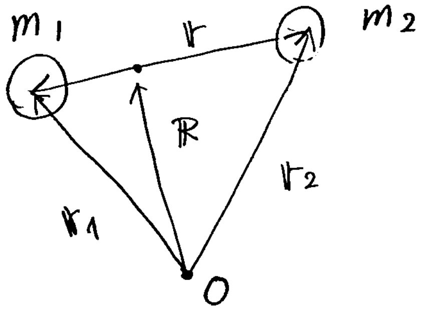
4. 水素原子（束縛状態）

4.1. 2粒子系：重心運動と相対運動

$$H = \frac{\mathbb{P}_1^2}{2m_1} + \frac{\mathbb{P}_2^2}{2m_2} + V(\mathbb{r}_1, \mathbb{r}_2)$$



重心座標 $\mathbb{R} = \dfrac{m_1\mathbb{r}_1 + m_2\mathbb{r}_2}{m_1 + m_2}$，$m_1 + m_2 \equiv M$

相対座標 $\mathbb{r} = \mathbb{r}_1 - \mathbb{r}_2$

を導入．

・$\mathbb{R}, \mathbb{r}$ に共役な運動量？

$$\mathbb{P} = \alpha\, \mathbb{P}_1 + \beta\, \mathbb{P}_2$$

$$\rightarrow [\mathbb{R}, \mathbb{P}] = \left(\frac{m_1}{M}\alpha + \frac{m_2}{M}\beta\right)\cdot i\hbar \qquad (M = m_1 + m_2)$$
$$[\mathbb{r}, \mathbb{P}] = (\alpha - \beta)\cdot i\hbar$$

$[\mathbb{R}, \mathbb{P}] = i\hbar$，$[\mathbb{r}, \mathbb{P}] = 0$ となるように

α, β を決めると $\alpha = \beta = 1$

すなわち $\mathbb{P} = \mathbb{P}_1 + \mathbb{P}_2$ （全運動量）

同様に $\mathbb{p} = \alpha' \mathbb{P}_1 + \beta' \mathbb{P}_2$ として

$$[\mathbb{R}, \mathbb{p}] = 0, \quad [\mathbb{r}, \mathbb{p}] = i\hbar$$

となるように α', β' を選ぶと

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$$\begin{cases} \alpha' - \beta' = 1 \\ m_1 \alpha' + m_2 \beta' = 0 \end{cases} \quad \rightarrow \quad \begin{aligned} \alpha' &= -\frac{m_2}{m_1}\beta' \\ \left(-\frac{m_2}{m_1} - 1\right)\beta' &= 1 \\ \beta' &= -\frac{m_1}{M} \\ \alpha' &= +\frac{m_2}{M} \end{aligned}$$

$$\therefore \quad \mathbf{p} = \frac{m_2}{M}\mathbf{p}_1 - \frac{m_1}{M}\mathbf{p}_2$$

(note)

$$\begin{pmatrix} \mathbb{P} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{m_2}{M} & -\frac{m_1}{M} \end{pmatrix} \begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{m_2}{M} & -\frac{m_1}{M} \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{P} \\ \mathbf{p} \end{pmatrix} = - \begin{pmatrix} -\frac{m_1}{M} & -1 \\ -\frac{m_2}{M} & 1 \end{pmatrix} \begin{pmatrix} \mathbb{P} \\ \mathbf{p} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{m_1}{M}\mathbb{P} + \mathbf{p} \\ \frac{m_2}{M}\mathbb{P} - \mathbf{p} \end{pmatrix}$$

$$\therefore$$

$$\begin{aligned} H &= \frac{1}{2m_1}\left(\frac{m_1}{M}\mathbb{P} + \mathbf{p}\right)^2 + \frac{1}{2m_2}\left(\frac{m_2}{M}\mathbb{P} - \mathbf{p}\right)^2 + V(\mathbf{r}_1, \mathbf{r}_2) \\ &= \frac{1}{2}\left(\frac{m_1}{M^2} + \frac{m_2}{M^2}\right)\mathbb{P}^2 + \frac{1}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\mathbf{p}^2 + \left(\frac{1}{M} - \frac{1}{M}\right)\mathbb{P}\cdot\mathbf{p} + V \\ &= \frac{\mathbb{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + V(\mathbf{r}_1, \mathbf{r}_2) \end{aligned}$$

$$\mu = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)^{-1} \qquad (\text{換算質量})$$

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もし ポテンシャル V が $\mathbf{r}_1 - \mathbf{r}_2$ のみの関数だとしたら重心運動と相対運動は完全に分離：

$$H = \underbrace{\frac{\mathbb{P}^2}{2M}}_{H_{cm}} + \underbrace{\frac{\mathbf{p}^2}{2\mu} + V(\mathbf{r})}_{H_{rel}}$$

$\uparrow$

"自由粒子"

全系の波動関数は $\Psi(\mathbf{r}, \mathbb{R}) = \psi(\mathbf{r})\, e^{i\mathbb{P}\cdot\mathbb{R}/\hbar}$

$\psi(\mathbf{r})$ は

$$\left[\frac{\mathbf{p}^2}{2\mu} + V(\mathbf{r})\right]\psi(\mathbf{r}) = \underbrace{\left(E_{tot} - \frac{\mathbb{P}^2}{2M}\right)}_{E_{cm}}\psi(\mathbf{r})$$

に従う。

(重心固定系でのエネルギー)

(note) $\mathbf{p} = \mu\dot{\mathbf{r}} = \dfrac{m_1 m_2}{m_1+m_2}(\dot{\mathbf{r}}_1 - \dot{\mathbf{r}}_2)$

$$= \frac{1}{M}(m_2\cdot m_1\dot{\mathbf{r}}_1 - m_1\cdot m_2\dot{\mathbf{r}}_2)$$

$$= \frac{1}{M}(m_2\mathbf{p}_1 - m_1\mathbf{p}_2)$$

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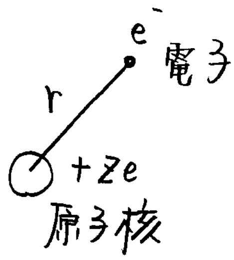
4.2. "水素"原子 の束縛状態



$$V(r) = -\frac{Ze^2}{r}$$

$$\psi(\mathbf{r}) = R_\ell(r)\, Y_{\ell m}(\hat{\mathbf{r}})$$

$$\downarrow$$

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right)\right] R_\ell(r) = 0.$$

$$\rho \equiv \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r \quad \rightarrow \quad \frac{1}{r} = \sqrt{\frac{8\mu|E|}{\hbar^2}} \cdot \frac{1}{\rho}$$

$$\downarrow$$

$$\left[\frac{8\mu|E|}{\hbar^2}\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{\ell(\ell+1)}{\rho^2}\right) + \underbrace{\frac{2\mu}{\hbar^2}\left(\underset{\substack{\| \\ -|E|}}{E} + \sqrt{\frac{8\mu|E|}{\hbar^2}} \cdot \frac{Ze^2}{\rho}\right)}_{=\ \frac{2\mu}{\hbar^2}|E|\left(\underset{\substack{\| \\ 4\lambda}}{\left(\sqrt{\frac{8\mu}{\hbar^2|E|}} \cdot Ze^2\right)}\frac{1}{\rho} - 1\right)}\right] R_\ell(\rho) = 0$$

$$\downarrow$$

$$\boxed{\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{\ell(\ell+1)}{\rho^2} + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)\right] R_\ell(\rho) = 0}$$

$$\lambda = \frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2|E|}} = Z \cdot \underset{\substack{\| \\ \alpha = \frac{1}{137}}}{\left(\frac{e^2}{\hbar c}\right)} \sqrt{\frac{\mu c^2}{2|E|}}$$

・ $\rho \to \infty$ での振るまい

$$\frac{d^2}{d\rho^2} R_\ell - \frac{1}{4} R_\ell = 0$$

$\downarrow$

$$R_\ell(\rho) \sim e^{-\frac{\rho}{2}}$$

・ $\rho \to 0$ での振るまい

$$\frac{d^2}{d\rho^2} R_\ell + \frac{2}{\rho}\frac{d}{d\rho} R_\ell - \frac{\ell(\ell+1)}{\rho^2} R_\ell = 0$$

$\downarrow$

$$R_\ell \sim \rho^\ell$$

$$\left(R_\ell'' - \frac{2}{\rho} R_\ell' = \ell(\ell-1)\rho^{\ell-2} + 2\ell\rho^{\ell-2} = \ell(\ell+1)\rho^{\ell-2} \right)$$

$\downarrow$

$\boxed{R_\ell(\rho) = e^{-\frac{\rho}{2}} G(\rho) = e^{-\frac{\rho}{2}} \rho^\ell H(\rho)}$ とおいてみる。

$\downarrow$

$$R_\ell' = -\frac{1}{2} e^{-\frac{\rho}{2}} G + e^{-\frac{\rho}{2}} G'$$

$$R_\ell'' = \frac{1}{4} e^{-\frac{\rho}{2}} G - e^{-\frac{\rho}{2}} G' + e^{-\frac{\rho}{2}} G''$$

$\downarrow$

$$\left[\cancel{\frac{1}{4}} G - G' + G'' - \frac{1}{\rho} G + \frac{2}{\rho} G' - \frac{\ell(\ell+1)}{\rho^2} G + \left(\frac{\lambda}{\rho} - \cancel{\frac{1}{4}} \right) G \right] \times e^{-\frac{\rho}{2}} = 0$$

$\downarrow$

$$G'' - \left(1 - \frac{2}{\rho}\right) G' + \left(\frac{\lambda - 1}{\rho} - \frac{\ell(\ell+1)}{\rho^2} \right) G = 0.$$

$$\sum_{k=0}^{\infty} a_k k(k-1)\rho^{k-2} = 2a_2 + 6a_3\rho + \cdots$$

$$\sum_{k=0}^{\infty} a_{k+1} \cdot k(k+1)\rho^{k-1} = 2a_2 + 6a_3\rho + \cdots$$

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$$G(\rho) = \rho^l H(\rho)$$

$\downarrow$

$$G' = l\rho^{l-1}H + \rho^l H'$$
$$G'' = l(l-1)\rho^{l-2}H + 2l\rho^{l-1}H' + \rho^l H''$$

$\downarrow$

$$\cancel{l(l-1)\rho^{l-2}}H + 2l\rho^{l-1}H' + \rho^l H'' - l\rho^{l-1}H - \rho^l H'$$
$$+ 2\cancel{l\rho^{l-2}}H + 2\rho^{l-1}H' - \cancel{l(l+1)\rho^{l-2}}H$$
$$+ \frac{\lambda-1}{\rho}\rho^l H = 0$$

$\downarrow$

$$\boxed{H'' + \left(\frac{2l+2}{\rho} - 1\right)H' + \frac{\lambda-l-1}{\rho}H = 0}$$

$$H(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$ と展開してみる

$\downarrow$

$$\sum_{k=0}^{\infty} a_k \left[\underline{k(k-1)\rho^{k-2}} + k\left(\underline{\frac{2l+2}{\rho}} - 1\right)\rho^{k-1} + (\lambda-l-1)\rho^{k-1} \right] = 0$$

$k \to k+1$ $\qquad$ $k \to k+1$

$\downarrow$

$$\sum_{k=0}^{\infty} \Big(a_{k+1}\,\underline{(k+1)}\cdot k\cdot\rho^{k-1} + \underline{(k+1)}(2l+2)\rho^{k-1}a_{k+1}$$
$$- k a_k \rho^{k-1} + (\lambda-l-1)\rho^{k-1}a_k \Big) = 0$$

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$$\therefore \sum_{k=0}^{\infty} \rho^{k-1} \left[(k+1)(k+2l+2) a_{k+1} + (\lambda - l - 1 - k) a_k \right] = 0$$

$$\therefore \boxed{(k+1)(k+2l+2) a_{k+1} + (\lambda - l - 1 - k) a_k = 0}$$

漸化式

$\because$ (note) $\dfrac{a_{k+1}}{a_k} = - \dfrac{\lambda - l - 1 - k}{(k+1)(k+2l+2)} \longrightarrow \dfrac{1}{k}$

$\therefore a_k \sim \dfrac{1}{k!}$

$\therefore$

もし k のシリーズが無限に続けば

$$H(\rho) = \sum_{k=0}^{\infty} a_k \rho^k \sim \sum_{k=0}^{\infty} \frac{\rho^k}{k!} = e^{\rho}$$

この時

$\because$

$$R_l(\rho) \sim \rho^l e^{\rho} \cdot e^{-\frac{\rho}{2}}$$
$$= \rho^l e^{\frac{\rho}{2}} \quad (\text{発散})$$

$\rightarrow$ このようにならないためには和がどこかで止まる必要がある。

$\therefore$

$\boxed{\lambda = l + 1 + n_r}$ という条件が満たされれば

$$a_k = 0 \qquad (k \geq n_r + 1)$$

$\rho = \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r$

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$n = n_r + l + 1$ とおくと

- $n \geq l + 1$
- n は整数
- エネルギーは

$$\lambda = \frac{Ze^2}{\hbar c}\sqrt{\frac{\mu c^2}{2|E|}} = n$$

$\frac{e^2}{\hbar c} = \alpha$

↓

$$E = -|E| = -\frac{(Z\alpha)^2}{2n^2}\cdot\mu c^2$$

$$\rho = \sqrt{\frac{8\mu}{\hbar^2}\cdot\frac{(Z\alpha)^2}{2n^2}\cdot\mu c^2}\; r = \frac{2\mu c\, Z\alpha}{n\hbar}\cdot r$$

$$= \frac{2Z}{na_0} r \;;\; a_0 \equiv \frac{\hbar}{\mu c\alpha}$$

(ボーア半径)

▨ スペクトル

エネルギーは n にしかよらない。
⟷ 同じ n を持つ l, m の組は同じエネルギーを持つ。

- 基底状態 ($n = 1$)

$$n_r = l = 0$$

$$E = -\frac{(Z\alpha)^2}{2}\cdot\mu c^2$$

$\mu c^2 = 0.51\ \mathrm{MeV},\ Z = 1$ とすると

$$E = -\frac{1}{2}\cdot\left(\frac{1}{137}\right)^2\cdot 0.51 = 1.36\times10^{-5}\ \mathrm{MeV}$$
$$= 13.6\ \mathrm{eV}$$

波動関数 : $\underbrace{R_{10}}_{nl}(r) \propto e^{-\frac{\rho}{2}} = e^{-Zr/a_0}$