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

To: Group 63 Engineers

From: Arthur L. Loeb, Dudley A. Buck, Norman Menyuk

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In the previous meeting the Hartree and Hartree-Fock methods of arriving at a self-consistent field determination were discussed. Both methods are essentially similar in that calculations involving either the Hartree or Hartree-Fock method involve the same five steps outlined at the previous meeting. The methods differ only in that the Hartree-Fock method involves a more sophisticated first approximation of the average field in which the electrons move.

Hartree considers the j^{th} electron and the average field in which it moves, arriving at the equation

$$-\frac{\hbar^2}{2m}\nabla_j^2\psi_j + \left[V_j(\vec{r_i}) + \sum_i{}' e^2 \int \frac{|\psi_i|^2}{r_{ij}}\, d\tau\right]\psi_j = 0$$

The first two terms represent the ordinary Schroedinger equation for the isolated j^{th} electron. The final term,

$$\sum_i{}' e^2 \int \frac{|\psi_i|^2}{r_{ij}}\, d\tau$$

represents the charge density in the region of the j^{th} electron due to the action of all the other electrons.

Fock further considered the fact that the other electrons are influenced by the fact that the j^{th} electron is at the point at which it is assumed to be located. This involves spin considerations since, assuming the j^{th} electron to have a particular spin orientation, it will tend to exclude electrons of like spin orientation from the immediate vicinity. Furthermore, the ψ's must be mutually orthogonal and orthogonal to ψ_j.

The question arises as to where the Zener model fits into the general scheme discussed at the previous meeting. Since this model considers the d shell electrons as bound, its viewpoint is basically atomistic, and in this respect is most closely comparable with the Heitler-London model. However, it may be recalled (meeting XXXVI) that the energy

$$E = \frac{1}{2}\alpha S_d^2 - \beta S_c S_d + \frac{1}{2}\gamma S_c^2$$

was minimized as a function of S_c. This is tantamount to considering one conduction electron spin S_c in the field due to the other atoms. In this respect the Zener model, with its strong s-d coupling corresponds to the model used in the Hartree-Fock calculation, with an electron in the average field due to the d shell and s bands. The exclusion principle is considered implicitly in finding the average potential.

A talk was given by Dudley Buck on alloys of the approximate composition 75% nickel, 25% iron. According to S. Kaya* there is a considerable difference in the magnetic properties of permalloy (76% Ni - 24% Fe) in the ordered and disordered state. In the disordered state a square hysteresis loop is obtained, as indicated in figure 82a. The ordered state of permalloy gives rise to a constricted hysteresis loop of the type shown in figure 82b.

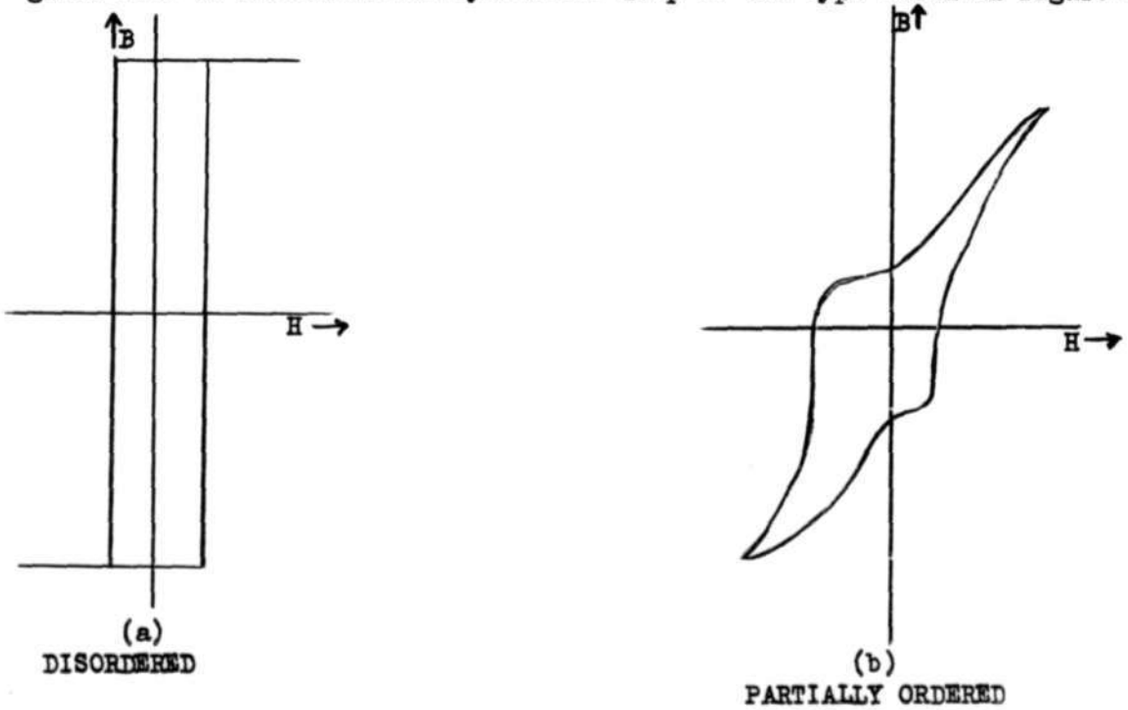
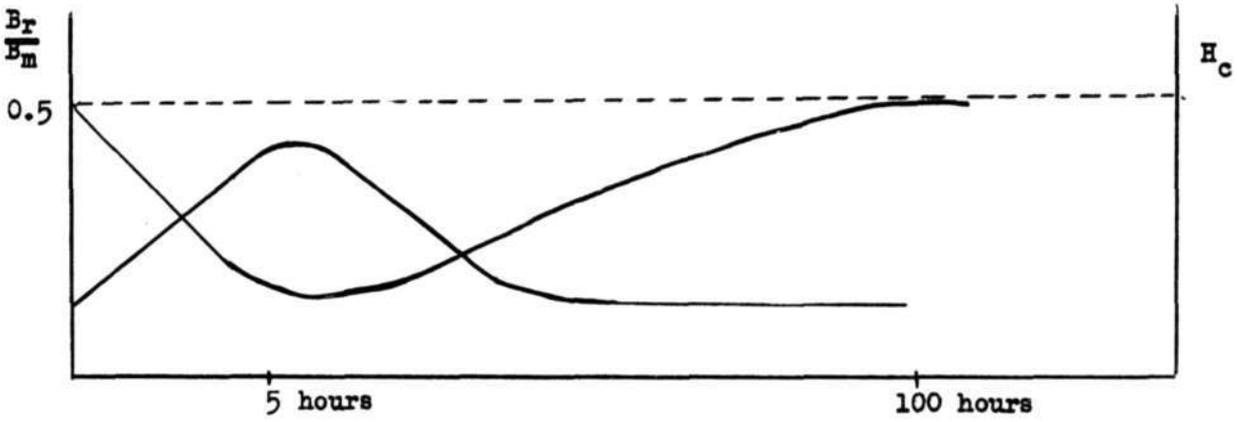


FIGURE 82

* Kaya, S., Washington Conference on Magnetism, Univ. of Maryland, Maryland. (1952)

The ordered system is obtained by annealing at 490°C for five hours after having previously quenched the permalloy at 600°C. The ordering temperature is approximately 510°C.

The ratio of the remanence to maximum flux density as well as the coercive force was found to depend upon the annealing time. This dependence is shown in figure 83. $\frac{B_r}{B_M}$ is found to be a minimum and H_c a maximum for an annealing time of approximately five hours. This is believed to be associated with the formation of short range ordering. At longer annealing times long range ordering takes place.



ANNEALING TIME

FIGURE 83

According to J. E. Goldman, the specific heat of the disordered state is about twice that of the ordered state.

At the same conference D. I. Gordon investigated the variation in the Barkhausen noise in 4-79 molybdenum-permalloy as a function of the initial permeability. The experimental equipment was set up as shown in figure 84. The permanent magnet, rotating at 33 rpm, reverses the magnetization of the mo-permalloy. The output or noise is read on the output meter, and according to Gordon this is due the the Barkhausen jumps occurring during the magnetization reversal. The results are shown in figure 85.

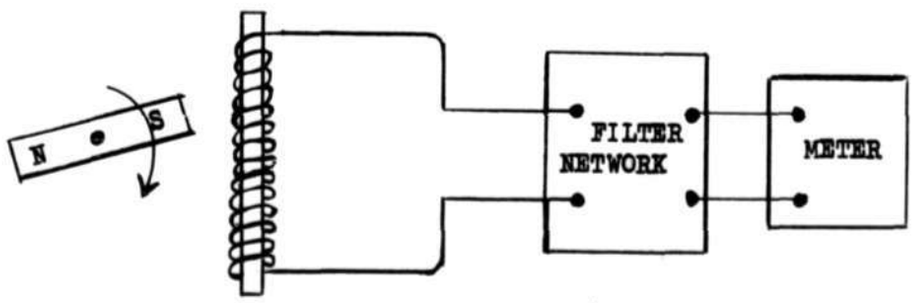


FIGURE 84

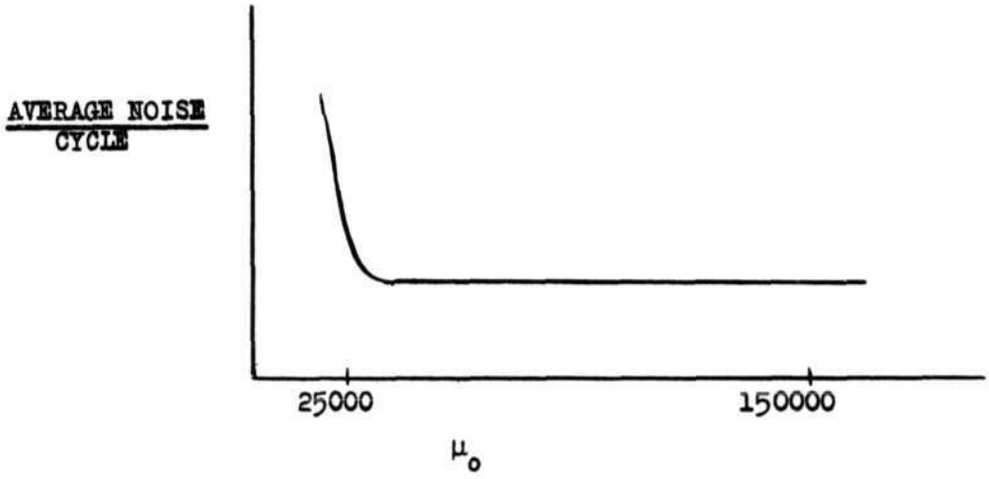


FIGURE 85

It is of interest to try to tie in the ordered Ni_3Fe alloy with the Zener model. The three nickel and one iron atoms are originally in the state described by figure 86a. However, in view of the tendency for the atoms to become ions with either full or half full shells, as discussed at meeting 39, one can assume the two extra iron electrons are transferred to two nickel ions, thereby filling their 3d shells and leaving the iron 3d shell half full. In view of the large increase in the number of exchange pairs involved, it has further been assumed that one 4s electron per molecule is demoted to the 3d shell. Figure 86a then goes over to the form shown in figure 86b. The ionic charge listed here is based on the assumption that the demoted electron is taken equally from the four atoms.

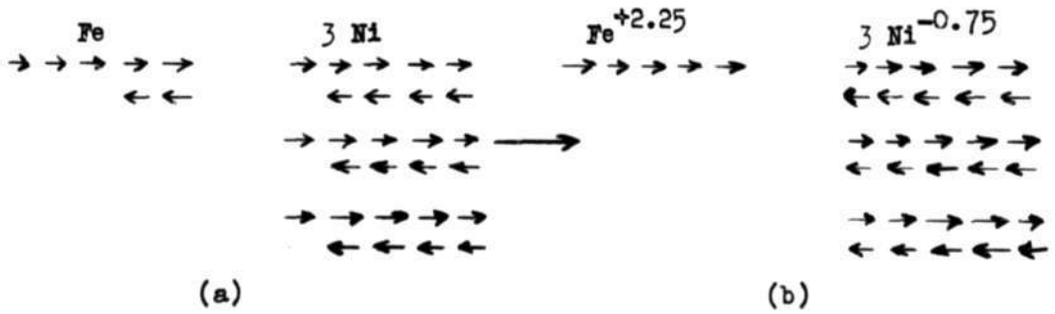


FIGURE 86

According to this model, the iron ion contributes 5 μ_B and the nickel ions contribute no magnetic moment. This gives a resultant of 5/4 or 1.25 μ_B per atom. This compares favorably with the experimental value 1.2μ_B per atom.

However, according to the results obtained by Shull from neutron diffraction experiments, iron contributes 2.6 μ_B and each nickel atom contributes 0.7 μ_B. This yields the resultant value $\frac{4.7}{4}$ or 1.175 μ_B per atom.

On the basis of similar experiments Corliss and Hastings obtained a contribution of 2.0 μ_B from the iron atom and 0.8 μ_B from each nickel atom. This leads to the value $\frac{4.4}{4} = 1.1\ \mu_B$ per atom.

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ALL/DAB/NM:jrt

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