

must have a solution such that  $\Pi_{ij}^h = \Pi_{ji}^h$ ,  $\Pi_{hh}^h = 0$  and which will transform according to the law of transformation of the coefficients of projective connection. By repeated application of (4.2) and (4.3) we find that (4.4) are completely integrable and although in general the solutions will not be coefficients of projective connection,  $\infty \frac{n(n-1)(n+2)}{2}$  of them will satisfy all the conditions of the problem.

The same set of vectors  $\xi_{(\alpha)}^i$  can serve as the components for a simply transitive group of affine collineations, as the equations

$$\frac{\partial \Gamma_{ij}^h}{\partial x^k} = \frac{\partial R_{ik}^h}{\partial x^j} - R_{im}^h R_{jk}^m - \Gamma_{ij}^m R_{mk}^h + \Gamma_{im}^h R_{jk}^m + \Gamma_{mj}^h R_{ik}^m \quad (4.5)$$

are also completely integrable. The general solutions of (4.5) are coefficients of *asymmetric connection*,  $\infty \frac{n^2(n+1)}{2}$  of them being coefficients of affine connection. There exists only one manifold, its coefficients of connection being  $R_{jk}^i$ , with respect to which each of the given vectors  $\xi_{(\alpha)}^i$  is a parallel vector field.

<sup>1</sup> Eisenhart, L. P., and Knebelman, M. S., these PROCEEDINGS, 13, 1927, p. 38.

<sup>2</sup> Eisenhart, L. P., *Ibid.*, 8, 1922, p. 236.

<sup>3</sup> Veblen, O., and Thomas, J. M., *Ann. Math.*, 27, 1926, p. 287.

<sup>4</sup> *Loc. cit.*, pp. 288-291.

<sup>5</sup> Eisenhart, L. P., *Riemannian Geometry*, 1926, Chap. VI.

## REMARKS ON THE QUANTUM THEORY OF DIFFRACTION

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1. *On Fraunhofer Diffraction Phenomena.*—Before attacking the Fresnel problems we shall restate some of the considerations of our last paper, dealing with the Fraunhofer diffraction in a new form suitable for generalization.<sup>2</sup> The main question discussed in that paper was as to the intensity of light diffracted by any optical structure at a given angle to the incident beam. We saw there that the "electronic intensity,"  $\rho$  of the diffracting system is a function of the space which may be referred to any system of coördinates. Let us use a rectangular cartesian system  $x, y, z$  and denote the cosines of the angles between the axes and the direction of the incident ray by  $\alpha_0, \beta_0, \gamma_0$ .

The general expression for the electronic density can then be given in terms of a three-fold Fourier integral

$$\rho(x, y, z) = \int_{-\infty}^{+\infty} d\omega_1 \int_{-\infty}^{+\infty} d\omega_2 \int_{-\infty}^{+\infty} A_{\omega_1\omega_2\omega_3} \cos(\omega_1x + \omega_2y + \omega_3z - \delta_{\omega_1\omega_2\omega_3}) d\omega_3, \quad (1)$$

where

$$A_{\omega_1\omega_2\omega_3} e^{i\delta_{\omega_1\omega_2\omega_3}} = \frac{1}{8\pi^3} \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} dv \int_{-\infty}^{+\infty} \rho(u, v, w) \cos(\omega_1u + \omega_2v + \omega_3w) dw. \quad (2)$$

This means that the actual electronic density can be always built up by a superposition of a three-fold infinity of sinusoidal elementary lattices. Each elementary lattice consisting of uniform plane layers perpendicular to the direction  $(\omega_1x + \omega_2y + \omega_3z)/\sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2}$ .

On the other hand we have seen in section 3 of the paper referred to that, from a classical point of view, the mean amplitude of the secondary radiation emitted in a direction  $\alpha, \beta, \gamma$  is the modulus of

$$S(\alpha, \beta, \gamma) = C \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} \rho e^{\frac{2\pi}{\lambda} [x(\alpha - \alpha_0) + y(\beta - \beta_0) + z(\gamma - \gamma_0)]} dz. \quad (3)$$

We see that the expressions of  $A$  and  $S$  become identical (apart from the constant  $C$ ), when

$$\omega_1 = 2\pi(\alpha - \alpha_0)/\lambda, \quad \omega_2 = 2\pi(\beta - \beta_0)/\lambda, \quad \omega_3 = 2\pi(\gamma - \gamma_0)/\lambda. \quad (4)$$

This means that out of our infinity of lattices only that one is responsible for the reflected beam (3) for which the coefficients  $\omega_1, \omega_2, \omega_3$  satisfy relations (4). In fact, let us consider the special case when our structure is of such a constitution that  $A$  has a finite value only for the arguments (4) and is zero for all other values of  $\omega_1, \omega_2, \omega_3$ . From the comparison of (2) and (3) it follows that the diffracted intensity will have a finite value only for the direction  $\alpha, \beta, \gamma$  and will vanish for all other directions. The general case can be regarded as a superposition of such special cases, so that each elementary lattice throws its whole intensity in only one direction.

It is useful to adapt the system of coordinates to the direction of the diffracted ray under consideration. Let us consider the directions of the primary and the secondary ray as known and including an angle  $2\varphi$ , and let us choose as  $x$ -axis the bisectrix of the angle between the secondary ray and the negative direction of the primary, as  $y$ -axis the bisectrix of the adjacent angle (between the positive directions of the primary and the secondary ray) and as  $z$ -axis the perpendicular to  $x$  and  $y$ . We will have then  $\alpha = \cos \varphi, \alpha_0 = -\cos \varphi, \beta = \beta_0 = \sin \varphi, \gamma = \gamma_0 = 0$ . Equations (4) take the form

$$\omega_1 = 4\pi \cos \varphi/\lambda, \quad \omega_2 = 0, \quad \omega_3 = 0 \quad (5)$$

This means that the plane layers of the responsible lattice are at right angles to the  $x$ -axis and in a position with respect to the primary and secondary ray corresponding to a regular reflection from those layers. The spacing  $a$  of this lattice is connected with  $\omega_1$  by the relation  $2\pi/a = \omega_1$  and satisfies, therefore, the Bragg relation

$$2a \cos \varphi = \lambda. \quad (6)$$

The expression (3) for the reflected intensity assumes the simpler form

$$S = C \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} \rho e^{i\omega_1 x} dz. \quad (7)$$

It was shown in paper I (section 2) that in the act of reflection the  $x$ -component of the momentum carried by the light wave is changed by the amount  $h/a$  for every energy quantum  $h\nu$ .

2. *Fresnel Diffraction from the Classical Point of View.*—We shall use the same degree of accuracy that is used in most text books<sup>3</sup> developing the Huyghens principle. That is, we shall assume that the amplitude of the primary wave at a distance  $r$  from the source of light  $O$  is given by  $e^{ikr}/r$ . If this wave falls on a diffracting structure having the electronic density  $\rho$ , every element of this structure becomes a secondary source emitting light according to the same law. In a second point  $O'$  the intensity of the scattered or diffracted light is, therefore, represented by the modulus of the well-known expression

$$S = C \iiint \frac{e^{i\frac{2\pi}{\lambda}(r+r')}}{rr'} \rho dx dy dz \quad (8)$$

where  $r$  denotes the distance from  $O$  to the scattering element  $dx dy dz$ ,  $r'$  the distance from that element to  $O'$ , and where the integral is to be extended over the whole volume of the diffracting structure.

We can construct an analogy with formula (7) of the last section if we introduce instead of the cartesian coördinates  $x, y, z$  a new system of curvilinear variables, so that  $r + r' = \xi$  is one of them. This can be done in the following way. Let us denote the distance  $OO'$  by  $f$ , let us choose the origin of the cartesian system in the middle of that distance, and the  $x$ -axis coinciding with the line  $OO'$ . The new coördinates  $\xi, \eta, \varphi$  will then be given by the relations

$$\begin{aligned} x &= \frac{1}{2f} \xi \eta, & y &= \frac{1}{2f} \sqrt{\xi^2 - f^2} \cdot \sqrt{f^2 - \eta^2} \cos \varphi, \\ z &= \frac{1}{2f} \sqrt{\xi^2 - f^2} \cdot \sqrt{f^2 - \eta^2} \sin \varphi. \end{aligned} \quad (9)$$

The surfaces  $\xi = \text{const.}$  are a family of confocal stretched ellipsoids of rotation while the surfaces  $\eta = \text{const.}$  are the orthogonal family of confocal hyperboloids. We have further

$$\xi = r + r', \quad \eta = r - r' \tag{10}$$

The line elements in the respective directions  $\xi, \eta, \varphi$  are given by

$$ds_\xi = \frac{1}{2} \sqrt{\frac{\xi^2 - \eta^2}{\xi^2 - f^2}} d\xi, \quad ds_\eta = \frac{1}{2} \sqrt{\frac{\xi^2 - \eta^2}{f^2 - \eta^2}} d\eta, \tag{11}$$

$$ds_\varphi = \frac{1}{2f} \sqrt{\xi^2 - f^2} \cdot \sqrt{f^2 - \eta^2} d\varphi.$$

The volume element, correspondingly,

$$dV = \tau(\xi, \eta, \varphi) d\xi d\eta d\varphi = \frac{1}{8f} (\xi^2 - \eta^2) d\xi d\eta d\varphi. \tag{12}$$

Finally the angle  $\psi$  between  $r$  and the normal to the ellipsoid  $\xi = \text{const.}$

$$\cos \psi = \sqrt{\frac{\xi^2 - f^2}{\xi^2 - \eta^2}}. \tag{13}$$

With these substitutions  $\tau/rr' = 1/2f$ , so that (8) becomes

$$S = \frac{C}{2f} \int_f^{+\infty} d\xi \int_{-f}^{+f} d\eta \int_0^{2\pi} \rho e^{i\frac{2\pi}{\lambda}\xi} d\varphi. \tag{14}$$

The analogy with the case of the last section is a far reaching one. As there by formula (1), we can represent  $\rho$  by a Fourier expression. The only difference is that, due to the finite variability of  $\eta$  (from  $-f$  to  $+f$ ) and  $\varphi$  (from 0 to  $2\pi$ ), two of the integrations must be replaced by summations:

$$\rho(\xi, \eta, \varphi) = \int_{-\infty}^{+\infty} d\omega_1 \sum_{-\infty}^{+\infty} n_2 \sum_{-\infty}^{+\infty} n_3 A_{\omega_1 n_2 n_3} \cos(\omega_1 \xi + \frac{\pi}{f} n_2 \eta + n_3 \varphi - \delta_{\omega_1 n_2 n_3}) \tag{15}$$

$$A_{\omega_1 n_2 n_3} = e^{i\delta_{\omega_1 n_2 n_3}} = \frac{1}{8\pi^2 f} \int_{-\infty}^{+\infty} du \int_{-f}^{+f} dv \int_0^{2\pi} \rho(u, v, w) e^{i(\omega_1 u + \frac{\pi}{f} n_2 v + n_3 w)} dw. \tag{16}$$

Again we see that the distribution of density can be represented by superposition of a three-fold infinity of curved elementary lattices. The comparison of (16) and (14) shows, in close analogy to section 1, that for the secondary pencil only that elementary lattice is responsible for which

$$\omega_1 = 2\pi/\lambda, \quad n_2 = 0, \quad n_3 = 0. \tag{17}$$

This means that the responsible lattice represents a sinusoidal succession of uniform layers characterized by the condition  $\xi = \text{const.}$  That is, the layers are ellipsoids of rotation having all the common focal line  $OO'$ . As the spacing of a lattice is given by the relation  $\omega = 2\pi/a$  we see that in this case

$$a = \lambda. \quad (18)$$

From layer to layer the parameter  $\xi$  increases by a constant amount, equal to the wave-length. Such a lattice has the property of converting a divergent wave emitted in  $O$  into one converging toward  $O'$ .

3. *Momentum of the Primary and Secondary Waves.*—In this section we shall carry the analogy with the Fraunhofer case still farther and show that in the act of reflection from our ellipsoidal lattice there prevails a transformation of momentum quite similar to that discovered by Duane for the plane lattice. We shall call  $\xi$ -momentum the Lagrangean momentum conjugated with the variable  $\xi$ . The amount of  $\xi$ -momentum carried by the primary wave can be found in the following way. Let us consider an element  $d\sigma$  of one of the ellipsoids  $\xi = \text{const.}$  and let us ask how much  $\xi$ -momentum  $dp_\xi$  passes through it in the short time  $dt$ , due to the primary wave motion. If this element of area suddenly became perfectly absorbing, it would absorb all of the radiation falling on it and acquire, in this way, the momentum  $dp_\xi$  in the time  $dt$ . As the momentum is the time integral of a force, we have

$$dp_\xi = f_\xi dt \quad (19)$$

if we denote by  $f_\xi$  the Lagrangean generalized force exercised by the primary wave on the absorbing element. If under the action of this force the element is displaced in the direction  $\xi$  so that the parameter  $\xi$  experiences an increase  $d\xi$ , the work of the force is given by

$$dW = f_\xi d\xi. \quad (20)$$

On the other hand, the same work in terms of the ordinary cartesian force  $F_\xi$  acting on the element in the normal direction, due to the light pressure, will be

$$dW = F_\xi ds_\xi. \quad (21)$$

Comparing the two expressions for  $dW$  we find  $f_\xi = F_\xi ds_\xi/d\xi$  and

$$dp_\xi = F_\xi dt ds_\xi/d\xi. \quad (22)$$

The force  $F_\xi$  is known in theory of light pressure<sup>4</sup> to be  $F_\xi dt = \cos \psi dE/c$ , where  $dE$  denotes the energy falling on the area  $d\sigma$  in the time  $dt$  and  $\psi$  the angle with the normal as in (13). It follows

$$dp_{\xi} = \frac{\cos \psi}{c} \frac{ds_{\xi}}{d\xi} dE. \quad (23)$$

Formulae (11) and (13) of section 2 show us that  $\cos \psi ds_{\xi}/d\xi = 1/2$ , so that

$$dp_{\xi} = dE/2c. \quad (24)$$

As this relation is true for any pencil, it is true for any finite portion of the primary wave:

$$p_{\xi} = E/2c. \quad (25)$$

This is a portion of the primary wave having an energy  $E$  carries a  $\xi$ -momentum proportional to this energy, the constant of proportionality being  $1/2c$ .

Turning from the primary wave to the secondary, we notice that the conditions in the latter have a perfect symmetry with those in the former, the only difference being that the secondary wave is a convergent one so that the  $\xi$ -momentum has the opposite sign. We can, therefore, write

$$p'_{\xi} = -E/2c. \quad (26)$$

If the energy  $E$ , originally contained in the primary wave, by reflection from the elements of the grating, goes over to the convergent secondary wave, this act of reflection is connected with a change of  $\xi$ -momentum  $p_{\xi} - p'_{\xi} = E/c$ . In the special case, when we consider an amount of reflected energy  $E = h\nu$ , we have

$$\Delta p_{\xi} = h\nu/c = h/\lambda. \quad (27)$$

We have seen in section 2 that  $\gamma = a$ : the wave-length is equal to the spacing of the responsible lattice. The last relation, therefore, can be written

$$\Delta p_{\xi} \cdot a = h \quad (28)$$

in which form it shows a complete analogy with Duane's rule for the change of translatory momentum in the case of the Fraunhofer diffraction.

4. *Interpretation in Terms of Light Quanta.*—Let us regard the problem sketched in the beginning of section 2 from the point of view of light quanta. Light quanta of the frequency  $\nu$  are emitted by the source  $O$ . They can be reflected in many different ways by the elements of the optical structure surrounding the source and having the electronic density distribution  $\rho$ . If, however, the analogy with the case discussed in section 1 holds still in the applications of the correspondence principle, we must expect that the probability of the light quanta being reflected into the point  $O'$  is associated with the same term in our Fourier expression (15)

which is responsible in the classical theory for converting the primary wave into a secondary wave converging towards  $O'$ . Speaking more definitely, the principles laid down in paper I let us expect that this probability will be proportional to the square of the amplitude  $A_{\omega_1, \nu_1, m_1}$  of the responsible lattice, defined by the conditions (16) and (17).

The "mechanism" of this reflection can be described in the following way. Let us assume that our optical system is capable of a motion in which all the surfaces  $\xi = \text{const.}$  move in a normal direction so that each surface remains a confocal ellipsoid. The light quantum collisions of the above-considered type are such that they impart to our optical structure just such a motion. For the  $\xi$ -momentum  $\Delta p_\xi$  which the system can pick up in a collision with a light quantum we have to introduce the same quantum restriction as in the case of paper I

$$\int \Delta p_\xi d\xi = h$$

where the integral must be extended over a period of the corresponding lattice equal to  $a = \lambda$ , according to (18). We get again relation (28)

$$\Delta p_\xi \cdot a = h. \quad (28)$$

The mechanical meaning of the  $\xi$ -momentum possessed by our structure is the following. Let  $m$  be the mass density in any point of our structure, then the kinetic energy of a volume element  $dV$  in its motion in the  $\xi$ -direction will be

$$T = \frac{m}{2} (ds_\xi/dt)^2 dV = \frac{1}{2} m (ds_\xi/d\xi)^2 \dot{\xi}^2 dV.$$

The  $\xi$ -momentum of this element is, therefore,  $\partial T/\partial \dot{\xi} = m(ds_\xi/d\xi)^2 \dot{\xi} dV$ , while the total  $\xi$ -momentum becomes

$$p_\xi = \int m (ds_\xi/d\xi)^2 \dot{\xi} dV,$$

the integration being extended over the whole volume of the structure.

Since the momentum acquired by the diffracting structure is supplied by the light quantum, the latter loses an amount of  $\xi$ -momentum equal to  $\Delta p_\xi = h/a = h/\lambda = h\nu/c$ . As we have seen in section 2, the ordinary cartesian momentum  $M_\xi$  in the direction  $\xi$  is connected with the  $\xi$ -momentum by the relation  $M_\xi ds_\xi/d\xi = p_\xi$ , so that the light quantum undergoes in the collision a change of the  $\xi$ -component of its cartesian momentum which, on account of the relation  $ds_\xi/d\xi \cos \psi = 1/2$ , can be written

$$\Delta M_\xi = 2 \cos \psi \Delta p_\xi = 2h\nu \cos \psi/c. \quad (29)$$

The light quantum possesses a rectilinear momentum  $h\nu/c$  in the direction of its motion. In the moment when it crosses a surface  $\xi = \text{const.}$  the normal component to this surface is  $h\nu \cos \psi/c$ , the tangential com-

ponent  $h\nu \sin \psi/c$ . Equation (29) shows us that in a collision the tangential component remains unchanged, while the normal loses the amount  $2h\nu \cos \psi/c$  and becomes, therefore,  $-h\nu \cos \psi/c$  or oppositely equal to its value before the collision. This change corresponds to a regular reflection from a surface  $\xi = \text{const.}$  and brings, therefore, the quantum to the second focus  $O'$  of the surface.

These considerations show us that if we had a structure just consisting of the elementary ellipsoidal lattice, all the light quanta going out of the focus  $O$  would be reflected into the focus  $O'$ . In section 2 we have seen that exactly the same conditions prevail in the case of light waves following the classical theory. If we have a more complicated structure, the principle of correspondence suggests that the probability of light quanta behaving in this way will be proportional to the square of the amplitude  $A_{\omega_1 n_2 n_3}$  of the responsible lattice. On the other hand, according to formula (14), the intensity of the wave converging into  $O'$  will be expressed just by the same quantity  $A_{\omega_1 n_2 n_3}^2$ . It follows that the classical theory and the above-sketched adaptation of the quantum theory give identical results.

5. *Limitations of the Theory.*—At first sight it could seem that the agreement between the classical theory and the quantum theory is just as good in the case of Fresnel diffraction as in the case of Fraunhofer diffraction. A closer examination shows, however, that there is a considerable difference between the two cases. To account for the Fraunhofer phenomena we represent the electronic density as a superposition of elementary lattices which is *unique and independent of the incident and reflected radiation*. The different types of reflection we could interpret as collisions with the individual elementary lattices. On the other hand, describing the Fresnel phenomena, we adapted the Fourier integral (15) to the special positions of the source of light and the point of observation. The system of elementary lattices is no longer unique, and even if we keep the source of light in a constant position, we still have a different system for every point in which we observe the intensity. An attempt to solve this difficulty by attributing to all these systems equal probability and by postulating collisions with the constituent lattices of all of them fails for the following reasons. The number of these lattices is an infinity of higher order and, if only one of them should contribute to the reflection we are interested in, the intensity of this reflection must be infinitely small. On the other hand, through every point in our space there pass light quanta reflected to an infinity of other points and the question arises why they do not contribute to the intensity in the first point. It is, therefore, clear that the phenomena of the Fresnel diffraction cannot be explained by purely corpuscular considerations. It is necessary to attribute to the light quanta properties of phase and coherence similar to those of the waves of the classical theory.<sup>5</sup>



<sup>1</sup> The publication of this paper, written in 1924, was delayed because the authors were busy with other work. The recent discovery made by Davisson and Germer (*Nature*, 119, p. 558, 1927) gives to the problem of corpuscular diffraction a new interest and importance.

<sup>2</sup> P. S. Epstein and P. Ehrenfest, these PROCEEDINGS, 10, p. 133, 1924.

<sup>3</sup> Cf., for instance, *Enzyklopädie der Math.*, Wiss.

<sup>4</sup> M. Planck, "Theorie der Wärmestrahlung," Formula (64). The factor 2 in Planck's formula arises from his considering a perfectly reflecting element, while we have a perfectly absorbing one.

<sup>5</sup> Since this was written, the work of de Broglie and Schroedinger has brought us much nearer to the solution of these problems.

## ABSOLUTE INTENSITIES IN THE HYDROGEN-CHLORIDE ROTATION SPECTRUM

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The development of new quantum theories which purport to furnish a means for the prediction of the absolute intensities of spectral lines makes it important to determine these intensities experimentally in such cases as may be theoretically treated. One of these few is the pure rotation spectrum as, for example, that of hydrogen chloride recently determined in absorption by Czerny.<sup>1</sup> This spectrum was used by Tolman and Badger<sup>2</sup> in the calculation of integral absorption coefficients, and so for the determination of the experimental  $B_{ij}$ 's or the probabilities of transition from one energy state of rotation to the next higher in the presence of radiation which may be absorbed. Since, however, this spectrum was investigated with a spectrometer of not very great resolving power, this process may have led to somewhat inaccurate results. In the present article are described new experimental measurements on the same spectrum, and an improved method whereby they are used to determine absolute absorption coefficients.

If the absorption is measured at several pressures, keeping the path length constant, an indirect method can be used for evaluating  $\int \alpha(\nu) d\nu$ , which avoids the difficulties due to low resolving power. Suppose that the intensity of the background radiation used in the absorption experiments is the function of wave-length  $I_0(\lambda)$ . If now the center of the spectrometer slit is set on the wave-length  $\lambda_s$ , radiation of other wave lengths between the limits of say  $\lambda_s + S$  and  $\lambda_s - S$  will be falling on the thermocouple due to the finite slit width. We may make the reasonable assumption that the intensity of such light of wave-length  $\lambda_s + \delta$  will