A General Derivation of the Formula for the Diffraction by a Perfect Grating

CARL ECKART, *University of Chicago*

(Received April 29, 1933)

I. INTRODUCTION AND ABSTRACT

The present use of ruled gratings for the absolute measurement of x-ray wave-lengths makes it necessary to investigate the possibility of systematic deviations from the simple formula for the diffraction from a perfect grating. A perfect grating is understood to have the following properties: (1) It is ruled on a continuum—its material has no atomic properties. (2) The optical properties of its material are completely determined by a refractive index (which may be complex). (3) It is ruled on a perfectly plane surface. (4) Its lines are truly parallel, identical, and uniformly spaced. (5) It is infinite in extent. (6) It is so oriented that the plane of incidence and diffraction is perpendicular to the rulings (this makes the problem two-dimensional). Of these properties, only (6) is non-essential and could be eliminated at the expense of a slight complication. The property (5) results in an infinite resolving power: theoretically, the resolving power of a finite portion of a perfect grating may be calculated in a manner which is discussed. It might seem that any derivation based on the foregoing simplifications could be no more general than the usual elementary derivation. However, the latter neglects the following factors: (a) The influence of multiple scattering; (b) Refraction, if the material of the grating is transparent. (This is really a particular case of (a)); (c) Shadows cast by one ruling on its neighbors; (d) Surface waves, similar to those arising on total reflection at a plane surface. In this case, these are the high order spectra for which $\sin \theta_n > 1$. A. H. Compton[1] has given an elementary derivation which takes account of the factors (a), (b) and (c). The present calculation confirms his result that these factors do not influence the calculation of the wave-length, and extends it to include the factor (d).

II. THE CALCULATION

BECAUSE of the properties (1), (2), and (6), the basis of the discussion may be taken to be the wave equation

$$(\partial^2 u/\partial x^2)+(\partial^2 u/\partial y^2)+k^2 u=0, \qquad (1)$$

where u is the wave function and

$$k=2\pi\mu/\lambda, \qquad (2)$$

λ being the wave-length in vacuo and μ the refractive index. The refractive index may vary from point to point, and may or may not be continuous. It may also be complex (opaque medium) at some points and real (transparent medium) at others. The rulings are taken to be parallel to the z-axis, and x-z is the plane of the grating.

Because of the properties (3), (4) and (5), the function μ will be periodic in x, with the period a = grating space:

$$\mu(x+a,\ y)=\mu(x,\ y). \qquad (3.1)$$

The dependence on y may be supposed such that

$$\mu(x,\ +\infty)=\mu', \quad k=k', \qquad (3.2)$$

$$\mu(x,\ -\infty)=\mu'', \quad k=k'', \qquad (3.3)$$

where μ' and μ'' are real constants.

The boundary conditions subject to which Eq. (1) is to be solved are, firstly, those of finiteness, continuousness, and single-valuedness. Secondly, it may be supposed that there is a single plane wave incident on the grating (coming from $y=+\infty$) and an infinite number of reflected and transmitted waves. Taking Eqs. (3.2) and (3.3) into account, this means that when $y \gg 0$

$$u(x,\ y)=\exp\left[ik'(x\sin\varphi-y\cos\varphi)\right] + \sum A_n \exp\left[ik'(x\sin\theta_n+y\cos\theta_n)\right], \qquad (4.1)$$

and when $y \ll 0$

$$u(x,\ y)=\sum B_n \exp\left[ik''(x\sin\varphi_n-y\cos\varphi_n)\right]. \qquad (4.2)$$

In Eq. (4.1), the first term is the incident wave and the others are the reflected waves; Eq. (4.2) contains the transmitted waves. Hence all angles are to be taken between $-\pi/2$ and $+\pi/2$ if they are real; however $\sin\theta_n$ and $\sin\varphi_n$ may be greater than unity if, as is to be expected, they are

[1] A. H. Compton, J. Frank. Inst. **208**, 605 (1929).

related to $\sin\varphi$ by the simple grating formulae. In this case, the definition

$$\cos\theta = +i(\sin^2\theta - 1)^{\frac{1}{2}}, \quad \sin\theta > 1, \tag{5}$$

is to be used. The choice of the sign for this radical is such that u remains finite for large values of y.

The periodicity of the refractive index, expressed by Eq. (3.1) has the following consequence: if $u=f(x, y)$ be a solution of Eq. (1), so is $u=f(x+a, y)$. From this it follows that for certain real constants α, it is possible to find solutions satisfying the equation

$$u(x+a, y) = u(x, y)\exp(i\alpha). \tag{6}$$

For, let $f(x, y)$ be a solution which does not satisfy this equation; then

$$v(x, y) = (1/N)\sum_{m=0}^{N-1} f(x+ma, y)\exp(-im\alpha)$$

is also a solution and satisfies the equation

$$v(x+a, y) = v(x, y)\exp(i\alpha) + (1/N)[f(x+Na, y)\exp(-iN\alpha) - f(x, y)].$$

Hence

$$u(x, y) = \lim_{N=\infty} v(x, y)$$

is a solution which satisfies Eq. (6). It would seem that this process can be carried out for every value of α; this is true, but the resulting u may be the trivial solution $u\equiv 0$.

It therefore remains to determine the values of α which are consistent with Eqs. (4). From these it is found that when $y\gg 0$:

$$u(x+a, y) = \exp[ik'a\sin\varphi]\{\exp[ik'(x\sin\varphi - y\cos\varphi)] + \sum A_n\exp[ik'a(\sin\theta_n - \sin\varphi)]\exp[ik'(x\sin\theta_n + y\cos\theta_n)]\},$$

and when $y\ll 0$:

$$u(x+a, y) = \exp[ik'a\sin\varphi]\{\sum B_n\exp[ik''a\sin\varphi_n - ik'a\sin\varphi]\exp[ik''(x\sin\varphi_n - y\cos\varphi_n)]\}.$$

When these are compared with the original Eqs. (4), it is seen that Eq. (6) can be satisfied only if

$$\alpha = k'a\sin\varphi \quad (\text{mod } 2\pi), \tag{7.1}$$

$$ak'(\sin\theta_n - \sin\varphi) = 2\pi n, \tag{7.2}$$

$$ak''\sin\varphi_n - ak'\sin\varphi = 2\pi n, \tag{7.3}$$

where n is an integer which may be identified with the index on the angles.

III. Discussion of the Significance of Eq. (6)

The last two equations above are the ordinary grating formulae. They are seen to follow directly from the requirement that Eq. (6) be satisfied by the solution of the wave equation. The question of the necessity of this requirement arises immediately.

Its physical significance may be seen from the fact that Eq. (6) implies that the intensity $|u|^2$ is periodic in x, with the same period as the grating itself. But this should be a result of the calculation and not a condition to be imposed *a priori*. Also, the requirement of a periodic intensity distribution does not in turn imply the Eq. (6). The latter can not therefore be a consequence of physical considerations. Nor is it a mathematical necessity. The difficulty is the same one which arises each time Fourier's solution of the problem of the stretched string is explained to a beginner. It is not possible to prove that *every* solution of this problem *must* have the form

$$\sin(nx)\sin(nct + \text{const.}).$$

But the need to prove the impossible vanishes when Fourier's theorem shows that it is possible to express the general solution as a series of *particular* solutions which *do* have this form.

In the present case, the solutions u form a complete orthogonal set in terms of which every solution of Eq. (1) can be expressed as a generalized Fourier integral.[2] The orthogonality is readily proved from Eq. (6) and the completeness may be inferred from the fact that the set reduces to a known complete set when the index of refraction has the special form $\mu=$ constant.

As a particular case, it would be possible to

[2] This is strictly true only when another set of functions representing waves incident from $y=-\infty$ is included.

build up a solution representing a finite beam of radiation incident on the infinite grating. This would be the physical equivalent of the omission of property (5) from the definition of the perfect grating. I believe that it would be feasible to make this calculation but that the result would very likely be the same formulae for the resolving power, etc., of a plane grating (used without collimator and telescope) which Stauss and Porter have already obtained by simpler methods.[3]

---

[3] A. W. Porter, Phil. Mag. **5**, 1067 (1928). H. E. Stauss, Phys. Rev **34**, 1601 (1929).