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

To: Group 63 Staff

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Before going further into the subject of magnetism, we must become familiar with quantum mechanics.* In this meeting we will consider the factors that led to the new hypotheses for mechanics in this century.

The duality of waves and particles led Schroedinger to formulate his equation, and so will be discussed first. Until this century it had been generally accepted that light was a wave motion and matter corpuscular. Newton had held that light was corpuscular. However, on the basis of wave motion, Huygens was able to explain the diffraction of light at a slit and the refraction of light at the boundary of a new medium. The wave theory of light was therefore accepted and the corpuscular theory of light fell into disrepute. The corpuscular theory of matter was generally accepted.

In the 19th Century, Hamilton pointed out the analogy of particle motion to light motion in geometric optics. This led Hamilton to formulate his principle of least action.

At the start of the twentieth century, Planck tried to find the energy distribution of black-body radiation as a function of frequency. The result obtained by purely classical methods was at variance with experimental evidence. In order to overcome this, Planck found a mathematical equation to fit the data which implied that radiant energy was emitted or absorbed by metals in discrete quanta of energy rather than continuously.

Einstein went beyond this. According to his hypothesis of light quanta (photons), light consists of quanta, of energy $h\nu$, which are corpuscular. On the basis of this hypothesis he successfully explained the photoelectric effect. According to Einstein's explanation, the entire energy of a photon impinging upon a metal is transferred to a single electron in the metal. Upon leaving the surface of the metal, the electron will have

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* Read Eckl, D. J., "Some Remarks on Quantum Mechanics", Digital Computer Laboratory, Engineering Note E-463

a kinetic energy

$$1/2\ mv^2 = h\nu - \phi \,. \qquad \text{XIX-1}$$

where ϕ = work function of the metal; (see figure 40). If the frequency of the impinging radiation is brought below ν_0, where $h\nu_0 = \phi$, the photons will not give up enough energy to the electrons to enable them to leave the surface. Thus there is a frequency ν_0 below which the photoelectric effect stops; ν_0 is known as the threshold frequency.

From the photoelectric effect we see radiant energy exhibits corpuscular as well as wave characteristics. In 1924 De Broglie hypothesized that this dual wave and corpuscular character should be exhibited by particles as well as by radiation. On the basis of the De Broglie hypothesis (see Appendix III), the wavelength associated with a particle is:

$$\lambda = \frac{h}{p}$$

where h = Planck's constant = 6.6×10^{-27} erg-sec
p = particle momentum

One might ask why this wave nature had never been noticed before. It should be noted that diffraction effects occur when a wave passes through a slit of the same order of magnitude as the wavelength. For a particle of finite dimensions, e.g. mass m = 1 gram, velocity = 1000 cm. per second, we find that $\lambda = 6.6 \times 10^{-30}$ cm. Since no slit this small is obtainable, it is impossible to observe any diffraction effect for so large a particle. Even for an electron, the wavelength is of the order of interatomic distances in a crystal. A mechanically built grating cannot be made with spacings that small, but crystals are used and the interference effect has been seen.

The relative magnitude of the wavelength and the system dimensions is of extreme importance in all problems. To point this up, a problem arising in classical optics is given as an example.*

For an optical examination of thin metal films the metal is evaporated onto a thin, transparent film; to compute the reflection and transmission of such a system, the reflection and transmission of the backing must be calculated. Some backings, e.g. glass, have a thickness that is very large compared to the wavelength of the incident radiation, while others, e.g. cellulose backings, have a thickness of the order of the wavelength of the incident radiation. For the latter case optical interference is observed, and amplitude addition must be employed in the calculation. For the case of a relatively heavy backing (glass), intensity superposition of reflected and incident radiation is used in the backing. This latter calculation is simple and was generally accepted until questioned by Koller. Harris, Beasley and Loeb (op. cit.) have analyzed the situation and concluded that when the dimensions of the backing are large compared to the wavelength, the uncertainties in the measurement of thickness and wavelength necessitate averaging over a finite range of the measured quantities; this calculation showed that for the case of glass backing intensity addition is justified.

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* Harris, Beasley, and Loeb, "Reflection and Transmission of Radiation by Metal Films and the Influence of Nonabsorbing Backings", Journal of the Optical Society of America, 41, September, 1951, P. 604.

In quantum mechanics the situation is analogous: when the dimensions of the medium are large compared to the wavelength of the particle, classical theory is sufficient, but for small media quantization (amplitude addition) is necessary.

The Heisenberg uncertainty principle is most frequently seen in the form

$$\Delta p \, \Delta q \sim h \quad \text{or} \quad \Delta \varepsilon \, \Delta t \sim h \qquad \text{XIX-2}$$

However, it is possible to derive from purely classical wave theory, the relations

$$\Delta \nu \, \Delta t \sim 1 \qquad \Delta\left(\frac{1}{\lambda}\right) \Delta q \sim 1 \qquad \text{XIX-3}$$

wherein:

Δp = uncertainty in momentum
Δq = uncertainty in coordinate
$\Delta \varepsilon$ = uncertainty in energy
Δt = uncertainty in time
$\Delta \nu$ = uncertainty in frequency
$\Delta \lambda$ = uncertainty in wavelength

If we apply the relations

$$\varepsilon = h\nu \qquad \text{and} \qquad \lambda = \frac{h}{p},$$

we see the two sets of equations above are equivalent. In order to derive equations XVIII-3 for a wave packet, it would be necessary to express the packet in terms of a Fourier series. We shall not derive the equations here, but in order to better understand them, let us consider a packet of white light, which consists of a single maximum and is zero elsewhere, as shown in figure 41 (a).

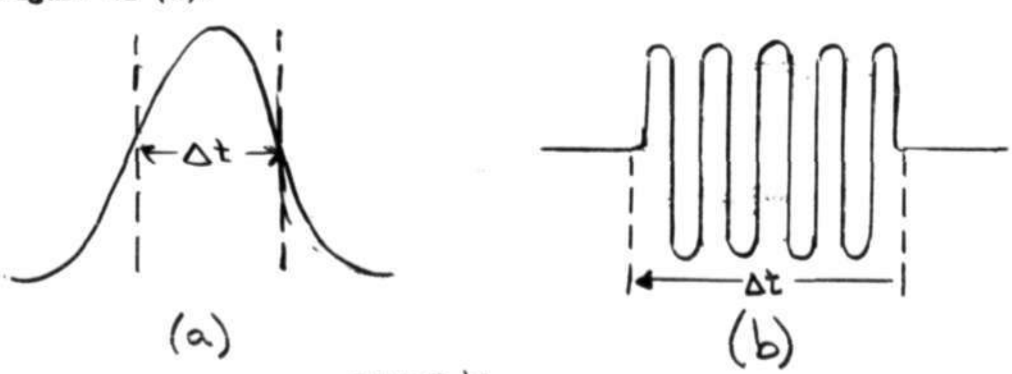

FIGURE 41

In order to produce this type of packet a number of Fourier components will have to be added. The frequency spread involved will be $\Delta\nu$. It is impossible to localize the time to any greater extent than Δt as shown in the figure. If $\Delta t \longrightarrow 0$ (figure 41, becoming a sharp spike) then the spread of frequencies required to produce this packet would be infinite. Similarly, if $\Delta\nu \rightarrow 0$ (monochromatic light) then $\Delta t \longrightarrow \infty$ and the radiation would continue indefinitely. If monochromatic waves are admitted by opening a slit and cut off by closing this slit a time t later, it has definite bounds, as in figure 41 (b), and Fourier components must be introduced to give a zero resultant beyond the region of finite amplitude. Thus, though the frequency within this region may be monochromatic, the frequency uncertainty of the packet is finite.

A similar analysis may be made of the relation between the location of the packet in space and the inverse of the wavelength.

One of the fundamental concepts of modern physics is the correspondence principle. One of the conclusions to be drawn from this principle is that systems in a high quantum state should behave classically. For example, consider a particle in a box; if the energy is low and the associated wavelength is of the order of the box dimensions, the system must be solved using quantum mechanics. However, if the particle is in a high quantum state (higher energy), the wavelength is decreased. If the box dimensions are then much greater than the wavelength, the system may be treated classically.

To arrive at a fundamental equation which would be valid for atomic systems, Schroedinger introduced a wave function Ψ. This function describes the state of the system in question.

The Schroedinger equation is a hypothesis. As such, it cannot be derived from some more fundamental equation or equations. When formulating his equation, Schroedinger used the notation of Hamilton, who had reformulated Newton's law. Hamilton introduced a quantity called the Hamiltonian $\underline{H}$ which is a function of momentum and coordinates. The Hamiltonian of a system is equal to the total energy of that system. Expressed mathematically,

$$H = H(p,q) = E$$

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Approved DRB

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