量子力学3 まとめレポート 6/2分

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spin-orbital function スピン軌道関数

Zeeman effect より $\vec{B} \neq 0$ では $\Delta H \sim \vec{L}\cdot\vec{B}$, $\vec{\mu}\cdot\vec{B}$ $(\vec{\mu} \sim \vec{S})$

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

また $\begin{cases} S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle \\ S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle \end{cases}$

$\longrightarrow$ $H = H_0 - \frac{e}{2m} g \vec{B}\cdot\vec{S}$ $\longrightarrow$ $\uparrow, \downarrow$ の自由度が出てきた

今までは. $i\hbar \frac{\partial}{\partial t}\psi = H_0\psi$ これから

$H_0 = -\frac{\hbar}{2m}\Delta + V(\vec{r})$ $\longrightarrow$ $|\psi(r)\rangle = \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{pmatrix}$

2 components

internal degree of random 内部自由度

この $\psi_\mu(r)$: spin-orbital function.

$\mu = \uparrow, \downarrow$

(復習) Time-reversal operator $\Theta = i\sigma_y K$ K : complex conjugate

$i\sigma_y = i\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$: real unitary

$K^\dagger$: anti-unitary tr.

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

$= i\sigma_y(\vec{r})^*(i\sigma_y)^{-1} = \vec{r}^* = \vec{r}$. coordinate $\vec{r}$: invariant.

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

$\Theta : \vec{p} \longmapsto -\vec{p}$

$\vec{L} = \vec{r}\times\vec{p}$: $\Theta\vec{L}\Theta^{-1} = \Theta\vec{r}\Theta^{-1}\times\Theta\vec{p}\Theta^{-1} = \vec{r}\times(-\vec{p}) = -\vec{L}$.

$\Theta : \vec{L} \longmapsto -\vec{L}$

$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ では? $(i\sigma_y)^{-1} = i^{-1}\sigma_y^{-1} = -i\sigma_y$

$\Theta\sigma_x\Theta^{-1} = i\sigma_y\sigma_x^*(-i\sigma_y) = i\sigma_y\sigma_z = i^2\sigma_x = -\sigma_x$

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

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

以上から.

$$\Theta \vec{\sigma} \Theta^{-1} = -\vec{\sigma} \quad \therefore \quad \Theta \vec{S} \Theta^{-1} = -\vec{S} \qquad \Theta : \vec{S} \mapsto -\vec{S}.$$

Zeeman effect より.

$$H = H_0 - \frac{e}{2m}\vec{B}(\vec{L}+g\vec{S})$$ であった。(Dirac eq. の $(\frac{v}{c})$ のオーダー)

もし $\vec{B}\neq\vec{0}$ なら $\Theta H \Theta^{-1} \neq H$ であり. $\vec{B}$: time-reversal breaking.

$H_{so} = f\vec{L}\cdot\vec{S}$: spin-orbital interaction ($(\frac{v}{c})^2$ のオーダー)

→ Important for heavy atom  peridic table (周期表).

$$\left.\begin{aligned} &\Theta H_{so}\Theta^{-1} = f(-\vec{L})\cdot(-\vec{S}) = H_{so} \\ &H_0 = \frac{\vec{p}^2}{2m} + V(\vec{r}) \underset{\Theta}{\mapsto} \frac{(-\vec{p})^2}{2m}+V(\vec{r}) = H_0. \end{aligned}\right) \text{ time reversal invariant.}$$

$\Theta H \Theta^{-1} = H$ time-reversal inv. のとき ($H\psi = E\psi$ から)

$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$ となる $\Psi = \begin{pmatrix}\Psi_\uparrow\\ \Psi_\downarrow\end{pmatrix}$ を考える.

$\Psi(\vec{r},t) = e^{-\frac{iEt}{\hbar}}\psi(\vec{r})$: stationary state (定常状態).

また $H\psi_j = E_j\psi_j$

⇒ $\Theta H^{-1}\Theta = H$ → degeneracy　Kramers degeneracy
クラマーズ縮退

ただし, $i\neq j$　$E_i = E_j$

ex) spin orbit

$$H = -\frac{\hbar^2}{2m}\Delta + V(r) + f(r)\left(\vec{r}\times\frac{\hbar}{i}\nabla\right)\cdot\vec{S}$$ である.

これは系の詳細に依らない。 independent of the detail.

$\Theta(H\psi) = E\Theta\psi$ を考える.

$= \underbrace{\Theta H \Theta^{-1}}_{=H}\Theta\psi$

$\rightarrow$ $H\Theta\psi = E\Theta\psi$ $\qquad \psi^{\Theta} \equiv \Theta\psi$

$H\psi^{\Theta} = E\psi^{\Theta}$

$$\begin{cases} \psi \longleftrightarrow E \\ \psi^{\Theta} \longleftrightarrow E \end{cases} \longrightarrow \text{degenerate ?}$$

(for any op. Θ)

if ψ and ψ^{Θ} are different, $\longrightarrow$ degeneracy

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

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

$\rightarrow \langle\psi|\psi^{\Theta}\rangle = (\psi_\uparrow^*, \psi_\downarrow^*)\begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix} = \psi_\uparrow^*\psi_\downarrow^* - \psi_\downarrow^*\psi_\uparrow^* = 0.$

$\Rightarrow$ orthogonal each other

$\|\psi\|^2 = \|\psi^{\Theta}\|^2 = 1$. $\qquad$ $\underline{\longrightarrow \text{degenerate} \Rightarrow \text{Kramers deg.}}$

<u>Another view</u>

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

$\langle\Theta\psi|\Theta\phi\rangle$ を考える。

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

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

<u>$\phi = \Theta\psi$ のとき</u>.

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

$\Theta^2 = (i\sigma_y K)^2 = \left(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}K\right)^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -E_2 \equiv -1$.

$\Theta^2 \equiv -1$

$= -\langle\Theta\psi|\psi\rangle$ $\qquad \therefore \langle\Theta\psi|\psi\rangle = 0.$

$|\psi\rangle \longleftrightarrow |\Theta\psi\rangle$: orthogonal multiple of spins and orbital angular momentum.

(多数のスピン).

if $\vec{S_1}, \vec{S_2}, \cdots \vec{S_N}$ $\qquad \vec{S_1} \leftrightarrow |\sigma_1\rangle \quad \sigma_1 = \uparrow, \downarrow$

state $\underset{(\sigma_1=\uparrow,\downarrow}{|\sigma_1\rangle} \otimes \underset{\sigma_2=\uparrow,\downarrow}{|\sigma_2\rangle} \otimes \cdots \otimes \underset{\sigma_N=\uparrow,\downarrow)}{|\sigma_N\rangle} = |\sigma_1, \cdots \sigma_N\rangle$: N spin state.

$\rightarrow \Theta = (i\sigma_y^1) \otimes (i\sigma_y^2) \otimes \cdots \otimes (i\sigma_y^N) K.$

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

$= (-1)^N$ only if N : odd $\rightarrow \Theta^2 = -1 \leftrightarrow$ Kramers deg.

☆ 2 spins (independent)

$\vec{S_1} = \frac{\hbar}{2}\vec{\sigma_1}$, $\vec{S_2} = \frac{\hbar}{2}\vec{\sigma_2} \longrightarrow \vec{S} = \vec{S_1} + \vec{S_2}$: addition of spins.

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

$\vec{S_2} : |\uparrow\rangle_2, |\downarrow\rangle_2, \quad |m\rangle_2.$

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

$\vec{S_1}|m_1, m_2\rangle = (\vec{S_1}|m_1\rangle_1)|m_2\rangle_2 = (\vec{S_1}|m_1\rangle) \otimes |m_2\rangle = (\vec{S_1}|m_1\rangle)|m_2\rangle.$

同様に.

$\vec{S_2}|m_1, m_2\rangle = |m_1\rangle \vec{S_2}|m_2\rangle$

$(\vec{S_1} + \vec{S_2})|m_1, m_2\rangle = \vec{S_1}|m_1\rangle|m_2\rangle + |m_1\rangle\vec{S_2}|m_2\rangle$

また $S^z = S_1^z + S_2^z$

$S^z|\uparrow\uparrow\rangle = (S_1^z|\uparrow\rangle)|\uparrow\rangle + |\uparrow\rangle S_2^z|\uparrow\rangle$

$= \frac{\hbar}{2}|\uparrow\rangle|\uparrow\rangle + |\uparrow\rangle\frac{\hbar}{2}|\uparrow\rangle = (\frac{\hbar}{2} + \frac{\hbar}{2})|\uparrow\uparrow\rangle = \hbar|\uparrow\uparrow\rangle$

加えて $S^z|M\rangle = \hbar|M\rangle$ より. $|\uparrow\uparrow\rangle = |M(=1)\rangle$

$\rightsquigarrow S_z \geq 1$ $\quad$ S_z : Angular momentum.

$$[S_1^i, S_1^j] = i\hbar\,\varepsilon^{ijk} S_1^k$$
$$[S_2^i, S_2^j] = i\hbar\,\varepsilon^{ijk} S_2^k$$
$$\rightarrow [S_1^i, S_2^j] = 0$$

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

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

$\vec{S} = \vec{S}_1 + \vec{S}_2 \quad [S^i, S^j] = i\hbar\,\varepsilon^{ijk} S^k$

$\vec{S}$: angular momentum

Addition of angular momentum