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

To: Group 63 Engineers

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In an attempt to justify the assumption of invariance of the spin direction of the conduction (s) electrons let us consider the different states that may exist for a system of two d shells and one s electron. Consider the three states shown in figure 64 (a). In the first two cases, the d shell spins (large arrow) are anti-parallel, and in the third state they are parallel. The dotted arrows represent two possible states for the conduction electron. The conduction electron spin direction (small arrow) is considered invariant in the first and third cases, while in the second case the possibility of the spin flipping is considered. The analogy between this problem and that of the double wall is used, and the corresponding potential for each case is shown in figure 64 (b).

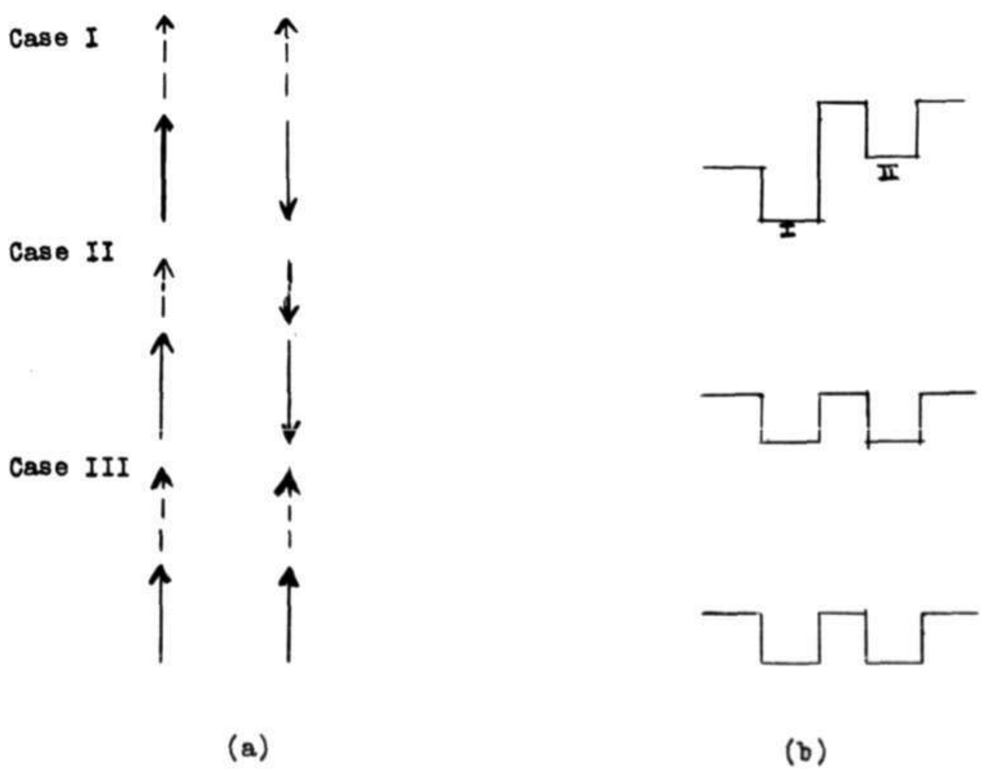

FIGURE 64

Let us consider the energy associated with each state

Case I

In accordance with the exclusion principle the conduction electron will spend less time near the shell with spin aligned parallel to itself than it will near the shell with which it is aligned anti-parallel. The energies of these two possible electron positions are therefore different, as indicated in the figure. The energies will be

$$\mathcal{E}_1 = H_I - \frac{{H'_{I\,II}}^2}{H_{II} - H_I}$$

$$\mathcal{E}_2 = H_{II} + \frac{{H'_{I\,II}}^2}{H_{II} - H_I}$$

The second term on the right hand side of the above equations represents the perturbation energy which arises from the interaction. Since $H'_{I\,II}$ is small and $H_{II} - H_I$ is relatively large, this term will be small. The probability of resonance will be small but finite. The matrix describing this configuration is

	ψ_1	ψ_2
ψ_1	H_I	$H'_{I\,II}$
ψ_2	$H'_{I\,II}$	H_{II}

Case II

In this case, the energies are equal. Furthermore, since there is no interaction of the spins, $H' = 0$, and there is no possibility of resonance.

$$\mathcal{E}_1 = \mathcal{E}_2 = H,$$

or in matrix form

	ψ_1	ψ_2
ψ_1	H	0
ψ_2	0	H

Case III

Here the unperturbed energy levels will be equal, but because of the spin interaction H' has a finite value. Thus

$$\mathcal{E}_1 = H + H'$$

$$\mathcal{E}_2 = H - H'$$

In matrix form

	ψ_1	ψ_2
ψ_1	H	H'
ψ_2	H'	H

Comparing the results we see the third case, which leads to ferromagnetism, leads to the greatest possibility of resonance. In the case of an electron with flipping spin there is no possibility of resonance. For the cases of parallel spin, the first case has a resonance energy

$$\frac{{H'_{I\,II}}^2}{H_{II} - H_I}$$

whereas the third case has a resonance energy H'. If $H' \sim H'_{I\,II}$ and $H'_{I\,II} << H_{II} - H_I$, then

$$\frac{H'_{I\,II}}{H_{II} - H_I} << H',$$

so the resonance for the third case is the greatest.

At the previous meeting we discussed some of the magnetic properties of manganese. Zener considered the effect of the distance between the manganese atoms as had been done before, but he also took the effect of the conduction electron into account. In addition, Zener considers the distribution of the manganese atoms in the pure state, and proposes a face centered tetragonal lattice with spins oriented as shown in figure 65.

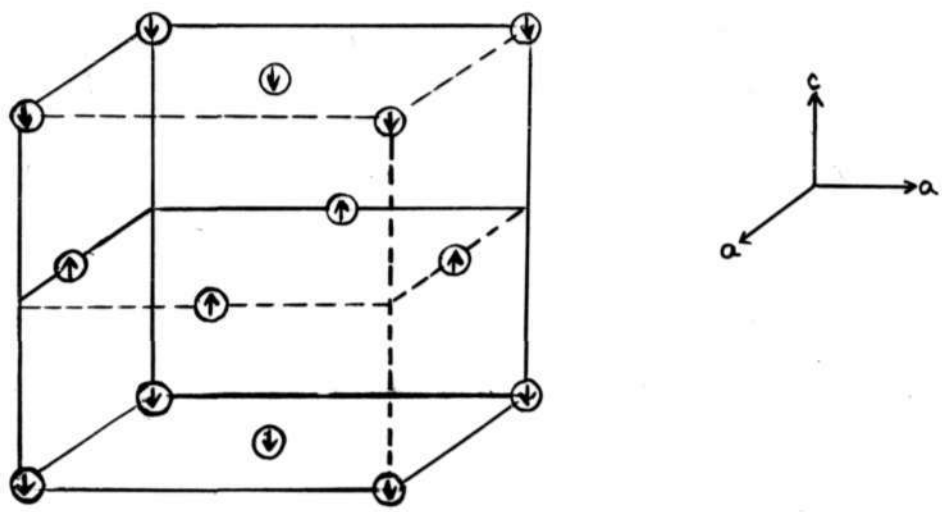

FIGURE 65

According to this postulated spin arrangement an exchange repulsion will exist between nearest neighbors in the same a a plane. On the other hand, no exchange repulsion will exist between nearest neighbors in the same c a plane. Therefore this spin arrangement will produce a distortion from a cubic lattice and will lead to a tetragonal lattice with a c/a ratio smaller than unity. The γ-phase of manganese appears to follow this arrangement, being a face centered tetragonal with a c/a ratio of 0.94.

Emmeration of various energies involved:

1. d-d coupling energy

2. d-s coupling energy

3. Fermi (s-s) energy

The d-d coupling energy can be represented as $1/2 \alpha S_d^2$ per atom, where S_d is the mean component per atom, in units of Bohr magnetons, of the net spin of the d shells in the magnetization direction. α is always positive, and decreases with increasing separation of d shells.

The d-s coupling energy may be represented by $-\beta S_c S_d$ per atom, where S_c is the net magnetization per atom of the conduction electron in units of Bohr magnetons. β is always positive and can be determined with the help of spectroscopic data.

The Fermi energy of the conduction electrons arises from the unbalanced spin distribution of conduction electrons, and is zero when there is an equal number of conduction electron spins in either direction. This energy can be represented by $1/2\gamma S_c^2$ per atom for a small imbalance. In this equation

$$\gamma = \frac{2\epsilon}{3n}$$

where $\underline{\epsilon}$ is the kinetic energy at the top of the Fermi distribution and $\underline{n}$ is the number of conduction electrons per atom. The total spin energy is therefore

$$E_{spin} = \frac{1}{2}\alpha S_d^2 - \beta S_c S_d + \frac{1}{2}\gamma S_c^2 \qquad \text{XXXVI-1}$$

To find the value of S_c for which E_{spin} is a minimum,

$$\frac{\partial E_{spin}}{\partial S_c} = 0 = -\beta S_d + \gamma S_c$$

$$S_c = \left(\frac{\beta}{\gamma}\right) S_d \qquad \text{XXXVI-2}$$

Substituting XXXVI-2 into XXXVI-1 to obtain the minimum E_{spin},

$$E_{spin} = \frac{1}{2}\left\{\alpha - \left(\frac{\beta^2}{\gamma}\right)\right\} S_d^2 \qquad \text{XXXVI-3}$$

The term $\left\{\alpha - \left(\frac{\beta^2}{\gamma}\right)\right\}$ corresponds to Weiss' inner field; and

$\beta^2 \gtrless \alpha\gamma$ indicates ferromagnetism / antiferromagnetism

Signed Arthur L. Loeb
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