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§. 中心力ポテンシャルの問題

Dirac 方程式

$$i\hbar\left(\frac{\partial}{\partial t}+\frac{i}{\hbar}g\varphi(\mathbf{r},t)\right)\psi=\left[-i\hbar c\vec{\alpha}\cdot\left(\nabla-\frac{ig}{\hbar}A(\mathbf{r},t)\right)+\beta mc^2\right]\times\psi$$

ディラック表示 $\vec{\alpha}=\begin{pmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix}$, $\beta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

$g\varphi(\mathbf{r},t)=V(r)$, $A(\mathbf{r},t)=0$ のとき:

$$i\hbar\frac{\partial}{\partial t}\psi=\left[-i\hbar c\vec{\alpha}\cdot\nabla+\beta mc^2+V(r)\right]\psi$$

$\rightarrow$ $\psi(\mathbf{r},t)=\psi(\mathbf{r})e^{-iEt/\hbar}$ として

$$\underbrace{\left(c\vec{\alpha}\cdot\vec{p}+\beta mc^2+V(r)\right)}_{\equiv H}\psi(\mathbf{r})=E\psi(\mathbf{r})$$

(note) $\vec{J}=\vec{L}+\vec{S}$; $\vec{S}=\frac{\hbar}{2}\vec{\Sigma}=\frac{\hbar}{2}\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}$

$$[H,J^2]=0$$

$$[H,J_z]=0$$

$[J_z, H] = 0$ の証明

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

$$[J_z, \beta mc^2 + V(r)] = [L_z, V(r)] = 0$$

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

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

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

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

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

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

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

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

$$\boxed{[L_z + S_z, H] = 0.}$$

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

$\downarrow$

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

$\vec{\sigma}\cdot\vec{p}$ はパリティを変える演算子

$\longrightarrow$ ψ_A, ψ_B は異なるパリティを持つ

$\vec{J}$ は保存 $\longrightarrow$ $l = j \pm \frac{1}{2}$ のどちらかを ψ_A
どちらかを ψ_B

例） $S_{1/2}$ と $P_{1/2}$

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

(note) $\left(\frac{\vec{\sigma}\cdot\vec{r}}{r}\right)^2 = 1$

$\downarrow$ $\frac{\vec{\sigma}\cdot\vec{r}}{r}|\mathcal{Y}_{j,j+\frac{1}{2},m}\rangle = -|\mathcal{Y}_{j,j-\frac{1}{2},m}\rangle$

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

(note). $j^2|\mathcal{Y}_{jlm}\rangle = j(j+1)|\mathcal{Y}_{jlm}\rangle$, $l^2|\mathcal{Y}_{jlm}\rangle = l(l+1)|\mathcal{Y}_{jlm}\rangle$
$j_z|\mathcal{Y}_{jlm}\rangle = m|\mathcal{Y}_{jlm}\rangle$

$$\begin{cases} \nabla = \mathbf{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \mathbf{e}_\theta \frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta} \mathbf{e}_\varphi \frac{\partial}{\partial \varphi} \\ \mathbf{r} = r\mathbf{e}_r \end{cases}$$

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

$$\Updownarrow \quad \sigma\cdot\mathbf{p} = \frac{(\sigma\cdot\mathbf{r})^2}{r^2}(\sigma\cdot\mathbf{p}) = \frac{\sigma\cdot\mathbf{r}}{r^2}\left(\frac{\hbar}{i} r\frac{\partial}{\partial r} + i\hbar\,\sigma\cdot\boldsymbol{\ell}\right)$$

(note) $\mathbf{j} = \boldsymbol{\ell} + \mathbf{s}$
$$\rightarrow \mathbf{j}^2 = \boldsymbol{\ell}^2 + \mathbf{s}^2 + 2\boldsymbol{\ell}\cdot\mathbf{s} = \boldsymbol{\ell}^2 + \mathbf{s}^2 + \boldsymbol{\ell}\cdot\sigma$$

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

$$= -\frac{1}{r}\left(\frac{\hbar}{i} r\frac{\partial}{\partial r} + i\hbar\left(j-\frac{1}{2}\right)\right)|\mathcal{Y}_{j,\ell=j+\frac{1}{2},m}\rangle$$

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

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$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_A(\mathbf{r}) \\ \psi_B(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \frac{1}{r} G(r)\, \mathcal{Y}_{jlm}(\hat{\mathbf{r}}) \\ i \frac{1}{r} F(r)\, \mathcal{Y}_{jl'm}(\hat{\mathbf{r}}) \end{pmatrix}$$

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

$$\begin{cases} \hbar c \left(\frac{dF}{dr} - \frac{\kappa}{r} F \right) = -(E - V(r) - mc^2)\, G \\ \hbar c \left(\frac{dG}{dr} + \frac{\kappa}{r} G \right) = (E - V(r) + mc^2)\, F \end{cases}$$

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

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(note) $\frac{1}{r}\boldsymbol{\sigma}\cdot\mathbf{r}\;|\mathcal{Y}_{j,l=j-\frac{1}{2},m}\rangle = -\,|\mathcal{Y}_{j,l=j+\frac{1}{2},m}\rangle$ の証明

$$\begin{cases} x_{\pm1} \equiv \mp\frac{1}{\sqrt{2}}(x \pm iy) = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1\pm1} \\ x_0 = z = \sqrt{\frac{4\pi}{3}}\, r\, Y_{10} \\ \sigma_{\pm1} = \mp\frac{1}{\sqrt{2}}(\sigma_x \pm i\sigma_y),\ \sigma_0 = \sigma_z \end{cases}$$

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

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

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

$$= \sqrt{\frac{4\pi}{3}}\,(-)^{l+\frac{1}{2}+j}\,\delta_{j,j'}\,\delta_{m,m'}\begin{Bmatrix} j & 1/2 & l' \\ 1 & l & 1/2 \end{Bmatrix}$$ (see Edmonds, eq. 7.1.6)

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

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

$$\begin{Bmatrix} j=l+\frac{1}{2} & 1/2 & l'=l\pm1 \\ 1 & l & 1/2 \end{Bmatrix} = \begin{cases} \frac{1}{\sqrt{6l'}} & (l'=l+1) \\ 0 & (l'=l-1) \end{cases}$$

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

$$= \begin{cases} -1 & (j'=j,\ l'=j+\frac{1}{2},\ m'=m) \\ 0 & (\text{それ以外}) \end{cases}$$

四 水素様原子

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

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

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

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

(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)