

—量子力学第2 プリント 角運動量—

軌道角運動量の固有関数 - 例 - 立方調和関数 -

$$(\ell = 0 : s - wave) \quad \varphi_{00}(x, y, z) = \frac{1}{\sqrt{4\pi}}$$

$$(\ell = 1 : p - wave) \quad \varphi_{1x} = \frac{\sqrt{3}}{2\sqrt{\pi}}x, \quad \varphi_{1y} = \frac{\sqrt{3}}{2\sqrt{\pi}}y, \quad \varphi_{1z} = \frac{\sqrt{3}}{2\sqrt{\pi}}z$$

$$\varphi_{11} = -\frac{1}{\sqrt{2}}(\varphi_{1x} + i\varphi_{1y}) = -\sqrt{\frac{3}{8\pi}}(x + iy) = -\sqrt{\frac{3}{8\pi}}r \sin\theta e^{i\phi},$$

$$\varphi_{10} = \varphi_{1z} = \sqrt{\frac{3}{4\pi}}z = \sqrt{\frac{3}{4\pi}}r \cos\theta,$$

$$\varphi_{1-1} = \frac{1}{\sqrt{2}}(\varphi_{1x} - i\varphi_{1y}) = \sqrt{\frac{3}{8\pi}}(x - iy) = \sqrt{\frac{3}{8\pi}}r \sin\theta e^{-i\phi}$$

$$(\ell = 2 : d - wave)$$

$$\varphi_{2,3z^2-r^2} = \sqrt{\frac{5}{16\pi}}(3z^2 - r^2) = \sqrt{\frac{5}{16\pi}}r^2(3\cos^2\theta - 1),$$

$$\varphi_{2,x^2-y^2} = \sqrt{\frac{15}{16\pi}}(x^2 - y^2) = \sqrt{\frac{15}{16\pi}}r^2 \sin^2\theta \cos 2\phi,$$

$$\varphi_{2,yz} = \sqrt{\frac{15}{4\pi}}yz = \sqrt{\frac{15}{4\pi}}r^2 \sin\theta \cos\theta \sin\phi,$$

$$\varphi_{2,zx} = \sqrt{\frac{15}{4\pi}}zx = \sqrt{\frac{15}{4\pi}}r^2 \sin\theta \cos\theta \cos\phi,$$

$$\varphi_{2,xy} = \sqrt{\frac{15}{4\pi}}xy = \sqrt{\frac{15}{4\pi}}r^2 \sin^2\theta \sin 2\phi.$$

$$\varphi_{22} = \frac{1}{\sqrt{2}}(\varphi_{2,x^2-y^2} + i\varphi_{2,xy}) = \frac{\sqrt{15}}{4\sqrt{2\pi}}r^2 \sin^2\theta e^{2i\phi},$$

$$\varphi_{21} = -\frac{1}{\sqrt{2}}(\varphi_{2,zx} + i\varphi_{2,yz}) = -\frac{\sqrt{15}}{2\sqrt{2\pi}}r^2 \sin\theta \cos\theta e^{i\phi},$$

$$\varphi_{20} = \varphi_{2,3z^2-r^2} = \frac{\sqrt{5}}{2\sqrt{4\pi}}r^2(3\cos^2\theta - 1),$$

$$\varphi_{2-1} = \frac{1}{\sqrt{2}}(\varphi_{2,zx} - i\varphi_{2,yz}) = \frac{\sqrt{15}}{2\sqrt{2\pi}}r^2 \sin\theta \cos\theta e^{-i\phi},$$

$$\varphi_{2-2} = \frac{1}{\sqrt{2}}(\varphi_{2,x^2-y^2} - i\varphi_{2,xy}) = \frac{\sqrt{15}}{4\sqrt{2\pi}}r^2 \sin^2\theta e^{-2i\phi}$$

軌道角運動量の固有関数 - 球関数 -

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dP_{\ell m}(\cos \theta)}{d\theta} \right) + \left(\ell(\ell + 1) - \frac{m^2}{\sin^2 \theta} \right) P_{\ell m}(\cos \theta) = 0.$$

ルジャンドル (Legendre) の陪微分方程式

$$\frac{d}{d\omega} \left[(1 - \omega^2) \frac{dP_{\ell m}(\omega)}{d\omega} \right] + \left(\ell(\ell + 1) - \frac{m^2}{1 - \omega^2} \right) P_{\ell m}(\omega) = 0$$

ルジャンドルの微分方程式

$$\frac{d}{d\omega} \left[(1 - \omega^2) \frac{dP_{\ell}(\omega)}{d\omega} \right] + \ell(\ell + 1) P_{\ell}(\omega) = 0$$

$$P_{\ell}(\omega) = \frac{1}{2^{\ell} \ell!} \frac{d^{\ell}}{d\omega^{\ell}} (\omega^2 - 1)^{\ell} = \frac{(-1)^{\ell}}{2^{\ell} \ell!} \frac{d^{\ell}}{d\omega^{\ell}} (1 - \omega^2)^{\ell}$$

$$P_{\ell m}(\omega) = (1 - \omega^2)^{|m|/2} \frac{d^{|m|}}{d\omega^{|m|}} P_{\ell}(\omega)$$

$$N_{\ell m} = \sqrt{\frac{2\ell + 1}{2} \frac{(\ell - |m|)!}{(\ell + |m|)!}}$$

軌道角運動量 $\hat{\ell}^2$ および $\hat{\ell}_z$ の固有関数 (球関数)

$$Y_{\ell m}(\theta, \phi) = \Theta_{\ell m}(\theta) \Phi_m(\phi),$$

$$\Theta_{\ell m}(\theta) = (-1)^{\frac{m+|m|}{2}} \left[\frac{2\ell + 1}{2} \frac{(\ell - |m|)!}{(\ell + |m|)!} \right]^{1/2} P_{\ell m}(\cos \theta)$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$\hat{\ell}^2 Y_{\ell m} = \hbar^2 \ell(\ell + 1) Y_{\ell m}$$

$$\hat{\ell}_z Y_{\ell m} = \hbar m Y_{\ell m}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta Y_{\ell' m'}(\theta, \phi)^* Y_{\ell m}(\theta, \phi) = \delta_{\ell' \ell} \delta_{m' m}$$

上昇演算子および下降演算子と角運動量演算子の行列要素

軌道角運動量演算子の具体的な形

$$\hat{\ell}_{\pm} Y_{\ell m}(\theta, \phi) = \hbar \sqrt{(\ell \mp m)(\ell \pm m + 1)} Y_{\ell m \pm 1}(\theta, \phi)$$