$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right)\psi(\mathbf{r}) = 0$$

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

$\downarrow$

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

$$\psi(\mathbf{r}) = \underbrace{\boxed{\frac{u_\ell(r)}{r}}}_{=R_\ell(r)}\, Y_{\ell m}(\theta,\varphi) \qquad とすると$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)\hbar^2}{2mr^2}+V(r)-E\right]u_\ell(r)=0$$

$$u_\ell(r) \sim r^{\ell+1} \qquad (r\sim 0)$$

$$1 = \int_0^\infty r^2 dr\, |R_\ell(r)|^2 = \int_0^\infty dr\, |u_\ell(r)|^2$$

3.5. 球対称調和振動子

$$V(r) = \frac{1}{2} m\omega^2 r^2 = \frac{1}{2} m\omega^2 (x^2+y^2+z^2)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} u_\ell(r) + \left(\frac{\ell(\ell+1)\hbar^2}{2mr^2} + \frac{1}{2} m\omega^2 r^2 - E\right) u_\ell(r) = 0$$

$$\rho = \sqrt{\frac{m\omega}{\hbar}}\, r, \quad \varepsilon = \frac{2E}{\hbar\omega}$$

$\downarrow$

$$-\frac{\hbar^2}{2\cancel{m}} \cdot \frac{\cancel{m}\omega}{\cancel{\hbar}} \frac{d^2}{d\rho^2} u_\ell(\rho) + \left(\frac{\cancel{m}\omega}{\cancel{\hbar}} \cdot \frac{\ell(\ell+1)\cancel{\hbar^2}}{2\cancel{m}\rho^2} + \frac{1}{2}\cancel{m}\omega^{\cancel{2}}\rho^2 \cdot \frac{\hbar}{\cancel{m\omega}} - E\right) u_\ell(\rho) = 0$$

$\downarrow$

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

$\rho \to 0$ での振るまい ： $u_\ell(\rho) \sim \rho^{\ell+1}$

$\rho \to \infty$ での振るまい ：

$$\frac{d^2}{d\rho^2} u_\ell(\rho) - \rho^2 u_\ell(\rho) = 0$$

$\downarrow$

$$u_\ell(\rho) \sim e^{-\rho^2/2}$$

$$\left(u_\ell' = -\rho e^{-\rho^2/2} \right.$$
$$\left. u_\ell'' = -e^{-\rho^2/2} + \rho^2 e^{-\rho^2/2} \sim \rho^2 e^{-\rho^2/2} \right)$$

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$$u_l(\rho) = \rho^{l+1} e^{-\rho^2/2} S(\rho)$$ とおくと

$$u_l' = (l+1)\rho^l e^{-\rho^2/2} S - \rho^{l+2} e^{-\rho^2/2} S + \rho^{l+1} e^{-\rho^2/2} S'$$

$$\begin{aligned} u_l'' = {} & l(l+1)\rho^{l-1} e^{-\rho^2/2} S - (l+1)\rho^{l+1} e^{-\rho^2/2} S \\ & + (l+1)\rho^l e^{-\rho^2/2} S' \\ & - (l+2)\rho^{l+1} e^{-\rho^2/2} S + \rho^{l+3} e^{-\rho^2/2} S - \rho^{l+2} e^{-\rho^2/2} S' \\ & + (l+1)\rho^l e^{-\rho^2/2} S' - \rho^{l+2} e^{-\rho^2/2} S' + \rho^{l+1} e^{-\rho^2/2} S'' \end{aligned}$$

$$= \rho^{l+1} e^{-\rho^2/2} \left[\frac{l(l+1)}{\rho^2} S - (2l+3) S + (2l+2)\cdot\frac{1}{\rho} S' - 2\rho S' + \rho^2 S + S'' \right]$$

↓

$$\cancel{\frac{l(l+1)}{\rho^2}} S - (2l+3) S + \frac{2l+2}{\rho} S' - 2\rho S' + \cancel{\rho^2 S} + S''$$

$$- \cancel{\frac{l(l+1)}{\rho^2}} S + (\varepsilon - \cancel{\rho^2}) S = 0$$

↓

$$S'' + \left(\frac{2l+2}{\rho} - 2\rho\right) S' + (\varepsilon - 2l - 3) S = 0$$

さらに $x = \rho^2$ とおくと

$$\frac{d}{d\rho} = 2\rho \frac{d}{dx}, \quad \frac{d^2}{d\rho^2} = 2\frac{d}{dx} + 4\rho^2 \frac{d^2}{dx^2}$$

↓

$$4x \frac{d^2 S}{dx^2} + 2\frac{dS}{dx} + \left(\frac{2l+2}{\rho} - 2\rho\right) \cdot 2\rho \frac{dS}{dx} + (\varepsilon - 2l - 3) S = 0$$

↓

$$x \frac{d^2 S}{dx^2} + \left(l + \frac{3}{2} - x\right) \frac{dS}{dx} + \frac{1}{4}(\varepsilon - 2l - 3) S = 0$$

cf. 1次元の調和振動子

$$H(\rho)=\sum_n b_n \rho^n$$

$$(n+2)(n+1)\,b_{n+2}=(2n-\varepsilon+1)\,b_n$$

$$S(x)=\sum_{n=0}^{\infty} a_n x^n \quad \text{とおくと}$$

$$x\frac{d^2S}{dx^2}=\sum_{n=0}^{\infty} n(n-1)\,a_n\,x^{n-1}$$

$$=\sum_{n=0}^{\infty} n(n+1)\,a_{n+1}\,x^n$$

$$\frac{dS}{dx}=\sum_{n=0}^{\infty} n\,a_n\,x^{n-1}=\sum_{n=0}^{\infty}(n+1)\,a_{n+1}\,x^n$$

$$\downarrow$$

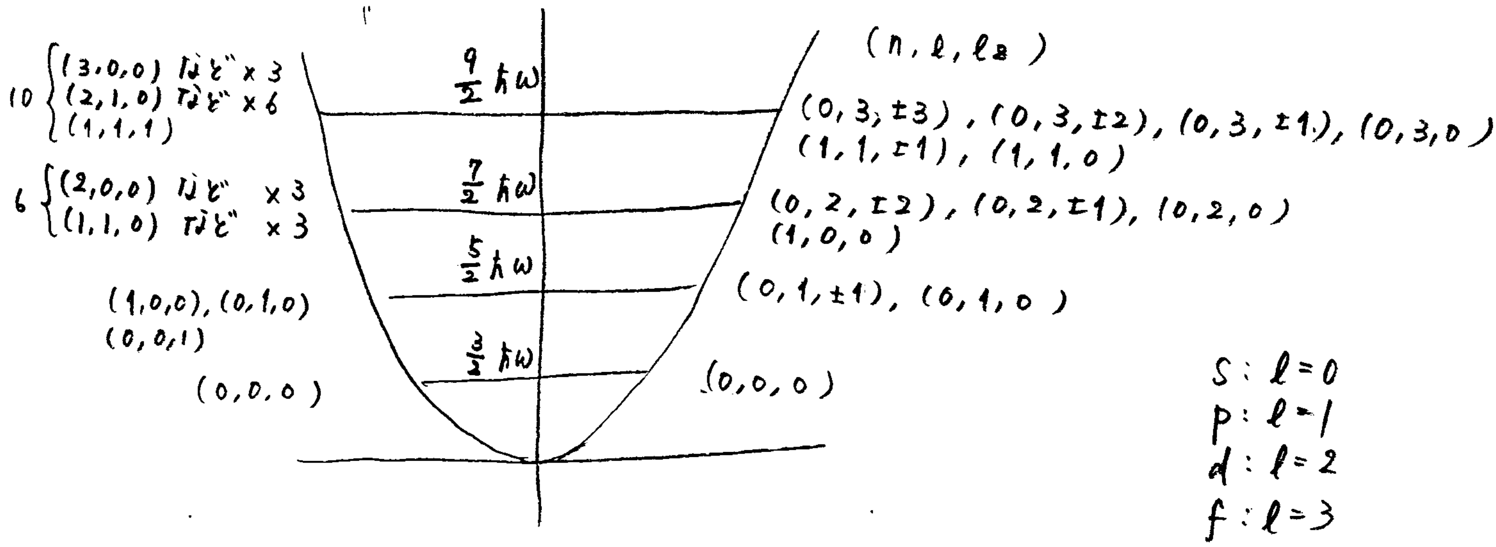
$$\sum_{n=0}^{\infty}\Big[n(n+1)a_{n+1}+\left(l+\tfrac{3}{2}\right)(n+1)a_{n+1}-n a_n+\frac{1}{4}(\varepsilon-2l-3)a_n\Big]x^n=0$$

$$\downarrow$$

$$a_{n+1}=\frac{\frac{1}{4}(\varepsilon-2l-3-4n)}{\left(l+\frac{3}{2}+n\right)(n+1)}\,a_n$$

和が有限で切れるためには

$$\varepsilon=4n+2l+3 \quad\rightarrow\quad E=\left(2n+l+\tfrac{3}{2}\right)\hbar\omega$$



$s: l=0$
$p: l=1$
$d: l=2$
$f: l=3$
……

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(note) ソニン多項式

$$x \frac{d^2}{dx^2} S_n^{(\alpha)} + (\alpha+1-x)\frac{d}{dx} S_n^{(\alpha)} + n S_n^{\alpha} = 0$$

$$S_0^{(\alpha)}(x) = 1$$

$$S_1^{(\alpha)}(x) = \alpha + 1 - x$$

$$S_2^{(\alpha)}(x) = \frac{1}{2}\left\{ (\alpha+1)(\alpha+2) - 2(\alpha+2)x + x^2 \right\}$$

など.

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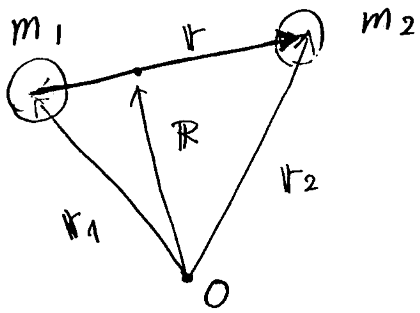
4. 水素原子の束縛状態

4.1. 2粒子系：重心運動と相対運動

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



重心座標 $\mathbf{R} = \dfrac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{\underbrace{m_1 + m_2}_{\equiv M}}$

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

を導入.

・$\mathbf{R}$, $\mathbf{r}$ に共役（キョウヤク）な運動量？

$[\mathbf{r}_i, \mathbf{p}_j] = i\hbar\delta_{ij}$
$(i, j = 1, 2)$

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

(x, y, z の各成分で)

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

$$[\mathbf{r}, \mathbf{P}] = (\beta - \alpha)\cdot i\hbar$$

$[\mathbf{R}, \mathbf{P}] = i\hbar$, $[\mathbf{r}, \mathbf{P}] = 0$ となるように
α, β を決めると $\alpha = \beta = 1$
すなわち $\underline{\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2}$ （系の全運動量）

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

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

となるように α', β' を選ぶと

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

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

(note)

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

$\downarrow$

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

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

$\therefore$

$$H = \frac{1}{2m_1}\left(\frac{m_1}{M}\mathbb{P} - \boldsymbol{p}\right)^2 + \frac{1}{2m_2}\left(\frac{m_2}{M}\mathbb{P} + \boldsymbol{p}\right)^2 + V(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

$$= \frac{1}{2}\left(\frac{m_1}{M^2} + \frac{m_2}{M^2}\right)\mathbb{P}^2 + \frac{1}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\boldsymbol{p}^2 + \cancel{\left(\frac{1}{M} - \frac{1}{M}\right)}\mathbb{P}\cdot\boldsymbol{p} + V$$

$$= \frac{\mathbb{P}^2}{2M} + \frac{\boldsymbol{p}^2}{2\mu} + V(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

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

もし ポテンシャル V が $\mathbf{r}_2 - \mathbf{r}_1$ 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：

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

↑
"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

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

に従う。

（重心固定系でのエネルギー）

(note) $$\mathbf{p} = \mu\dot{\mathbf{r}} = \frac{m_1 m_2}{m_1+m_2}(\dot{\mathbf{r}}_2 - \dot{\mathbf{r}}_1)$$
$$= \frac{1}{M}(m_1 \cdot m_2 \dot{\mathbf{r}}_2 - m_2 \cdot m_1 \dot{\mathbf{r}}_1)$$
$$= \frac{1}{M}(m_1 \mathbb{P}_2 - m_2 \mathbb{P}_1)$$

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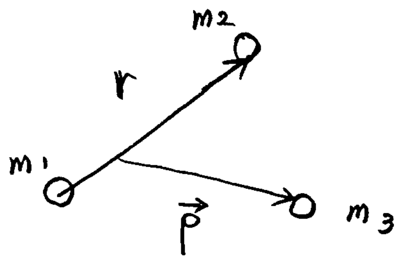
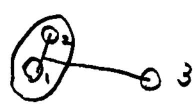
cf. 3体系の場合（ヤコビ座標）



$$\begin{cases} \mathbf{R} = \dfrac{1}{m_1+m_2+m_3}\left(m_1\mathbf{r}_1 + m_2\mathbf{r}_2 + m_3\mathbf{r}_3\right) \\[2ex] \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \\[2ex] \vec{\rho} = \mathbf{r}_3 - \dfrac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1+m_2} \end{cases}$$



これらに共役な運動量は

$$\begin{cases} \mathbb{P} = \mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 \\[1ex] \mathbf{p} = \dfrac{m_1}{m_1+m_2}\mathbf{p}_2 - \dfrac{m_2}{m_1+m_2}\mathbf{p}_1 \\[2ex] \mathbf{p}_\rho = \dfrac{m_1+m_2}{m_1+m_2+m_3}\mathbf{p}_3 - \dfrac{m_3}{m_1+m_2+m_3}(\mathbf{p}_1+\mathbf{p}_2) \end{cases}$$

↓

$$\begin{cases} \mathbf{p}_1 = \dfrac{m_1}{M}\mathbb{P} - \mathbf{p} - \dfrac{m_1}{m_{12}}\mathbf{p}_\rho \\[2ex] \mathbf{p}_2 = \dfrac{m_2}{M}\mathbb{P} + \mathbf{p} - \dfrac{m_2}{m_{12}}\mathbf{p}_\rho \\[2ex] \mathbf{p}_3 = \dfrac{m_3}{M}\mathbb{P} + \mathbf{p}_\rho \end{cases}$$

$$M = m_1 + m_2 + m_3$$
$$m_{12} = m_1 + m_2$$

↓

$$\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + \frac{\mathbf{p}_3^2}{2m_3}$$

$$= \frac{1}{2m_1}\left(\frac{m_1^2}{M^2}\mathbb{P}^2 + \mathbf{p}^2 + \frac{m_1^2}{m_{12}^2}\mathbf{p}_\rho^2 - \cancel{\frac{2m_1}{M}\mathbb{P}\cdot\mathbf{p}} - \frac{2m_1^2}{M m_{12}}\mathbb{P}\cdot\mathbf{p}_\rho + \cancel{\frac{2m_1}{m_{12}}\mathbf{p}\cdot\mathbf{p}_\rho}\right)$$

$$+ \frac{1}{2m_2}\left(\frac{m_2^2}{M^2}\mathbb{P}^2 + \mathbf{p}^2 + \frac{m_2^2}{m_{12}^2}\mathbf{p}_\rho^2 + \cancel{\frac{2m_2}{M}\mathbb{P}\cdot\mathbf{p}} - \frac{2m_2^2}{M m_{12}}\mathbb{P}\cdot\mathbf{p}_\rho - \cancel{\frac{2m_2}{m_{12}}\mathbf{p}\cdot\mathbf{p}_\rho}\right)$$

$$+ \frac{1}{2m_3}\left(\frac{m_3^2}{M^2}\mathbb{P}^2 + \mathbf{p}_\rho^2 + \cancel{\frac{2m_3}{M}\mathbb{P}\cdot\mathbf{p}_\rho}\right)$$

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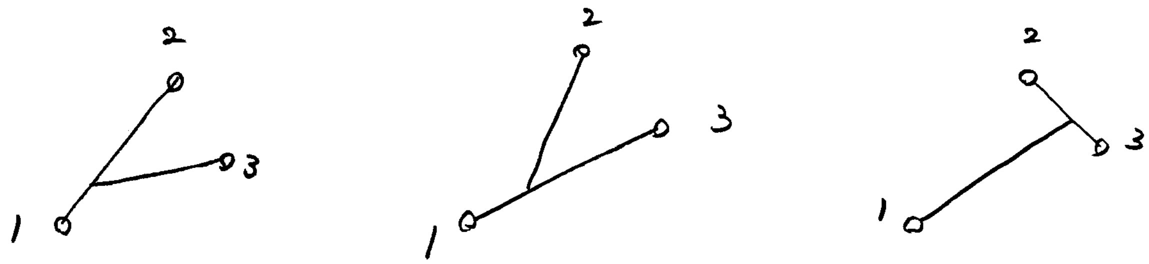
$$= \frac{1}{2M^2}(m_1+m_2+m_3)\,\mathbb{P}^2 + \frac{1}{2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\mathbb{p}^2 + \frac{1}{2}\left(\frac{m_1}{m_{12}^2}+\frac{m_2}{m_{12}^2}+\frac{1}{m_3}\right)\mathbb{p}_\rho^2$$

$$= \frac{\mathbb{P}^2}{2M} + \frac{\mathbb{p}^2}{2\mu_{12}} + \frac{1}{2\mu_{12-3}}\mathbb{p}_\rho^2$$

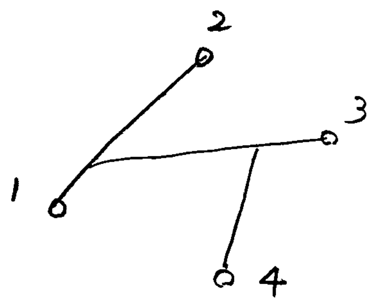
$$\frac{1}{\mu_{12}} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$\frac{1}{\mu_{12-3}} = \frac{1}{m_{12}} + \frac{1}{m_3}$$

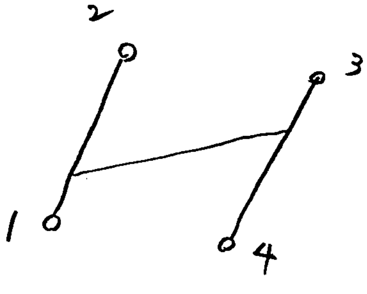
ヤコビ座標 → 重心運動の分離



(4体系の場合)



など



など

※どの組み方を選ぶのかはそれぞれの問題に応じて
↓
いずれの場合も全体の重心運動は完全に分離。