THE QUANTUM THEORY OF THE FRAUNHOFER DIFFRACTION

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1. *Introductory.*—In an important paper published on the pages of these PROCEEDINGS, W. Duane[1] makes a successful "attempt to formulate a theory of the reflection of X-rays by crystals, based on quantum ideas without reference to interference laws." A. H. Compton,[2] enlarging upon a hint contained in Duane's paper, has recently pointed out that the latter's hypothesis can be justified by the application of the general rules of the theory of quanta to the translatory motions of a crystal lattice.

Both these authors are dealing with the case of parallel beams of incident and reflected light (Fraunhofer diffraction) and of infinite lattices giving absolutely sharp pencils of reflected rays of different order. The purpose of the following lines is to study the problems with respect to finite gratings and other diffracting systems, again with restriction to the case of the Fraunhofer reflection.[3]

A finite grating, as the most extreme case of which we can regard the totality of only two reflecting points, can be regarded as a superposition of infinite gratings according to Fourier's theorem. Mathematically, therefore, our problem is reduced to a Fourier analysis. On the other hand, a finite grating produces a more or less continuous spectrum, and in the quantum theory the intensity corresponding to any given angle of deflection of the rays by the grating must be expressed in terms of the probability of the light quanta undergoing such a deflection. These circumstances suggest *the principle of correspondence* as a suitable instrument for carrying through our investigation.

2. *The Duane-Compton Rules of Quantization.*—We state here the Duane-Compton rules in a generalized form bringing out the invariancy of the result for any choice of axes. Let us consider a three dimensional infinite triclinic lattice with the spacings a_1, a_2, a_3 in the respective directions of its chief axes. The contention of Compton is that in a collision with a light quantum such a lattice can only pick up a linear momentum the orthogonal projections of which p_1, p_2, p_3 on the directions q_1, q_2, q_3 of the chief axes satisfy the fundamental conditions of the quantum theory

$$\int p_1 dq_1 = n_1 h, \qquad \int p_2 dq_2 = n_2 h, \qquad \int p_3 dq_3 = n_3 h \qquad (1)$$

n_1, n_2, n_3 are three integral numbers and h denotes Planck's constant of action. The periodicity of the lattice is given by its spacings a_1, a_2, a_3 so that the first integral is to be extended from q_1 to $q_1 + a_1$, and the others correspondingly. We obtain, therefore,

$$p_1 = hn_1/a_1, \quad p_2 = hn_2/a_2, \quad p_3 = hn_3/a_3. \qquad (2)$$

On the other hand the momentum of a light quantum of the frequency ν is given by $h\nu/c = h/\lambda$, where c is the velocity of light and λ the wave-length in vacuo corresponding to the frequency ν. If the direction of propagation of the light includes with its main axes angles the cosines of which are, before its collision with the lattice, α_0, β_0, γ_0, and after its reflection α, β, γ, each light quantum loses in the collision a momentum the projections of which on our main axes are $h(\alpha - \alpha_0)/\lambda$, $h(\beta - \beta_0)/\lambda$, $h(\gamma-\gamma_0)/\lambda$.

The principle of conservation of momentum requires, therefore, the relations

$$\alpha-\alpha_0 = \lambda n_1/a_1, \qquad \beta-\beta_0 = \lambda n_2/a_2, \qquad \gamma-\gamma_0 = \lambda n_3/a_3, \tag{3}$$

which are identical with those derived by von Laue from the theory of interference.

However, the choice of the main axes is arbitrary and we can remove this arbitrariness only by proving that if the lattice acquires in a collision a momentum in the direction of any straight line connecting two of its points (following Bragg we shall call such a direction a "crystal avenue"), this momentum must satisfy a condition analogous to (2)

$$p.a = nh \tag{4}$$

where a is the smallest distance between two points in that line. Referred to the main axes, a will be the diagonal of a parallelepipedon with the edges m_1a_1, m_2a_2, m_3a_3, if m_1, m_2, m_3 are three integers prime to each other. It is easy to see that in terms of these edges

$$a = m_1a_1 \cos(a_1a) + m_2a_2 \cos(a_2a) + m_3a_3 \cos(a_3a)$$

Applying conditions (2) we get

$$p \cos (a_1a) = \lambda n_1/a_1, \quad p \cos (a_2a) = \lambda n_2/a_2, \quad p \cos (a_3a) = \lambda n_3/a_3.$$

Multiplying the three equations by m_1a_1, m_2a_2, m_3a_3, respectively, and adding them we receive

$$pa = (m_1n_1 + m_2n_2 + m_3n_3)\lambda$$

As m_1, m_2, m_3 are prime to each other, the parenthesis, according to a well known theorem of theory of numbers, by a suitable choice of positive or negative integral values for n_1, n_2, n_3, can be made equal to any integer n.

We see, therefore, that relation (4) is contained in our conditions (2) or, in other words, that the latter conditions may be imposed on the orthogonal projections of the momentum on any three crystal avenues.

3. *Infinite Linear Grating.*—Let us begin our considerations with the single case of a one dimensional grating the elements of which are arranged in a straight line. In this line (the distance in which from a fixed point we denote by x) the material points with which the light quanta may collide are distributed with a certain density ρ. We shall call ρ for short

the "*electronic density*," and the notion of a grating involves that this electronic density is a periodic function of x with a period a called "the spacing of the grating."

If the grating is moving at a constant velocity in the direction x relatively to a resting point in this line, the density in that point will change as a periodic function of the time and return to its original value after the grating has moved through the distance a or a multiple of it. That is the reason why Compton regards the spacing a as the region over which the quantum integral $\int pdq = nh$ must be extended (cf. section 2), giving the relation

$$p = hn/a \tag{4}$$

If the distribution of electronic density was a sinusoidal one represented by the formula

$$\rho = A \sin (2\pi x/a + \delta) \tag{5}$$

the change of density in a fixed point, due to the motion of the grating, would be a simple harmonic oscillation. By means of the Fourier theorem any distribution of electronic density can be built up of sinusoidal terms, in other words, any grating, infinite or finite, can be represented as a superposition of infinite sinusoidal gratings of the type (5). This case deserves, therefore, a particularly close study. The principle of correspondence tells[4] us that to every harmonic term in the expression of ρ there corresponds a quantum change of motion accompanied by a change of momentum p given by our equation (4) if we substitute in it for n/a the coefficient of $2\pi x$ in the argument of the sine.

If, therefore, the Duane-Compton relation[4] tells us that a grating can only pick up momentum in multiples of the quantity h/a, the principle of correspondence permits us to go farther and to say that a *sinusoidal grating of the constitution (5) will experience only changes of momentum in amounts* $\pm h/a$ *and not in multiples of it.*[5]

The general expression for ρ in an infinite grating is

$$\rho = \sum_{0}^{\infty} n \; A_n \sin(2\pi nx/a + \delta) \tag{6}$$

To a term of this series with the coefficient n/a of the argument $2\pi x$ there corresponds a change of momentum given by the same value of the coefficient of h in equation (4). In a lattice of such a constitution momentum can be, therefore, picked up in a large variety of ways. Moreover, the principle of correspondence gives us additional information with respect to the relative frequency of the different possible changes of momentum: the probability of the grating's picking up the momentum nh/a is proportional to the square of the coefficient of the corresponding term of our series, that is to A_n^2.

As stated in section 2 the change of momentum experienced by a grating in its collision with a light quantum determines the direction of emergence of the light quantum according to the equation

$$\alpha - \alpha_0 = \lambda n/a. \tag{7}$$

The above statement on the probabilities of momenta means, therefore, that the intensity of the spectrum of the n^{th} order will be proportional to A_n^2.

In order to show that these conditions are in agreement with the interference theory of gratings we have only to prove that a sinusoidal grating produces the same effect from the point of view of the latter theory, that is that a distribution of electronic density represented by the formula

$$\rho = A_m \sin 2\pi mx/a \tag{8}$$

will give two absolutely sharp reflected beams at angles following from (7) by putting $n = \pm m$ with intensities proportional to A_m^2. The proof is easily given: An element dx of the grating gives a contribution to the amplitude of light, emitted in a direction α, which is proportional to the modulus of the expression

$$\rho e^{i\frac{2\pi}{\lambda}x(\alpha-\alpha_0)} dx \tag{9}$$

The total amplitude in that direction is, therefore

$$S = C.A_m \int \sin 2\pi m \frac{x}{a} . e^{i\frac{2\pi}{\lambda}x(\alpha-\alpha_0)} \tag{10}$$

We shall evaluate this expression first for a finite grating taking as limits of integration $\pm Na$ and then go over to $N = \infty$.

$$S = \frac{iCA_m}{2\pi}\left\{\frac{\sin\left(\frac{m}{a}-\frac{\alpha-\alpha_0}{\lambda}\right)Na}{\frac{m}{a}-\frac{\alpha-\alpha_0}{\lambda}} - \frac{\sin\left(\frac{m}{a}+\frac{\alpha-\alpha_0}{\lambda}\right)Na}{\frac{m}{a}+\frac{\alpha-\alpha_0}{\lambda}}\right\}.$$

We see that the amplitude is proportional to A_m and that it has two maxima in the two directions $\alpha - \alpha_0 = \pm m\lambda/a$. Moreover, the maximum amplitude is proportional to N, and when N becomes infinite the intensity in the maximum completely dominates so that the whole energy is thrown into the directions of the maxima and the latter become absolutely sharp. There is, therefore, a complete identity in the Fraunhofer diffraction produced by an infinite sinusoidal grating from the point of view of the classical theory and from the point of view of the theory of light quanta sketched above. As any linear diffracting system can be built up by infinite sinusoidal gratings this identity will hold for the totality of all phenomena of Fraunhofer reflection. *The considerations of the first half of this section contain, therefore, the complete translation of the theory of Fraunhofer diffrac-*

tion into the language of the quantum theory. The following section contains only the application of these principles to one or two special cases.

4. *The linear Point Lattice.*—From the mathematical point of view the sinusoidal grating treated in the preceding section is the simplest. However, such a grating cannot be realized physically, because in some points its density becomes negative producing a reflection connected with a change of phase by half a period. The grating that is considered as the fundamental one in most text books is the *point grating:* the graphical representation of the electronic density ρ of such a grating as a function of x being a succession of equidistant peaks, very narrow compared with the spacing a.

Infinite Point Lattice.—Analytically we can express the distribution in this case by a Fourier series. Computed in the well known way, the coefficients of all the terms of lower order turn out to be the same. If C is the height of a peak and c its breadth we get for ρ the series (6) with $A_0 = Cc/a$, $A_n = 2Cc/a$. *This means that the spectra of different order produced by such a grating are all of the same intensity,* as the intensity of the n^{th} order is proportional to A_n^2. It need not disturb us that the above expressions for A_n do no longer hold for large numbers n, because the corresponding terms have no physical significance: the corresponding change of momentum, though theoretically possible, will never take place because the impinging light quantum does not possess enough momentum to realize it.

Finite Point Lattice.—In this case we have to use the Fourier integral instead of the Fourier series. If we choose as origin ($x = 0$) the centre of the grating, the expression for the electronic density will be

$$\rho(x) = \int_0^{\infty} A(\omega) \cos 2\pi\omega x d\omega \tag{11}$$

$$A(\omega) = \frac{2}{\pi}\int_{-\infty}^{+\infty} \rho(\beta) \cos 2\pi \omega\beta \, d\beta \tag{12}$$

This grating appears, therefore, as a superposition of an infinite number of sinusoidal gratings with the respective spacings $a' = 1/\omega$. According to section 3 such a grating will produce a reflected ray in a direction given by the relation

$$\alpha - \alpha_0 = \lambda/a' = \omega\lambda, \tag{13}$$

while the relative intensity of this ray is given by the square of $A(\omega)$. This intensity is easily computed from (12): as $\rho(\beta)$ is different from zero only in the positions of the peaks $\beta = ma$, we get

$$A(\omega) = \frac{2}{\pi}\frac{Cc}{a}\sum_{-U}^{+U} \cos 2\pi m\omega a = \frac{2}{\pi}\frac{Cc}{a}\frac{\sin N\pi a\omega.}{\sin \pi a\omega}$$

if we denote by $N = 2U + 1$ the total number of peaks in our grating. To express the intensity produced by the grating as a function of the direction we have only to substitute into the square of A the expression of ω from equation (13)

$$A^2 = 4\frac{C^2c^2}{\pi^2a^2}\frac{\sin^2 N\pi a(\alpha-\alpha_0)/\lambda}{\sin^2 \pi a(\alpha-\alpha_0)/\lambda}, \quad (14)$$

in complete agreement with the classical interference formula.

In the special case, when $N = 2$, we obtain from (14) the well known distribution due to the interference of two dipoles

$$A^2 = 16\cos^2 \pi a(\alpha-\alpha)_0/\lambda. \quad (15)$$

5. *The Space Lattice.*—The generalization for the three-dimensional case does not involve any new ideas. If we denote the three crystal avenues of a triclinic lattice chosen as main axes by x_1, x_2, x_3, the distribution of electronic density in any lattice of this type and, in fact, in any other system can be built up of terms of the type

$$\rho_{m_1m_2m_3} = A_{m_1m_2m_3}\sin\left(2\pi m_1\frac{x_1}{a_1} + \delta_{m_1}\right)\sin\left(2\pi m_2\frac{x_2}{a_2} + \delta_{m_2}\right)\cdot\sin\left(2\pi m_3\frac{x_3}{a_3} + \delta_{m_3}\right) \quad (16)$$

therefore it is sufficient to discuss the distribution of density given by this equation.

Applying the principle of correspondence in the same way as in the case of the linear grating, we conclude that such a lattice can pick up only a momentum the orthogonal projections of which on the directions x_1, x_2, x_3 are given by equations (2) with $n_1 = \pm m_1$, $n_2 = \pm m_2$, $n_3 = \pm m_3$. According to the analysis of such a motion in section 2 this means that our lattice can only acquire momentum directed in one of the four crystal avenues with the oblique components $\pm m_1a_1$, $\pm m_2a_2$, $\pm m_3a_3$ and in each of these directions with only one definite velocity (both ways, positive and negative).

The direction of the light quantum after the collision, is given by equations (3). As α, β, γ are not independent, we see that a collision can only occur if λ satisfies the von Laue-Bragg condition with absolute sharpness. In this case the lattice will give us with equal probability eight different directions of the reflected rays.

In order to prove the complete equivalence of the quantum theory with the classical treatment for three dimensional distributions, we have only to show that the interference theory leads to the same results in the case of distribution (16). In the classical theory the mean amplitude in a direction α, β, γ is proportional to the modulus of the expression

$$\iiint \rho e^{i\frac{2\pi}{\lambda}[x_1(\alpha - \alpha_0) + x_2(\beta - \beta_0) + x_3(\gamma - \gamma_0)]} dx_1 dx_2 dx_3. \qquad (17)$$

Introducing for ρ the distribution (16) we see that expression (17) is the product of three factors of the type given by formula (10) and discussed in section 3. It follows from that discussion that the whole reflected energy will be thrown into the same eight directions which were found on the basis of the quantum theory. This proves in a general way the complete identity of results in both treatments for any possible system, and it is not necessary to enter into special examples.

6. *Conclusion.*—The above considerations are restricted to the case of the Fraunhofer diffraction and neglect the small change of the wave-length due to the Compton effect. Moreover they are dealing only with the linear momentum without reference to the possible changes of angular momentum and other quantic conditions of the system. The last restriction seems natural as only the linear momentum has a direct connection with the direction of motion of the light quantum which is the only important element of our discussion. On the contrary the restriction to Fraunhofer phenomena does not appear to be a necessary one and we hope to extend our theory to more general cases.

The situation in optics appears, therefore, to be thus:

1. The photoelectric phenomenon and the Compton effect can be explained only by the action of light quanta.

2. The phenomena of Fraunhofer diffraction can be treated as well on the basis of the wave theory of light as by a combination of the concept of light quanta with Bohr's principle of correspondence.

3. The phenomena of coherence resist all attempts of the quantum theory.

However, it must be remembered that Bohr's principle of correspondence contains the essential features of the wave theory in a form suitable for the quantum theory. Our treatment, therefore, means rather a readjustment than a complete abandoning of the wave theory.

[1] W. Duane. *Proc. Nat. Acad. Sci., Washington,* **9**, p. 159 (1923).

[2] A. N. Compton. *Ibid.,* **9**, p. 359 (1923).

[3] Moreover we neglect the slight changes of the wave-length due to the Compton effect.

[4] Strictly speaking the principle of correspondence must be applied to the totality of the grating and the incident light wave, because without an exciting wave the uniform motion of a grating does not produce any radiation.

[5] We have to include the sign minus because (5) can be written also $\rho = -A \sin(-2\pi\, x/a - \delta)$.