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

To: Group 63 Staff

From: Arthur L. Loeb and Norman Menyuk

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Suggested Reading: 1 - "The Electronic Structure of Metals", R. Kronig, Physica XV, No. 1-2, April 1949, 1.

2 - "Introduction to the Theory of Semi-conductors III, Conductors in Metals, Field Free Case". D. J. Eckl, Digital Computer Laboratory, Engineering Note E-474.

Structure of Metals

The structure of metals is of importance to us because the theories and models evolved in the study of metals must be used for the study of ferromagnetism.

An exact solution of a problem in physics is generally unattainable, and approximation methods must be used. Even so small a system as one consisting of two protons and two electrons (H_2 molecule) cannot be solved exactly, and perturbation methods must be applied. There are two models which are commonly taken as the unperturbed systems. For the case of the two proton-two electron system they would be:

1 - The first model is that of one electron moving in an average field due to the two protons and the other electron. Consideration of the motion of the second electron must lead to a result consistent with that of the first. This approach is known as the self-consistent field method. The approximation arrived at with this model is not very good for large internuclear distances, but produces results consistent with those obtained for the helium atom when the internuclear distance vanishes (the helium nucleus has twice the charge of one hydrogen nucleus).

2 - The second model assumes two hydrogen atoms far apart, the solutions of which are known. These atoms are then moved close together and their interaction is considered a perturbation analogous to the coupling of two harmonic oscillators. This is the Heitler-London method, which yields good results for fairly large interatomic distances. The approximation is not too good for the atoms close together; specifically, it does not reduce to the helium atom when the internuclear distance vanishes, as does the result of method 1.

The first five pages of the Kronig article mentioned above were read, and certain passages were amplified.

Kronig discusses the classical background of the electronic theory of metals, and the need for a simplifying model. This led to the model of the free electron gas which considered the free electrons as independent particles, exerting no forces upon each other. However, interactions with metallic ions exist in the form of short range forces. With this model it was possible to derive velocity distributions arising in various metals due to the action of external fields.

On this basis, Ohm's law and the Wiedemann-Franz law were derived. The Wiedemann-Franz law relates the electrical conductivity and the thermal conductivity due to free electron motion. In conductors, almost all the thermal conductivity is due to this motion. However, this model did not suffice to explain specific heat; and as we have previously stated, it leads to a zero para and diamagnetism.

The advent of quantum mechanics has made it possible to clear up these as well as other unexplained phenomena. The model of the free electron gas without force field was carried over to quantum mechanics; but it was insufficient to explain the subdivision of solids into conductors, semi-conductors, and insulators. Furthermore, this model could not explain the optical properties of metals.

With respect to the optical behavior we might note that in our discussion of the subject (meeting 11) we were able to explain dispersion only by assuming a restoring force acting on the electrons.

Bloch and Brillouin replaced the model of the free electron gas without force field with the model of an electron gas in a periodic potential with the periodicity of the crystal lattice. The electrons are still treated as independent particles. With this model, for a given direction of motion, the permissible energy values of an electron lie in certain allowed energy intervals. These allowed ranges are separated from each other by forbidden intervals.

It might be noted that the mathematical problem of setting up disturbances in a transmission line of an infinite set of four terminal networks is very similar.* Here waves of certain frequencies are attenuated and others are not. In an analagous way for our case of periodic potential, we have certain ranges of energy in which propagations occur. Between these ranges the wave is attenuated, falling off so rapidly that we can say that these regions of energy are forbidden. On this basis, with the help of figure 24, a physical explanation of the difference between conductors, semi-conductors, and insulators may be made.

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* Slater, "Quantum Theory of Matter", McGraw-Hill and Co., 1st Edition, New York, Page 261.

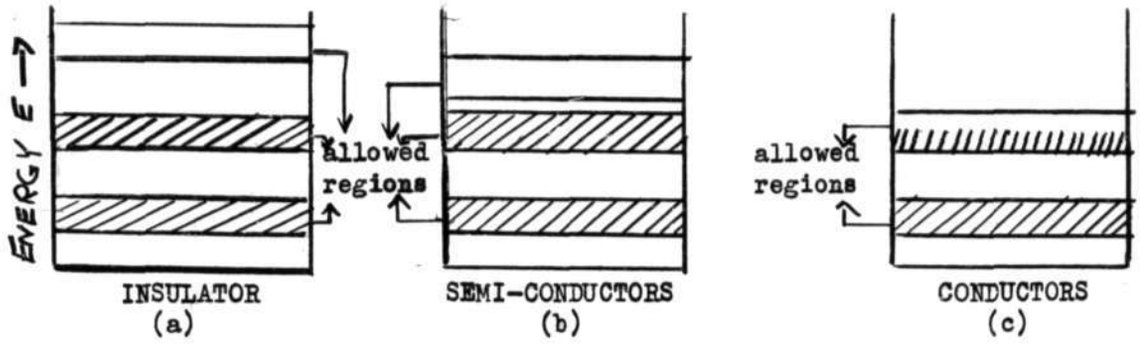

FIGURE 25

In figure 25(a) we see that the lower allowed energy regions are full, and the one above is empty. In order for an electron to increase its energy, it must jump to an energy level which is not already occupied by an electron. Since the lowest unoccupied level is in the upper region, a tremendous amount of energy is needed to cause an electron to bridge the forbidden region.

For the case of the semi-conductors (figure 25(b)), the lower energy levels are filled, but the highest filled region is separated from the lowest empty region by only a small forbidden zone. Thermal agitation of the electrons in the upper level can permit some of them to jump to an energy level in the unfilled region. We find, in support of this hypothesis, that conductivity of a semi-conductor increases as the temperature increases.

In a conducting medium (figure 25(c)) the upper allowed region is only partially occupied by electrons. Therefore, on the application of an electric field the electrons in the unfilled region can easily move to a higher permissible energy level and current will occur.

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