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THE QUANTUM INTEGRAL AND DIFFRACTION BY A CRYSTAL

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Duane has recently pointed out[1] that if the momentum of a crystal grating perpendicular to the crystal face is nh/a, where n is an integer, h is Planck's constant and a is the distance between successive atomic layers, and if the momentum of the incident radiation quantum is $h\nu/c$, then Bragg's diffraction formula $n\lambda = 2a \sin\theta$ is a necessary consequence. It is worth while to point out that the general statement of the quantum postulate, $\int p\,dq = nh + \eta$, leads directly to the result that the momentum of the crystal changes by integral multiples of h/a as Duane assumes.

Let us express our quantum postulate in the form

$$\bar{p} \equiv \frac{\int p\,dq}{\int dq} = \frac{nh}{q_1} + \gamma, \qquad (1)$$

where $\bar{p}$ is the displacement average of the momentum, $q_1 = \int dq$ is the displacement necessary to bring the system back to its original condition, and the constant γ, corresponding for example to the zero point energy of an oscillator according to Planck's second radiation formula, represents the minimum value of the average momentum. Applying this expression to the case of a beam of infinite plane waves of wave-length λ, it is clear that after the beam has propagated itself through a complete wave-length it is again in its original condition. Thus $q_1 = \lambda$. The momentum of the beam in the direction of propagation is therefore

$$p = nh/\lambda + \gamma.$$

This corresponds, according to the relativity theory, to an energy

$$\epsilon = pc = nhc/\lambda + \gamma c = nh\nu + \gamma c.$$

If $n = 1$ and $\gamma = 0$, we thus have $\epsilon = h\nu$, which is in accord with the results of photoelectric experiments. Thus the momentum of the light ray is

$$p = h/\lambda. \qquad (2)$$

Let us consider in a similar manner the motion of an infinite three dimensional grating, such as a crystal. If a_x is the distance between the layers of atoms in the X-direction, the condition of the grating after it has moved a distance a_x is indistinguishable from its original condition, since layers of atoms again occupy the original positions. Thus in equation (1), $q_1 = a_x$, and hence

$$\bar{p}_x = n_x h/a_x + \gamma_x = p_x, \tag{3}$$

since $p_x = \bar{p}_x$ for uniform motion. Just as in the case of the light ray, where p was the momentum of the whole ray, so here p represents the momentum of the whole crystal. The constant γ_x in this equation assumes different values according to the motion of the axes relative to which the momentum of the crystal is measured. This equation states that the momentum of the crystal along the X-axis changes by integral multiples of h/a_x, i.e., that

$$\delta p_x = \frac{h}{a_x}\,\delta n_x, \tag{4a}$$

where δp_x is the change in the X component of the momentum, and δn_x is an integer. Similarly, if a_y and a_z are the distances between the layers of atoms along the Y and Z axes, respectively,

$$\delta p_y = \frac{h}{a_y}\,\delta n_y \quad \text{and} \quad \delta p_z = \frac{h}{a_z}\,\delta n_z. \tag{4b, c}$$

These expressions (4) ascribe a momentum to the crystal which is quantized in precisely the manner asumed by Duane. He had shown that the dimensions of the equations demanded a length in the denominator of the right-hand members, and the lengths a were the only ones which appeared suitable; but the constant of proportionality, unity, remained arbitrary. We now see that this quantized momentum of the crystal is a direct consequence of the fundamental quantum postulate.

We shall now proceed with the discussion of the passage of radiation through the crystal according to the method suggested by Duane, though in somewhat greater detail. Let l_x, l_y, l_z be the direction cosines of the incident ray, and l_x', l_y', l_z' the direction cosines of the diffracted ray. If λ is the wave-length of the incident ray and λ' that of the diffracted ray, the increase in the X component of the momentum of the ray by the diffraction is $hl_x'/\lambda' - hl_x/\lambda$. By the principle of the conservation of momentum, this change in the momentum of the radiation must be balanced by the change in the momentum of the crystal, i.e., $hl_x'/\lambda' - hl_x/\lambda + h\delta n_x/a_x = 0$. Thus

$$\frac{l_x'}{\lambda'} - \frac{l_x}{\lambda} + \frac{\delta n_x}{a_x} = 0, \quad \frac{l_y'}{\lambda'} - \frac{l_y}{\lambda} + \frac{\delta n_y}{a_y} = 0, \quad \frac{l_z'}{\lambda'} - \frac{l_z}{\lambda} + \frac{\delta n_z}{a_z} = 0. \tag{5}$$

The total change in momentum of the crystal is $(\delta p_x^2 + \delta p_y^2 + \delta p_z^2)^{1/2}$, or

$$\delta p = h \left\{ \left(\frac{\delta n_x}{a_x}\right)^2 + \left(\frac{\delta n_y}{a_y}\right)^2 + \left(\frac{\delta n_z}{a_z}\right)^2 \right\}^{1/2}. \quad (6)$$

From the principle of the conservation of energy it follows that the change in energy of the radiation is balanced by the change in kinetic energy of the crystal. In order to avoid changes of wave-length due to the Doppler effect, we must suppose that the initial velocity of the crystal is zero, and hence also that the initial value of $p = 0$. The energy equation is then

$$\frac{hc}{\lambda'} - \frac{hc}{\lambda} + \frac{(\delta p)^2}{2M} = 0. \quad (7)$$

Substituting the value of δp given in equation (6), and using in this equation the values of $\delta\eta/a$ given by expression (5), equation (7) becomes

$$\frac{hc}{\lambda} - \frac{hc}{\lambda'} = \frac{h^2}{2M} \left\{ \left(\frac{l_x}{\lambda} - \frac{l_x'}{\lambda'}\right)^2 + \left(\frac{l_y}{\lambda} - \frac{l_y'}{\lambda'}\right)^2 + \left(\frac{l_z}{\lambda} - \frac{l_z'}{\lambda'}\right)^2 \right\}. \quad (8)$$

On multiplying both sides by λ/hc we obtain

$$1 - \frac{\lambda}{\lambda'} = \frac{h/\lambda c}{2M} \left\{ \left(l_x - l_x' \frac{\lambda}{\lambda'}\right)^2 + \left(l_y - l_y' \frac{\lambda}{\lambda'}\right)^2 + \left(l_z - l_z' \frac{\lambda}{\lambda'}\right)^2 \right\}. \quad (9)$$

In this expression $h/\lambda c = h\nu/c^2$ is the mass of the incident quantum of radiation, which is very small indeed compared with the mass M of the crystal. Hence we have almost exactly

$$1 - \lambda/\lambda' = 0, \text{ or } \lambda' = \lambda. \quad (10)$$

When the value of λ' given by equation (10) is substituted in equations (5), we obtain

$$l_x - l_x' = \delta n_x \frac{\lambda}{a_x}, \quad l_y - l_y' = \delta n_y \frac{\lambda}{a_y}, \quad l_z - l_z' = \delta n_z \frac{\lambda}{a_z}. \quad (11a, b, c)$$

These expressions are exactly those obtained on the theory of interference for the angles at which the ray of wave-length λ may be diffracted by a crystal. Here, however, they are based upon the energy and momentum principles and the quantum postulate.

In order to put this result in the more familiar form known as Bragg's law, let us suppose that the incident ray lies in the XY plane, and that momentum is imparted only along the X axis, i.e., we assume $l_z = 0$, $\delta n_y = 0$ and $\delta n_z = 0$. It follows from equation (11c) that $l_z' = 0$, meaning that the diffracted ray also lies in the XY plane. If we call θ the glancing angle of incidence of the ray as it strikes the YZ plane of the crystal

and θ' the glancing angle of emergence, we have $l_x = \sin\theta$, $l_x' = -\sin\theta'$, $l_y = \cos\theta$ and $l_y' = \cos\theta'$. Equation (11b) thus becomes

$$\cos\theta - \cos\theta' = 0,$$

whence $\theta' = \pm\theta$. If $\theta' = -\theta$, we find from (11a) that $\delta n_x = 0$, whence if the ray is undeflected no momentum is imparted to the crystal. If, however, a number $\delta n_x = n$ quanta of momentum are imparted to the crystal, we must have $\theta_1 = \theta$, and equation (11a) becomes

$$n\lambda = 2a_x \sin\theta. \qquad (12)$$

This is identical with Bragg's expression, derived from the usual interference considerations, in which n represents the order to the diffracted beam.

It will be noted that this derivation of equations (11) and (12) has assumed infinitely long trains of waves, and a diffracting crystal which is infinite in extent. The same assumptions are also used (at least implicitly) when these expressions are derived on the interference theory. In both cases the modifications for finite wave-trains and finite crystals may be made by considering these finite quantities as the Fourier integrals of infinite wave-trains or gratings. The equations thus resulting from the quantum postulate have been given by G. Breit;[2] though in accord with the viewpoint of the present paper, we should consider the momentum of the crystal itself to be quantized rather than Breit's suggestion of some disturbance traversing the crystal.

The argument leading to equation (9) is precisely similar to that used by the writer in calculating the change in wave-length when X-rays are scattered by individual electrons,[3] except that in the latter case the mass $h/\lambda c$ of the radiation is comparable with the mass m of the scattering electron, so that the change in wave-length becomes appreciable. The fact that equation (9) indicates no measurable change in wave-length for the diffracted ray suggests that it is scattering by large groups of electrons, such as atoms or minute crystals, which gives rise to the scattered X-ray of unmodified wave-length.[4]

Attention may well be called to the fact that the present quantum conception of diffraction is far from being in conflict with the wave theory. In fact we were able to quantize the incident radiation only in view of the fact that it repeats itself at regular space intervals. Thus even from the quantum viewpoint electromagnetic radiation is seen to consist of waves.

[1] W. Duane, *Proc. Nat. Acad. Sci.*, May, 1923.

[2] G. Breit, *Ibid.*, July, 1923.

[3] A. H. Compton, *Physic. Rev.*, May, 1923.

[4] A. H. Compton, *Ibid.*, July, 1923; P. A. Ross, *Proc. Nat. Acad. Sci.*, July, 1923.