

Digital Computer Laboratory  
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SUBJECT: GROUP 63 SEMINAR ON MAGNETISM, XXX

To: Group 63

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Date: February 10, 1953

Since no interaction exists between different spin functions, there can be no transition from symmetrical to anti-symmetric space functions or vice versa.

Having examined the spin function at the previous meeting, let us now consider the space functions at and near the ground state.

Example I. Helium

(A)  $\left. \begin{array}{l} \text{Anti-symmetric Space State} \\ \text{Symmetric Spin State} \end{array} \right\}$  (triplets)

Lowest state ( $n = 1, \ell = m_\ell = 0$ )

$$= \psi_{100}(1) \psi_{100}(2) - \psi_{100}(2) \psi_{100}(1) = 0$$

Therefore, there is no possibility of an anti-symmetric space state (triplet) in the ground state of helium.

Next lowest state ( $n = 2, \ell = 0, m_\ell = 0$ )

$$= \psi_{100}(1) \psi_{200}(2) - \psi_{100}(2) \psi_{200}(1)$$

This is a possible state for helium, but it represents a higher energy level than the previous state. Other states for which  $n = 2$  are also possible, involving different values of  $\ell$  and  $m_\ell$ .

(B)  $\left. \begin{array}{l} \text{Symmetric Space State} \\ \text{Anti-Symmetric Spin State} \end{array} \right\}$  (singlets)

Ground state

$$= \psi_{100}(1) \psi_{100}(2) + \psi_{100}(2) \psi_{100}(1)$$

$$= 2 \psi_{100}(1) \psi_{100}(2)$$

This is a possible state and can be shown to be the ground state. It is the only possible state in which both electrons are in  $n=1$  states, and thus corresponds to lower energy than states with not more than one electron in the  $n=1$  level. The ground state of helium is therefore a singlet.

Low perturbed state

Perturbed singlet states can also exist. They will have a higher energy than the ground states; e.g., for  $n=2$

$$\psi_{100}(1) \psi_{200}(2) + \psi_{100}(2) \psi_{200}(1)$$

Example II. Beryllium

Beryllium has atomic number 4. It consists of a nucleus and four electrons. Two of these electrons lie in the  $n=1$  level. This fills the K shell ( $n=1$ ). The two outer electrons therefore are in the field due to the combined effect of the nucleus and the inner electrons.

Therefore, for an outer electron of beryllium in the ground state,  $n=2$ .

The outer electrons can therefore be in a large number of possible quantum states without being perturbed sufficiently to go to the next shell ( $n=3$ ). Using the notation

$$\psi_{100}(1) \psi_{200}(2) \pm \psi_{200}(1) \psi_{100}(2) = (100, 200)_{\substack{(s) \\ (a)}}$$

the possible states for  $n=2$  are:

1. For symmetric space states (anti-symmetric spin states)

$$(200, 200), (200, 211), (200, 210), (200, 21\bar{1}), (211, 211) \\ (211, 210), (211, 21\bar{1}), (210, 210), (210, 21\bar{1}), (21\bar{1}, 21\bar{1})$$

2. For anti-symmetric space states (symmetric spin states)

$$(200, 211), (200, 210), (200, 21\bar{1}), (211, 210) \\ (211, 21\bar{1}), (210, 21\bar{1})$$

wherein  $\bar{1} = -1$ .

The reduction in the number of permissible levels for anti-symmetric space functions must occur if the Pauli exclusion principle is to hold since, according to this principle, two electrons in the same spin state cannot exist in the same space state.

We can set up  $10 \times 10$  and  $6 \times 6$  matrices for the symmetric and anti-symmetric space states respectively to deal with the exchange elements  $H^i_{ml}$  amongst the various states of the beryllium atom for which  $n=2$ . A theorem which we will not prove here states that exchange occurs only between states for which  $m_l(1) + m_l(2)$  are the same.

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Therefore, if we identify a non-zero matrix element by an asterisk, the matrix for the anti-symmetric space function is as follows:

	<u>(200, 211)</u>	<u>(200, 210)</u>	<u>(200, 21<math>\bar{1}</math>)</u>	<u>(211, 210)</u>	<u>(211, 21<math>\bar{1}</math>)</u>	<u>(210, 21<math>\bar{1}</math>)</u>
(200, 211)	*	0	0	*	0	0
(211, 210)	0	*	0	0	*	0
(200, 21 $\bar{1}$ )	0	0	*	0	0	*
(211, 210)	*	0	0	*	0	0
(211, 21 $\bar{1}$ )	0	*	0	0	*	0
(210, 21 $\bar{1}$ )	0	0	*	0	0	*

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Interactions involving electrons in the identical space state is allowed for symmetric space wave functions. The matrix for the symmetric space function is therefore:

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	(200, 200)	(200, 211)	(200, 210)	(200, 21 $\bar{1}$ )	(211, 211)	(211, 210)	(211, 21 $\bar{1}$ )	(210, 210)	(210, 21 $\bar{1}$ )	(21 $\bar{1}$ , 21 $\bar{1}$ )
(200, 200)	*	0	*	0	0	0	*	*	0	0
(200, 211)	0	*	0	0	0	*	0	0	0	0
(200, 210)	*	0	*	0	0	0	*	*	0	0
(200, 21 $\bar{1}$ )	0	0	0	*	0	0	0	0	*	0
(211, 211)	0	0	0	0	*	0	0	0	0	0
(211, 210)	0	*	0	0	0	*	0	0	0	0
(211, 21 $\bar{1}$ )	*	0	*	0	0	0	*	*	0	0
(210, 210)	*	0	*	0	0	0	*	*	0	0
(210, 21 $\bar{1}$ )	0	0	0	*	0	0	0	0	*	0
(21 $\bar{1}$ , 21 $\bar{1}$ )	0	0	0	0	0	0	0	0	0	*

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