}$ $\partial_\phi \mathbf{e}_\phi = \begin{pmatrix} -\cos\phi \\ -\sin\phi \\ 0 \end{pmatrix}$

$\mathbb{L}^2 = -\hbar^2(\mathbf{e}_\phi\partial_\theta - \mathbf{e}_\theta\frac{1}{\sin\theta}\partial_\phi)(\mathbf{e}_\phi\partial_\theta - \mathbf{e}_\theta\frac{1}{\sin\theta}\partial_\phi)$

$\partial_\phi \mathbf{e}_\theta = \begin{pmatrix} -\sin\phi\cos\theta \\ \cos\phi\cos\theta \\ 0 \end{pmatrix}$ $\partial_\theta \mathbf{e}_\phi = 0$ $\mathbf{e}_\theta \cdot \partial_\phi \mathbf{e}_\theta = 0$

$\mathbf{e}_\phi \cdot \partial_\theta \mathbf{e}_\theta = 0$

$$= -\hbar^2\Big[(\mathbf{e}_\phi\cdot\mathbf{e}_\phi)\partial_\theta^2 + \underbrace{(\mathbf{e}_\phi\cdot\partial_\theta\mathbf{e}_\phi)}_{=0}\partial_\theta - \underbrace{(\mathbf{e}_\phi\cdot\mathbf{e}_\theta)}_{=0}\partial_\theta\frac{1}{\sin\theta}\partial_\phi - \underbrace{(\mathbf{e}_\phi\cdot\partial_\theta\mathbf{e}_\theta)}_{=0}\frac{1}{\sin\theta}\partial_\phi$$

$$- \underbrace{(\mathbf{e}_\theta\cdot\mathbf{e}_\phi)}_{=0}\frac{1}{\sin\theta}\partial_\phi\partial_\theta - (\mathbf{e}_\theta\cdot\partial_\phi\mathbf{e}_\phi)\frac{1}{\sin\theta}\partial_\theta + (\mathbf{e}_\theta\cdot\mathbf{e}_\theta)\frac{1}{\sin^2\theta}\partial_\phi^2 + \underbrace{(\mathbf{e}_\theta\cdot\partial_\phi\mathbf{e}_\theta)}_{=0}\frac{1}{\sin^2\theta}\partial_\phi\Big]$$

$$= -\hbar^2\Big[\underbrace{(\mathbf{e}_\phi\cdot\mathbf{e}_\phi)}_{=1}\partial_\theta^2 - \underbrace{(\mathbf{e}_\theta\cdot\partial_\phi\mathbf{e}_\phi)}_{=-\cos\theta}\frac{1}{\sin\theta}\partial_\theta + \underbrace{(\mathbf{e}_\theta\cdot\mathbf{e}_\theta)}_{=1}\frac{1}{\sin^2\theta}\partial_\phi^2\Big]$$

$$= -\hbar^2\Big[\partial_\theta^2 + \frac{\cos\theta}{\sin\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\Big] = -\hbar^2\Big[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\phi^2\Big]$$

$\mathbb{L}^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}$ より、$Y_{\ell m} = (2\pi)^{-\frac{1}{2}} e^{im\phi}\Theta_{\ell m}(\theta)$ であるから

$$\Big[-\frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d}{d\theta}) + \frac{m^2}{\sin^2\theta}\Big]\Theta_{\ell m} = \ell(\ell+1)\Theta_{\ell m}$$

$$\Big[-\frac{d}{d\cos\theta}(\sin^2\theta\frac{d}{d\cos\theta}) + \frac{m^2}{\sin^2\theta}\Big]\Theta_{\ell m}$$

$t=\cos\theta$ として $\Big[-\frac{d}{dt}((1-t^2)\frac{d}{dt}) + \frac{m^2}{1-t^2}\Big]P_\ell^m(t) = \ell(\ell+1)P_\ell^m(t)$

→ ルジャンドルの陪関数は次のルジャンドルの陪微分方程式を満たす。

$$\frac{d}{dt}((1-t^2)\frac{d}{dt})\frac{dP_\ell^m(t)}{dt} + \Big[\ell(\ell+1) - \frac{m^2}{1-t^2}\Big]P_\ell^m(t) = 0$$

特に $m=0$ として $\frac{d}{dt}((1-t^2)\frac{d}{dt})\frac{dP_\ell(t)}{dt} + \ell(\ell+1)P_\ell(t) = 0$

球面調和関数 $Y_{\ell m}$ と $Y_{\ell' m}$ との直交関係から

$$\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}\int_{-1}^{1} d(\cos\theta)\, P_{\ell'}^m(\cos\theta) P_\ell^m(\cos\theta) = \delta_{\ell'\ell}$$

$$\rightarrow \frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}\int_{-1}^{1} dt\, P_{\ell'}^m(t) P_\ell^m(t) = \delta_{\ell'\ell}$$

特に $m=0$ のとき

$$\frac{2\ell+1}{2}\int_{-1}^{1} dt\, P_{\ell'}(t) P_\ell(t) = \delta_{\ell'\ell}$$

5、多重極展開

ロドリゲスの公式から多重極展開を導く

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{\sqrt{r^2+r'^2-2\mathbf{r}\cdot\mathbf{r}'}} = \frac{1}{r_>}\frac{1}{\sqrt{1-2\left(\frac{r_<}{r_>}\right)\cos\theta+\left(\frac{r_<}{r_>}\right)^2}} = \sum_{l=0}^{\infty}\frac{r_<^{\,l}}{r_>^{\,l+1}}P_l(\cos\theta)$$

$$P_l(t) = \frac{1}{2^l l!}\frac{d^l}{dt^l}(t^2-1)^l \underset{\text{グルサの定理}}{=} \frac{1}{2^l l!}\frac{l!}{2\pi i}\int_{C_t^+}d\xi\,\frac{(\xi^2-1)^l}{(\xi-t)^{l+1}} = \frac{1}{2\pi i}\int_{C_t^+}d\xi\left[\frac{\xi^2-1}{2(\xi-t)}\right]^l\frac{1}{\xi-t}$$

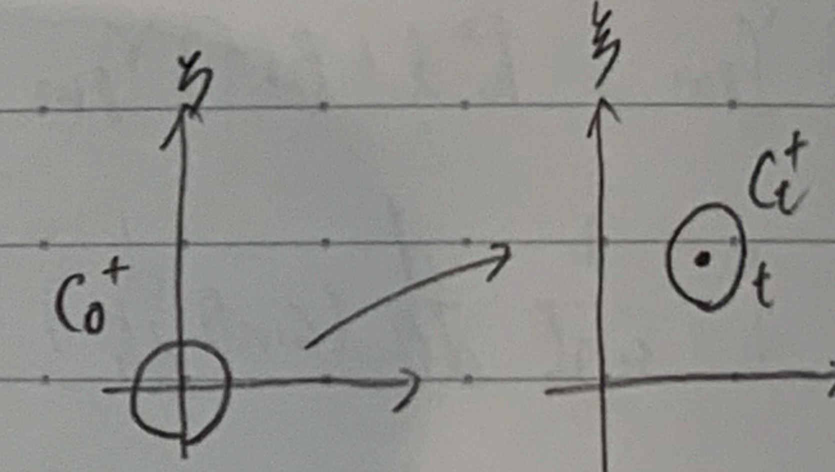
$f(z) = \frac{1}{2\pi i}\int_{C_z^+}d\xi\,\frac{f(\xi)}{\xi-z}$ これをn回ビブンして $f^{(n)}(z) = \frac{n!}{2\pi i}\int_{C_z^+}d\xi\,\frac{f(\xi)}{(\xi-z)^{n+1}}$ ：グルサの定理

$\frac{1}{\zeta} = \frac{\xi^2-1}{2(\xi-t)}$ として $\xi\to\zeta$ の変数変換を考える.

$\zeta\xi^2-\zeta = 2\xi-2t$ ∴ $\zeta\xi^2-2\xi+2t-\zeta=0$ 　$\xi = \left(1\pm\sqrt{1-2t\zeta+\zeta^2}\right)/\zeta$

$\xi = \frac{1\pm R}{\zeta}$ 　$R=\sqrt{1-2t\zeta+\zeta^2}$ とかくと.

$\zeta\to 0$ のとき $R\to 1-t\zeta+\frac{1}{2}\zeta^2$, $\xi\to\frac{1\pm(1-t\zeta+\frac{1}{2}\zeta^2)}{\zeta}$ なので



$\xi=\frac{1-R}{\zeta}$ の分枝をとれば $\zeta\to 0$ のとき $\xi\to t-\frac{1}{2}\zeta$

$$\xi=\frac{1-R}{\zeta} \to d\xi = \frac{-d\zeta}{\zeta^2}(1-R)-\frac{1}{\zeta}\frac{-2t+2\zeta}{2R}d\zeta = \frac{-R+R^2+t\zeta-\zeta^2}{\zeta^2 R}d\zeta$$

$$= \frac{-R-t\zeta+1}{\zeta^2 R}d\zeta = \frac{\xi-t}{\zeta R}d\zeta \qquad \to \frac{d\xi}{\xi-t} = \frac{d\zeta}{R\zeta}$$

よって

$$P_l(t) = \frac{1}{2\pi i}\int_{C_0^+}d\zeta\,\frac{1}{R\zeta^{l+1}} \underset{\text{グルサの定理}}{=} \frac{1}{l!}\frac{d^l}{d\zeta^l}\frac{1}{R}\Big|_{\zeta=0} = \frac{1}{l!}\frac{d^l}{d\zeta^l}\frac{1}{\sqrt{1-2t\zeta+\zeta^2}}\Big|_{\zeta=0}$$

これは $\frac{1}{R}$ を ζ の周りでテイラー展開するとみれば.

$$\frac{1}{R} = \frac{1}{\sqrt{1-2t\zeta+\zeta^2}} = \sum_{l=0}^{\infty}P_l(t)\zeta^l$$

これをルジャンドル関数の母関数展開とよぶ

これを用いて.

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{\sqrt{r^2+r'^2-2\mathbf{r}\cdot\mathbf{r}'}} = \frac{1}{r_>}\frac{1}{\sqrt{1-2\left(\frac{r_<}{r_>}\right)\cos\theta+\left(\frac{r_<}{r_>}\right)^2}}$$

$$= \sum_{l=0}^{\infty}\frac{r_<^{\,l}}{r_>^{\,l+1}}P_l(\cos\theta)$$

ここで $\mathbf{r}$ と $\mathbf{r}'$ がなす角の大きさが θ であり、$r_>$ は $|\mathbf{r}|$ と $|\mathbf{r}'|$ の大きい方、$r_<$ は小さい方である.