量子力学3 まとめレポート　5/29分

A

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(前回) $\vec{B}$ finite,

$\vec{L}$ circular motion 円運動
$\sim$ magnetization 磁化

$$\Delta E \sim -\overbrace{\frac{e}{2m}}\vec{L}\cdot\vec{B}$$

orbital magnetization
軌道磁化.

To be consistent with exp., : $\vec{L} \to \vec{L} + g\vec{S}$ $(g \sim 2)$

$\vec{S}$: $[S_i, S_j] = i\hbar\,\varepsilon_{ijk} S_k$, $\vec{S}^\dagger = \vec{S}$

$S^2 = \hbar^2 s(s+1)$, $s = 1/2$ $\longrightarrow$ spin 」.

☆ spin and Pauli matrix (パウリ行列).

$\vec{S}^2 |s.M\rangle = \hbar^2 s(s+1) |s.M\rangle$ $(s = 1/2)$

$S_z |s.M\rangle = \hbar M |s.M\rangle$, $M = -s, \underbrace{-s+1}_{=s} = -1/2, 1/2$

$\langle j.m+1 | J_+ | jm\rangle = \hbar\sqrt{(j-m)(j+m+1)}$ (*1)

$\langle j\,m-1 | J_- | jm\rangle = \hbar\sqrt{(j+m)(j-m+1)}$ (*2)

$$\begin{cases} M = +1/2, \uparrow \\ M = -1/2, \downarrow \end{cases}$$ として.

(*1) $\rightarrow$ $(j = 1/2,\ m = -1/2)$ $\langle\uparrow | S_+ | \downarrow\rangle = \hbar\sqrt{(\frac{1}{2}-(-\frac{1}{2}))(\frac{1}{2}-\frac{1}{2}+1)} = \hbar$, $S_+|\uparrow\rangle = 0$

(*2) $\rightarrow$ $(j = 1/2,\ m = 1/2)$ $\langle\downarrow | S_- | \uparrow\rangle = \hbar\sqrt{(\frac{1}{2}+\frac{1}{2})(\frac{1}{2}-\frac{1}{2}+1)} = \hbar$, $S_-|\downarrow\rangle = 0$

$S_z|\uparrow\rangle = \hbar M|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$ $(M = 1/2)$

$S_z|\downarrow\rangle = \hbar M|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$ $(M = -1/2)$

ここで行列表示

$$\begin{pmatrix}\langle\uparrow| \\ \langle\downarrow|\end{pmatrix} S_z \left(|\uparrow\rangle, |\downarrow\rangle\right) = \begin{pmatrix}\langle\uparrow|S_z|\uparrow\rangle & \langle\uparrow|S_z|\downarrow\rangle \\ \langle\downarrow|S_z|\uparrow\rangle & \langle\downarrow|S_z|\downarrow\rangle\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix} \equiv \frac{\hbar}{2}\sigma_z$$

$\sigma_z = \begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}$ (one of) the Pauli matrix

$\therefore\ S_z = \frac{\hbar}{2}\sigma_z .$

$\vec{S} = \frac{\hbar}{2}\vec{\sigma}\ ,\quad S_x = \frac{\hbar}{2}\sigma_x\ ,\quad S_y = \frac{\hbar}{2}\sigma_y$

$$S_\pm = S_x \pm i S_y \quad \longrightarrow \quad \begin{cases} S_x = \frac{1}{2}(S_+ + S_-) \\ S_y = \frac{1}{2i}(S_+ - S_-) \end{cases}$$

$$\begin{pmatrix} \langle\uparrow| \\ \langle\downarrow| \end{pmatrix} S_\pm \left(|\uparrow\rangle, |\downarrow\rangle\right) = \begin{pmatrix} \langle\uparrow|S_\pm|\uparrow\rangle^{=0} & \langle\uparrow|S_\pm|\downarrow\rangle^{\mp\left\{\substack{\hbar \\ 0}\right.} \\ \langle\downarrow|S_\pm|\uparrow\rangle_{\pm\left\{\substack{0 \\ \hbar}\right.} & \langle\downarrow|S_\pm|\downarrow\rangle_{=0} \end{pmatrix}$$

$$\left(\langle\uparrow|\downarrow\rangle = \langle \tfrac{1}{2}|-\tfrac{1}{2}\rangle = 0 \quad , \quad \langle\downarrow|\uparrow\rangle = 0 \right)$$

$$= \begin{cases} \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & (S_+) \\ \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & (S_-) \end{cases}$$

$$\longrightarrow S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y \qquad \sigma_y = \frac{1}{i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli matrix

$$\vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \ ,\quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ,\quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} ,\quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Vector of matrices

～基本的性質～

$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = E_2$ 　 2×2 unit matrix

$\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} -i\cdot i & 0 \\ 0 & i\cdot(-i) \end{pmatrix} = E_2$

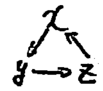
$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = E_2$ 　　　 $\underline{\therefore\ \sigma_i^2 = E_2}$

$\sigma_x\sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\sigma_z$

$\sigma_y\sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = i\sigma_x$

$\sigma_z\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = i\sigma_y$

C.P. cyclic permutation 循環置換



$\sigma_x^\dagger = \sigma_x\ ,\quad \sigma_y^\dagger = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^* = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y\ ,\quad \sigma_z^\dagger = \sigma_z$

$\vec{\sigma}^\dagger = \vec{\sigma}$ 　　　 $\vec{\sigma}$: hermite

$$\begin{pmatrix} (\sigma_x\sigma_y)^\dagger = (i\sigma_z)^\dagger \\ \sigma_y^\dagger\sigma_x^\dagger = -i\sigma_z^\dagger \\ \sigma_y\sigma_z = -i\sigma_z \end{pmatrix} \longrightarrow \sigma_i\sigma_j = -\sigma_j\sigma_i \quad (i \neq j)$$

$\sigma_i^2 = E_2$ であったから、

$(i \neq j)$ $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k$

$$\left.\begin{matrix} \mathrm{Tr}\,\sigma_x = 0 \\ \mathrm{Tr}\,\sigma_y = 0 \\ \mathrm{Tr}\,\sigma_z = 0 \end{matrix}\right) \longrightarrow \mathrm{Tr}\,\vec{\sigma} = \vec{0}$$

$$\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = \begin{cases} E_2 + E_2 = 2E_2 & i = j \\ 0 & i \neq j \end{cases} \qquad \therefore \{\sigma_i, \sigma_j\} = 2\delta_{ij}E_2$$

For a genetic 2×2 matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$,

4 real numbers a, b, c, d

(notation $E_2 \equiv \sigma_0 \to \sigma_x = \sigma_1, \sigma_y = \sigma_2, \sigma_z = \sigma_3$)

対応するはず..

$A = A_0\sigma_0 + A_1\sigma_1 + A_2\sigma_2 + A_3\sigma_3$

A_1, A_2, A_3, A_4, : 4

$$A = \sum_{i=0}^{3} A_i\sigma_i$$

$$\mathrm{Tr}\,A\sigma_0 = \mathrm{Tr}\,A = \sum_{i=0}^{3}\mathrm{Tr}(A_0\sigma_0^2 + A_1\underbrace{\sigma_1\sigma_0}_{\sigma_1} + A_2\underbrace{\sigma_2\sigma_0}_{\sigma_2} + A_3\underbrace{\sigma_3\sigma_0}_{\sigma_3})$$

$$= A_0\,\mathrm{Tr}\,\sigma_0 = 2A_0$$

$$\mathrm{Tr}\,A_1\sigma_1 = \sum_{i=0}^{3}\mathrm{Tr}(A_0\sigma_0\sigma_1 + A_1\sigma_1^2 + A_2\underbrace{\sigma_2\sigma_1}_{-i\sigma_3} + A_3\underbrace{\sigma_3\sigma_1}_{i\sigma_2})$$

$$= A_1\,\mathrm{Tr}\,\sigma_1^2 = 2A_1$$

....

$$\longrightarrow \begin{pmatrix} A_1 = \frac{1}{2}\mathrm{Tr}\,A\sigma_1 \\ A_2 = \frac{1}{2}\mathrm{Tr}\,A\sigma_2 \\ A_3 = \frac{1}{2}\mathrm{Tr}\,A\sigma_3 \end{pmatrix}$$

$$A = A_0\sigma_0 + A_1\sigma_1 + A_2\sigma_2 + A_3\sigma_3 = A_0\sigma_0 + \vec{A}\cdot\vec{\sigma} \qquad \vec{A} = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}$$

$$A_i = \frac{1}{2}\mathrm{Tr}\,A\sigma_i \qquad i = 0, 1, 2, 3$$

$$\vec{A}\cdot\vec{\sigma} = A_1\sigma_1 + A_2\sigma_2 + A_3\sigma_3$$

$$= A_1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + A_2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + A_3\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} A_3 & A_1 - iA_2 \\ A_1 + iA_2 & -A_3 \end{pmatrix}$$

$A_0 = \mathrm{Tr}A$

$\to$ if $\mathrm{Tr}A = 0$, $A = \vec{A}\cdot\vec{\sigma}$ となる $\exists\vec{A}$ $\quad A^\dagger = A$, $\vec{A}$: real $(\vec{\sigma}^\dagger = \vec{\sigma})$

A, B : 2×2 matrix

$A = (\vec{A}\cdot\vec{\sigma})$, $B = (\vec{B}\cdot\vec{\sigma})$

$A\cdot B = (\vec{A}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma}) = \vec{A}\cdot\vec{B}\,\sigma_0 + i\vec{\sigma}(\vec{A}\times\vec{B})$ (Dirac) formula

product of the matrices 行列の積

$$(\because)\ (\vec{A}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma}) = A_i\sigma_i B_j\sigma_j \qquad i=1\sim3,\ j=1\sim3,$$

$$= A_i B_j \sigma_i\sigma_j$$

$$= \sum_{i=j} A_iB_i\sigma_i^2 + \sum_{i\neq j} A_iB_j \underbrace{\sigma_i\sigma_j}_{i\varepsilon_{ijk}\sigma_k}$$

$$= \sum_{i=0}^{3} A_iB_i\sigma_0 + \sum_{i,j,k} \underbrace{A_iB_j\, i\,\varepsilon_{ijk}}_{i(A\times B)_k}\sigma_k$$

$$= (\vec{A}\cdot\vec{B})\sigma_0 + i\vec{\sigma}\cdot(\vec{A}\times\vec{B}) \qquad \blacksquare$$

ex) $H = -\mu\underbrace{\vec{S}\cdot\vec{B}}_{\text{scalor}}$ のエネルギーは?

$\vec{B}/\!/\vec{z}$

$$H = -\mu \underbrace{S_z}_{\frac{\hbar\sigma_z}{2}} B = -\frac{\mu B\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \begin{pmatrix}-\frac{\hbar}{2}\mu B & 0\\ 0 & \frac{\hbar}{2}\mu B\end{pmatrix} \longrightarrow \pm\frac{1}{2}\hbar\mu B.$$

<u>another way</u>

$$\mathrm{Tr}\,H = -\mu\,\mathrm{Tr}\,\vec{S}\cdot\vec{B} = -\mu\hbar\vec{B}\cdot\mathrm{Tr}\,\vec{\sigma} = 0$$

eigen value E_1, E_2

$$\mathrm{Tr}\,H = E_1 + E_2 = 0 \qquad E_2 = -E_1$$

$$H^2 = \left(\frac{\mu\hbar}{2}\vec{B}\cdot\vec{\sigma}\right)^2 = \left(\frac{\mu\hbar}{2}\right)^2(\vec{B}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma})$$

$$= \left(\frac{\mu\hbar}{2}\right)^2\left(\vec{B}\cdot\vec{B}\sigma_0 + i\vec{\sigma}\cdot\underbrace{\vec{B}\times\vec{B}}_{0}\right)$$

$$= \left(\frac{\mu\hbar}{2}\right)^2|\vec{B}|^2\sigma_0 \qquad E_1 = \frac{\mu\hbar}{2}|\vec{B}| \ /\!/ \ \lrcorner$$

☆ Time reversal symmetry　時間反転対称性

symmetry operation 対称操作 $\longleftrightarrow$ unitary operator

Time reversal $\longleftrightarrow$ anti-unitary operation

$$\Theta = \underbrace{i\sigma_2}_{\text{unitary}} \underbrace{K}_{\text{complex conjugate}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} K \qquad i\sigma_2 = i\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$(i\sigma_2)^\dagger = -i\sigma_2^\dagger = -i\sigma_2$$

$$(i\sigma_2)^\dagger i\sigma_2 = (-i\sigma_2)(i\sigma_2) = \sigma_2^2 = E_2 . \qquad i\sigma_2 : \text{unitary}$$

Θ : time reversal operator

$$\Theta\sigma_1\Theta^{-1} = i\sigma_2(\sigma_1)^*(-i\sigma_2) = \sigma_2\sigma_1^*\sigma_2 = \sigma_2\sigma_1\sigma_2 = i\sigma_2\sigma_3 = i^2\sigma_1 = -\sigma_1$$

$$\Theta\sigma_2\Theta^{-1} = i\sigma_2(\sigma_2)^*(-i\sigma_2) = \sigma_2\sigma_2^*\sigma_2 = -\sigma_2^3 = -\sigma_2$$

$$\Theta\sigma_3\Theta^{-1} = i\sigma_2(\sigma_3)^*(-i\sigma_2) = \sigma_2\sigma_3^*\sigma_2 = \sigma_2\sigma_3\sigma_2 = i\sigma_1\sigma_2 = i^2\sigma_3 = -\sigma_3$$

$$\Theta\vec{\sigma}\Theta^{-1} = -\vec{\sigma}$$

$$\Theta\vec{S}\Theta^{-1} = -\vec{S}$$

cf) $\vec{L} = \vec{r}\times\vec{p}$

$$\left.\begin{aligned} \Theta\vec{r}\Theta^{-1} &= \vec{r} \\ \Theta\vec{p}\Theta^{-1} &= \Theta\frac{\hbar}{i}\nabla\Theta^{-1} = -\vec{p} \end{aligned}\right) \quad \Theta\vec{L}\Theta^{-1} = -\vec{L}$$

$$\Theta\vec{L}\cdot\vec{S}\Theta^{-1} = (-\vec{L})\cdot(-\vec{S}) = \vec{L}\cdot\vec{S}$$

spin orbit interaction invariant

Θ invariant