量子力学3 6/1　　　　　　　　　　　　201310873 田村 啓

授業の記録【事実・知識】　　　　　　　　メモ【考え・気持ち・自主学習】

Spin-orbital function スピン軌道関数

Zeeman effect. $\vec{B} \neq \vec{0}$

$\Delta H \sim \vec{L}\cdot\vec{B}$, $\vec{\mu} \sim \vec{S}$

$\vec{\mu}\cdot\vec{B}$　　$\vec{S}^2 = S(S+1)$

$S = \frac{1}{2}$

$S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$

$S_z|\downarrow\rangle = \frac{\hbar}{2}|\downarrow\rangle$

$H = H_0 - \frac{e}{2m} g \vec{B}\cdot\vec{S}$

$i\hbar \frac{\partial}{\partial t}\psi = H_0 \psi$

$H_0 = -\frac{\hbar^2 \Delta}{2m} + V(\vec{r})$

$\psi(\vec{r}) \longrightarrow |\psi(\vec{r})\rangle = \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{pmatrix}$

internal degree of freedom
内部自由度

$\psi_\mu(r)$　$\mu = \uparrow, \downarrow$　spin-orbital fn.

- Time-reversal operator Θ : $i\sigma_y K$

K : c.c.

Unitary transformation　　$i\sigma_y = i\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

K^+ 反ユニタリ
Anti-unitary

$\vec{r}$: $\Theta \vec{r} \Theta^{-1} = i\sigma_y K(\vec{r})(i\sigma_y)^{-1}K^{-1}$　　$K^{-1} = K$, $KK^{-1} = 1$

$= i\sigma_y (\vec{r})^* (i\sigma_y)^{-1} = \vec{r}^* = \vec{r}$

座標　　　不変
coordinate $\vec{r}$: invariant

$\Theta \vec{p} \Theta^{-1} = i\sigma_y (\vec{p})^* (i\sigma_y)^{-1} = \vec{p}^* = \frac{\hbar}{-i}\vec{\nabla} = -\vec{p}$

$\Theta \vec{L} \Theta^{-1} = \Theta \vec{r} \Theta^{-1} \times \Theta \vec{p} \Theta^{-1}$

$= \vec{r} \times (-\vec{p}) = -\vec{L}$

$\vec{S} = \frac{\hbar}{2}\sigma$　　$\sigma_x^* = \sigma_x$　$\sigma_x \sigma_y = i\sigma_z$

$\Theta \sigma_x \Theta^{-1} = i\sigma_y \sigma_x^* (-i\sigma_y) = \sigma_y \cdot i\sigma_z = -\sigma_x$

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

$\Theta \sigma_z \Theta^{-1} = i\sigma_y \sigma_z (-i\sigma_y) = i\sigma_x \sigma_y = -\sigma_z$

$\Theta \vec{\sigma} \Theta^{-1} = -\vec{\sigma}$,　$\Theta \vec{S} \Theta^{-1} = -\vec{S}$
$(\Theta : \vec{S} \to -\vec{S})$

Zeeman effect $\vec{B} \neq \vec{0}$
$H = H_0 - \frac{e}{2m}\vec{B}\cdot(\vec{L} + g\vec{S})$

$\Theta H \Theta^{-1} \neq H$

$\vec{B}$: time reversal breaking

$H_{SO} = f \cdot \vec{L}\cdot\vec{S}$
↑ spin orbit interaction
important for heavy atom
(周期表の下の方の原子)

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

H_{SO} : time reversal invariant

$H_0 = \frac{\vec{p}^2}{2m} + V(r) \longrightarrow \frac{(-\vec{p})^2}{2m} + V(r) = H_0$
invariant

$i\hbar \frac{\partial}{\partial t}\Psi = H\Psi$

$\Psi(r) = \begin{pmatrix} \Psi_\uparrow \\ \Psi_\downarrow \end{pmatrix}$　　$\leftrightarrow H\psi = E\psi$

$\Psi(\vec{r}, t) = e^{-Et/\hbar}\psi(\vec{r})$
stationary state 定常状態

$H\psi_j = E_j \psi_j$

$\Theta H \Theta^{-1} = H \longrightarrow$ degeneracy 縮退

$i \neq j$. $E_i = E_j$　Kramers degeneracy (クラマース)

$H = -\frac{\hbar^2}{2m}\Delta + V(r) + f(r)(\vec{r} \times \frac{\hbar}{i}\vec{\nabla})\cdot\vec{S}$
independent of the detail 詳細によらない

$H\psi = E\psi$

$\Theta(H\psi) = \Theta H \Theta^{-1}\Theta\psi = E\Theta\psi$

$\psi^\Theta \equiv \Theta\psi$ とすると $\begin{cases} H\psi = E\psi \\ H\psi^\Theta = E\psi^\Theta \end{cases}$

degenerate?
for any operator (Θ)

作成年月日:　　年　　月　　日

ψとψ^{Θ}が異なるなら縮退しているということで

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

$$\psi^{\Theta} = \Theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = i\sigma_2 K \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_\uparrow^* \\ \psi_\downarrow^* \end{pmatrix}$$

$$= \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}$$

$$\langle \psi | \psi^* \rangle = (\psi_\uparrow^*, \psi_\downarrow^*) \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}$$

$$= \psi_\uparrow^* \psi_\downarrow^* - \psi_\downarrow^* \psi_\uparrow^* = 0$$

orthogonal each other

$\|\psi\|^2 = \|\psi^{\Theta}\|^2 = 1$ $\downarrow$

Kramers deg.

Another view $\quad \Theta = i\sigma_2 K = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} K$

$\forall |\psi\rangle, |\phi\rangle$

$$|\Theta\psi\rangle = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}, \quad |\Theta\phi\rangle = \begin{pmatrix} \phi_\downarrow^* \\ -\phi_\uparrow^* \end{pmatrix}$$

$$\langle \Theta\psi | \Theta\phi \rangle = (\psi_\downarrow, -\psi_\uparrow) \begin{pmatrix} \phi_\downarrow^* \\ -\phi_\uparrow^* \end{pmatrix}$$

$$= \phi_\downarrow^* \psi_\downarrow + \phi_\uparrow^* \psi_\uparrow$$

$$= \langle \phi | \psi \rangle$$

ここで

$\phi = \Theta\psi$ とすると

$$\langle \Theta\psi | \Theta^2 \psi \rangle = \langle \Theta\psi | \psi \rangle$$

$$\Theta^2 = (i\sigma_2 K)^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^2 = -E$$

$$= -1$$

$$\Rightarrow \quad -\langle \Theta\psi | \psi \rangle = \langle \Theta\psi | \psi \rangle = 0$$

$\therefore$ $|\psi\rangle$ と $|\Theta\psi\rangle$ は直交

- multiple of spins and orbital angular momenta

if $\vec{S}_1, \vec{S}_2, \cdots, \vec{S}_N$

$\downarrow \quad \downarrow$

$|\sigma_1\rangle, |\sigma_2\rangle, \cdots \qquad \sigma_i = \uparrow, \downarrow$

state $|\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \cdots \otimes |\sigma_N\rangle$

$$= |\sigma_1 \, \sigma_2 \, \cdots \, \sigma_N\rangle$$

$\uparrow \; \uparrow \; \cdots \; \uparrow$

$\downarrow \; \downarrow \; \cdots \; \downarrow$ $\quad$ N spin state

$$\Theta = (i\sigma_y) \otimes (i\sigma_y^2) \otimes \cdots \otimes (i\sigma_y^N) K$$

$$\Theta^2 = \underbrace{(i\sigma_2)^2}_{-1} \otimes \underbrace{(i\sigma_2^2)^2}_{-1} \otimes \cdots \otimes \underbrace{(i\sigma_2^N)^2}_{-1} \underbrace{K^2}_{1} = (-1)^N$$

$\Theta^2 = (-1)^N$

only if N: odd

$\Theta^2 = -1 \longrightarrow$ Kramers deg.

★ 2 spins (independent)

$\vec{S}_1 = \frac{\hbar}{2}\vec{\sigma}_1$

$\vec{S}_2 = \frac{\hbar}{2}\vec{\sigma}_2$ $\qquad \vec{S} = \vec{S}_1 + \vec{S}_2$ $\quad$ addition of spins

$\vec{S}_1 = |\uparrow\rangle_1, |\downarrow\rangle_1 \qquad \vec{S}_1 : |m\rangle_1$

$\vec{S}_2 = |\uparrow\rangle_2, |\downarrow\rangle_2 \qquad \vec{S}_2 : |m\rangle_2$

$$|m_1, m_2\rangle \equiv |m_1\rangle_1 |m_2\rangle_2$$
$$= |m_1\rangle_1 \otimes |m_2\rangle_2$$

$$\vec{S}_1 |m_1 m_2\rangle = (\vec{S}_1 |m_1\rangle_1) |m_2\rangle_2$$
$$= (\vec{S}_1 |m_1\rangle \otimes |m_2\rangle$$
$$= (\vec{S}_1 |m_1\rangle) |m_2\rangle$$

$$\vec{S}_2 |m_1 m_2\rangle = |m_1\rangle \vec{S}_2 |m_2\rangle$$

$$(\vec{S}_1 + \vec{S}_2)|m_1 m_2\rangle = \vec{S}_1 |m_1\rangle |m_2\rangle + |m_1\rangle \vec{S}_2 |m_2\rangle$$

$$S^2 = S_1^2 + S_2^2$$

$$S^2 |\uparrow\uparrow\rangle = (S_1^2 |\uparrow\rangle) |\uparrow\rangle + |\uparrow\rangle S_2^2 |\uparrow\rangle$$
$$= \frac{\hbar}{2} |\uparrow\rangle |\uparrow\rangle + |\uparrow\rangle \frac{\hbar}{2} |\uparrow\rangle$$
$$= \hbar |\uparrow\rangle |\uparrow\rangle = \hbar |\uparrow\uparrow\rangle$$

$S^2 |M\rangle = \hbar |M\rangle, \quad |\uparrow\uparrow\rangle = |M = 1\rangle$

$\rightarrow S \geq 1 \qquad \vec{S}$: Angular momentum?

$$\left.\begin{aligned} [S_1^i, S_1^j] &= i\hbar \varepsilon^{ijk} S_1^k \\ [S_2^i, S_2^j] &= i\hbar \varepsilon^{ijk} S_2^k \end{aligned}\right\} \rightarrow [S_1^i, S_2^j] = 0$$

$\vec{S}_1, \vec{S}_2$: independent

$$[S_1^i + S_2^i, \; S_1^j + S_2^j] = [S_1^i, S_1^j] + [S_2^i, S_2^j]$$
$$= i\hbar \varepsilon^{ijk} (S_1^k + S_2^k)$$

$\vec{S} = \vec{S}_1 + \vec{S}_2$ $\quad$ addition of angular momentum

$$[S^i, S^j] = i\hbar \varepsilon^{ijk} S^k$$

$\vec{S}$: angular momentum