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SUBJECT: GROUP 63 SEMINAR ON MAGNETISM, XXXI

To: Group 63

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We may rearrange the rows and columns of the determinants listed at the previous meeting to obtain the following forms:

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

TABLE I

ANTI SYMMETRIC SPIN FUNCTION
SYMMETRIC SPACE FUNCTION
} (singlets)

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

TABLE II

SYMMETRIC SPIN FUNCTION
ANTI-SYMMETRIC SPIN FUNCTION (triplets)

Table I shows that the 10 x 10 matrix for anti-parallel spins can be arranged in a number of sub-matrices. It has been split up into a quartic array involving four energy levels, two quadratic arrays involving two energy levels each, and two linear arrays corresponding to a single energy level each.

States with the same value of n and ℓ, but different values of m_ℓ are degenerate in the absence of an applied field. Therefore, in table I, the two quadratic arrays correspond to the same energies with no external field present. The same is true of the two linear arrays. However, upon application of an external field, this degeneracy is removed.

Table II, describing parallel spin, has fewer elements; hence parallel spin gives rise to a spectrum involving considerably fewer spectral lines.

It can be shown that the state corresponding to the lowest energy is the (200, 200) state, which only exists for the symmetric space state. Therefore, the most stable state of the atom is an anti-parallel spin state.

The exclusion principle is extremely useful in that it correctly predicts which otherwise permissible spectral lines are forbidden. No exceptions to the exclusion principle have ever been noted. The electron behavior described by the exclusion principle is identical with the behavior which would occur if a repulsive force existed between electrons with parallel spins.

The light elements, for which the principal quantum number n is low (n = 1,2) have relatively few space states in their outer shell. On the other hand, heavier elements have a larger number of possible space states within a given outer shell (n = 3,4). Therefore, there is a greater possibility of electrons of the heavier elements having their spins aligned without having to be excited to a higher shell. Therefore, one would expect ferromagnetism to occur in the heavier materials more readily than in the light elements.

Let us consider the next simplest case of two nuclei with two electrons (e.g. 2 hydrogen atoms). In meeting 26 we dealt with the problem of two nuclei and one electron, and found

$$\Psi = c\,(\psi_I^{\circ} \pm \psi_{II}^{\circ})$$

where roman numeral subscripts are used to denote nuclear coordinates.

This led to a Ψ_S and a Ψ_A, with subscripts S and A referring respectively to symmetry and anti-symmetry in the nuclear coordinates. These arose purely from perturbation considerations, and it was found that Ψ_S was a stabler state than Ψ_A. This was in no way connected with the Pauli exclusion principle which is concerned only with electron coordinates, not nuclear ones.

Now, if a second electron is added to the system interactions between the electrons will occur. Unless sufficient excitation is introduced to raise the electrons to the n = 2 shell, both electrons will be in 1S states. The four possible solutions will then be as follows:

	Space	Spin	
1.	$1s_S, 1s_S$	↑↓	Singlet
2.	$1/\sqrt{2}\,(1s_S, 1s_A - 1s_A, 1s_S)$	↑↑	Triplet
3.	$1/\sqrt{2}\,(1s_S, 1s_A + 1s_A, 1s_S)$	↑↓	Singlet
4.	$1s_A, 1s_A$	↑↓	Singlet

The subscripts S and A refer to the nuclear coordinates. Since states 1, 3, and 4 are symmetric space states they are singlet states. Space state 2 is an anti-symmetric space state, and so gives rise to a triplet corresponding to the three symmetric spin states.

Of the four possible solutions, only solution 1 corresponds to the nuclei in the symmetric state. Since this was found to be the most stable state, it is the most probable state for formation of a hydrogen molecule H_2.

On combining two lithium atoms the two outer electrons are in the n = 2 state, so without going to a higher shell the possible states are $2s_I$, $2s_{II}$, $2p_I$, $2p_{II}$. Since $2p_I$ and $2p_{II}$ each represent 3 states (m_ℓ = 1, 0, -1) there are sixteen possible solutions. A great deal of resonance can occur, and double lines appear. As a third lithium atom is brought into system, the number of resonances is further increased, and triple lines appear. As the number of lithium atoms introduced into the system is increased, the lines become bands, and the increased possibility for exchange makes the system stabler. The difference between lithium and hydrogen is that in the former case there is considerable exchange for the valence electron (n = 2), so that a crystal can be formed, while the addition of a third H atom to the H_2 molecule can only produce resonance possibilities at the

expense of energy necessary to raise the third electron from an n = 1 to an n = 2 state. The state thus produced is less stable than the H_2 molecule so that hydrogen does not normally exist in crystalline form.

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