Digital Computer Laboratory
Massachusetts Institute of Technology
Cambridge, Massachusetts

SUBJECT: GROUP 63 SEMINAR ON MAGNETISM, XXXIX

To: Group 63 Engineers

From: Arthur L. Loeb and Norman Menyuk

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In the fourth of his series of articles on ferromagnetism, Zener discusses the structure sensitivity of the magnetic properties of iron. Iron can exist in a body centered or face centered lattice. The body centered iron exhibits ferromagnetism while the face centered lattice is not ferromagnetic.

While the face centered phase of iron can only exist above the Curie temperature, the lack of ferromagnetic coupling cannot be dismissed on this basis. From the face centered phase of nickel iron and cobalt iron, one finds the extrapolated Curie temperature of the pure iron face centered phase lies in the vicinity of absolute zero at best.

Néel interpreted this difference of magnetic properties in terms of the atomic separation in the two phases. In body-centered iron the separation between nearest and next-nearest neighbors are 2.48 and 2.86 angstron units respectively. In face-centered iron these separations are 2.52 and 3.58 Å respectively. Interpreting these figures in terms of the Heisenberg theory, with the exchange integral changing sign in a particular separation region (see figure 5 - meeting VI), only the distance 2.86 Å lies in the region of ferromagnetic coupling. Thus no ferromagnetic coupling exists in the face centered lattice, and exists between next-nearest neighbors in the body centered lattice.

Zener finds this line of reasoning artificial. Instead, he considers the first transition period from nickel to cobalt, as shown in table I.

TABLE I

Element	V	Cr	Mn	Fe	Co	Ni
Atomic Number	23	24	25	26	27	28
Electron Distribution	d^4s	d^5s	d^6s	d^7s	d^8s	d^9s

The electron distribution in the above table differs from that given in table I of meeting XXXV because the above considers only one electron remaining in the 4s shell after demotion to the 3d shell.

According to Zener's theory, as discussed previously, direct exchange coupling of the d shells always tends to align the spins of adjacent d shells anti-parallel. In nickel and cobalt the d shells are relatively far apart, so the d - d coupling is slight (see figure 67 a) and the s - d coupling in these elements leads to ferromagnetism. In the chromium and vanadium atoms, the overlap of the d shells is much greater (see figure 67 b) so the anti-ferromagnetic coupling predominates. Iron and manganese lie between these ferromagnetic and anti-ferromagnetic regions. That is, the d - d coupling of these elements, tending toward antiferromagnetic alignment, is approximately equal to the s - d coupling tending toward ferromagnetic alignment, so the crystal structure plays the deciding role. The complete absence of ferromagnetism in face-centered iron leads Zener to believe that iron would not be ferromagnetic were it not for an inherent flexibility of the body centered lattice.

It has long been established that atoms tend to lose or gain electrons so as to have complete outer shells. Zener further states, from exchange energy considerations, that there will also be a tendency toward a half-filled d shell in the transition elements.

As an example, consider the iron configuration $3d^7 4s$. If two such atoms were brought together they would be lined up, in accordance with Hund's rule and the exclusion principle, as shown in figure 69 a.

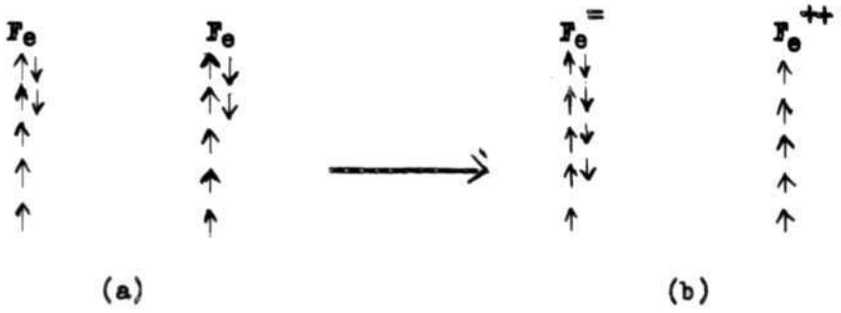

FIGURE 69

According to Zener, the configuration of figure 69 b would be more favorable from an exchange point of view, since the exchange energy in the positive half-shells (↑) is unchanged, while the total number of pairs of the negative half shells (↓) is changed from 2 to 6 on going from configuration (a) to configuration (b).

The iron atoms are now ionized. The Fe^{++} ions have saturation magnetic moment of $2.5\mu_B$ (Bohr magnetons), and the $Fe^{=}$ ions have a saturation magnetic moment of $0.5\ \mu_B$.

If the Fe^{++} and $Fe^{=}$ ions arrange themselves as nearest neighbors in a body centered lattice, as in figure 70, the saturation magnetic moment per atom is $2.0\ \mu_B$, as compared to the observed value $2.2\ \mu_B$. This difference can arise from the polarization of the conduction electrons.

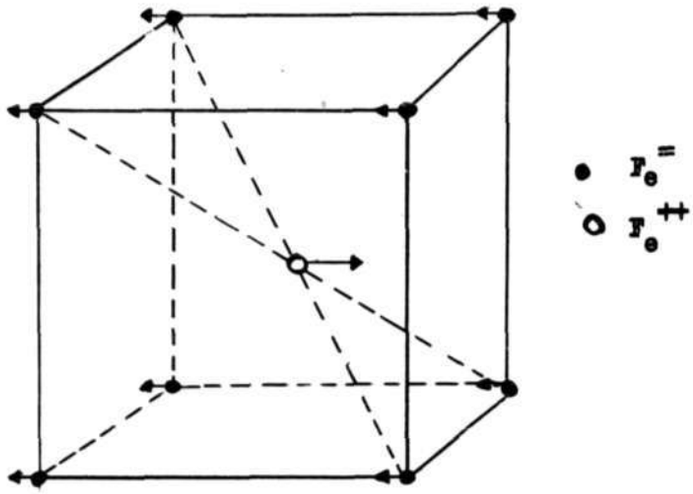

FIGURE 70

The electrostatic energy will be lowest for a body centered lattice as shown in the above figure. One objection to this model may be that the gain in exchange energy in such a lattice may be more than offset by the rise in the electrostatic energy. However, calculations by Zener show that the electrostatic energy might be lower than the exchange energy.

A second objection arises from the fact that localized net electron spin should be detected by neutron diffraction experiments. Dr. Shull has performed such experiments and failed to observe this effect. Zener is able to retain this model by considering the polar lattice as one in which the polarity of a given atom fluctuates rapidly.

Signed Arthur L. Loeb
Arthur L. Loeb

Norman Menyuk
Norman Menyuk

Approved DRB
David R. Brown

ALL/NM:jrt

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