Projection theorem revised

The statement is

$$\langle \alpha' j' m' | \vec{V}_{(q)} | \alpha j m \rangle = \frac{\langle \alpha' j' m' | \vec{J}_{(q)} | \alpha j m \rangle}{j(j+1)} \langle \alpha j n | \vec{J} \cdot \vec{V} | \alpha j n \rangle$$

From Wigner - Eckart theorem we know

$$\langle \alpha' j m' | \vec{V}_{(q)} | \alpha j m \rangle = \langle j 1 ; m q | j m' \rangle \frac{\langle \alpha' j \| \vec{V} \| \alpha j \rangle}{\sqrt{2j+1}}$$

Similarly,

$$\langle \alpha' j m' | \vec{J}_{(q)} | \alpha j m \rangle = \langle j 1 ; m q | j m' \rangle \frac{\langle \alpha' j \| \vec{J} \| \alpha j \rangle}{\sqrt{2j+1}}$$

Therefore

$$\langle \alpha' j m' | \vec{V}_{(q)} | \alpha j m \rangle = \langle \alpha' j m' | \vec{J}_{(q)} | \alpha j m \rangle \frac{\langle \alpha' j \| \vec{V} \| \alpha j \rangle}{\langle \alpha' j \| \vec{J} \| \alpha j \rangle}$$

To know the ratio of reduced matrices:

$$\langle \alpha' j n | \vec{J}_\alpha \vec{V}_\alpha | \alpha j n \rangle = \sum_{n'} \langle \alpha' j n | J_\alpha | \alpha' j n' \rangle \langle \alpha' j n' | V_\alpha | \alpha j n \rangle$$

$$= \underbrace{\sum_{n'} \langle \alpha' j n | J_\alpha | \alpha' j n' \rangle \langle \alpha' j n' |}_{=\mathbb{1}} J_\alpha | \alpha j n \rangle \frac{\langle \alpha' j \| \vec{V} \| \alpha j \rangle}{\langle \alpha' j \| \vec{J} \| \alpha j \rangle}$$

$$= \langle \alpha' j n | J_\alpha^2 | \alpha j n \rangle \frac{\langle \alpha' j \| \vec{V} \| \alpha j \rangle}{\langle \alpha' j \| \vec{J} \| \alpha j \rangle}$$

Since α' is arbitrary, we choose $\alpha' = \alpha$

$$\langle \alpha j n | \vec{J} \cdot \vec{V} | \alpha j n \rangle = j(j+1) \frac{\langle \alpha j \| \vec{V} \| \alpha j \rangle}{\langle \alpha' j \| \vec{J} \| \alpha j \rangle}$$

Thus prove the projection theorem $\boxed{\vec{A} \rightarrow \frac{\vec{J} \langle \vec{J} \cdot \vec{A} \rangle}{j(j+1)}}$

Lande - g factor

Magnetic moment

$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_s$ sum of the orbital moment and the spin moment

$\vec{\mu}_L = -g_L \mu_B \vec{L}$ $\vec{\mu}_s = -g_s \mu_B \vec{S}$ $\mu_B \equiv \frac{e\hbar}{2m_e}$

The resultant g_J - factor is defined by

$$\langle \alpha j m | \vec{\mu} | \alpha j m' \rangle = -g_J \langle \alpha j m | \vec{J} | \alpha j m' \rangle \mu_B$$

$$\vec{\mu} = -(g_L \vec{L} + g_s \vec{S}) \mu_B$$

by the projection theorem

$$\langle | \vec{\mu} | \rangle = -g_L \mu_B \frac{\langle | (\vec{L}\cdot\vec{J})\vec{J} | \rangle}{j(j+1)} - g_s \mu_B \frac{\langle | (\vec{S}\cdot\vec{J})\vec{J} | \rangle}{j(j+1)}$$

$\vec{J} = \vec{L} + \vec{S}$

$$\left.\begin{aligned} \vec{S}^2 &= \vec{J}^2 + \vec{L}^2 - 2\vec{J}\cdot\vec{L} \\ \vec{L}^2 &= \vec{J}^2 + \vec{S}^2 - 2\vec{J}\cdot\vec{S} \end{aligned}\right\} \quad \begin{aligned} \vec{J}\cdot\vec{L} &= \tfrac{1}{2}\left(j(j+1) + \ell(\ell+1) - s(s+1) \right] \\ \vec{J}\cdot\vec{S} &= \tfrac{1}{2}\left(j(j+1) + s(s+1) - \ell(\ell+1) \right] \end{aligned}$$

$$= -\frac{g_L \mu_B}{2} \frac{j(j+1) + \ell(\ell+1) - s(s+1)}{j(j+1)} \langle | \vec{J} | \rangle$$
$$- \frac{g_s \mu_B}{2} \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{j(j+1)} \langle | \vec{J} | \rangle$$

$$= \left[-\frac{g_L + g_s}{2} + \frac{(g_L - g_s)[s(s+1) - \ell(\ell+1)]}{2j(j+1)} \right] \langle | \vec{J} | \rangle \mu_B$$

Namely, $g_J = +\frac{g_L + g_s}{2} + \frac{(g_s - g_L)[s(s+1) - \ell(\ell+1)]}{2j(j+1)}$

Input $g_L = 1$, $g_s = 2$

$$\Rightarrow \quad g_J = \frac{3}{2} + \frac{s(s+1) - \ell(\ell+1)}{2j(j+1)} = \boxed{1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}}$$

Nucleon Magnetic moments

Proton : $\underbrace{uu}d$ S-wave $\ell = 0$

Neutron : $u\underbrace{dd}$ $J = S_1 + S_2 + S_3$

identical particles, since color WF is totally antisymmetrical

$\Rightarrow$ exchange uu (or dd in n) spin $\rightarrow$ symmetrical

$\Rightarrow$ uu (or dd in n) is in the spin triplet state.

✩ $S_{uu} = 1$ (or $S_{dd} = 1$), denoted as aab, S_{aa}

$$\vec{\mu} = 2\cdot\frac{g_a e\hbar}{2m_a c}\vec{S}_{a_1} + 2\frac{g_a e\hbar}{2m_a c}\vec{S}_{a_2} + 2\frac{g_b e\hbar}{2m_b c}\vec{S}_b \quad , \quad \text{take } m_a = m_b = m_q$$

$$\Rightarrow \langle\vec{\mu}\rangle = \frac{e\hbar}{m_q c}\left\langle g_a(\vec{S}_{a_1} + \vec{S}_{a_2}) + g_b(\vec{S}_b)\right\rangle$$

$$= \frac{e\hbar}{m_q c}\frac{1}{j(j+1)}\left[g_a\langle(\vec{S}_{aa}\cdot\vec{J})\vec{J}\rangle + g_b\langle(\vec{S}_b\cdot\vec{J})\vec{J}\rangle\right]$$

since $\vec{J} = \vec{S}_{aa} + \vec{S}_b$, $j = \frac{1}{2}$, $S_{aa} = 1$, $S_b = \frac{1}{2}$

$$= \frac{e\hbar}{m_q c}\frac{\langle\vec{J}\rangle}{j(j+1)}\left[g_a\frac{j(j+1) + S_{aa}(S_{aa}+1) - S_b(S_b+1)}{2} + g_b\frac{j(j+1) + S_b(S_b+1) - S_{aa}(S_{aa}+1)}{2}\right]$$

$$= \frac{e\hbar}{m_q c}\frac{\langle\vec{J}\rangle}{\left(\frac{1}{2}\cdot\frac{3}{2}\right)}\left[\frac{g_a}{2}\left(\frac{1}{2}\cdot\frac{3}{2} + 1\cdot 2 - \frac{1}{2}\cdot\frac{3}{2}\right) + \frac{g_b}{2}\left(\frac{1}{2}\cdot\frac{3}{2} + \frac{1}{2}\cdot\frac{3}{2} - 1\cdot 2\right)\right]$$

$$= \frac{e\hbar}{m_q c}\frac{2}{3}\langle\vec{J}\rangle\left[2g_a - \frac{g_b}{2}\right] = \frac{2}{3}\frac{e\hbar}{2(m_q c)}\langle\vec{J}\rangle\left[4g_a - g_b\right]$$

For proton, $a = u$, $g_a = +\frac{2}{3}$, $g_b = -\frac{1}{3}$ $\quad g_p = 2\left[4\cdot\frac{2}{3} - \left(-\frac{1}{3}\right)\right] = 2(3)\left(\frac{m_N}{3m_q}\right)$

neutron $a = d$ " $-\frac{1}{3}$ " $+\frac{2}{3}$ $\quad g_N = 2\left[4\left(-\frac{1}{3}\right) - \left(\frac{2}{3}\right)\right] = 2(-2)\left(\frac{m_N}{3m_q}\right)$

$$\frac{g_p}{g_N} = -1.5$$

c.f. $g_p = 2\cdot(2.79)$

$g_N = 2\cdot(-1.91)$

$$\boxed{\text{exp } \frac{g_p}{g_N} = -1.46}$$

Identical particles

Symmetric and anti-symmetric WFs

2 identical particles with $\vec{r}_1, \vec{r}_2$ and WF $u(\vec{r}_1, \vec{r}_2)$

($\vec{r}_i$ may include spin), The system is governed by Hamiltonian

$H(\vec{r}_1, \vec{r}_2)$.

Since the 2 particles are identical,

$$H(\vec{r}_1, \vec{r}_2) = H(\vec{r}_2, \vec{r}_1)$$

We may take this as the definition of "identical" or "indistinguishable".

Then,

$$H(\vec{r}_1, \vec{r}_2)\, u(\vec{r}_1, \vec{r}_2) = E\, u(\vec{r}_1, \vec{r}_2)$$

also

$$H(\vec{r}_2, \vec{r}_1)\, u(\vec{r}_1, \vec{r}_2) = E\, u(\vec{r}_1, \vec{r}_2)$$

or one can rename $\vec{r}_1 \Leftrightarrow \vec{r}_2$,

$$\Rightarrow H(\vec{r}_1, \vec{r}_2)\, u(\vec{r}_2, \vec{r}_1) = E\, u(\vec{r}_2, \vec{r}_1)$$

Both $u(\vec{r}_1, \vec{r}_2)$ and $u(\vec{r}_2, \vec{r}_1)$ are solutions of the Schrödinger Eq with the same energy.

$\Rightarrow$ ① They are linearly independent $\Rightarrow$ degenerate

② or $u(\vec{r}_1, \vec{r}_2) = c\, u(\vec{r}_2, \vec{r}_1)$, c is a constant

If case-②, we do a second interchange

$$\Rightarrow u(\vec{r}_1, \vec{r}_2) = c\, u(\vec{r}_2, \vec{r}_1) = c^2 u(\vec{r}_1, \vec{r}_2)$$

Thus, $c^2 = 1$, or $c = \pm 1$.

When $C=+1$, we have the symmetric solution.

$$\Rightarrow \quad \psi_S = \frac{1}{\sqrt{2}}\left[u(\vec{r}_1, \vec{r}_2) + u(\vec{r}_2, \vec{r}_1) \right]$$

and when $C=-1$, " anti-sym "

$$\Rightarrow \quad \psi_A = \frac{1}{\sqrt{2}}\left[u(\vec{r}_1, \vec{r}_2) - u(\vec{r}_2, \vec{r}_1) \right]$$

These are the only possible non-degenerate solutions.

- It's easy to generalize the discussion to $n > 2$ identical particles.
- Aagain Hamiltonian is symmetric under any # of particle pair-exchange
- n - particles $\Longrightarrow$ $n!$ permutations (can be built up by many pair-exchanges)

$$\Rightarrow \quad \frac{n!}{2} \text{ even permutation } (P_E)$$

$$\frac{n!}{2} \text{ odd permutation } (P_O)$$

- Thus

$$H[\vec{r}_1, \vec{r}_2 \cdots \vec{r}_n] = H[P(\vec{r}_1, \vec{r}_2, \cdots \vec{r}_n)]$$

- If $u(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_n)$ is a solution to $Hu = Eu$

then $u(P(\vec{r}_1 \cdots \vec{r}_n))$ is also a solution for the <u>same</u> energy.

- For the nondegenerate case, we find that

$$u(P_E(\vec{r}_1 \cdots \vec{r}_n)] = u(\vec{r}_1 \cdots \vec{r}_n)$$

$$u(P_O(\vec{r}_1 \cdots \vec{r}_n)] = \pm u(\vec{r}_1 \cdots \vec{r}_n)$$

For the "+" sign,

$$\Rightarrow \psi_S = \frac{1}{\sqrt{n!}} \sum_{i=1}^{n!} u[P_i(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_n)]$$ (for both Even and Odd permutation)

If the sign is "−", we have the antisymmetrical solution

$$\Rightarrow \psi_A = \frac{1}{\sqrt{n!}} \sum_{i=1}^{n!} \varepsilon_i \, u[P_i(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_n)]$$

$\varepsilon_i = \pm 1$ for $\begin{matrix}\text{even} \\ \text{odd}\end{matrix}$ permutations

These are the only non-degenerate solutions.

Experimental facts:

If the identical particals have integral spin

$\Rightarrow$ WF is always symmetric under exchange, — Bose-Einstein statistics $\Rightarrow$ Boson

While If the spin is half-integral

$\Rightarrow$ WF is always antisymmetric " — Fermi-Dirac statistics $\Rightarrow$ Fermion

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The time-dependent Schrödinger Eq.

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$ preserve the symmetry

$\because$ H, (Permutation) $= H$, ψ and $\frac{\partial \psi}{\partial t}$ have the same symmetry.

Need Quantum Field Theory, first pointed out by Pauli (1940)

no good understanding yet —

The Pauli Exclusion Principle

- consider n electrons.
- In some certain approximation we can ignore the interactions between the electrons.
- Hamiltonian = sum of 1-particle Hamiltonian.

$$\Rightarrow H(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_n) = H_0(\vec{r}_1) + H_0(\vec{r}_2) + \cdots + H_0(\vec{r}_n)$$

- The wave function before antisymmetrization.

$$\psi = \varphi_{N_1}(\vec{r}_1) \times \varphi_{N_2}(\vec{r}_2) \cdots \varphi_{N_n}(\vec{r}_n)$$

N_i $i = 1, 2 \cdots n$ label the quantum numbers of the 1-particle WF φ, we can simply write it as: (usually reffered as 1-P orbitals)

$$\psi = \varphi_1(\vec{r}_1)\, \varphi_2(\vec{r}_2) \cdots \varphi_n(\vec{r}_n)$$

- Now, taking into account of the exchange symmetry

$$\psi = \frac{1}{\sqrt{n!}} \begin{vmatrix} \varphi_1(\vec{r}_1) & \varphi_1(\vec{r}_2) & \cdots & \varphi_1(\vec{r}_n) \\ \varphi_2(\vec{r}_1) & \varphi_2(\vec{r}_2) & & \varphi_2(\vec{r}_n) \\ \vdots & & \ddots & \vdots \\ \varphi_n(\vec{r}_1) & \varphi_n(\vec{r}_2) & & \varphi_n(\vec{r}_n) \end{vmatrix}$$

This is called a "Slater determinant".

e.g.

$$\frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_1(r_1) & \varphi_1(r_2) \\ \varphi_2(r_1) & \varphi_2(r_2) \end{vmatrix} = \frac{1}{\sqrt{2!}} \left(\varphi_1(r_1)\varphi_2(r_2) - \varphi_1(r_2)\varphi_2(r_1) \right)$$

$$\frac{1}{\sqrt{3!}} \begin{vmatrix} \varphi_1(r_1) & \varphi_1(r_2) & \varphi_1(r_3) \\ \varphi_2(r_1) & \varphi_2(r_2) & \varphi_2(r_3) \\ \varphi_3(r_1) & \varphi_3(r_2) & \varphi_3(r_3) \end{vmatrix} = \frac{1}{\sqrt{6}} \left(\begin{array}{l} \varphi_1(r_1)\varphi_2(r_2)\varphi_3(r_3) + \varphi_1(r_2)\varphi_2(r_3)\varphi_3(r_1) + \varphi_1(r_3)\varphi_2(r_1)\varphi_3(r_2) \\ - \varphi_1(r_3)\varphi_2(r_2)\varphi_3(r_1) - \varphi_1(r_1)\varphi_2(r_3)\varphi_3(r_2) - \varphi_3(r_3)\varphi_2(r_1)\varphi_1(r_2) \end{array} \right)$$

Since a determine always vanishes if any two rows or columns are equal,

⇒ the quantum numbers (orbitals) must be distinct.

⇒ no two φ_s can have exactly the same quantum numbers. (including spin)

⇒ This is the <u>Pauli exclusion principle</u> !

☆ We shall emphasize that the exclusion principle only has meaning in the approximation of a separable Hamiltonian (negligible particle-particle interactions) !

☆ Antisymmetric is more fundamental.

☆ No restriction applies for bosons,

unlimited # of photons can exist in the same EM mode.