The derivation is similar to that of equation (21) of Becker & Dunstetter (1984).

Configuration III

The geometry of configuration II is shown in Fig. 18 with $b = \overline{S n_1}$. One obtains:
for M_1 in domain 1

$$D_h^1 = i\chi J_0[2\chi(xy)^{1/2}];$$

for M_s in domain 2,

$$D_h^2(x, y) = D_h^1(x, y) - i\chi \times J_0[2\chi\{(x-b)[y+(\beta_0/\beta_h)b]\}^{1/2}]. \quad (A2)$$

Equation ($A2$) is obtained in the same way as equation (23) of Becker & Dunstetter (1984).

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Diffraction by a Randomly Distorted Crystal. I. The Case of Short-Range Order

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Abstract

Kato's statistical theory of diffraction [Kato (1980). *Acta Cryst.* A**36**, 763-769, 770-778] is reformulated in a self-consistent manner. The local displacement field $\mathbf{u}(\mathbf{r})$ occurs through the phase factor $\varphi(\mathbf{r}) = \exp[2\pi i\mathbf{h}\,.\,\mathbf{u}(\mathbf{r})]$. The present paper is concerned with the limiting case where $\langle\varphi(\mathbf{r})\rangle = E = 0$: this corresponds to the situation where only secondary extinction is present. There are two correlation lengths in the problem, the first one τ for the phase factor φ, the second one Γ for the wave-field amplitudes. Kato assumed $\Gamma \gg \tau$. It is shown in the present paper that $\Gamma \simeq \tau$, a property which has important consequences for the general theory, where $E \neq 0$, to be discussed in the second paper of this series.

I. Introduction

Kato (1980*a*) has proposed a statistical theory that describes the propagation of X-rays and neutrons in a distorted crystal. This theory covers the whole range of perfection from purely dynamical (perfect crystal) to purely kinematical (mosaic crystal) diffraction. It thus fills the gap between secondary and primary extinction that were treated independently in previous approaches.

The application of this theory has been discussed by Kato (1980*b*) and an improved solution was recently proposed by the authors (Al Haddad & Becker, 1988) that led to a fair description of experimental data on silicon (Olekhnovich, Karpei, Olekhnovich & Puzenkova, 1983). This modification was confirmed by Guigay (1989).

The theory involves long-range- and short-range-order parameters. The effective short-range correlation length introduced by Kato has been questioned in the literature (Olekhnovich *et al.*, 1983) and relies on non-trivial assumptions.

In this series of papers, we intend to discuss the statistical hypothesis in detail, and to propose an improved self-consistent formulation of the problem. In order to discuss separately the various approximations, we shall start in the present paper by the particular case where long-range order is negligible (secondary extinction only). The general theory will be presented in a second paper, together with a practical solution.

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II. Takagi's equations and the statistical hypothesis

For simplicity, we shall consider a non-absorbing and centrosymmetric crystal.

A. Let s_0 be a coordinate along the direction of the incident beam. Let us assume Bragg scattering to occur at the reciprocal-lattice point **h**. We denote the coordinate along the scattered direction by s_h. If D_0 and D_h are the amplitudes of the waves in the incident and scattered directions respectively, their propagation obeys Takagi's equations:

$$\frac{\partial D_0}{\partial s_0} = i\chi\varphi D_h, \quad \frac{\partial D_h}{\partial s_h} = i\chi\varphi^* D_0, \qquad (1)$$

where

$$\chi = (\lambda a C/V)F = 1/\Lambda. \qquad (2)$$

F is the structure factor for the Bragg reflection **h**, supposed here to be real (centrosymmetric crystal). λ is the wavelength, V the volume of the unit cell, a equals 1 pm for neutrons, 0·28 pm for X-rays. Λ is the 'extinction length', the distance above which multiple scattering (dynamical effects) becomes important, C = polarization factor for X-rays.

φ is a phase shift which accounts for the local displacement from perfection. If $\mathbf{u}(\mathbf{r})$ is the displacement field in the crystal:

$$\varphi = \exp[2\pi i \mathbf{h}\,.\,\mathbf{u}(\mathbf{r})]. \qquad (3)$$

The situation is depicted in Fig. 1. We assume a crystal to be totally illuminated by an incident beam. A typical optical route is shown in this figure; the beam enters the crystal at S and exits at M. The amplitude at M will depend on the phases φ_i at the points m_i where scattering has occurred.

The practical solution of (1) is impossible in the general case, even if $\mathbf{u}(\mathbf{r})$ is known at each point. In most situations, the displacement field $\mathbf{u}(\mathbf{r})$ is unknown and some assumptions have to be formulated before (1) can be solved.

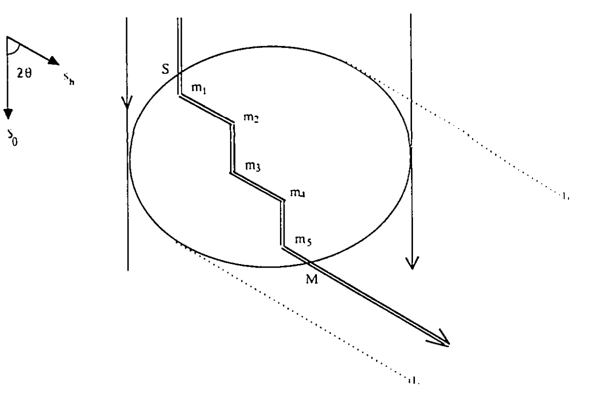


Fig. 1. Schematic representation of the scattering processes. —— incident beam; · · · · scattered beam; ══ a typical optical path through the crystal. θ: Bragg angle.

Equations (1) have been proved by Takagi (1962, 1969) and Taupin (1964) and reformulated by Kato (1973).

They can be viewed as very general propagation equations for waves in the presence of a scattering potential. χ is the amplitude of the scattering process, and φ a local phase shift that will be considered as a random quantity.

B. Given a crystal, it is possible to analyse the displacement field **u** in terms of its probability distribution function $P(\mathbf{u})$ (Becker & Al Haddad, 1989).

It is possible to consider φ as a random variable. Kato introduced the quantity

$$E = \langle\varphi(\mathbf{r})\rangle_\mathbf{r} = \int_v \varphi(\mathbf{r})\,\mathrm{d}v, \qquad (4)$$

where v is the volume of the crystal, which can also be written as

$$E = \int P(\mathbf{u}) \exp(2\pi i \mathbf{h}\,.\,\mathbf{u})\,\mathrm{d}\mathbf{u}. \qquad (5)$$

E is the long-range-order parameter of the problem. It is equivalent to a static Debye–Waller factor. It is reasonable to assume a Gaussian distribution for $P(\mathbf{u})$ if the displacements are random enough. Assuming an isotropic distribution, one gets

$$E = \exp[-(2\pi^2/3)h^2\langle u^2\rangle], \qquad (6)$$

where $\langle u^2\rangle$ is the mean square displacement over the crystal under study. Equation (6) also shows the dependence of E on the Bragg angle $[|\mathbf{h}| = 2(\sin\theta)/\lambda$ where 2θ is the scattering angle]. For a perfect crystal, $E = 1$.

If $\langle u^2\rangle^{1/2}$ becomes larger than the reticular plane interspacing $d = 1/h$, E becomes very small and will often be neglected. The limit $E \to 0$ corresponds to the purely 'mosaic' crystal.

Kato also introduced a short-range-order parameter through the pair-correlation function:

$$f(\mathbf{t}) = \langle\varphi^*(\mathbf{r}+\mathbf{t})\varphi(\mathbf{r})\rangle_\mathbf{r}. \qquad (7)$$

This function is assumed to be real and symmetric. If we write

$$\varphi = E + \delta\varphi, \qquad (8)$$

where $\delta\varphi$ is the phase fluctuation, we get

$$f(\mathbf{t}) = E^2 + \langle\delta\varphi^*(\mathbf{r}+\mathbf{t})\delta\varphi(\mathbf{r})\rangle_\mathbf{r}.$$

Since $f(0) = 1$,

$$f(\mathbf{t}) = E^2 + (1-E^2)g(\mathbf{t}), \qquad (9)$$

where $g(0) = 1$ and $g(\mathbf{t})$ is a decreasing function that describes the phase correlation between two points separated by the vector **t**.

We are interested in the solution of (1) in the case where $\mathbf{u}(\mathbf{r})$ has a known distribution. The statistical hypothesis is thus introduced at this particular stage: the diffracted power does not depend on the details of the displacement field $\{\mathbf{u}(\mathbf{r})\}$.

One may expect that there exist many hypothetical crystals with different displacement fields $\{\mathbf{u}_1\}\ldots\{\mathbf{u}_p\}$ but having the same diffraction spectrum. These crystals must have the same distribution function $p(\mathbf{u})$ and the same correlation function $g(\mathbf{t})$.

If such an assumption is valid, it becomes possible to describe the intensities of the incident and diffracted beams as an ensemble average over all the crystals that would give the same diffraction spectrum: this would also correspond to studying the scattering by a homogeneously distorted crystal defined as an average among crystal 1, crystal 2, ..., crystal p.

It is obvious that one of the conditions to be fulfilled is that the actual dimension l of the sample be large compared to any characteristic length, such as Λ or τ,

$$l \gg \tau, \quad l \gg \Lambda. \tag{10}$$

Write the intensities in the incident and diffracted directions as

$$I_0 = \langle |D_0|^2 \rangle, \quad I_h = \langle |D_h|^2 \rangle, \tag{11}$$

the brackets having the meaning of an ensemble average.

If the phase sequence along an optical route such as shown in Fig. 1 can be approximated by a Markov chain, and if $\mathbf{t} = x\mathbf{u}_0 + y\mathbf{u}_h$ (where $\mathbf{u}_0$ and $\mathbf{u}_h$ are the unit vectors along the incident and diffracted beams), one can show (Becker & Al Haddad, 1989) that

$$g(\mathbf{t}) = \exp(-\mathbf{a}\,.\,\mathbf{t}). \tag{12a}$$

If, moreover, the incident and diffracted directions are supposed to be equivalent for the correlation

$$g(\mathbf{t}) = \exp[-(x+y)/\tau], \tag{12b}$$

we note that

$$\begin{aligned} g(x, y) &= g(x)g(y) \\ g(0, y) &= g(y), \\ g(x, 0) &= g(x). \end{aligned} \tag{12c}$$

Correlation lengths τ_n are defined as

$$\tau_n = \int_0^\infty [g(t)]^n \, \mathrm{d}t, \quad \tau_1 = \tau. \tag{13}$$

τ measures the width of the pair-correlation function g, and represents the distance over which two routes lose their mutual phase coherence.

Higher-order correlation functions can be introduced but the present theory will only take pair correlation into consideration. The implications of such a constraint will be discussed later.

C. In the present paper, we shall restrict the discussion to the case where E is very small, thus neglecting long-range order. We shall use the following simplifications:

$$\begin{aligned} \langle \varphi \rangle &= 0 \\ \langle \varphi^*(\mathbf{r}+\mathbf{t})\varphi(\mathbf{r}) \rangle &= f(\mathbf{t}) = g(\mathbf{t}). \end{aligned} \tag{14}$$

The second paper of this series will deal with the general case (Becker & Al Haddad, 1990).

Before solving (1) under the conditions (14), we shall make a further assumption concerning the scattering geometry and boundary conditions for the beams. This is summarized in Fig. 2.

Let S be a point illuminated on the crystal surface. S can be considered as a point source, emitting a spherical wave. Suppose the diffracted beam exits at M. Let

$$\overline{Sm} = s_0, \quad \overline{mM} = s_h.$$

We suppose that the parallelogram $(SmMp)$ is totally inside the crystal (transmission geometry).

This approximation has been shown to be fair in many situations (Becker & Coppens, 1974; Becker & Dunstetter, 1984), especially for small scattering angles (the most important situations for multiple scattering). We assume a unit intensity for the incident beam, which leads to the boundary condition.

$$D_0^0 = \delta(s_h). \tag{15}$$

One calculates the solution for this point source (Green function of the problem). It is then necessary to integrate over the exit surface from the crystal, and over all the source points, in order to get the integrated diffracted power that is recorded in an experiment. The integrated diffracted power for a homogeneous incident beam is shown to be (Kato, 1976; Becker, 1977):

$$P = (\lambda/\sin 2\theta) \int_v I_h(m) \, \mathrm{d}v, \tag{16}$$

where $I_h(m)$ is the intensity of the diffracted beam at M originating from the source S: notice that any point m inside the crystal defines uniquely the pair (S, M).

III. Propagation equations for the intensities

Takagi's equations can be transformed into integral equations, as proposed by Kato:

$$D_h(s_0, s_h) = i\chi \int_0^{s_h} \varphi^*(s_0, \eta) D_0(s_0, \eta) \, \mathrm{d}\eta \tag{17a}$$

$$D_0(s_0, s_h) = \delta(s_h) + i\chi \int_0^{s_0} \varphi(\xi, s_h) D_h(\xi, s_h) \, \mathrm{d}\xi. \tag{17b}$$

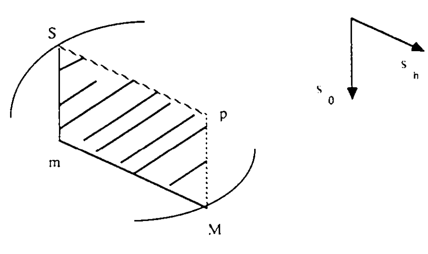
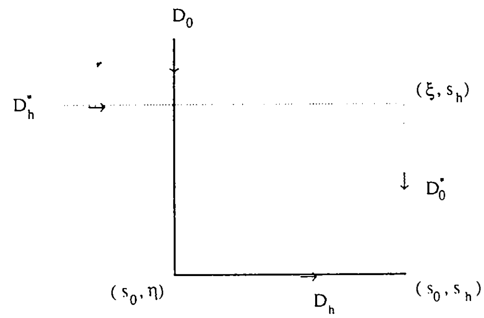


Fig. 2. Assumed geometry for the diffraction.

It is easy to write the propagation equations for I_0 or I_h:

$$\frac{\partial I_0}{\partial s_0} = -\frac{\partial I_h}{\partial s_h} = i\chi\{\langle D_0^* \varphi D_h\rangle - \langle D_h^* \varphi^* D_0\rangle\}. \quad (18)$$

Equation (18) correlates D_0 and D_h at the same point. In order to estimate this quantity, we must take into account the fact that the actual values of D_0 and D_h at a given point are defined by the scattering events which have occurred at preceding points: this is achieved with (17). The situation is schematized in the following diagram where horizontal lines refer to the diffracted direction and vertical lines to the incident direction: the two routes join at (s_0, s_h) and correspond to the evaluation of $D_0^*(s_0, s_h) D_h(s_0, s_h)$.



Let us consider the term $\langle D_0^* \varphi D_h\rangle$. Through (17*a*), one creates a correlation between $D_0^*(s_0, s_h)$ and $D_0(s_0, \eta)$. Through (17*b*), one gets a correlation between $D_h(s_0, s_h)$ and $D_h^*(\xi, s_h)$. Since these two correlations are independent, one must add the two processes. The term $\delta(s_h)$ in (17*b*) does not correspond to a scattering event and can be discarded. We get

$$\begin{aligned}\frac{\partial I_0}{\partial s_0} = \chi^2 \int_0^{s_0} & \mathrm{d}\xi \langle D_h^*(\xi, s_h) D_h(s_0, s_h) \\ & \times \varphi^*(\xi, s_h) \varphi(s_0, s_h)\rangle + \text{c.c.} \\ -\chi^2 \int_0^{s_h} & \mathrm{d}\eta \langle D_0^*(s_0, s_h) D_0(s_0, \eta) \\ & \times \varphi^*(s_0, \eta) \varphi(s_0, s_h)\rangle + \text{c.c.} \quad (19)\end{aligned}$$

Assuming the brackets to be real, we get

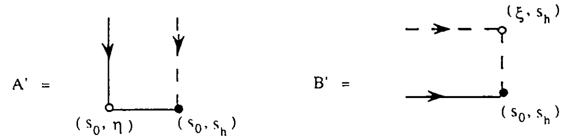
$$\frac{\partial I_0}{\partial s_0} = -\frac{\partial I_h}{\partial s_h} = 2\chi^2 [B' - A'] \quad (20)$$

with

$$A' = \int_0^{s_h} \mathrm{d}\eta \langle D_0^*(s_0, s_h) D_0(s_0, \eta) \varphi^*(s_0, \eta) \varphi(s_0, s_h)\rangle \quad (21)$$

$$B' = \int_0^{s_0} \mathrm{d}\xi \langle D_h(s_0, s_h) D_h^*(\xi, s_h) \varphi^*(\xi, s_h) \varphi(s_0, s_h)\rangle.$$

A' and B' can be represented by the following diagrams:



where • : φ o : φ*

It should be recalled that D_0 or D_h only change their value at a scattering point. $D_0^*(s_0, s_h) D_0(s_0, \eta)$ is defined by scattering events taking place earlier on the routes, for example:

We wish now to evaluate (21). We will restrict the discussion to the pair-correlation assumption. Therefore (Feller, 1970), the average of the product of an even number of random quantities, each of which has a zero mean value, can be written as the sum of all the independent products of pair correlations. Take $\langle a_1 a_2 a_3 a_4\rangle$. It can be written, in the pair-correlation approximation:

$$\begin{aligned}\langle a_1 a_2 a_3 a_4\rangle = \langle a_1 a_2\rangle\langle a_3 a_4\rangle + \langle a_1 a_3\rangle\langle a_2 a_4\rangle \\ + \langle a_1 a_4\rangle\langle a_2 a_3\rangle. \quad (22)\end{aligned}$$

If $\langle a_i\rangle = 0$, this expression is exact when the random variables a_i have a Gaussian multivariate distribution.

Furthermore, (17) can be used iteratively and leads to

$$D_h(s_0, s_h) = i\chi\varphi^*(s_0, 0) + \hat{L} D_h,$$

where

$$\hat{L} f = -\chi^2 \int_0^{s_0} \mathrm{d}\xi \int_0^{s_h} \mathrm{d}\eta\, \varphi^*(s_0, \eta) \varphi(\xi, \eta) f(\xi, \eta). \quad (23)$$

From this, we get

$$\begin{aligned}\langle D_h\rangle &= \sum_0^{\infty} (-1)^n \langle \hat{L}^n [i\chi\varphi^*(s_0, 0)]\rangle \\ &= \sum_0^{\infty} (-1)^n i\chi(-\chi^2)^n \int_0^{s_0} \mathrm{d}\xi_1 \int_0^{s_h} \mathrm{d}\eta_1 \ldots \\ &\quad \times \int_0^{\xi_{n-1}} \mathrm{d}\xi_n \int_0^{\eta_{n-1}} \mathrm{d}\eta_n \langle \varphi^*(s_0, \eta_1) \varphi(\xi_1, \eta_1) \ldots \\ &\quad \times \varphi^*(\xi_{n-1}, \eta_n) \varphi(\xi_n, \eta_n) \varphi^*(\xi_n, 0)\rangle.\end{aligned}$$

The bracket involves the average of a product of an odd number of quantities whose mean value is zero. If the displacement field is such that $\hat{\mathbf{h}}.\mathbf{u}(\mathbf{r}_1) \ldots \hat{\mathbf{h}}.\mathbf{u}(\mathbf{r}_n)$ has approximately a multivariate Gaussian distribution (Feller, 1970; Becker & Al

Haddad, 1989), each term in the preceding expansion is zero and we conclude that

$$\langle D_h\rangle = 0. \tag{24a}$$

Similarly, if we consider only the part of the incident beam which corresponds to multiple scattering,

$$\langle D_0\rangle = 0. \tag{24b}$$

There is a total lost of phase coherence along a given route. As a result, the only contribution to the intensity must come from the correlation between different routes originating from S and joining at (s_0, s_h). That is equivalent to saying that the only non-vanishing terms in (21) are

$$\langle D_0^*(s_0, s_h)D_0(s_0, \eta)\rangle\langle\varphi^*(s_0, \eta)\varphi(s_0, s_h)\rangle$$

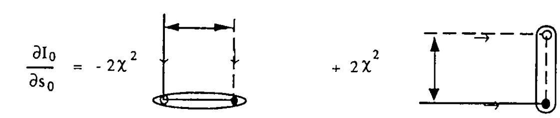
and

$$\langle D_h(s_0, s_h)D_h^*(\xi, s_h)\rangle\langle\varphi^*(\xi, s_h)\varphi(s_0, s_h)\rangle.$$

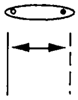
The term $\langle D_0^*(s_0, s_h)\varphi(s_0, s_h)\rangle\langle D_0(s_0, \eta)\varphi^*(s_0, \eta)\rangle$ is zero since each bracket is proportional to $\partial\langle D_h^*\rangle/\partial s_h$ and $\partial\langle D_h\rangle/\partial\eta$: remember that $\langle D_h\rangle = 0$. The term $\langle D_0^*(s_0, s_h)\varphi^*(s_0, \eta)\rangle\langle D_0(s_0, \eta)\varphi(s_0, s_h)\rangle$ would, by the use of (17), involve non-first-neighbour phase correlation, which is neglected in the present approach. Thus, phase and amplitude couplings can be separated, and one gets

$$A' = \int_0^{s_h} \mathrm{d}\eta\, g(s_h - \eta)\langle D_0^*(s_0, s_h)D_0(s_0, \eta)\rangle$$
$$B' = \int_0^{s_0} \mathrm{d}\xi\, g(s_0 - \xi)\langle D_h(s_0, s_h)D_h^*(\xi, s_h)\rangle. \tag{25}$$

The diagrammatic version of (25) is



where  stands for a phase correlation

and  stands for a transverse amplitude correlation.

a. Kato's approximation

To estimate A' and B', Kato made the assumption that the transverse correlation length (Γ) of the amplitude is much larger than τ, the phase correlation length. Γ is the distance over which $\langle D_0^*(s_0, s_h)D_0(s_0, s_h - \Gamma\rangle$ becomes negligible. Then $\langle D_0^*(s_0, s_h)D_0(s_0, \eta)\rangle$ can thus be replaced by $I_0(s_0, s_h)$ in (25). This leads to a very simple solution:

$$A' = \tau I_0(s_0, s_h), \quad B' = \tau I_h(s_0, s_h). \tag{26}$$

Thus, the propagation equations take the simple form:

$$\partial I_0/\partial s_0 = -\partial I_h/\partial s_h = 2\chi^2\tau[I_h - I_0], \tag{27}$$

which is familiar in secondary-extinction theories (Zachariasen, 1967; Becker & Coppens, 1974), where the quantity $(2\chi^2\tau)$ plays the role of a specific scattering cross section.

Earlier, Kato (1976) proposed a theory for secondary extinction, based on a detailed study of all the possible coupling schemes between two optical routes. This theory, precise but quite complicated, cannot be generalized if $E \neq 0$. It leads to

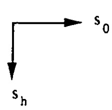
$$\partial I_0/\partial s_0 = -\partial I_h/\partial s_h = 2\chi^2\tau_2[I_h - I_0]. \tag{28}$$

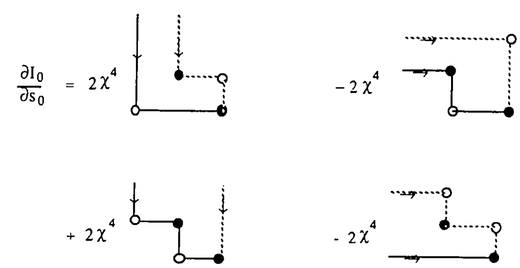
The only difference from (27) is the occurrence of τ_2 instead of τ and seems minor.

In fact, we shall see that it is related to the approximation leading to (26), which has to be critically discussed. The difference between (27) and (28) will be shown to be quite fundamental in terms of the physics background.

b. Self-consistent approach

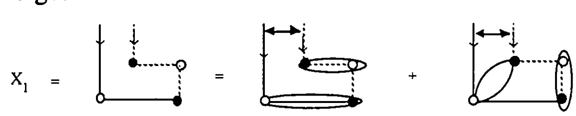
We must consider A' and B' without making any *a priori* approximation. If we wish to calculate them directly, this will involve quantities such as $\langle D_0^*(s_0, s_h)D_0(s_0, \eta)\rangle$, which has to be expanded in terms of preceding scattering events. We must therefore consider an expansion of $\partial I_0/\partial s_0$ at least to order χ^4.





$$= 2\chi^4[X_1 + X_2 + X_3 + X_4]. \tag{29}$$

In evaluating X_i, we will again separate phase and amplitude correlations, following arguments leading to (22). Taking into account all the pair correlations, we get



$$X_1 = \int_0^{s_h} \mathrm{d}\eta \int_0^{s_0} \mathrm{d}\xi' \int_0^{s_h} \mathrm{d}\eta'\{g(s_h - \eta)g(s_h - \eta')$$
$$+ g(s_0 - \xi')g(s_0 - \xi', \eta - \eta')\}$$
$$\times\langle D_0(s_0, \eta)D_0^*(\xi', \eta')\rangle. \tag{30}$$

We shall use two more approximations:

(1) it is shown in the Appendix that $\langle D_0(s_0, \eta) D_0^{*}(\xi', \eta')\rangle$ can be replaced by $\langle D_0(\xi', \eta) D_0^{*}(\xi', \eta')\rangle$ (long longitudinal amplitude correlation);

(2) if $x, y > 0$,

$$g(x+y) \simeq g(x)g(y) \tag{31}$$

(Becker & Al Haddad, 1989).

$$\begin{aligned} X_1 = {} & 2\int_0^{s_h} g^2(s_h-\eta)\,\mathrm{d}\eta \int_0^{s_0}\mathrm{d}\xi' \int_0^{\eta}\mathrm{d}\eta'\, g(\eta-\eta') \\ & \times \langle D_0(\xi', \eta) D_0^{*}(\xi', \eta')\rangle \\ & + 2\int_0^{s_0}\mathrm{d}\xi'\, g^2(s_0-\xi') \int_0^{s_h}\mathrm{d}\eta \int_0^{\eta}\mathrm{d}\eta'\, g(\eta-\eta') \\ & \times \langle D_0(\xi', \eta) D_0^{*}(\xi', \eta')\rangle \\ = {} & 2\tau_2 \int_0^{s_0}\mathrm{d}\xi\, A'(\xi, s_h) + 2\tau_2 \int_0^{s_h}\mathrm{d}\eta\, A'(s_0, \eta), \end{aligned} \tag{32}$$

where use was made of the fact that A' has slow variations on a distance of order τ.

By similar arguments:

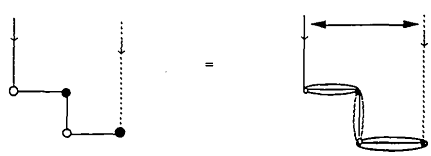
$X_2 =$

$$= -2\tau_2 \int_0^{s_0}\mathrm{d}\xi\, B'(\xi, s_h) - 2\tau_2 \int_0^{s_h}\mathrm{d}\eta\, B'(s_0, \eta). \tag{33}$$

We then consider X_3. We notice that the former scattering events occur on the same optical route and correlations between adjacent pairs cannot be factored out.

$$\begin{aligned} & \langle \varphi(s_0, s_h)\varphi^{*}(s_0, \eta)\varphi(\xi', \eta)\varphi^{*}(\xi', \eta')\rangle \\ & \quad = g(s_h-\eta)g(\eta-\eta')G(s_0-\xi'), \end{aligned}$$

where $G(s_0-\xi')$ correlates the two horizontal pairs on a distance of order τ:



as a consequence, $X_3/X_1 \simeq \tau/s_0$. X_3 can be neglected. Similarly X_4 is neglected.

Finally, we get

$$\frac{\partial I_0}{\partial s_0} = 4\chi^4\tau_2 \left\{ \int_0^{s_0} \mathrm{d}\xi [A'-B'](\xi, s_h) + \int_0^{s_h} \mathrm{d}\eta [A'-B'](s_0, \eta) \right\}. \tag{34}$$

From (20), this can be transformed into

$$\begin{aligned} \frac{\partial I_0}{\partial s_0} & = 2\chi^2\tau_2 \left[-\int_0^{s_0} \frac{\partial I_0}{\partial s_0}(\xi, s_h)\,\mathrm{d}\xi + \int_0^{s_h} \frac{\partial I_h}{\partial s_h}(s_0, \eta)\,\mathrm{d}\eta \right] \\ & = 2\chi^2\tau_2[I_h - I_0] \end{aligned}$$

and

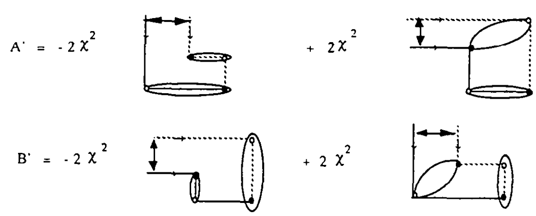
$$\frac{\partial I_h}{\partial s_h} = 2\chi^2\tau_2[I_0 - I_h]. \tag{35}$$

The correlation length τ_2 is retrieved and we find agreement with Kato's (1976) theory.

The previous results can be written as

$$A' = \tau_2 I_0, \quad B' = \tau_2 I_h, \tag{36}$$

as can be seen by an expansion of (22):



(37)

Equation (36) shows that the transverse amplitude correlation length Γ is of the same order as the phase correlation length τ, a result which differs significantly from Kato's predictions.

This difference will also have a strong influence on the theory when there is long-range order ($E \neq 0$).

IV. Solution

The solution of (28) or (35) is well known (Becker, 1977; Kato, 1976, 1980*b*): it depends on the boundary values for I_0 and I_h.

A simple use of (15) and (17) would lead to

$$I_0(\varepsilon, s_h) \sim 0, \quad I_h(s_0, \varepsilon) \sim \chi^2 \tag{38}$$

for $\varepsilon \ll s_0$, s_h but $\varepsilon \gg \tau$. Equations (38) are the effective boundary conditions for kinematical theory (single scattering).

However, this single scattering can occur at any $x < s_0$: the incident beam at s_0 is thus reduced by an effective absorption factor $\exp(-2\chi^2\tau_2 s_0)$. The effective boundary values have to be taken as (Al Haddad & Becker, 1988):

$$I_0(\varepsilon, s_h) \sim 0, \quad I_h(s_0, \varepsilon) \sim \chi^2 \exp(-2\chi^2\tau_2 s_0). \tag{39}$$

The solution is then

$$\begin{aligned} I_0(s_0, s_h) & = \chi^2(s_0/s_h)^{1/2} \\ & \quad \times \mathrm{I}_1[2\sigma(s_0 s_h)^{1/2}] \exp[-\sigma(s_0+s_h)] \\ I_h(s_0, s_h) & = \chi^2 \mathrm{I}_0[2\sigma(s_0 s_h)^{1/2}] \exp[-\sigma(s_0+s_h)], \end{aligned} \tag{40}$$

where

$$\sigma = 2\chi^2 \tau_2 \qquad (41)$$

is the specific scattering cross section and I_0, I_1 stand for modified Bessel functions of the first kind.

The kinematical diffracted power (16) is

$$P_k = (\lambda/\sin 2\theta)\chi^2 v. \qquad (42)$$

The measured power is

$$P = P_k y, \qquad (43)$$

where y is the extinction factor. We get

$$y = v^{-1} \int_v \exp[-\sigma(s_0 + s_h)] I_0[2\sigma(s_0 s_h)^{1/2}]\, dv, \qquad (44)$$

an expression of great use in secondary-extinction theory.

V. Concluding remarks

We have shown, in the case of negligible long-range order, that the correlation functions for the amplitudes in the transverse direction can be calculated without any *a priori* approximation. The correlation length of the amplitudes is of the same order as the correlation length for the phase, a result which is consistent with the detailed calculation of Kato (1976), but which discards Kato's (1980*a*, *b*) assumptions concerning the general statistical theory. This result is important for the general theory to be presented in a following paper.

APPENDIX

Longitudinal correlation of the beams

Let us consider the quantity

$$a = \int_0^{s_h} \langle D_h^*(s_0, s_h) D_0(s_0, \eta) \varphi^*(s_0, \eta) \rangle \, d\eta. \qquad (A1)$$

We take its derivative with respect to s_h applying the same method as in the text:

$$\begin{aligned} \frac{\partial a}{\partial s_h} &= \langle D_h^* \varphi^* D_0 \rangle \\ &\quad - i\chi \int_0^{s_h} \langle D_0^*(s_0, s_h) D_0(s_0, \eta) \rangle g(s_h - \eta)\, d\eta \\ &= i\chi[B' - 2A'] \qquad (A2) \end{aligned}$$

since $\langle D_h^* \varphi^* D_0 \rangle = i\chi[B' - A']$.

We can also expand ($A1$) as

$$\begin{aligned} a &= i\chi \int_0^{s_h} d\eta \int_0^{s_h} d\xi \langle D_h^*(s_0, s_h) D_h(\xi, \eta) \rangle g(s_0 - \xi) \\ &\quad - i\chi \int_0^{s_h} d\eta \int_0^{s_h} d\eta' \langle D_0^*(s_0, \eta') D_0(s_0, \eta) \rangle g(\eta - \eta'). \end{aligned} \qquad (A3)$$

The second term is

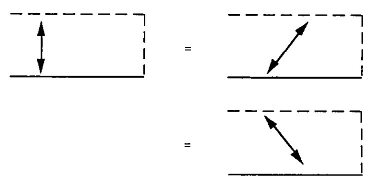
$$-2i\chi \int_0^{s_h} d\eta A'(s_0, \eta).$$

If we replace $\langle D_h^*(s_0, s_h) D_h(\xi, \eta) \rangle$ by $\langle D_h^*(s_0, \eta) \times D_h(\xi, \eta) \rangle$ in the first term, we get

$$a = i\chi \int_0^{s_h} d\eta [B'(s_0, \eta) - 2A'(s_0, \eta)] \qquad (A4)$$

and $\partial a/\partial s_h = i\chi[B' - 2A']$, a result similar to ($A2$).

It is therefore legitimate to replace $\langle D_h^*(s_0, s_h) \times D_h(\xi, \eta) \rangle$ by $\langle D_h^*(s_0, \eta) D_h(\xi, \eta) \rangle$. Thus, we can consider that the longitudinal correlation of the amplitudes is large and only the transverse correlation plays an important role in the theory. This is related to the fact that the amplitudes change only their values due to scattering.



The amplitude correlation function between two parallel routes depends only on the distance between the two routes, and not on the particular position on each route.

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