A CONDITION FOR MOMENTUM TRANSFER IN DIFFRACTION EFFECTS

By B. Makiej

Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław*

(*Received December 1, 1972*)

Emphasizing the corpuscular aspect, the phenomenon of light diffraction can be treated as a process of transfer of complex momenta between a photon beam and a macroscopic diffracting arrangement. This arrangement can bestow upon the photon beam only such complex momenta that appear in its transferable momenta spectrum. We show this as an example, on X-ray beam diffraction in a crystal and on photon beam diffraction on the edge of an aperture in an opaque screen.

It was shown recently [1] that in the case of the Fraunhofer diffraction the phenomenon can be treated as a result of complex momenta transfer between the diaphragm and photons. Such a description of the phenomenon, emphasizing the corpuscular aspect, leads to practically the same results as the classical Kirchhoff theory in the formulation of Rubinowicz [2]. The question arises, whether more general regularities appear during the exchange of complex momenta between the photon beam and the diffracting arrangement.

In all cases of an interaction between two systems, one of them can be treated as the "donor", and the other as the "receiver" of any definite physical quantity. The value of the transferred physical quantity should depend on the transferable value in the first (donor) system and on the strength of the interaction between the systems (this strength depending, among other factors, on the receiving ability of the second system). Where the transferable quantity disappears the transferred quantity should also disappear.

Let us draw our attention to a relatively simple kind of interaction: elastic scattering of an X-ray beam on a perfect crystal lattice. Let all lattice points be identical, their coordinates being described by the lattice vectors

$$\boldsymbol{l} = \sum_i l_i \boldsymbol{a}_i \tag{1}$$

* Address: Zakład Badań Nadprzewodnictwa, Instytut Niskich Temperatur i Badań Strukturalnych PAN, Próchnika 95, 53-529 Wrocław, Poland.

where $\boldsymbol{a}_i$ are basic vectors of the crystal unity cell and l_i are integers. The vector of the reciprocal lattice

$$\boldsymbol{g} = \sum_i g_i \boldsymbol{b}_i \tag{2}$$

is determined by the basic vectors of the reciprocal lattice $\boldsymbol{b}_i$ and by the Miller indices g_i of the Bragg planes. Let us try to determine a function which will express the interaction ability of the crystal lattice with the X-ray beams. In a recent paper [3] a function was introduced which has the meaning of the ability of the system to transfer physical quantities, namely the "transferability". In the case of a system consisting of microsystems the density of the transferability is a complex function ψ which is called the density of activity. The last, as it was proved, possesses all main features of a quantum-mechanical wave function.

Basing on the above statements we assume that the sites of the crystal lattice represent regions of concentration of the density of activity. Considering the presumption that all the lattice sites are identical, we see that the density of activity for a fixed time $t = 0$ is a periodical function $\psi(\boldsymbol{r}+\boldsymbol{l}) = \psi(\boldsymbol{r})$ for all space points $\boldsymbol{r}$ and for all the lattice translations $\boldsymbol{l}$. Hence, this function can be represented by means of a Fourier series

$$\psi(\boldsymbol{r}) = \sum_g \psi_g(\boldsymbol{r}); \qquad \psi_g = A_g \exp(i2\pi \boldsymbol{g}\boldsymbol{r}), \tag{3}$$

where the summation is performed over the indices g_x, g_y, g_z and ψ_g is the component of the density of activity corresponding to the wave vector $2\pi\boldsymbol{g}$. The coefficients of the expansion are given by

$$A_g = \frac{1}{V_{\text{cell}}} \int\limits_{\text{cell}} \psi(\boldsymbol{r}) \exp(-i2\pi \boldsymbol{g}\boldsymbol{r}) d\tau \tag{4}$$

where the integration is performed over the basic cell of the lattice.

Our interpretation of the wave function of quantum mechanics [1, 3] enables us to ascribe a meaning to the expression $-i\hbar\nabla\psi(\boldsymbol{r})$, namely, to consider it as the density of the transferable complex momenta, *i. e.* momenta that could under certain conditions be transferred to another system. As follows from (3), the density of the transferable complex momenta of the crystal lattice is:

$$-i\hbar\nabla\psi(\boldsymbol{r}) = 2\pi\hbar \sum_g \boldsymbol{g}\psi_g(\boldsymbol{r}), \tag{5}$$

where the coefficients of $\psi_g(\boldsymbol{r})$ are the momenta. Thus only discrete momenta $2\pi\hbar\boldsymbol{g}$ proportional to the vectors of the reciprocal lattice appear in the spectrum of the transferable momenta of the crystal. Therefore, when we pass a uniform monochromatic beam of photons with wave vector $\boldsymbol{k}_0$ through a crystal, photons obtain additional momenta due to elastic scattering in the crystal lattice. It seems quite natural that the values of the transferred momenta should belong to the set of the transferable momenta. Hence, upon changing the direction of the wave vector from $\boldsymbol{k}_0$ to $\boldsymbol{k}_1$

the relation

$$k_1 - k_0 = 2\pi g; \; |k_1| = |k_0| \tag{6}$$

should hold which is identical with the Bragg condition. Denoting the angle between k_0 and k_1 by θ, we get from (6) $2d \sin \theta/2 = 2\pi n/|k_0|$ where n is an integer and $d = n/|g|$. In the case when the wavelength of the X-ray fulfils the condition $\lambda > 2d$, the Bragg conditions cannot be satisfied as momenta smaller than a certain boundary value do not appear in the momentum spectrum of the crystal lattice.

In the above formulation of the Bragg condition we have based on a rule that can be expressed as follows: a system can transfer a certain complex momentum only when this momentum appears in the spectrum of the complex momenta of the transferring system. Let us make use of that rule — the rule determining the possibility of momentum transfer — to describe light diffraction on an edge of an aperture in a screen. For simplicity, we consider a thin, opaque planar screen with a small opening, lying in the $X0Y$-plane of the Cartesian coordinate system. A uniform monochromatic beam of photons with wave vector k_0 falls on the aperture 0 perpendicularly to the plane of the screen and interacts with the screen. The photons passing near the edges of the aperture obtain additional transverse complex momenta, *i. e.* a change in the direction of the motion of photons — diffraction occurs.

Let us find the spectrum of the complex momenta of a planar screen with an aperture. For that purpose we ascribe to the fixed uniform screen (at the moment $t = 0$) the density of activity ψ equal 1 everywhere outside the aperture and equal to 0 inside it. For the complementary screen the density of activity ψ_0 is 1 in the region of the opening and 0 everywhere else. Consider the Fourier expansion

$$\psi = \int A_k \exp (ikr) dk. \tag{7}$$

The Fourier transform

$$A_k = \int_{\text{screen}} \psi \exp(-kr) d\sigma \tag{8}$$

is the amplitude of the component of the density of activity $\psi_k = A_k \exp(ikr)$. The k-component of the density of the complex momentum is given by the expression $-i\hbar \nabla \psi_k$.

In the special case of a screen with an aperture together with the complementary diaphragm (*i. e.* the opening closed), the density of activity of such a full screen is equal 1 in the whole $X0Y$-plane. The Fourier transform of the function $\psi + \psi_0 = 1$ is expressed by the product $\delta(k_x)\,\delta(k_y)$, where k_x and k_y denote projections of the wave vector on the directions of the $0Y$ and $0X$, respectively. As we are interested in the motion of photons which obtain additional transverse momenta different from zero, *i. e.* when $|k| \neq 0$,we have for that case:

$$\int_{\text{screen}} \psi \exp(-ikr) d\sigma + \int_{\text{aperture}} \psi_0 \exp(-ikr) d\sigma = 0. \tag{9}$$

Hence the spectral distribution of the components of the density of activity of a screen with an aperture is equal to the spectral distribution — with opposite sign — of the components of the density od activity of the complementary screen. Thus the integral over the infinite area (the screen) can be replaced by the integral over the area of the aperture. We will make use of this result further on. The distribution of the density of activity of the photon beam may be calculated assuming elastic scattering in the edge region of the aperture; thus, photons with initial momentum $\hbar \boldsymbol{k}_0$ and final (after diffraction) momentum $\hbar \boldsymbol{k}_1$ (where $|\boldsymbol{k}_1| = |\boldsymbol{k}_0|$) obtain additional transversal momenta (perpendicular to $\boldsymbol{k}_0$), $\hbar(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp = \hbar \boldsymbol{k}$, originating from the screen. We assume also that the spectrum of the complex momenta transferred from the screen to the photons during elastic scattering has approximately the same shape as that of the transferable complex momenta of the screen[1]. Considering the above, in the case of the Fraunhofer diffraction — when a parallel photon beam with a fixed wave wector $\boldsymbol{k}_1$ is observed, the Fourier transform of the function ψ has, according to (9), the form

$$A_{k_1} = - \int_{\text{aperture}} \exp\left[-i(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp \boldsymbol{r}\right] d\sigma \tag{10}$$

and gives us a quantity proportional to the amplitude of the density of activity of the investigated beam (the case of a homogeneous falling beam).

In the investigation of Fresnel diffraction of light in a point P which is at a finite distance R from the screen, contributions from all photons arriving from the scattering region to the place of observation should be added. In that case $(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp$ in the expression for the amplitude of the density of activity is not constant, unlike that for the case of Fraunhofer diffraction of light. Therefore, on performing the integration one must consider: 1° the dependence of the number of photons arriving at P on the position of the surface element $d\sigma$, and 2° the change of the angle between the constant vector $\boldsymbol{k}_0$ and the vector $\boldsymbol{k}_1$ directed to the point of observation with the coordinates $(0,0,R)$.

Such a choice of the origin of the coordinate-system makes the directions of the vectors $(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp$ and $\boldsymbol{r}$ opposite to each other and

$$|(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp| = k_0 \sin(\boldsymbol{k}_0, \boldsymbol{k}_1). \tag{11}$$

The relations (10) and (11) may be used to calculate the radiation density of activity in the point P after introducing some simplifying assumptions mentioned below. Let us assume that the number of photons directed to the point P does approximately not depend on the position of the scattering element $d\sigma$. Further, experiments show that a diffraction pattern is observed only near the geometrical shadow, *i. e.*, only for small deviation angles of the light beam deflected from its original direction $\boldsymbol{k}_0$. The following assumption is thus justified:

$$\frac{|\boldsymbol{r}|}{R} \ll 1, \tag{12}$$

with the resulting approximation $|(\boldsymbol{k}_1 - \boldsymbol{k}_0)_\perp| \cong k_0 |\boldsymbol{r}|/R$. Hence, basing on (10), the amplitude of the density of activity of the photon beam at the point R will be approximately

$$A_p = \text{const} \int_{\text{aperture}} \exp\left(ik_0 |\boldsymbol{r}|^2/R\right) d\sigma. \tag{13}$$

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[1] With this assumption, the Babinet rule can be obtained from (9).

In addition, the size of the aperture 0 does not have to be very small which may be concluded from the accepted condition (12), because an integral of the form (13) is, as it is well known, quickly convergent and the contributions from large values of $|\boldsymbol{r}|/R$ do not influence significantly the result of the calculations [4].

Owing to the simplifying assumptions made when considering the problem of Fresnel diffraction we obtain a result similar to that evaluated on the base of the Kirchhoff theory which proves the usefulness of our simple model describing the phenomenon of diffraction without making use of Huygens principle.

In the presented description of the phenomenon of diffraction as a process of scattering and exchange of the momenta of X-ray photons with the crystal lattice, or the exchange of the momenta of light photons with the screen it becomes obvious that the values of the complex momenta transferred to the photons depend on the Fourier distribution of the density of activity of the diffracting arrangement. As a consequence the values of transversal momenta transferred to photons do not depend on the initial values of the photon momenta (if no fundamental change arises in the mechanism of interaction with the change of initial values), but they depend on the distribution of the scattering elements.

The author is much indebted to Dr J. Petykiewicz for reading the manuscript and for valuable remarks.

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