# §. 中心力ポテンシャルの問題

$$H = c\vec{\alpha}\cdot\vec{p} + \beta mc^2 + V(r)$$

(note) $[L_z, H] = [x p_y - y p_x, \ c\alpha_1 p_x + c\alpha_2 p_y + c\alpha_3 p_z]$

$$= i\hbar c\alpha_1 p_y - i\hbar c\alpha_2 p_x$$

$$= i\hbar c(\vec{\alpha}\times\vec{p})_z$$

$$\vec{S} = \frac{\hbar}{2}\vec{\Sigma} = \frac{\hbar}{2}\begin{pmatrix}\vec{\sigma} & 0 \\ 0 & \vec{\sigma}\end{pmatrix}$$

$$[S_z, H] = \frac{\hbar c}{2}\left[\begin{pmatrix}\sigma_z & 0 \\ 0 & \sigma_z\end{pmatrix}, \begin{pmatrix}0 & \sigma_i \\ \sigma_i & 0\end{pmatrix}\right] p_i$$

$$= \frac{\hbar c}{2} p_i \left[\begin{pmatrix}\sigma_z & 0 \\ 0 & \sigma_z\end{pmatrix}\begin{pmatrix}0 & \sigma_i \\ \sigma_i & 0\end{pmatrix} - \begin{pmatrix}0 & \sigma_i \\ \sigma_i & 0\end{pmatrix}\begin{pmatrix}\sigma_z & 0 \\ 0 & \sigma_z\end{pmatrix}\right]$$

$$= \frac{\hbar c}{2} p_i \begin{pmatrix}0 & [\sigma_z, \sigma_i] \\ [\sigma_z, \sigma_i] & 0\end{pmatrix}$$

$$= \frac{\hbar c}{2} p_i \begin{pmatrix}0 & 2i\varepsilon_{3ij}\sigma_j \\ 2i\varepsilon_{3ij}\sigma_j & 0\end{pmatrix} = \hbar c\cdot i\varepsilon_{3ij} p_i \alpha_j$$

$$= -i\hbar c(\vec{\alpha}\times\vec{p})_z$$

$\therefore$

$$[L_z + S_z, H] = 0$$

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$\downarrow \begin{cases} c(\vec{\sigma}\cdot\vec{p})\psi_B = (E - V(r) - mc^2)\psi_A \\ c(\vec{\sigma}\cdot\vec{p})\psi_A = (E - V(r) + mc^2)\psi_B \end{cases}$$

(note) $\frac{1}{r}(\vec{\sigma}\cdot\vec{r})\,|\mathcal{Y}_{j,l=j-1/2,m}\rangle = -|\mathcal{Y}_{j,l=j+1/2,m}\rangle$

$$\frac{1}{r}(\vec{\sigma}\cdot\vec{r})\,|\mathcal{Y}_{j,l=j+1/2,m}\rangle = -\left(\frac{\vec{\sigma}\cdot\vec{r}}{r}\right)^2 |\mathcal{Y}_{j,l=j-1/2,m}\rangle$$

$$= -|\mathcal{Y}_{j,l=j-1/2,m}\rangle$$

derivation:

$$x_{\pm1} = \mp\frac{1}{\sqrt{2}}(x \pm iy) = \sqrt{\frac{4\pi}{3}}\, r Y_{\pm1}$$

$$x_0 = z = \sqrt{\frac{4\pi}{3}}\, r Y_{10}$$

$$\sigma_{\pm1} = \mp\frac{1}{\sqrt{2}}(\sigma_x \pm i\sigma_y), \quad \sigma_0 = \sigma_z$$

$$\downarrow$$

$$\vec{\sigma}\cdot\vec{r} = \sigma_0 x_0 - \sigma_1 x_{-1} - \sigma_{-1} x_1 = \vec{\sigma}\cdot\vec{x}$$

$$= \sqrt{\frac{4\pi}{3}}\, r\, \sigma\cdot Y_1$$

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$$\langle \mathcal{Y}_{j'l'm'} | \frac{1}{r} \vec{\sigma} \cdot \vec{r} | \mathcal{Y}_{jlm} \rangle = \langle \mathcal{Y}_{j'l'm'} | \sqrt{\frac{4\pi}{3}}\, \sigma \cdot Y_1 \, | \mathcal{Y}_{jlm} \rangle$$

$$= \sqrt{\frac{4\pi}{3}} (-)^{l+\frac{1}{2}+j} \delta_{j,j'} \delta_{m,m'} \begin{Bmatrix} j & 1/2 & l' \\ 1 & l & 1/2 \end{Bmatrix}$$

$$\times \underbrace{\langle l' \| Y_1 \| l \rangle}_{= (-)^{l'} \frac{\hat{l} \hat{l'} \sqrt{3}}{\sqrt{4\pi}} \begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix}} \underbrace{\langle \tfrac{1}{2} \| \sigma \| \tfrac{1}{2} \rangle}_{= \sqrt{6}}$$

(see Edmonds, eq. 7.1.6)

$$\begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix} \to l' = l \pm 1$$

$$\begin{Bmatrix} j=l+1/2 & 1/2 & l'=l+1 \\ 1 & l & 1/2 \end{Bmatrix} = \frac{1}{\sqrt{6}} \cdot \frac{1}{\sqrt{l'}}$$

$$\begin{Bmatrix} j=l+1/2 & 1/2 & l'=l-1 \\ 1 & l & 1/2 \end{Bmatrix} = 0$$

$$\begin{pmatrix} l+1 & 1 & l \\ 0 & 0 & 0 \end{pmatrix} = (-)^{l-1} \sqrt{\frac{l+1}{(2l+3)(2l+1)}}$$

$$\langle \mathcal{Y}_{j,l=j+1/2,m} | \frac{1}{r} \vec{\sigma} \cdot \vec{r} | \mathcal{Y}_{j,l=j-1/2,m} \rangle = \begin{cases} -1 & \\ 0 & \text{otherwise} \end{cases}$$

(note)
$$(\vec{\sigma}\cdot\vec{r})(\vec{\sigma}\cdot\vec{p}) = \mathbf{r}\cdot\mathbf{p} + i\vec{\sigma}\cdot(\vec{r}\times\vec{p})$$
$$= \mathbf{r}\cdot\mathbf{p} + i\hbar\,\vec{\sigma}\cdot\vec{\ell} = \frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\vec{\sigma}\cdot\vec{\ell}$$

$\Downarrow$
$$\vec{\sigma}\cdot\vec{p} = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}(\vec{\sigma}\cdot\vec{r})(\vec{\sigma}\cdot\vec{p})$$
$$= \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\,\vec{\sigma}\cdot\vec{\ell}\right)$$

(note) $j = \vec{\ell} + \vec{s}$
$\Downarrow$
$$j^2 = \ell^2 + s^2 + 2\vec{\ell}\cdot\vec{s} = \ell^2 + s^2 + \vec{\ell}\cdot\vec{\sigma}$$

$$(\vec{\sigma}\cdot\vec{p})\,|\mathcal{Y}_{j,\ell=j-1/2,m}\rangle = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\,(j^2-\ell^2-s^2)\right)|\mathcal{Y}_{j\ell m}\rangle$$
$$= \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\,\underbrace{\left(j(j+1)-\ell(\ell+1)-\frac{3}{4}\right)}_{\ell\,=\,j-1/2}\right)|\mathcal{Y}_{j,\ell=j-1/2,m}\rangle$$
$$= -\frac{1}{r}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\,(j-1/2)\right)|\mathcal{Y}_{j,\ell=j+1/2,m}\rangle$$

$$(\vec{\sigma}\cdot\vec{p})\,|\mathcal{Y}_{j,\ell=j+1/2,m}\rangle = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\,\underbrace{\left(j(j+1)-\ell(\ell+1)-\frac{3}{4}\right)}_{-\ell-1\,=\,-j-\frac{3}{2}}\right)|\mathcal{Y}_{j\ell m}\rangle$$
$$= -\frac{1}{r}\left(\frac{\hbar}{i}r\frac{\partial}{\partial r} + i\hbar\left(-j-\frac{3}{2}\right)\right)|\mathcal{Y}_{j,\ell=j-1/2,m}\rangle$$

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$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_A(\mathbf{r}) \\ \psi_B(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g(r)\, \mathcal{Y}_{jlm}(\hat{\mathbf{r}}) \\ i f(r)\, \mathcal{Y}_{jl'm}(\hat{\mathbf{r}}) \end{pmatrix}$$

$$l' = 2j - l = \begin{cases} j - \frac{1}{2} & (l = j + \frac{1}{2}) \\ j + \frac{1}{2} & (l = j - \frac{1}{2}) \end{cases}$$

• $j = l_A + \frac{1}{2} \quad \rightarrow \quad l_A = j - \frac{1}{2}, \quad l_B = j + \frac{1}{2}$

$$c(\vec{\sigma}\cdot\vec{p})\, \mathcal{Y}_B = -\frac{c}{r}\left(\frac{\hbar}{i} r \frac{\partial}{\partial r} + i\hbar\left(-j - \frac{3}{2}\right)\right) \mathcal{Y}_A$$

$$c(\vec{\sigma}\cdot\vec{p})\, \mathcal{Y}_A = -\frac{c}{r}\left(\frac{\hbar}{i} r \frac{\partial}{\partial r} + i\hbar\left(j - \frac{1}{2}\right)\right) \mathcal{Y}_B$$

$$\begin{cases} -\frac{ic}{r}\left(\frac{\hbar}{i} r f' + i\hbar\left(-j - \frac{3}{2}\right) f\right) = (E - V(r) - mc^2)\, g \\ -\frac{c}{r}\left(\frac{\hbar}{i} r g' + i\hbar\left(j - \frac{1}{2}\right) g\right) = i(E - V + mc^2) f \end{cases}$$

or
$$\begin{cases} -\hbar c f' + \hbar c\left(-j - \frac{3}{2}\right)\frac{f}{r} = (E - V(r) - mc^2)\, g \\ \hbar c g' - \hbar c\left(j - \frac{1}{2}\right)\frac{g}{r} = (E - V(r) + mc^2) f \end{cases}$$

• $j = l_A - \frac{1}{2} \quad \rightarrow \quad l_A = j + \frac{1}{2}, \quad l_B = j - \frac{1}{2}$

$$\begin{cases} -\hbar c f' + \hbar c\left(j - \frac{1}{2}\right)\frac{f}{r} = (E - V(r) - mc^2)\, g \\ \hbar c g' - \hbar c\left(-j - \frac{3}{2}\right)\frac{g}{r} = (E - V(r) + mc^2) f \end{cases}$$

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$$f \equiv \frac{F}{r}, \quad g \equiv \frac{G}{r}$$

$$\longrightarrow \quad f' = \frac{F'}{r} - \frac{F}{r^2}, \quad g' = \frac{G'}{r} - \frac{G}{r^2}$$

$j = l_A + \frac{1}{2}$ :

$$\begin{cases} -\hbar c F' + \hbar c \left(-j - \frac{1}{2}\right) \frac{F}{r} = \left(E - V(r) - mc^2\right) G \\ \hbar c G' - \hbar c \left(j + \frac{1}{2}\right) \frac{G}{r} = \left(E - V(r) + mc^2\right) F \end{cases}$$

$j = l_A - \frac{1}{2}$ :

$$\begin{cases} -\hbar c F' + \hbar c \left(j + \frac{1}{2}\right) \frac{F}{r} = \left(E - V - mc^2\right) G \\ \hbar c G' - \hbar c \left(-j - \frac{1}{2}\right) \frac{G}{r} = \left(E - V + mc^2\right) F \end{cases}$$

$$\begin{cases} \hbar c \left(F' - \frac{k}{r} F\right) = -\left(E - V(r) - mc^2\right) G \\ \hbar c \left(G' + \frac{k}{r} G\right) = \left(E - V(r) + mc^2\right) F \end{cases}$$

$$k = \begin{cases} -j - \frac{1}{2} & \left(j = l_A + \frac{1}{2}\right) \\ j + \frac{1}{2} & \left(j = l_A - \frac{1}{2}\right) \end{cases}$$

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・原点付近でのふるまい

$$F \sim a r^s, \quad G \sim b r^t \quad \text{とすると}$$

$$\begin{cases} (s-\kappa)\, a r^{s-1} = -\frac{1}{\hbar c}(E - V_0 - mc^2)\, b r^t \\ (t+\kappa)\, b r^{t-1} = \frac{1}{\hbar c}(E - V_0 + mc^2)\, a r^s \end{cases}$$

i) $s = t - 1 \quad \rightarrow \quad s - 1 = t - 2$
$\rightarrow \quad r^{s-1} \gg r^t$

$\Downarrow$

$$(s-\kappa)\, a r^{s-1} \sim 0 \quad \rightarrow s = \kappa$$

$$(\underbrace{t+\kappa}_{\kappa+1})\, b = \frac{1}{\hbar c}(E - V_0 + mc^2)\, a$$

$\Downarrow$

$$F \sim a r^\kappa, \quad G \sim \frac{1}{2\kappa+1} \cdot \frac{1}{\hbar c}(E - V_0 + mc^2)\, a r^{\kappa+1}$$

$$(\kappa > 0, \quad \kappa + 1 = l_A + 1, \quad \kappa = l_B + 1)$$

ii) $t = s - 1$

$$(t+\kappa)\, b r^{t-1} \sim 0$$

$$(s-\kappa)\, a = -\frac{1}{\hbar c}(E - V_0 - mc^2)\, b$$

$\Downarrow$

$$G \sim b r^{-\kappa}, \quad F \sim -\frac{1}{-2\kappa+1} \cdot \frac{1}{\hbar c}(E - V_0 - mc^2)\, b r^{-\kappa+1}$$

$$(\kappa < 0, \quad -\kappa + 1 = l_B + 1, \quad -\kappa = l_A + 1)$$

・遠方でのふるまい

$$\begin{cases} F' \sim -\frac{1}{\hbar c}(E-mc^2)G \\ G' \sim \frac{1}{\hbar c}(E+mc^2)F \end{cases}$$

$\Downarrow$

$$G'' = \frac{1}{\hbar c}(E+mc^2)F' = -\left(\frac{1}{\hbar c}\right)^2(E^2-m^2c^4)G$$

束縛状態　$E < mc^2$

$\Downarrow$

$$G \sim Ae^{-\frac{\sqrt{m^2c^4-E^2}}{\hbar c}r}$$

$$F' = -\frac{1}{\hbar c}(E-mc^2)\cdot Ae^{-\frac{\sqrt{m^2c^4-E^2}}{\hbar c}r}$$

$\Downarrow$

$$F \sim \frac{E-mc^2}{\sqrt{m^2c^4-E^2}}\cdot Ae^{-\frac{\sqrt{m^2c^4-E^2}}{\hbar c}r}$$

## 四 水素様原子

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

$$\rightarrow E = mc^2\left[1+\frac{Z^2\alpha^2}{\left(n'+\sqrt{(j+\frac{1}{2})^2-Z^2\alpha^2}\right)^2}\right]^{-1/2}$$

$$\sim mc^2\left[1+\frac{Z^2\alpha^2}{\left(n-\frac{Z^2\alpha^2}{2j+1}\right)^2}\right]^{-1/2} \qquad \left(n = n'+j+\frac{1}{2}\right)$$

$$\sim mc^2 - \underbrace{\frac{1}{2}mc^2Z^2\alpha^2\cdot\frac{1}{n^2}}_{\text{non-rel.}} \underbrace{- mc^2\cdot\frac{Z^4\alpha^4}{2j+1}\cdot\frac{1}{n^3}+\frac{3}{8}\cdot\frac{mc^2Z^4\alpha^4}{n^4}+\cdots}_{\text{相対論的補正}}$$

(note) for $n=1$, $j=\frac{1}{2}$ （1S 状態）

$$E_{1S} \sim mc^2(1+Z^2\alpha^2)^{-1/2} \sim mc^2\sqrt{1-Z^2\alpha^2}$$

$Z > \frac{1}{\alpha} = 137$ で原子は存在しなくなる

（実際には原子核の大きさを考慮すると $Z\sim 170$ くらいまで OK）

## §. 相対論的散乱問題の準備：非相対論的プロパゲータ

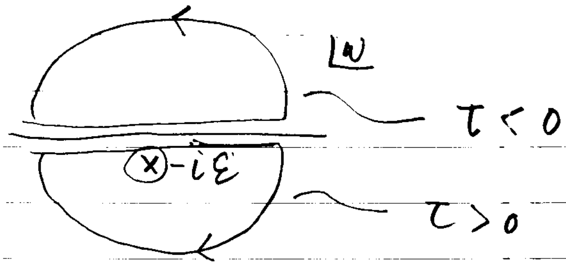
時刻 $t$ での波動関数 $\psi(x) = \psi(\mathbf{r}, t)$

→ 時刻 $t'$ $(> t)$ への時間発展：

$$\theta(t'-t)\,\psi(x') = i\int d^3x\; G(x'; x)\,\psi(x)$$

(note)

$$\theta(\tau) = \lim_{\varepsilon\to+0} \frac{-1}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}}{\omega+i\varepsilon}\,d\omega$$




↓

$$\frac{d\theta(\tau)}{d\tau} = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega\tau}\,d\omega = \delta(\tau)$$

$G(x'; x)$ ： プロパゲータ（伝搬関数），グリーン関数.

(note)

$$\left(i\hbar\frac{\partial}{\partial t'} - H(x')\right)\theta(t'-t)\,\psi(x')$$

$$= i\hbar\,\delta(t'-t)\,\psi(x') + \theta(t'-t)\underbrace{\left(i\hbar\frac{\partial}{\partial t'} - H(x')\right)\psi(x')}_{=0}$$

$$= i\hbar\,\delta(t'-t)\,\psi(x')$$

$$= i\int d\mathbf{r}\,\left[\left(i\hbar\frac{\partial}{\partial t'} - H(x')\right)G(x', x)\right]\psi(x)$$

$$\Leftrightarrow\quad \boxed{\left[i\hbar\frac{\partial}{\partial t'} - H(x')\right]G(x'; x) = \hbar\,\delta(t'-t)\,\delta(\mathbf{r}'-\mathbf{r})}$$

(note) 完全系： $\sum_n \psi_n(\mathbf{r}')\psi_n^*(\mathbf{r}) = \sum_n \langle \mathbf{r}'|\psi_n\rangle\langle\psi_n|\mathbf{r}\rangle$
$= \delta(\mathbf{r}-\mathbf{r}')$

$$G(x', x) = -i\,\theta(t'-t)\sum_n \psi_n(x')\psi_n^*(x)$$

(note) $\left(i\hbar\frac{\partial}{\partial t'} - H(x')\right)G(x', x)$ $\qquad$ $\left(i\hbar\frac{\partial}{\partial t'} - H(x')\right)\psi_n(x') = 0$

$$= \hbar\,\delta(t'-t)\sum_n \psi_n(x')\psi_n^*(x)$$
$$= \hbar\,\delta(t'-t)\sum_n \psi_n(\mathbf{r}', t)\psi_n^*(\mathbf{r}, t)$$
$$= \hbar\,\delta(t'-t)\,\delta(\mathbf{r}'-\mathbf{r})$$

・自由粒子の場合

$H = H_0 = -\frac{\hbar^2}{2m}\nabla^2 \longrightarrow$ 固有関数 $\varphi_p(x) = \dfrac{e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - \frac{p^2}{2m}t)}}{(2\pi\hbar)^{3/2}}$

(note) $\int d\mathbf{p}\; \varphi_p(\mathbf{r}', t)\varphi_p^*(\mathbf{r}, t) = \delta(\mathbf{r}'-\mathbf{r})$

$$G_0(x', x) = -i\,\theta(t'-t)\int d\mathbf{p}\;\varphi_p(x')\varphi_p^*(x)$$
$$= -i\,\theta(t'-t)\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\exp\left[\frac{i}{\hbar}\left(\mathbf{p}\cdot(\mathbf{r}'-\mathbf{r}) - \frac{p^2}{2m}(t'-t)\right)\right]$$

$$\parallel$$
$$-\frac{t'-t}{2m}\left(p^2 - \frac{2m}{t'-t}\,\mathbf{p}\cdot(\mathbf{r}'-\mathbf{r})\right)$$
$$\parallel$$
$$-\frac{t'-t}{2m}\left(\mathbf{p} - \frac{m(\mathbf{r}'-\mathbf{r})}{t'-t}\right)^2 + \frac{m(\mathbf{r}'-\mathbf{r})^2}{2(t'-t)}$$

$$= -i\,\theta(t'-t)\cdot\frac{1}{(2\pi\hbar)^3}\left(\frac{\pi\cdot 2m\hbar}{+i(t'-t)}\right)^{\frac{3}{2}} e^{\frac{im(\mathbf{r}'-\mathbf{r})^2}{2\hbar(t'-t)}}$$
$$= -i\,\theta(t'-t)\left(\frac{m}{2\pi i\hbar(t'-t)}\right)^{\frac{3}{2}}\exp\left(\frac{im(\mathbf{r}'-\mathbf{r})^2}{2\hbar(t'-t)}\right)$$