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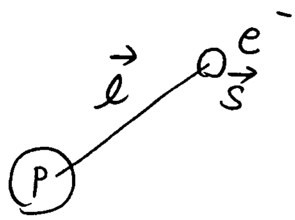
6.2. スピンと軌道角運動量の合成

例) 水素原子



$\mathbf{j} = \mathbf{l} + \mathbf{s}$

$\mathbf{s}$: $|\uparrow\rangle, |\downarrow\rangle$

$\mathbf{l}$: $|Y_{lm}\rangle \quad (-l \leq m \leq l)$

状態の分類 :

$m = l + \frac{1}{2}$:	$\vert Y_{ll}\rangle\vert\uparrow\rangle$	← 1つのみ
$m = l - \frac{1}{2}$:	$\vert Y_{l\,l-1}\rangle\vert\uparrow\rangle$, $\vert Y_{ll}\rangle\vert\downarrow\rangle$	← 2つの状態
$m = l - \frac{3}{2}$:	$\vert Y_{l\,l-2}\rangle\vert\uparrow\rangle$, $\vert Y_{l\,l-1}\rangle\vert\downarrow\rangle$	
$\vdots$		
$m = -l + \frac{1}{2}$:	$\vert Y_{l\,-l}\rangle\vert\uparrow\rangle$, $\vert Y_{l\,-l+1}\rangle\vert\downarrow\rangle$	
$m = -l - \frac{1}{2}$:	$\vert Y_{l\,-l}\rangle\vert\downarrow\rangle$	← 1つ

計 $(2l+1) \times 2$ こ の状態

→ $j = l + \frac{1}{2}$, $\quad -l - \frac{1}{2} \leq m \leq l + \frac{1}{2} \quad$ ($2l+2$ こ)

と $j = l - \frac{1}{2}$, $\quad -l + \frac{1}{2} \leq m \leq l - \frac{1}{2} \quad$ ($2l$ こ)

の状態に分類しなおす。

$(\mathbf{j}^2, j_z, \mathbf{l}^2, \mathbf{s}^2)$ の同時固有状態をつくる。

◦ (note) スピン・軌道力 : $V = \alpha \vec{l} \cdot \vec{s}$

$\mathbf{j}^2 = \mathbf{l}^2 + \mathbf{s}^2 + 2\mathbf{l}\cdot\mathbf{s} \quad \rightarrow \quad V = \frac{\alpha}{2}\left(\underline{\mathbf{j}^2} - \underline{\mathbf{l}^2} - \underline{\mathbf{s}^2}\right)$

$\Downarrow$

$\mathbf{j}^2$ と $\mathbf{l}^2$ と $\mathbf{s}^2$ の同時固有状態

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$$\vec{j}^2 |Y_{\ell\ell}\rangle|\uparrow\rangle = \hbar^2\left(\ell(\ell+1)+\frac{1}{2}\left(\frac{1}{2}+1\right)+2\ell\cdot\frac{1}{2}\right)|Y_{\ell\ell}\rangle|\uparrow\rangle$$
$$= \hbar^2\left(\ell^2+2\ell+\frac{3}{4}\right)|Y_{\ell\ell}\rangle|\uparrow\rangle$$
$$= \hbar^2\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right)|Y_{\ell\ell}\rangle|\uparrow\rangle$$

- $|j=\ell+\frac{1}{2},\ m=\ell+\frac{1}{2}\rangle = |Y_{\ell\ell}\rangle|\uparrow\rangle$

- $|j=\ell+\frac{1}{2},\ m=\ell-\frac{1}{2}\rangle \propto j_-\ |Y_{\ell\ell}\rangle|\uparrow\rangle$

$$= (\ell_-|Y_{\ell\ell}\rangle)|\uparrow\rangle + |Y_{\ell\ell}\rangle(s_-|\downarrow\rangle)$$
$$= \sqrt{(\ell-\ell+1)(\ell+\ell)}\ |Y_{\ell\ell-1}\rangle|\uparrow\rangle + |Y_{\ell\ell}\rangle|\downarrow\rangle$$
$$= \sqrt{2\ell}\ |Y_{\ell\ell-1}\rangle|\uparrow\rangle + |Y_{\ell\ell}\rangle|\downarrow\rangle$$

$\ell_-|Y_{\ell m}\rangle = \sqrt{\ell(\ell+1)-m(m-1)} \times |Y_{\ell m-1}\rangle$

- $|j=\ell+\frac{1}{2},\ m=\ell-\frac{1}{2}\rangle$ に直交する状態は $|j=\ell-\frac{1}{2},\ m=\ell-\frac{1}{2}\rangle$:

$$|j=\ell-\frac{1}{2},\ m=\ell-\frac{1}{2}\rangle \propto |Y_{\ell\ell-1}\rangle|\uparrow\rangle-\sqrt{2\ell}\,|Y_{\ell\ell}\rangle|\downarrow\rangle$$

- 一般の $|j=\ell+\frac{1}{2},\ m\rangle$ 及び $|j=\ell-\frac{1}{2},\ m\rangle$ は $|j=\ell\pm\frac{1}{2},\ m=\pm\frac{1}{2}\rangle$ に j_- を何回か作用して作ることができる。

$\downarrow$

$$|j=\ell\pm\frac{1}{2},\ m_\ell+\frac{1}{2}\rangle = \alpha_\pm\,|Y_{\ell m_\ell}\rangle|\uparrow\rangle+\beta_\pm\,|Y_{\ell m_\ell+1}\rangle|\downarrow\rangle.$$

$m \backslash j$	$\ell+\frac{1}{2}$	$\ell-\frac{1}{2}$
$\ell+\frac{1}{2}$	$|Y_{\ell\ell}\rangle|\uparrow\rangle$ $\boxed{\downarrow j_-}$	
$\ell-\frac{1}{2}$	$\sqrt{2\ell}\,|Y_{\ell\ell-1}\rangle|\uparrow\rangle + |Y_{\ell\ell}\rangle|\downarrow\rangle$ $\longrightarrow$ $\boxed{\downarrow j_-}$	$|Y_{\ell\ell-1}\rangle|\uparrow\rangle - \sqrt{2\ell}\,|Y_{\ell\ell}\rangle|\downarrow\rangle$ $\boxed{\downarrow j_-}$
$\ell-\frac{3}{2}$		

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$$l_- |Y_{11}\rangle = \sqrt{2}\,|Y_{10}\rangle$$
$$l_- |Y_{10}\rangle = \sqrt{2}\,|Y_{1-1}\rangle$$

例) $l=1$ と s の合成 : $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$

- $\left|\frac{3}{2}\ \frac{3}{2}\right\rangle = |Y_{11}\rangle|\uparrow\rangle$

- $j_- \left|\frac{3}{2}\ \frac{3}{2}\right\rangle = \sqrt{2}\,|Y_{10}\rangle|\uparrow\rangle + |Y_{11}\rangle|\downarrow\rangle$

$\downarrow$

$$\left|\frac{3}{2}\ \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\,|Y_{10}\rangle|\uparrow\rangle + \frac{1}{\sqrt{3}}\,|Y_{11}\rangle|\downarrow\rangle$$

- $\left|\frac{1}{2}\ \frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\,|Y_{10}\rangle|\uparrow\rangle - \sqrt{\frac{2}{3}}\,|Y_{11}\rangle|\downarrow\rangle$

- $j_- \left|\frac{3}{2}\ \frac{1}{2}\right\rangle = \frac{2}{\sqrt{3}}\,|Y_{1-1}\rangle|\uparrow\rangle + \sqrt{\frac{2}{3}}\,|Y_{10}\rangle|\downarrow\rangle \times \alpha$

$\downarrow$

$$\left|\frac{3}{2}\ -\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\,|Y_{1-1}\rangle|\uparrow\rangle + \sqrt{\frac{2}{3}}\,|Y_{10}\rangle|\downarrow\rangle$$

- $j_- \left|\frac{3}{2}\ -\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\,|Y_{1-1}\rangle|\downarrow\rangle + \frac{2}{\sqrt{3}}\,|Y_{1-1}\rangle|\downarrow\rangle$

$\downarrow$

$$\left|\frac{3}{2}\ -\frac{3}{2}\right\rangle = |Y_{1-1}\rangle|\downarrow\rangle$$

- $j_- \left|\frac{1}{2}\ \frac{1}{2}\right\rangle = \frac{\sqrt{2}}{\sqrt{3}}\,|Y_{1-1}\rangle|\uparrow\rangle + \frac{1}{\sqrt{3}}\,|Y_{10}\rangle|\downarrow\rangle - \frac{2}{\sqrt{3}}\,|Y_{10}\rangle|\downarrow\rangle$
$= \sqrt{\frac{2}{3}}\,|Y_{1-1}\rangle|\uparrow\rangle - \frac{1}{\sqrt{3}}\,|Y_{10}\rangle|\downarrow\rangle$

$\downarrow$

$$\left|\frac{1}{2}\ -\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\,|Y_{1-1}\rangle|\uparrow\rangle - \frac{1}{\sqrt{3}}\,|Y_{10}\rangle|\downarrow\rangle$$

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6.3. 一般の場合

$$\mathbb{J} = \boldsymbol{j}_1 + \boldsymbol{j}_2$$

① $|J = j_1 + j_2,\ M = j_1 + j_2\rangle = |j_1 j_1\rangle|j_2 j_2\rangle$
（これは一通りしかない）

② $|J = j_1 + j_2,\ M = j_1 + j_2 - 1\rangle \propto J_- |j_1 + j_2,\ j_1 + j_2\rangle$

③ $|j_1 + j_2,\ j_1 + j_2 - 1\rangle$ に直交する状態を作ると、それは
$|j_1 + j_2 - 1,\ j_1 + j_2 - 1\rangle$

④ $|j_1 + j_2,\ j_1 + j_2 - 2\rangle \propto J_- |j_1 + j_2, j_1 + j_2 - 1\rangle$
$|j_1 + j_2 - 1,\ j_1 + j_2 - 2\rangle \propto J_- |j_1 + j_2 - 1,\ j_1 + j_2 - 1\rangle$

⑤ これら２つの状態に直交する状態は
$|j_1 + j_2 - 2,\ j_1 + j_2 - 2\rangle$

⋮

↓

$$\left.\begin{array}{c} |j_1 - j_2| \le J \le j_1 + j_2 \\ -J \le M \le J \end{array}\right)$$
のすべての状態を作ることができる。

$$\boxed{|JM\rangle = \sum_{m_1, m_2} \underbrace{\langle j_1 m_1 j_2 m_2 | JM\rangle}_{} |j_1 m_1\rangle |j_2 m_2\rangle}$$

展開係数（クレブシュ・ゴルダン係数）

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(note) $J = j_1 + j_2$

$\Rightarrow$ $J^2 = j_1^2 + j_2^2 + 2 j_{1z} j_{2z} + (j_{1x} + i j_{1y})(j_{2x} - i j_{2y})$
$+ (j_{1x} - i j_{1y})(j_{2x} + i j_{2y})$

$\Rightarrow$

$$J^2 \,|j_1 j_1\rangle |j_2 j_2\rangle$$

$$= \hbar^2 \big(\underbrace{j_1(j_1+1) + j_2(j_2+1) + 2 j_1 j_2}_{} \big) |j_1 j_1\rangle |j_2 j_2\rangle$$

$$\| $$

$$j_1^2 + 2 j_1 j_2 + j_2^2 + j_1 + j_2$$

$$\| $$

$$(j_1 + j_2)^2 + j_1 + j_2$$

$$\| $$

$$(j_1 + j_2)(j_1 + j_2 + 1)$$

$\mathbb{J} = j_1 + j_2$

$J_z \backslash J$	j_1+j_2		j_1+j_2-1		j_1+j_2-2	$\cdots$	$\lvert j_1-j_2 \rvert$
j_1+j_2	$\lvert j_1 j_1\rangle \lvert j_2 j_2\rangle$						
	$\downarrow J_- = j_{1-} + j_{2-}$						
j_1+j_2-1	$\alpha \lvert j_1 j_1-1\rangle \lvert j_2 j_2\rangle + \beta \lvert j_1 j_1\rangle \lvert j_2 j_2-1\rangle$	$\xrightarrow{}$ 直交	$\beta \lvert j_1 j_1-1\rangle \lvert j_2 j_2\rangle - \alpha \lvert j_1 j_1\rangle \lvert j_2 j_2-1\rangle$				
	$\downarrow J_-$		$\downarrow J_-$				
j_1+j_2-2				$\xrightarrow{}$ 直交			
	$\downarrow J_-$		$\downarrow J_-$		$\downarrow J_-$		
						$\xrightarrow{}$ 直交	
	$\downarrow$		$\downarrow J_-$		$\downarrow J_-$		
$\vdots$	$\vdots$		$\vdots$		$\vdots$		
	$\downarrow$						
$-j_1-j_2$							

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例) $\ell_1 = 1$ と $\ell_2 = 1$ の合成: $\mathbb{L} = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2$

- $|22\rangle = |Y_{11}\rangle|Y_{11}\rangle$
- $L_-|22\rangle = \sqrt{2}\,|Y_{10}\rangle|Y_{11}\rangle + \sqrt{2}\,|Y_{11}\rangle|Y_{10}\rangle$

$\Downarrow$ $$|21\rangle = \frac{1}{\sqrt{2}}\left(|Y_{10}\rangle|Y_{11}\rangle + |Y_{11}\rangle|Y_{10}\rangle\right)$$

- $L_-|21\rangle \propto |Y_{1-1}\rangle|Y_{11}\rangle + |Y_{10}\rangle|Y_{10}\rangle \times 2 + |Y_{11}\rangle|Y_{1-1}\rangle$

$\Downarrow$ $$|20\rangle = \frac{1}{\sqrt{6}}\left(|Y_{1-1}\rangle|Y_{11}\rangle + 2|Y_{10}\rangle|Y_{10}\rangle + |Y_{11}\rangle|Y_{1-1}\rangle\right)$$

- $L_-|20\rangle \propto |Y_{1-1}\rangle|Y_{10}\rangle + 2|Y_{1-1}\rangle|Y_{10}\rangle + 2|Y_{10}\rangle|Y_{1-1}\rangle + |Y_{10}\rangle|Y_{1-1}\rangle$

$\Downarrow$ $$|2-1\rangle = \frac{1}{\sqrt{2}}\left(|Y_{10}\rangle|Y_{1-1}\rangle + |Y_{1-1}\rangle|Y_{10}\rangle\right)$$

- $|2-2\rangle = |Y_{1-1}\rangle|Y_{1-1}\rangle$

$$|11\rangle = \frac{1}{\sqrt{2}}\left(|Y_{10}\rangle|Y_{11}\rangle - |Y_{11}\rangle|Y_{10}\rangle\right)$$

- $L_-|11\rangle \propto |Y_{1-1}\rangle|Y_{11}\rangle + \cancel{|Y_{10}\rangle|Y_{10}\rangle} \cancel{- |Y_{10}\rangle|Y_{10}\rangle} - |Y_{11}\rangle|Y_{1-1}\rangle$

$\Downarrow$ $$|10\rangle = \frac{1}{\sqrt{2}}\left(|Y_{1-1}\rangle|Y_{11}\rangle - |Y_{11}\rangle|Y_{1-1}\rangle\right)$$

- $L_-|10\rangle \propto |Y_{1-1}\rangle|Y_{10}\rangle - |Y_{10}\rangle|Y_{1-1}\rangle$

$\Downarrow$ $$|1-1\rangle = \frac{1}{\sqrt{2}}\left(|Y_{1-1}\rangle|Y_{10}\rangle - |Y_{10}\rangle|Y_{1-1}\rangle\right)$$

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$$|00\rangle = \alpha\, |Y_{1-1}\rangle |Y_{11}\rangle + \beta\, |Y_{10}\rangle |Y_{10}\rangle + \gamma\, |Y_{11}\rangle |Y_{1-1}\rangle$$

$$\langle 20|00\rangle = 0 \rightarrow \alpha + 2\beta + \gamma = 0$$

$$\langle 10|00\rangle = 0 \rightarrow \alpha - \gamma = 0$$

$$\therefore \alpha = \gamma$$

$$\beta = -\alpha$$

$$\therefore$$

$$|00\rangle = \frac{1}{\sqrt{3}} \left(|Y_{1-1}\rangle |Y_{11}\rangle - |Y_{10}\rangle |Y_{10}\rangle + |Y_{11}\rangle |Y_{1-1}\rangle \right)$$