7-3 Dirac方程式による水素原子

水素原子のDirac方程式

$$\left[-i\alpha\cdot\nabla+\beta m-\frac{Ze^2}{r}\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r})$$

$$\left\{\begin{array}{l} m:\text{電子の質量} \\ \text{陽子の運動は無視する.} \end{array}\right.$$

$$\hat{H}=\hat{\mathbf{p}}\cdot\alpha+m\beta-\frac{Ze^2}{r}\quad(\text{Hamiltonian})$$

$$(\hat{\mathbf{p}}=-i\hbar\nabla)$$

$\Downarrow$

保存量は何か?

(非相対論: $\hat{\mathbb{L}}=\mathbf{r}\times\hat{\mathbf{p}}$ が保存量)

$\Updownarrow$ $\hat{\mathbb{L}}$ は保存量とならない!!

$$\left\{\begin{array}{l} \mathbb{J}\equiv\mathbb{L}+\frac{1}{2}\sigma \\ K\equiv\beta(\sigma\cdot\mathbb{L}+1) \end{array}\right.\quad\text{が保存量}$$

$\Updownarrow$

$$\left\{\begin{array}{l} [\hat{H},\mathbb{J}]=0 \\ [\hat{H},K]=0 \end{array}\right.\quad\text{が示される}$$

(a) $[\hat{H}, \mathbb{J}] = 0$ の証明

$$\begin{cases} \hat{H} = \hat{\mathbb{P}}\cdot\alpha + m\beta - \frac{Ze^2}{r} \\ \mathbb{J} = \mathbb{L} + \frac{1}{2}\sigma \end{cases}$$

(1) $$[\hat{H}, L_x] = [\hat{\mathbb{P}}\cdot\alpha + m\beta - \frac{Ze^2}{r}, L_x]$$

$$= [\hat{P}_x\alpha_x + \hat{P}_y\alpha_y + \hat{P}_z\alpha_z, y\hat{P}_z - z\hat{P}_y]$$

$$= \alpha_y[\hat{P}_y, y]P_z - \alpha_z[P_z, z]\hat{P}_y$$

$$= -i(\alpha \times \hat{\mathbb{P}})_x$$

(2) $$[\hat{H}, \frac{1}{2}\sigma_x] = \frac{1}{2}[\hat{\mathbb{P}}\cdot\alpha + m\beta, \sigma_x]$$

$$= \frac{1}{2}\left\{\begin{pmatrix} m & \hat{\mathbb{P}}\cdot\sigma \\ \hat{\mathbb{P}}\cdot\sigma & -m \end{pmatrix}\begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} - \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}\begin{pmatrix} m & \hat{\mathbb{P}}\cdot\sigma \\ \hat{\mathbb{P}}\cdot\sigma & -m \end{pmatrix}\right\}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & [\hat{\mathbb{P}}\cdot\sigma, \sigma_x] \\ [\hat{\mathbb{P}}\cdot\sigma, \sigma_x] & 0 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & -2i(\hat{\mathbb{P}}\times\sigma)_x \\ -2i(\hat{\mathbb{P}}\times\sigma)_x & 0 \end{pmatrix} = i(\alpha \times \mathbb{P})_x$$

よって $$[\hat{H}, \mathbb{J}_x] = [\hat{H}, L_x] + [\hat{H}, \frac{1}{2}\sigma_x] = 0$$

(b) $K = \beta(\sigma\cdot\mathbb{L}+1) = \beta\left(\sigma\cdot\mathbb{J}-\frac{1}{2}\right)$

$$[\hat{H}, K] = \left[\hat{\mathbb{P}}\cdot\alpha + m\beta - \frac{Ze^2}{r},\ \beta\sigma\cdot\mathbb{J} - \frac{1}{2}\beta\right]$$

$$= [\hat{\mathbb{P}}\cdot\alpha,\ \beta\sigma\mathbb{J}] - [\hat{\mathbb{P}}\cdot\alpha,\ \tfrac{1}{2}\beta]$$

$$= [\hat{\mathbb{P}}\cdot\alpha,\ \beta\sigma]\mathbb{J} - (\hat{\mathbb{P}}\cdot\alpha)\beta$$

(但し $[\mathbb{J}, \hat{H}]=0$ を用いた)

一方 $[\hat{\mathbb{P}}\cdot\alpha, \beta\sigma] = \begin{pmatrix} 0 & \sigma\cdot\hat{\mathbb{P}} \\ \sigma\cdot\hat{\mathbb{P}} & 0 \end{pmatrix}\begin{pmatrix} \sigma & 0 \\ 0 & -\sigma \end{pmatrix} - \begin{pmatrix} \sigma & 0 \\ 0 & -\sigma \end{pmatrix}\begin{pmatrix} 0 & \sigma\cdot\hat{\mathbb{P}} \\ \sigma\cdot\hat{\mathbb{P}} & 0 \end{pmatrix}$

$$= \begin{pmatrix} 0 & -(\sigma\cdot\hat{\mathbb{P}})\sigma - \sigma(\sigma\cdot\hat{\mathbb{P}}) \\ (\sigma\cdot\hat{\mathbb{P}})\sigma + \sigma(\sigma\cdot\hat{\mathbb{P}}) & 0 \end{pmatrix}$$

ここで $\begin{cases} (\sigma\cdot\hat{\mathbb{P}})\sigma = \hat{\mathbb{P}} + i\,\sigma\times\hat{\mathbb{P}} \\ \sigma(\sigma\cdot\hat{\mathbb{P}}) = \hat{\mathbb{P}} - i\,\sigma\times\hat{\mathbb{P}} \end{cases}$ より

$[\hat{\mathbb{P}}\cdot\alpha, \beta\sigma] = \begin{pmatrix} 0 & -2\hat{\mathbb{P}} \\ 2\hat{\mathbb{P}} & 0 \end{pmatrix}$ よって

$$[\hat{H}, K] = \begin{pmatrix} 0 & -2\hat{\mathbb{P}}\cdot\mathbb{J} \\ 2\hat{\mathbb{P}}\cdot\mathbb{J} & 0 \end{pmatrix} - (\hat{\mathbb{P}}\cdot\alpha)\beta$$

$$= \begin{pmatrix} 0 & -\hat{\mathbb{P}}\sigma \\ \hat{\mathbb{P}}\sigma & 0 \end{pmatrix} - \begin{pmatrix} 0 & -\hat{\mathbb{P}}\cdot\sigma \\ \hat{\mathbb{P}}\cdot\sigma & 0 \end{pmatrix} = 0$$

(但し $\hat{\mathbb{P}}\cdot\mathbb{J} = \frac{1}{2}\hat{\mathbb{P}}\cdot\sigma$ を用いた)

No.

Date

[Dirac方程式による水素原子](まとめ)

- $\hat{H} = \hat{p}\cdot\alpha + m\beta - \frac{Ze^2}{r}$

- 保存量： J^2, J_z, K

- エネルギー固有値 E_{nj}

$$E_{nj} = m\left[1 - \frac{(Z\alpha)^2}{n^2 + 2\left(n - \left(j+\frac{1}{2}\right)\right)\left\{\sqrt{\left(j+\frac{1}{2}\right)^2 - (Z\alpha)^2} - \left(j+\frac{1}{2}\right)\right\}}\right]^{\frac{1}{2}}$$

$$\begin{cases} n = 1, 2, 3, \cdots \\ j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots \\ 1s_{1/2} : \quad K = -1 \\ 2p_{1/2} : \quad K = 1 \end{cases}$$

【 $1S_{1/2}$ (基底状態) 】

$$\boxed{E_{1S_{1/2}} = m\sqrt{1-(\alpha Z)^2}}$$

$$\psi_{(r)} = \begin{pmatrix} f(r) \\ \\ -i(\sigma\cdot\hat{r})\, g(r) \end{pmatrix} \frac{1}{\sqrt{4\pi}} \chi_s$$

$$\begin{cases} f(r) = N\rho^{\gamma}\dfrac{e^{-\rho}}{\rho} \\ \\ g(r) = N\rho^{\gamma}\dfrac{e^{-\rho}}{\rho}\left(\dfrac{\epsilon(\gamma-1) - Z\alpha}{\gamma+1-Z\alpha\epsilon}\right) \end{cases}$$

但し

$$\begin{cases} \rho \equiv (Z\alpha)\, r \\ \\ \gamma \equiv \sqrt{1-(Z\alpha)^2} \\ \\ \epsilon \equiv \dfrac{1}{Z\alpha}(1-\gamma) \end{cases}$$

$$\alpha = \frac{1}{137}$$