Appendix

(A) １次元調和振動子の波動関数

エネルギー： $E_n = \left(n + \dfrac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2\cdots$

$$\alpha = \sqrt{\frac{m\omega}{\hbar}}$$

(a) $n = 0$

$$\psi_0(x) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha^2 x^2}$$

(b) $n = 1$

$$\psi_1(x) = \left(\frac{\alpha^2}{4\pi}\right)^{\frac{1}{4}} (2\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$

(c) $n = 2$

$$\psi_1(x) = \left(\frac{\alpha^2}{64\pi}\right)^{\frac{1}{4}} \left[4(\alpha x)^2 - 2\right] e^{-\frac{1}{2}\alpha^2 x^2}$$

(d) 一般の n

$$\psi_n(x) = \left(\frac{\alpha^2}{4^n \pi (n!)^2}\right)^{\frac{1}{4}} H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$

$H_0(\xi) = 1$

$H_1(\xi) = 2\xi$

$H_2(\xi) = 4\xi^2 - 2$

$H_3(\xi) = 8\xi^3 - 12\xi$

$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$

(B) 水素原子

Bohr 半径 : $a_0 = \dfrac{\hbar^2}{me^2}$

エネルギー： $E_n = -\dfrac{mZ^2e^4}{2n^2\hbar^2} = -\dfrac{m}{2n^2}\left(\dfrac{Z}{137}\right)^2$ ： $m = 0.51$ [MeV/c^2]

波動関数:

$$\psi(\boldsymbol{r}) = R_{n\ell}(r)Y_{\ell m}(\theta,\varphi)$$

(a) 1s 状態

$$R_{1s}(r) = \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} 2e^{-\frac{Zr}{a_0}}, \qquad Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

(b) 2p 状態

$$R_{2p}(r) = \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}} \frac{Zr}{\sqrt{3}a_0} e^{-\frac{Zr}{2a_0}}$$

$$\begin{cases} Y_{11}(\theta,\varphi) = -\sqrt{\dfrac{3}{8\pi}}\sin\theta e^{i\varphi} \\ Y_{10}(\theta,\varphi) = \sqrt{\dfrac{3}{4\pi}}\cos\theta \\ Y_{1-1}(\theta,\varphi) = \sqrt{\dfrac{3}{8\pi}}\sin\theta e^{-i\varphi} \end{cases}$$

(c) 2s 状態

$$R_{2s}(r) = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(2 - \frac{Zr}{a_0}\right)e^{-\frac{Zr}{2a_0}}, \qquad Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

(C) 積分公式

(a) Exponential の積分

$$\int_0^\infty e^{-\alpha x}dx = \frac{1}{\alpha}, \quad \int_0^\infty xe^{-\alpha x}dx = \frac{1}{\alpha^2}, \quad \int_0^\infty x^2e^{-\alpha x}dx = \frac{2}{\alpha^3}$$

$$\int_0^\infty x^n e^{-\alpha x}dx = (-1)^n\frac{\partial^n}{\partial\alpha^n}\frac{1}{\alpha} = \frac{n!}{\alpha^{n+1}}$$

(b) Gaussian の積分

$$\int_{-\infty}^\infty e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}, \quad \int_{-\infty}^\infty x^2e^{-\alpha x^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}, \quad \int_{-\infty}^\infty x^4e^{-\alpha x^2}dx = \frac{3}{4}\sqrt{\frac{\pi}{\alpha^5}}$$

$$\int_{-\infty}^\infty x^{2n}e^{-\alpha x^2}dx = (-1)^n\frac{\partial^n}{\partial\alpha^n}\sqrt{\frac{\pi}{\alpha}} = \frac{(2n-1)!!\sqrt{\pi}}{2^n\alpha^{n+\frac{1}{2}}}$$

[但し、$(2n-1)!! = 1\times3\times\cdots\times(2n-1)$]

(c) Gaussian の積分 (奇関数) [積分区間に注意]

$$\int_{-\infty}^\infty x^{2n+1}e^{-\alpha x^2}dx = 0$$

$$\int_0^\infty x^{2n+1}e^{-\alpha x^2}dx = \frac{1}{2}\frac{n!}{\alpha^{n+1}}$$