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共変微分：

$$i\hbar \frac{\partial}{\partial t} \to i\hbar\left(\frac{\partial}{\partial t} + \frac{i}{\hbar} q \varphi\right)$$

$$-i\hbar\nabla \to -i\hbar\left(\nabla - \frac{iq}{\hbar} A\right)$$

$\Downarrow$

$$i\hbar \frac{\partial}{\partial x^\mu} \to i\hbar\frac{\partial}{\partial x^\mu} - qA_\mu = i\hbar\left(\frac{\partial}{\partial x^\mu}+\frac{iq}{\hbar}A_\mu\right)$$

$$A_\mu = \left(\frac{\varphi}{c}, -A\right)$$

$$\frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial(ct)}, \nabla\right)$$

$\Downarrow$

$$\left[i\hbar\gamma^\mu \underbrace{\left(\frac{\partial}{\partial x^\mu} + \frac{iq}{\hbar}A_\mu\right)}_{\equiv D_\mu} - mc\right]\psi = 0$$

§. Dirac方程式の非相対論的極限

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

$A_\mu=\left(\frac{\varphi}{c},-A\right)$ が時間に依らないとして

$$\psi=\psi(x,t=0)\,e^{-iEt/\hbar}$$
$$=\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}e^{-iEt/\hbar}$$

とおく。

$$\downarrow\quad (E-q\varphi)\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}=\begin{pmatrix}mc^2 & c\vec{\sigma}\cdot(p-qA)\\ c\vec{\sigma}\cdot(p-qA) & -mc^2\end{pmatrix}\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix}$$

$$\psi_B=\frac{c}{E-q\varphi+mc^2}\vec{\sigma}\cdot(p-qA)\psi_A$$

$$[\vec{\sigma}\cdot(p-qA)]\frac{c^2}{E-q\varphi+mc^2}[\vec{\sigma}\cdot(p-qA)]\psi_A$$
$$=(E-q\varphi-mc^2)\psi_A$$

非相対論近似： $E\sim mc^2,\ |q\varphi|\ll mc^2$

$E_{NR}\equiv E-mc^2$

$$\downarrow\quad \frac{c^2}{E-q\varphi+mc^2}=\frac{c^2}{2mc^2+E_{NR}-q\varphi}=\frac{c^2}{2mc^2}\left(1-\frac{E_{NR}-q\varphi}{2mc^2}+\cdots\right)$$

$$(\nabla\times A + A\times\nabla)_k = \varepsilon_{ijk}(\partial_i A_j + A_i\partial_j)$$
$$= \varepsilon_{ijk}\left((\partial_i A_j) + A_j\partial_i + A_i\partial_j\right)$$
$$= \varepsilon_{ijk}(\partial_i A_j)$$

- leading order

$$\frac{c^2}{E - q\varphi + mc^2} \sim \frac{1}{2m}$$

$\downarrow$

$$\frac{1}{2m}\left[\vec{\sigma}\cdot(\mathbb{P} - q\mathbb{A})\right]^2 \psi_A = (E_{NR} - q\varphi)\psi_A$$

(note) $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot(\vec{A}\times\vec{B})$

$\downarrow$

$$[\vec{\sigma}\cdot(\mathbb{P} - qA)]^2 = (\mathbb{P} - qA)^2 + i\vec{\sigma}\cdot(\mathbb{P} - q\mathbb{A})\times(\mathbb{P} - q\mathbb{A})$$

$$(\mathbb{P} - q\mathbb{A})\times(\mathbb{P} - q\mathbb{A}) = \frac{\hbar}{i}\nabla\times(-q\mathbb{A}) - q\mathbb{A}\times\mathbb{P} = -\frac{\hbar q}{i}(\nabla\times A) = -\frac{\hbar q}{i}\mathbb{B}$$

$$= (\mathbb{P} - q\mathbb{A})^2 - \hbar q\,\vec{\sigma}\cdot\vec{B}$$

$\Downarrow$

$$\left[\frac{1}{2m}(\mathbb{P} - q\mathbb{A})^2 - \frac{\hbar q}{2m}\vec{\sigma}\cdot\vec{B} + q\varphi\right]\psi_A = E_{NR}\psi_A.$$

・the next order (簡単のため $A=0$ とする)

$$(\vec{\sigma}\cdot\vec{p})\,\frac{1}{2m}\left(1-\frac{E_{NR}-q\varphi}{2mc^2}\right)(\vec{\sigma}\cdot\vec{p})\,\psi_A=(E_{NR}-q\varphi)\,\psi_A$$

・ψ_A のみでは規格化されていない

$$\leftarrow \int dr\,(\psi_A^\dagger\psi_A+\psi_B^\dagger\psi_B)=1$$

・左辺に E_{NR} があって $H_{NR}(E_{NR})\psi_A=E_{NR}\psi_A$ の形になっている

・$i\hbar\,\mathbb{E}\cdot\mathbb{P}$ のような項が現われる(非エルミート)

(note) $\psi_B\sim\dfrac{\vec{\sigma}\cdot\vec{p}}{2mc}\psi_A$ なので規格化は

$$\int dr\;\psi_A^\dagger\left(1+\frac{p^2}{4m^2c^2}\right)\psi_A\sim 1$$

↓

ψ_A の代わりに $\Psi\equiv\underbrace{\left(1+\dfrac{\mathbb{P}^2}{8m^2c^2}\right)}_{\Omega}\psi_A$ を考える。

$$H_A\psi_A=E_{NR}\psi_A$$

$$\rightarrow\quad \Omega^{-1}H_A\,\Omega^{-1}\Psi=E_{NR}\,\Omega^{-1}\psi_A=E_{NR}\,\Omega^{-2}\Psi$$

(note)

$$\Omega^{-1} \sim 1 - \frac{\mathbb{P}^2}{8m^2c^2}$$

$$\Omega^{-2} \sim 1 - \frac{\mathbb{P}^2}{4m^2c^2}$$

$$\left(1-\frac{\mathbb{P}^2}{8m^2c^2}\right)\left[(\vec{\sigma}\cdot\vec{p})\frac{1}{2m}\left(1-\frac{E_{NR}-g\varphi}{2mc^2}\right)(\vec{\sigma}\cdot\vec{p})+g\varphi\right]\left(1-\frac{\mathbb{P}^2}{8m^2c^2}\right)\Psi$$

$$= E_{NR}\left(1-\frac{\mathbb{P}^2}{4m^2c^2}\right)\Psi$$

$$\Big[\frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}+g\varphi-\frac{\mathbb{P}^2}{8m^2c^2}\left(\frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}+g\varphi\right)-\left(\frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}+g\varphi\right)\frac{\mathbb{P}^2}{8m^2c^2}$$

$$-\frac{\vec{\sigma}\cdot\vec{p}}{2m}\left(\frac{E_{NR}-g\varphi}{2mc^2}\right)(\vec{\sigma}\cdot\vec{p})\Big]\Psi \sim E_{NR}\left(1-\frac{\mathbb{P}^2}{4m^2c^2}\right)\Psi$$

(note) $(\vec{\sigma}\cdot\vec{p})^2 = \vec{p}^{\,2}$

$$E_{NR}\,\mathbb{P}^2 = \frac{1}{2}\{E_{NR}, \mathbb{P}^2\}$$

$$\Big[\frac{\mathbb{P}^2}{2m}+g\varphi-\frac{\mathbb{P}^4}{8m^3c^2}+\frac{1}{8m^2c^2}\Big(\{\mathbb{P}^2, E_{NR}-g\varphi\}$$

$$-2(\vec{\sigma}\cdot\vec{p})(E_{NR}-g\varphi)(\vec{\sigma}\cdot\vec{p})\Big)\Big]\Psi$$

$$= E_{NR}\Psi.$$

(note)

$$\{A^2, B\} - 2ABA = [A, [A,B]]$$

$$A(AB-BA)-(AB-BA)A$$
$$= A^2B + BA^2 - 2ABA$$

$$y = (1+x)^{1/2}$$
$$y' = \frac{1}{2}(1+x)^{-\frac{1}{2}}$$
$$y'' = -\frac{1}{4}(1+x)^{-\frac{3}{2}}$$

$$\{ \mathbb{P}^2, E_{NR} - q\varphi \} - 2(\vec{\sigma}\cdot\vec{p})(E_{NR} - q\varphi)(\vec{\sigma}\cdot\vec{p})$$

$$= [(\vec{\sigma}\cdot\vec{p}), \underbrace{[\vec{\sigma}\cdot\vec{p}, E_{NR} - q\varphi]}_{= -\frac{\hbar}{i} q \vec{\sigma}\cdot \underbrace{\nabla\varphi}_{= -\mathbb{E}} = -i\hbar q \vec{\sigma}\cdot\vec{E}}]$$

$$= -i\hbar q (\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\vec{E}) + i\hbar q (\vec{\sigma}\cdot\vec{E})(\vec{\sigma}\cdot\vec{p})$$

$$= -i\hbar q (\vec{p}\cdot\vec{E}) + 2i\hbar q \cdot i\vec{\sigma}\cdot(\vec{E}\times\vec{p})$$

$$\uparrow$$

$$\nabla\times\mathbb{E} = 0$$

$$= -q\hbar^2(\nabla\cdot\mathbb{E}) - 2q\hbar\,\vec{\sigma}\cdot(\vec{E}\times\vec{p})$$

$$H_{NR} = \frac{\mathbb{P}^2}{2m} + q\varphi - \frac{\mathbb{P}^4}{8m^3c^2} - \frac{q\hbar\vec{\sigma}\cdot(\vec{E}\times\vec{p})}{4m^2c^2} - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\mathbb{E}$$

ダーウィン項

$$\uparrow$$

$$\sqrt{\mathbb{P}^2c^2 + m^2c^4} - mc^2$$
$$= \sqrt{m^2c^4\left(1 + \frac{\mathbb{P}^2}{m^2c^2}\right)} - mc^2$$
$$= mc^2\left(1 + \frac{\mathbb{P}^2}{2m^2c^2} - \frac{1}{8}\frac{\mathbb{P}^4}{m^4c^4} + \cdots\right) - mc^2$$
$$= \frac{\mathbb{P}^2}{2m} - \frac{\mathbb{P}^4}{8m^3c^2} + \cdots$$

中心ポテンシャル $g\varphi(r) = V(r)$ に対して

$$\mathbb{E} = -\nabla\varphi = -\frac{\mathbb{r}}{r}\frac{dV}{dr}\cdot\frac{1}{g}$$

$$-\frac{g\hbar}{4m^2c^2}\vec{\sigma}\cdot(\mathbb{E}\times\mathbb{p}) = \frac{\hbar}{4m^2c^2}\left(\frac{1}{r}\frac{dV}{dr}\right)\vec{\sigma}\cdot(\mathbb{r}\times\mathbb{p})$$

$$= \frac{1}{2m^2c^2}\left(\frac{1}{r}\frac{dV}{dr}\right)\vec{L}\cdot\vec{S}$$

スピン軌道力

§. 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) $[L_z, H] = [xp_y - yp_x,\ c\alpha_1 p_x + c\alpha_2 p_y + c\alpha_3 p_z]$

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

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

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

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

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

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

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

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

$\curvearrowright$

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

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

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

(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:

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

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

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

$$\downarrow$$

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

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

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

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

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

(see Edmonds, eq. 7.1.6)

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

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

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

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

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