

# 1) 174(s) : Derivation of the Pauli Exclusion Principle.

The H atom wavefunctions are combinations of the spin up and spin down states of the electron as follows:

$$\psi_1^R = F_1 |j m l - \rangle + i f_1 |j m l + \rangle \quad - (1)$$

$$\psi_2^R = F_2 |j m l - \rangle + i f_2 |j m l + \rangle \quad - (2)$$

$$\psi_1^L = F_1 |j m l - \rangle - i f_1 |j m l + \rangle \quad - (3)$$

$$\psi_2^L = F_2 |j m l - \rangle - i f_2 |j m l + \rangle \quad - (4)$$

w/:

$$(E - e\phi - mc^2) F - \hbar c \left( \frac{d}{dr} + \frac{j + 3/2}{r} \right) f = 0 \quad - (5)$$

$$(E - e\phi + mc^2) f + \hbar c \left( \frac{d}{dr} - \frac{j - 1/2}{r} \right) F = 0 \quad - (6)$$

The fundamental origin of the Pauli exclusion principle is that no two electrons can have the same set of quantum numbers by observation of spectra. In H there is only one electron occupying  $\pm$  spin states. It has been shown using the fermion equation that the correct H wavefunction must be the combinations (1) to (4). Applying parity,  $\hat{P}$ , means that:

$$\hat{P}(f) \rightarrow -f \quad - (7)$$

$$\hat{P}(F) \rightarrow F \quad - (8)$$

Eqs. (1) to (4) are the direct result of the most fundamental principle of special relativity, the

2) Lorentz transform. The latter is applied to the right and left Pauli spinors, which are interconvertible by parity.  
 $\hat{P}(\phi^R) = \phi^L$ ;  $\hat{P}(\phi^L) = \phi^R$ . — (9)

This procedure gives:

$$(E + c \underline{\sigma} \cdot \underline{\hat{p}}) \phi^L = mc^2 \phi^R \quad - (10)$$

$$(E - c \underline{\sigma} \cdot \underline{\hat{p}}) \phi^R = mc^2 \phi^L \quad - (11)$$

in which:  $E_0 = mc^2$ . — (12)

The words here is never negative energy is nature.  
 Make the mathematical transform:

$$\phi^L = \phi_S^R + \phi_S^L \quad - (13)$$

$$\phi^R = \phi_S^R - \phi_S^L \quad - (14)$$

where:

$$\phi_S^R = f |j m l_- \rangle \quad - (15)$$

$$\phi_S^L = -i f |j m l_+ \rangle \quad - (16)$$

Now use:

$$\hat{P}(\underline{\sigma} \cdot \underline{\hat{p}}) = - \underline{\sigma} \cdot \underline{\hat{p}} \quad - (17)$$

Eqs. (9) and (17) mean that eqs. (10) and (11) are interconvertible by parity. They are the correct equations to use. The transforms (13) and (14) define eqs. (1) to (4), i.e. the correct wavefunctions are the combinations of spin up and spin down for an electron. The transformations (13) to (14) give:

$$(E - mc^2) \phi_S^R + c \underline{\sigma} \cdot \underline{\hat{p}} \phi_S^L = 0 \quad - (18)$$

$$(E + mc^2) \phi_S^L - c \underline{\sigma} \cdot \underline{\hat{p}} \phi_S^R = 0 \quad - (19)$$

3) If parity is applied to eqs. (18) and (19) the same equations are obtained. Eqs. (18) and (19) are not interconverted by parity. This means that they are missing information because they do not use the fundamental Pauli spin of symmetry (a). Eqs. (10) and (11) produce, in the approximation:

$$E \rightarrow mc^2 \quad - (20)$$

the Schrodinger equation:

where  $\psi$  denotes either  $\psi^R$  or  $\psi^L$ . The (Coulomb potential of the H atom is introduced via the minimal prescription:

$$E \rightarrow E - e\phi \quad - (22)$$

so:

$$\hat{H} = mc^2 + e\phi + \frac{\hat{p}^2}{2m} - \frac{e}{4m^2c^2} \hat{\sigma} \cdot \hat{r} \phi \hat{\sigma} \cdot \hat{p} \quad - (23)$$

+ ...

The non-relativistic Schrodinger equation to spin is not considered, so:

$$\frac{\hat{p}^2}{2m} \psi = - \frac{\hbar^2 \nabla^2}{2m} \psi = (E - mc^2 - e\phi) \psi \quad - (24)$$

with

$$E - mc^2 \rightarrow \frac{1}{2}mv^2 = T. \quad - (25)$$

So the usual Schrodinger equation of H is obtained:

$$4) \quad \hat{H} \psi = (T + V) \psi. \quad - (26)$$

The total non-relativistic energy is denoted:

$$E = T + V \quad - (27)$$

and is the sum of the kinetic and potential energies.

The simplest example of an atom with more than one electron is Helium (He), which:

$$\psi(r_1, r_2) = \psi_{n_1 l_1 m_1}(r_1) \psi_{n_2 l_2 m_2}(r_2) \quad - (28)$$

If the electron spin is now considered, then exist the products:

$$\psi_1^R(A) \psi_1^R(B), \dots, \psi_1^L(A) \psi_2^L(B) \quad - (29)$$

where A and B denote different electrons. Denote:

$$F_i^-(A) = f_i |j m l - \rangle \quad - (30)$$

$$f_i^+(A) = f_i |j m l + \rangle \quad - (31)$$

and so on. Therefore:

$$\begin{aligned} \psi_1^R(A) \psi_1^R(B) &= (F_i^-(A) + i f_i^+(A)) (F_i^-(B) + i f_i^+(B)) \\ &= F_i^-(A) F_i^-(B) - f_i^+(A) f_i^+(B) + i (F_i^-(A) f_i^+(B) + f_i^+(A) F_i^-(B)) \end{aligned} \quad - (32)$$

- (32a)

Now apply parity:

$$\begin{aligned} \hat{P} (\psi_1^R(A) \psi_1^R(B)) &= F_i^-(A) F_i^-(B) - f_i^+(A) f_i^+(B) \\ &\quad - i (F_i^-(A) f_i^+(B) + f_i^+(A) F_i^-(B)) \end{aligned}$$

5) Finally use the algebraic result:

$$\begin{aligned} & (F_i^-(A) + i f_i^+(A))(F_i^-(B) + i f_i^+(B)) \\ &= (F_i^-(B) + i f_i^+(B))(F_i^-(A) + i f_i^+(A)) \end{aligned} \quad - (33)$$

Apply parity to the RHS:

$$\begin{aligned} & \hat{P} (F_i^-(B) + i f_i^+(B))(F_i^-(A) + i f_i^+(A)) \\ &= (F_i^-(B) - i f_i^+(B))(F_i^-(A) - i f_i^+(A)) \\ &= F_i^-(B)F_i^-(A) - f_i^+(B)f_i^+(A) \\ &\quad - i (F_i^-(B)f_i^+(A) + f_i^+(B)F_i^-(A)). \end{aligned} \quad - (34)$$

The Pauli Exclusion Principle is the result of the parity operations:

$$i (F_i^-(A)f_i^+(B) + f_i^+(A)F_i^-(B)) \quad - (35)$$

$$\rightarrow -i (F_i^-(B)f_i^+(A) + f_i^+(B)F_i^-(A))$$

The complete wave function is antisymmetric under exchange of A and B.

The origin of the Pauli exclusion principle is eqns. (1) to (4) of the fermion equation.