物理化学演習 I 小テスト第 5 回

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial x}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\Lambda^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

(1)　n=2 の時のエネルギーなので

l=0 → $m_l = 0$

l=1 → m_l=-1,0,1

従って三つ。

(2)　(略)

5.30×10^{-11} (m)

(3)　$\widehat{L^2}\psi(r,\theta,\phi) = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta$

$$= -\hbar^2\left(\frac{1}{\sin\theta}\cos\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial^2\theta}\right)\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta$$

$$= -\hbar^2\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\{-\cos\theta - \cos\theta\}$$

$$= -\hbar^2\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\{-2\cos\theta\}$$

$$= 2\hbar^2\psi$$

また、

$$\hat{L}_z\psi = -i\hbar\frac{\partial}{\partial\phi}\ \frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta$$

$$= i\hbar\ 0\ \frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}$$

従って固有値 0 の固有関数

(4) $\hat{H}\psi = -\frac{\hbar^2}{2m_e}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi$

$= -\frac{\hbar^2}{2m_e}\left(\frac{2}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial^2 r} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta -$

$\frac{e^2}{4\pi\epsilon_0 r}\ \frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta$

$$= -\frac{\hbar^2}{2m_e}\left(\frac{2}{r}\frac{1}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta - \frac{1}{a_0}\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta + \frac{1}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta\left(-\frac{1}{a_0}+\frac{r}{4a_0^2}\right) - \right.$$

$$\left.\frac{1}{r}\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta - \frac{1}{r}\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta + 0\right) - \frac{\hbar^2}{m_e r a_0}\psi$$

$$= -\frac{\hbar^2}{2m_e}\frac{r}{\sqrt{32\pi a_0^5}}e^{-\frac{r}{2a_0}}\cos\theta\left(\frac{2}{r} - \frac{1}{a_0\, r} - \frac{1}{a_0 r} + \frac{1}{4a_0^2} - \frac{1}{r} - \frac{1}{r} - \frac{2}{a_0 r}\right)$$

$$= -\frac{\hbar^2}{8m_e a_0^2}\ \psi$$

従って、 E= $-\frac{\hbar^2}{8m_e a_0^2}$ となる。

(5) $< r >= \int\int\int \psi^* \ \hat{r}\ \psi\ \ d\tau = \int_0^\infty\int_0^\pi\int_0^{2\pi}\frac{r^3}{32\pi a_o^5}\ e^{-\frac{r}{a_0}}\cos^2\theta\ r^2\sin\theta\ drd\theta d\phi$

$$= \frac{1}{32\pi a_o^5}\int_0^\infty r^5\ e^{-\frac{r}{a_0}}\ \int_0^\pi \cos^2\sin\theta\ d\theta\ \int_0^{2\pi} 1\ d\phi$$

$$= \frac{1}{32\pi a_o^5}\ 5!\, a_0^6 \times \frac{2}{3} \times 2\pi$$

$$= 5a_0$$

となる。