

第8回 量子力学3

Γ関数とβ関数

★Γ関数

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

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

$$\cdot \Gamma(1) = 1, \Gamma\left(\frac{1}{2}\right) = \pi^{1/2}$$

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

★β関数

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

$$= B(y, x)$$

$$\text{別の表式} = 2 \int_0^{\pi/2} d\theta \sin^{2x-1} \theta \cos^{2y-1} \theta$$

$$= \int_0^{\infty} du \frac{u^{x-1}}{(1+u)^{x+y}}$$

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

Y_{ℓℓ}の決定

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

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

L₊Y_{ℓℓ} = 0 から Θ_{ℓℓ} が満たす方程式を書けよ

$$\frac{\partial \Theta_{\ell\ell}}{\partial \theta} - \ell \cot \theta \Theta_{\ell\ell} = 0$$

$$\frac{d}{d\theta} \sin^{\ell} \theta = \ell \sin^{\ell-1} \theta \cdot \cos \theta = \ell \sin^{\ell} \theta \cot \theta$$

この解は Θ_{ℓℓ} = C_ℓ sin^ℓ θ とかける。規格化条件 $\int_0^{\pi} d\theta \sin \theta |\Theta_{\ell\ell}(\theta)|^2 = 1$ 定数 C_ℓ を求めれば C_ℓ = (-)^ℓ $\sqrt{\frac{(2\ell+1)!}{2 \cdot 2^{\ell} \ell!}}$ T: T_z = L_z C_ℓ = (-)^ℓ C'_ℓ, C'_ℓ > 0 と符号を選んだ。

$$Y_{\ell\ell}(\Omega) = (-)^{\ell} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(2\ell+1)!}{2}} \frac{1}{2^{\ell} \ell!} e^{i\ell\phi} \sin^{\ell} \theta$$

$$\begin{aligned} \int_0^{\pi} d\theta \sin \theta |\Theta|^2 &= C_{\ell}^2 \int_0^{\pi} d\theta \sin^{2\ell+1} \theta = C_{\ell}^2 \int_{-1}^1 d(-\cos \theta) (1-\cos^2 \theta)^{\ell} \quad (-\cos \theta = t) \\ &= 2C_{\ell}^2 \int_0^1 dt (1-t^2)^{\ell}, \quad t = s^{1/2}, \quad (dt = \frac{1}{2} s^{-1/2} ds) \\ &= C_{\ell}^2 \int_0^1 ds s^{-1/2} (1-s)^{\ell} = C_{\ell}^2 B\left(\frac{1}{2}, \ell+1\right) \\ &= C_{\ell}^2 \frac{\Gamma(1/2)\Gamma(\ell+1)}{\Gamma(\ell+3/2)} = C_{\ell}^2 \frac{\Gamma(1/2)\ell!}{(\ell+\frac{1}{2}) \cdots (1/2)\Gamma(1/2)} \\ &= C_{\ell}^2 \frac{2^{\ell+1} \ell!}{1 \cdot 3 \cdots (2\ell+1)} = C_{\ell}^2 \frac{2^{\ell+1} \ell! (2^{\ell} \ell!)}{(2\ell+1)!} \frac{2^{\ell} \ell!}{2^{\ell} \ell!} \\ &= C_{\ell}^2 \frac{(2^{\ell} \ell!)^2}{(2\ell+1)!} \cdot 2 \end{aligned}$$

$Y_{\ell 0}$ の決定

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

$$m=k \rightarrow \ell, f = \sin^{\ell} \theta, L_-^{\ell} [e^{i\ell\phi} \sin^{\ell} \theta] = \hbar^{\ell} \left(\frac{d}{d \cos \theta} \right)^{\ell} \sin^{2\ell} \theta$$

$$|j, m-k\rangle = \hbar^{-k} \left[\frac{(j+m-k)!}{(j+m)!} \frac{(j-m)!}{(j-(m-k))!} \right]^{1/2} (J_-)^k |j, m\rangle$$

$$j=m=k \rightarrow \ell, |\ell, 0\rangle = \hbar^{-\ell} \left[\frac{\ell!}{(2\ell)!} \frac{1!}{\ell!} \right]^{1/2} L_-^{\ell} |\ell, \ell\rangle_*$$

$$Y_{\ell 0}(\Omega) = (-)^{\ell} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(2\ell+1)!}{2}} \frac{1}{2^{\ell} \ell!} e^{i\ell\phi} \sin^{\ell} \theta$$

$$Y_{\ell 0}(\Omega) = \hbar^{-\ell} \sqrt{\frac{\ell!}{(2\ell)!}} \frac{1}{\ell!} L_-^{\ell} Y_{\ell \ell} = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos \theta)$$

ℓ 次のルジャンドル多項式

$$P_{\ell}(t) = \frac{1}{2^{\ell} \ell!} \frac{d^{\ell}}{dt^{\ell}} (t^2 - 1)^{\ell} \quad \text{ロビニエールの公式}$$

$$Y_{\ell 0}(\Omega) = (-)^{\ell} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(2\ell+1)!}{2}} \frac{1}{2^{\ell} \ell!} \left[\frac{d}{d \cos \theta} \right]^{\ell} \sin^{2\ell} \theta$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2\ell+1}{2}} \frac{1}{2^{\ell} \ell!} \left[\frac{d}{d \cos \theta} \right]^{\ell} (\cos^2 \theta - 1)^{\ell}$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2\ell+1}{2}} P_{\ell}(\cos \theta)$$

$Y_{\ell m}$ の決定

$(m \geq 0)$

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

$$m=0, k \rightarrow m, f = P_{\ell}, L_+^m [P_{\ell}] = (-\hbar)^m e^{im\phi} \sin^m \theta \left(\frac{d}{d \cos \theta} \right)^m P_{\ell}$$

$$|j, m+k\rangle = \hbar^{-k} \left[\frac{(j+m)!}{(j+m+k)!} \frac{(j-(m+k))!}{(j-m)!} \right]^{1/2} (J_+)^k |j, m\rangle$$

$$j \rightarrow \ell, m=0, k \rightarrow m, |\ell, m\rangle = \hbar^{-m} \left[\frac{\ell!(\ell-m)!}{(\ell+m)! \ell!} \right]^{1/2} L_+^m |\ell, 0\rangle$$

$$Y_{\ell 0}(\Omega) = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos \theta)$$

$m > 0$ に対し? $Y_{\ell m}$ を求めれば $Y_{\ell m} = \hbar^{-m} \sqrt{\frac{\ell!}{(\ell+m)!} \frac{(\ell-m)!}{\ell!}} L_+^m |\ell, 0\rangle$ だ!

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

Y_{lm}' の決定

(m' = -m, m ≥ 0)

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

$$k \rightarrow m, m \rightarrow 0, f = P_l, L^{-m} [P_l] = \hbar^m e^{-im\phi} \sin^m \theta \left(\frac{d}{d \cos \theta} \right)^m P_l$$

$$|j, m-k\rangle = \hbar^{-k} \left[\frac{(j+m-k)!}{(j+m)!} \frac{(j-m)!}{(j-(m-k))!} \right]^{1/2} (J_-)^k |j, m\rangle$$

$$j \rightarrow l, m=0, k \rightarrow m, |l, -m\rangle = \hbar^{-m} \left[\frac{(l-m)!}{l!} \frac{l!}{(l+m)!} \right]^{1/2} L^{-m} |l, 0\rangle$$

$$Y_{l0}(\Omega) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta)$$

m' = -m, m ≥ 0 に対して Y_{lm}' = Y_{l, -m} を求めたい

$$Y_{l, -m} = \hbar^{-m} \sqrt{\frac{(l-m)!}{l!} \frac{l!}{(l+m)!}} L^{-m} Y_{l0} \text{ (I)}$$

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

まとめ 軌道角運動量 $L = \hbar \times P = -i\hbar (\mathbf{e}_\theta \partial_\theta - \mathbf{e}_\phi \frac{1}{\sin \theta} \partial_\phi)$

球面調和関数

$$L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

$$L_z Y_{lm} = \hbar m Y_{lm}$$

$$L_+ Y_{l0} = L_- Y_{l, -2} = 0$$

$$(m \geq 0) Y_{lm}(\Omega) = (-)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \sin^m \theta \left[\frac{d}{d \cos \theta} \right]^m P_l(\cos \theta) e^{im\phi}$$

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

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

まとめで書けば

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

$$= (-)^{\frac{1}{2}(m+|m|)} \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{(|m|)}(\cos \theta) e^{im\phi} \quad \frac{1}{2}(m+|m|) = \begin{cases} m & (m \geq 0) \\ 0 & (m < 0) \end{cases}$$

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

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

全角運動量 L^2 について

$$L = -i\hbar(e_\phi \partial_\theta - e_\theta \frac{1}{\sin\theta} \partial_\phi)$$

$$e_\theta = \begin{pmatrix} \cos\phi \cos\theta \\ \sin\phi \cos\theta \\ -\sin\theta \end{pmatrix} \quad e_\phi = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}$$

$$\partial_\theta e_\theta = \begin{pmatrix} -\cos\phi \sin\theta \\ -\sin\phi \sin\theta \\ -\cos\theta \end{pmatrix} \quad \partial_\phi e_\phi = \begin{pmatrix} -\cos\phi \\ -\sin\phi \\ 0 \end{pmatrix}$$

$$\partial_\phi e_\theta = \begin{pmatrix} -\sin\phi \cos\theta \\ \cos\phi \cos\theta \\ 0 \end{pmatrix} \quad \begin{array}{l} \partial_\theta e_\phi = 0 \text{ (C)} \\ e_\theta \cdot \partial_\phi e_\theta = 0 \text{ (A)} \\ e_\phi \cdot \partial_\theta e_\theta = 0 \text{ (B)} \end{array}$$

$$L^2 = -\hbar^2 (e_\phi \partial_\theta - e_\theta \frac{1}{\sin\theta} \partial_\phi) (e_\phi \partial_\theta - e_\theta \frac{1}{\sin\theta} \partial_\phi)$$

$$\begin{aligned} &= -\hbar^2 [(e_\phi \cdot e_\phi) \partial_\theta^2 + (e_\phi \cdot \partial_\theta e_\phi) \partial_\theta - (e_\phi \cdot e_\theta) \partial_\theta \frac{1}{\sin\theta} \partial_\phi \\ &\quad - (e_\phi \cdot \partial_\theta e_\theta) \frac{1}{\sin\theta} \partial_\phi - (e_\theta \cdot e_\phi) \frac{1}{\sin\theta} \partial_\phi \partial_\theta - (e_\theta \cdot \partial_\phi e_\phi) \frac{1}{\sin\theta} \partial_\theta \\ &\quad + (e_\theta \cdot e_\theta) \frac{1}{\sin^2\theta} \partial_\phi^2 + (e_\theta \cdot \partial_\phi e_\theta) \frac{1}{\sin^2\theta} \partial_\phi] \end{aligned}$$

$$\begin{aligned} &= -\hbar^2 [(e_\phi \cdot e_\phi) \partial_\theta^2 - (e_\theta \cdot \partial_\phi e_\phi) \frac{1}{\sin\theta} \partial_\theta + (e_\theta \cdot e_\theta) \frac{1}{\sin^2\theta} \partial_\phi^2] \\ &\quad \underline{= -\cos^2\phi \cos\theta - \sin^2\phi \cos\theta} \\ &= -\cos\theta \end{aligned}$$

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

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

$$L^2 = -\hbar^2 [\frac{1}{\sin\theta} \partial_\theta (\sin\theta \partial_\theta) + \frac{1}{\sin^2\theta} \partial_\phi^2], \quad \Theta_{lm}(\theta) = \sqrt{\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)$$

$$\therefore L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm} \quad Y_{lm} = (2\pi)^{-1/2} e^{im\phi} \Theta_{lm}(\theta) \quad (l \geq |m|)$$

$$\left[-\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d}{d\theta} \right) + \frac{m^2}{\sin^2\theta} \right] \Theta_{lm} = l(l+1) \Theta_{lm}$$

$$\frac{d}{d\theta} = -\sin\theta \frac{d}{d\cos\theta}$$

$$\left[-\frac{d}{d\cos\theta} \left(\sin^2\theta \frac{d}{d\cos\theta} \right) + \frac{m^2}{\sin^2\theta} \right] \Theta_{lm} = l(l+1) \Theta_{lm}$$

↑から $t = \cos\theta$ と書くと

$$\left[-\frac{d}{dt} \left((1-t^2) \frac{d}{dt} \right) + \frac{m^2}{1-t^2} \right] P_l^m(t) = l(l+1) P_l^m(t)$$

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。

$$\frac{d}{dt} \left((1-t^2) \frac{dP_l^m(t)}{dt} \right) + \left[l(l+1) - \frac{m^2}{1-t^2} \right] P_l^m(t) = 0$$

特に $m=0$ とし

$$\frac{d}{dt} \left((1-t^2) \frac{dP_l(t)}{dt} \right) + l(l+1) P_l(t) = 0$$

球面調和関数 Y_{lm} と $Y_{l'm}$ との直交関係から

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

$$\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!} \int_{-1}^1 dt P_{l'}^m(t) P_l^m(t) = \delta_{ll'}$$

特に $m=0$ の時

$$\frac{2l+1}{2} \int_{-1}^1 dt P_{l'}(t) P_l(t) = \delta_{ll'}$$

ロドリゲスの公式から多重極展開を導く

$$\begin{aligned} \frac{1}{|r-r'|} &= \frac{1}{\sqrt{r^2+r'^2-2r \cdot r'}} = \frac{1}{r} \frac{1}{\sqrt{1-2\left(\frac{r'}{r}\right)\cos\theta + \left(\frac{r'}{r}\right)^2}} \\ &= \sum_{l=0}^{\infty} \frac{r'^l}{r^{l+1}} P_l(\cos\theta) \end{aligned}$$

グルサの定理

C_t^+ は $t \in \mathbb{R}$ に 対応する 十分小の π の 積分路

$$P_\ell(t) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dt^\ell} (t^2 - 1)^\ell \stackrel{\downarrow}{=} \frac{1}{2^\ell \ell!} \frac{\ell!}{2\pi i} \int_{C_t^+} d\xi \frac{(\xi^2 - 1)^\ell}{(\xi - t)^{\ell+1}} = \frac{1}{2\pi i} \int_{C_t^+} d\xi \frac{[\frac{\xi^2 - 1}{2(\xi - t)}]^\ell}{\xi - t}$$

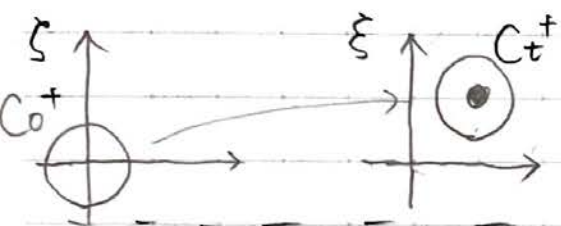
$\frac{1}{\xi} = \frac{\xi^2 - 1}{2(\xi - t)}$ とし $\xi \rightarrow \zeta$ の変数変換を考える.

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

$$\xi = \frac{1 \pm R}{\zeta}, R = \sqrt{1 - 2t\zeta + \zeta^2} \text{ と書けば}$$

$$\zeta \rightarrow 0 \text{ の時 } R \rightarrow 1 - t\zeta + \frac{1}{2}\zeta^2, \xi \rightarrow \frac{1 \pm (1 - t\zeta + \frac{1}{2}\zeta^2)}{\zeta} \text{ のうち}$$

$$\xi = \frac{1 - R}{\zeta} \text{ の分枝を とれば } \zeta \rightarrow 0 \text{ の時 } \xi \rightarrow t - \frac{1}{2}\zeta$$



ζ 平面の C_0^+ は ξ 平面の C_t^+ に向き
を保存して写る

コーシーの積分定理よりある関数 $f(z)$ が複素平面上正則な領域内 \mathcal{R} を正の向きに囲む閉曲線 C_z^+ に対して

$$f(z) = \frac{1}{2\pi i} \int_{C_z^+} d\xi \frac{f(\xi)}{\xi - z} \text{ これを } n \text{ 回微分して}$$

$$f^{(n)}(z) = \frac{n!}{2\pi i} \int_{C_z^+} d\xi \frac{f(\xi)}{(\xi - z)^{n+1}} = \text{グルサの定理}$$

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

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

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

$$\frac{d\xi}{\xi - t} = \frac{d\zeta}{R\zeta}$$

グリアの定理

$$\text{よって } P_l(t) = \frac{1}{2\pi i} \int_{C_0^+} d\zeta \frac{1}{R\zeta^{l+1}} \stackrel{\downarrow}{=} \frac{1}{l!} \frac{d^l}{d\zeta^l} \frac{1}{R} \Big|_{\zeta=0} = \frac{1}{l!} \frac{d^l}{d\zeta^l} \frac{1}{\sqrt{1-2t\zeta+\zeta^2}} \Big|_{\zeta=0}$$

これは $\frac{1}{R}$ を $\zeta=0$ の周りでテイラー展開するとみれば

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

これをルニヤ>ドリル関数の母関数展開と呼ぶ。

これを用いて

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

ここで r と r' が正角の大きさを θ であり、 $r >$ は $|r|$ と $|r'|$ の大きい方

$r <$ は小さい方