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Statistical Dynamical Theory of Crystal Diffraction. II. Intensity Distribution and Integrated Intensity in the Laue cases

BY NORIO KATO

Department of Crystalline Materials Science, Faculty of Engineering, Nagoya University, Nagoya, Japan

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Abstract

The theory described in the previous paper [Kato (1980). *Acta Cryst.* A36, 763–769] has been applied to calculating the intensity distribution in the topography of statistically homogeneous crystalline media. The integrated intensity for parallel-sided crystals is also presented. The formulae cover the whole range of crystal perfection. Primary and secondary extinctions can be treated on a unified theoretical base. A few numerical examples are given to demonstrate the variations of the integrated intensity as a function of the crystal thickness, the extinction distance and two parameters which characterize crystal perfection over short and long ranges compared with the extinction distance.

1. Introduction

Following the scheme described in the previous paper* (Kato, 1980*b*), we shall calculate the intensity distribution excited by the narrow incident wave $A\delta(s_g)$ in the Borrmann triangular fan. This is the first topic of this paper (§ 2). It turns out that the intensity field consists of four terms with weight factors depending on crystal perfection over a long range. One is the perfectly coherent component and another is the perfectly incoherent component. The two others are the mixed components and can be interpreted as due to a transformation of coherent waves to incoherent beams. The next topic is to calculate the integrated intensity for parallel-sided crystals (§§ 3 and 4) based on the results of § 2.

Only Laue cases are treated. The formulae obtained cover the whole range of crystal perfection by assigning a value between one and zero to a 'static' Debye–Waller factor E characterizing long-range perfection [equation (1.7)]. For a given E, the diffraction phenomena depend appreciably on the intrinsic correlation length τ which characterizes short-range perfection [equation (1.9)]. The details of the integrated intensities are discussed for the symmetrical Laue cases based on some numerical calculations (§ 4).

The results can be used for understanding diffraction topography when statistical considerations are necessary, as mentioned in the *Introduction* of paper 1. The results of §§ 3 and 4 can be used for understanding the nature of extinction when both primary and secondary extinctions are involved.

* This paper is referred to as paper 1. The previous series of papers having the title *On Extinction* (Kato, 1976*a*,*b*; 1979, 1980*a*) are referred to as I, II, III and IV.

2. The intensity distribution due to a narrow incident wave: $A\delta(s_g)$

Equations (1.26) can be solved immediately under the boundary conditions (1.33*a*) and (1.34*a*) from the results of equations (I.9) and (I.22) if μ_o and $\kappa_{\pm g}$ are replaced by μ_e and $E\kappa_{\pm g}$, respectively. The coherent part of the intensity, therefore, is given by

$$I_o^c = E^2|\kappa|^2 A^2 \left[\frac{s_o}{s_g}\right] |J_1(2\kappa E\sqrt{s_o s_g})|^2 \times \exp -\mu_e(s_o + s_g), \quad (1a)$$

$$I_g^c = E^2|\kappa_g|^2 A^2 |J_0(2\kappa E\sqrt{s_o s_g})|^2 \exp -\mu_e(s_o + s_g), \quad (1b)$$

where J_0 and J_1 are the Bessel functions of zeroth and first order, respectively.

Next, equations (1.28) without ⟦ ⟧ have to be solved under the boundary conditions (1.33*b*) and (1.34*b*). For this purpose, the method of two-dimensional Laplace transformation is useful. The Laplace transform of a function $F(s_o,s_g)$ is defined by

$$F(p,q) = \int_0^\infty\!\!\int F(s_o,s_g) \exp -(ps_o + qs_g)\, \mathrm{d}s_o\, \mathrm{d}s_g. \quad (2a)$$

Also, if $F(p,q)$ is given, the original function is obtained by the inverse transform as

$$F(s_o,s_g) = \left(\frac{1}{2\pi i}\right)^2 \int_{\gamma-i\infty}^{\gamma+i\infty}\!\!\int F(p,q) \exp (ps_o + qs_g)\, \mathrm{d}p\, \mathrm{d}q \quad (2b)$$

for $s_o,s_g \geq \varepsilon$.

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Here, we shall assume that $F(p,q)$ is regular in the domain of $\mathrm{Re}(p)$ and $\mathrm{Re}(q) \geq \gamma$, γ being called the radius of convergence.

The Laplace transform of equations (1.28) can be written as follows.

$$(p + \tilde{\mu}_e)I^i_o(p,q) = \tilde{\sigma}_{-g} I^i_g(p,q) + \sigma_{-g}(1 - E^2)I^c_g(p,q) \qquad (3a)$$

$$(q + \tilde{\mu}_e)I^i_g(p,q) = \tilde{\sigma}_g I^i_o(p,q) + \sigma_g(1 - E^2)I^c_o(p,q) + |\kappa_g|^2(1 - E^2)|A|^2(p + \tilde{\mu}_e)^{-1}. \qquad (3b)$$

The last term of (3b) is due to the boundary condition (1.33b), and it is the explicit form of

$$I^i_g(p,\varepsilon) = \int_\varepsilon^\infty I^i_g(s_o,\varepsilon) \exp - ps_o \, \mathrm{d}s_o. \qquad (4)$$

It is straightforward to solve $I^i_o(p,q)$ and $I^i_g(p,q)$ from (3). The results are

$$I^i_o(p,q) = [\sigma_g \tilde{\sigma}_{-g} I^c_o + \sigma_{-g}(q + \tilde{\mu}_e)I^c_g + \tilde{\sigma}_{-g}|\kappa_g|^2(p + \tilde{\mu}_e)^{-1}|A|^2]\,(1 - E^2)G(p,q), \qquad (5a)$$

$$I^i_g(p,q) = [\sigma_g(p + \tilde{\mu}_e)I^c_o + \sigma_{-g}\tilde{\sigma}_g I^c_g + |\kappa_g|^2|A|^2](1 - E^2)G(p,q), \qquad (5b)$$

where the arguments (p,q) are omitted in $\{I\}$ on the right side. The function G is defined by

$$G(p,q) = [(p + \tilde{\mu}_e)(q + \tilde{\mu}_e) - \tilde{\sigma}^2]^{-1}, \qquad (6)$$

where

$$\tilde{\sigma}^2 = \tilde{\sigma}_g \tilde{\sigma}_{-g}. \qquad (7)$$

If the Laplace transforms of $I^c_o(s_o,s_g)$ and $I^c_g(s_o,s_g)$ are given we shall have the Laplace transform $I^i_o(p,q)$ and $I^i_g(p,q)$. Using the relation (2b), in principle, we obtain the intensities $I^i_o(s_o,s_g)$ and $I^i_g(s_o,s_g)$.

Here, however, we shall write them down by the use of the convolution theorem of the Laplace transform, remembering that each term of the expressions for $I^i_o(p,q)$ and $I^i_g(p,q)$ of (5) is the product of $\{I\}$ and G multiplied by a function of $(p + \tilde{\mu}_e)$ or $(q + \tilde{\mu}_e)$. The final results are

$$I^i_o(s_o,s_g) = [\sigma_g\tilde{\sigma}_{-g}\kappa^2 E^2 I^{(1)}_o + \sigma_{-g}\tilde{\sigma}|\kappa_g|^2 E^2 I^{(2)}_o + |\kappa_g|^2(\tilde{\sigma}_{-g}/\tilde{\sigma})I^{(3)}_o]\,|A|^2(1 - E^2), \qquad (8a)$$

$$I^i_g(s_o,s_g) = [\sigma_g\tilde{\sigma}\kappa^2 E^2 I^{(1)}_g + \sigma_{-g}\tilde{\sigma}_g|\kappa_g|^2 E^2 I^{(2)}_g + |\kappa_g|^2 I^{(3)}_g]\,|A|^2(1 - E^2), \qquad (8b)$$

where $I^{(i)}_o$ and $I^{(i)}_g$ are the functions defined by

$$I^{(1)}_o = [I_0(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g)] * \left[\frac{s_o}{s_g}|J_1(2\kappa E\sqrt{s_o s_g})|^2 \exp -\mu_e(s_o + s_g)\right], \qquad (9a)$$

$$I^{(2)}_o = \left[\sqrt{\frac{s_o}{s_g}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g)\right] * [|J_0(2\kappa E\sqrt{s_o s_g})|^2 \exp -\mu_e(s_o + s_g)], \qquad (9b)$$

$$I^{(3)}_o = \sqrt{\frac{s_o}{s_g}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g), \qquad (9c)$$

$$I^{(1)}_g = \left[\sqrt{\frac{s_g}{s_o}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g)\right] * \left[\frac{s_o}{s_g}|J_1(2\kappa E\sqrt{s_o s_g})|^2 \exp -\mu_e(s_o + s_g)\right], \qquad (10a)$$

$$I^{(2)}_g = [I_0(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g)] * [|J_0(2\kappa E\sqrt{s_o s_g})|^2 \exp -\mu_e(s_o + s_g)], \qquad (10b)$$

$$I^{(3)}_g = I_0(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o + s_g). \qquad (10c)$$

Here, * implies the convolution of the functions on both sides. A few integrals of type (2b), which are required for deriving (8) from (5), are explained in Appendix A. It is worthwhile noting that $I^{(1)}_o$, $I^{(2)}_o$, $I^{(1)}_g$ and $I^{(2)}_g$ are defined by the convolution of the intensity distributions of perfectly coherent and incoherent cases. The position specified by the convolution variables, therefore, can be interpreted as a point where the coherent wave is converted to the incoherent beam. The physical meanings of each term of (8b) and (1b) are illustrated in Fig. 1. An analogous interpretation can also be given to (8a) and (1a).

3. The integrated intensities for parallel-sided crystals

(a) The perfectly coherent components, R^c_o and R^c_g

The intensity distributions are given by (1a) and (1b). The integrated intensities, therefore, are given by

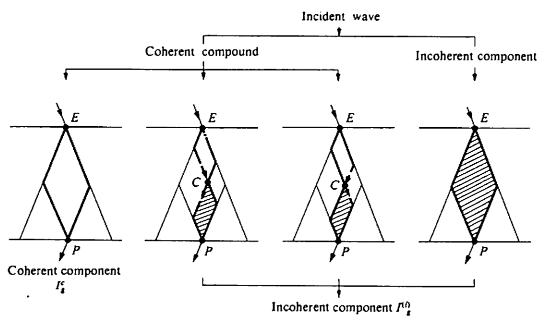

Fig. 1. Interpretation of the diffracted intensities I^c_g (equation 1b) and I^i_g (equation 8b). The last three drawings correspond to the three terms of $I^{(i)}_g$, respectively. E Entrance point. P Observation point. C The point where the coherent waves (white) are transformed to the incoherent beam (hatched). The arrows indicate the reflection processes of this transformation.

integrating the distributions over the exit surface.† As discussed in a previous paper (IV), it is convenient to multiply the results by the factor $[\lambda(\sin 2\theta_B)^{-2}]$ in order to represent them on the scale of unit angular and spatial distribution of the incident energy. Thus, one obtains the integrated intensities

$$R_o^c = E^2\, Q_o(t/\gamma_o)\exp(-Mt)w_o(t), \qquad (11a)$$

$$R_g^c = E^2\, Q(t/\gamma_o)\exp(-Mt)w_g(t), \qquad (11b)$$

where t is the thickness of the crystal and Q and Q_o are defined by

$$Q = \lambda(\sin 2\theta_B)^{-1}|\kappa_g|^2, \qquad (12a)$$

$$Q_o = \lambda(\sin 2\theta_B)^{-1}|\kappa_g\, \kappa_{-g}|. \qquad (12b)$$

The functions $w_o(t)$ and $w_g(t)$ are defined and calculated in Appendix B. Their expressions are given by

$$w_o(t) = \exp(-Nt) - \frac{1}{t}\{I_0(Nt)*J_0[(4Z^2 - N^2)^{1/2}t]\} + \frac{2N}{t}\{(\exp -Nt)*I_0(Nt) *J_0[(4Z^2 - N^2)^{1/2}t]\}, \qquad (13a)$$

$$w_g(t) = \frac{1}{t}\{I_0(Nt)*J_0[(4Z^2 - N^2)^{1/2}t]\}, \qquad (13b)$$

where $*$ implies the convolutional operation and the parameters M, N and Z are given as follows.

$$M = \tfrac{1}{2}\mu_e\left(\frac{1}{\gamma_o} + \frac{1}{\gamma_g}\right), \quad N = \tfrac{1}{2}\mu_e\left(\frac{1}{\gamma_o} - \frac{1}{\gamma_g}\right), \qquad (14a,b)$$

$$Z = \kappa E/\sqrt{\gamma_o\,\gamma_g}, \qquad (14c)$$

where γ_o and γ_g are the direction cosines between the normal of the crystal and the directions of s_o and s_g, respectively.

(b) *The perfectly incoherent components, R_o^i and R_g^i*

The incoherent components of the wave fields are composed of three terms, as discussed in the previous section [see (8a) and (8b)]; each third is a perfectly incoherent component. One can calculate the components immediately, as discussed in IV [equations (16) and (20)], by replacing μ_e and σ by $\tilde{\mu}_e$ and $\tilde{\sigma}$. The results are given in the form

$$R_o^i = (1 - E^2)Q_o(t/\sqrt{\gamma_o\,\gamma_g})\exp(-\tilde{M}t)u_o(t); \qquad (15a)$$

$$R_g^i = (1 - E^2)Q(t/\gamma_o)\exp(-\tilde{M}t)u_g(t), \qquad (15b)$$

where $u_o(t)$ and $u_g(t)$ are defined in Appendix B. The explicit forms are given by

$$u_o(t) = (1/\tilde{L}t)\{\cosh[(\tilde{N}^2 + \tilde{L}^2)^{1/2}t] - \tilde{N}(\tilde{N}^2 + \tilde{L}^2)^{-1/2}\sinh[(\tilde{N}^2 + \tilde{L}^2)^{1/2}t] - \exp(-\tilde{N}t)\}, \qquad (16a)$$

$$u_g(t) = \sinh[(\tilde{N}^2 + \tilde{L}^2)^{1/2}t]/[(\tilde{N}^2 + \tilde{L}^2)^{1/2}t]. \qquad (16b)$$

The parameters involved are defined by

$$\tilde{M} = \frac{1}{2}\left(\frac{1}{\gamma_o} + \frac{1}{\gamma_g}\right)\tilde{\mu}_e, \quad \tilde{N} = \frac{1}{2}\left(\frac{1}{\gamma_o} - \frac{1}{\gamma_g}\right)\tilde{\mu}_e, \qquad (17a,b)$$

$$\tilde{L} = \tilde{\sigma}/\sqrt{\gamma_o\,\gamma_g}. \qquad (17c)$$

(c) *The mixed components, $M_o^{(1)}$, $M_o^{(2)}$, $M_g^{(1)}$, $M_g^{(2)}$*

The next problems are to calculate the integrated intensities due to the first and second terms of (8a) and (8b). They already involve the convolutional integration $[J_c]$. The integral variables (s_o', s_g') can be transformed to (x', t'), being parallel and perpendicular coordinates to the crystal surface, by the transformations (IV.12). Also, it is worth noting the relation of the volume elements;

$$\mathrm{d}x'\,\mathrm{d}t' = \sin 2\theta_B\,\mathrm{d}s_o'\,\mathrm{d}s_g'. \qquad (18)$$

When the incident beam is sufficiently narrow, the required integrations are $[J_c]$ mentioned above and the integration over the exit surface $[J_a]$. If the incident beam is a homogeneous distribution of such a narrow beam, logically speaking, one needs additionally the integration $[J_e]$ over the entrance surface. Since, however, the result after taking the integration $[J_a]$ must be independent of the entrance position of the narrow beam, $[J_e]$ is redundant. In fact, this is the case for R^c and R^i where only the integration $[J_a]$ is needed.

In the cases of $M_o^{(1)}$, $M_o^{(2)}$, *etc.*, however, it is more convenient to exchange the order of $[J_c]$, $[J_a]$ and $[J_e]$. Fixing the integral variables (x', t'), we perform the integration $[J_e]$. Then, the integrand must be a function of t', $t - t'$ and $x - x'$. Next, we perform the integration $[J_a]$. The integrand then becomes a function of t' and $t - t'$. Thus, the integral can be given by a convolutional integration with respect to a single variable t', and the integration of x' can be regarded as redundant. From these considerations, one can write down the integrated intensities corresponding to the first and second terms of (8) as follows:

$$M_o^{(1)} = E^2(1 - E^2)Q_o\,\kappa^4\,\tau\tau_e(1/\gamma_o)^2\,[k_g*l_o]_t, \qquad (19a)$$

$$M_o^{(2)} = E^2(1 - E^2)Q_o\,\kappa^4\,\tau\tau_e(1/\gamma_o\sqrt{\gamma_o\,\gamma_g})\,[k_o*l_g]_t, \qquad (19b)$$

$$M_g^{(1)} = E^2(1 - E^2)Q\kappa^4\,\tau\tau_e(1/\gamma_o\sqrt{\gamma_o\,\gamma_g})\,[\bar{k}_o*l_o]_t, \qquad (19c)$$

$$M_g^{(2)} = E^2(1 - E^2)Q\kappa^4\,\tau\tau_e(1/\gamma_o)^2\,[k_g*l_g]_t, \qquad (19d)$$

† The procedures are similar to those used in deriving equations (IV.16) and (IV.20).

where the convolutional operation is defined by

$$[k*l]_t = \int_0^t k(t')l(t-t')\,dt' \tag{20}$$

and the functions k_o, k_g, l_o, *etc.* are defined and calculated in Appendix *B*. They involve M, N, Z defined by (14) as well as $\tilde{M}$, $\tilde{N}$ and $\tilde{L}$ defined by (17).

4. Symmetrical Laue cases

Although the integral intensities are given in analytical forms [(11), (15) and (19)], the expressions are rather complicated in general cases. To give physical meanings to these expressions, in this section we shall consider the simplest case: $N=0$ and $\tilde{N}=0$. Then, the functions w_o, w_g, *etc.* in (13), (16) and Appendix *B* are simplified as follows:

$$w_0 = (2Zt)^{-1}[(2Zt) - W(2Zt)], \tag{21a}$$

$$w_g = (2Zt)^{-1}\,W(2Zt), \tag{21b}$$

$$u_o = (\tilde{L}t)^{-1}[\cosh(\tilde{L}t) - 1], \tag{22a}$$

$$u_g = (\tilde{L}t)^{-1}\sinh(\tilde{L}t), \tag{22b}$$

$$l_o = (2Z)^{-1}[(2Zt) - W(2Zt)]\exp(-Mt), \tag{23a}$$

$$l_g = (2Z)^{-1}\,W(2Zt)\exp(-Mt), \tag{23b}$$

$$k_o = \bar{k}_o = (\tilde{L})^{-1}[\cosh(\tilde{L}t) - 1]\exp(-\tilde{M}t) \tag{24a}$$

$$k_g = (\tilde{L})^{-1}\sinh(\tilde{L}t)\exp(-\tilde{M}t), \tag{24b}$$

where

$$W(2Zt) = \int_0^{2Zt} J_0(\rho)\,d\rho \tag{25a}$$

$$= 2\sum_{n=0} J_{2n+1}(2Zt) \tag{25b}$$

is Waller's integral. In the following arguments, equation (1.37) is used for the expression of Γ, which is included in $\tilde{L}$ and $\tilde{M}$.

Substituting from (21) into (11), we have

$$R_o^c = EH_o\exp(-\mu_o T)\{2E(T/\Lambda) - W[2E(T/\Lambda)]\}$$
$$\times\exp\{-2(1-E^2)(\tau/\Lambda)(T/\Lambda)\}, \tag{26a}$$

$$R_g^c = EH_g\exp(-\mu_o T)W[2E(T/\Lambda)]$$
$$\times\exp\{-2(1-E^2)(\tau/\Lambda)(T/\Lambda)\}, \tag{26b}$$

where

$$H_o = H_g = \tfrac{1}{2}(\sin 2\theta_B)^{-1}(\lambda/\Lambda) \tag{27†}$$

† For avoiding complexity, $|\kappa_g| = |\kappa_{-g}|$ is assumed. In absorbing crystals H_o and H_g are slightly different.

and

$$\Lambda = |\kappa|^{-1}, \quad T = t/\cos\theta_B. \tag{28a,b}$$

Similarly, (15) and (22) give the results

$$R_o^i = (1-E^2)H_o\exp(-\mu_o T)(\tau_e/\Lambda)^{-1}$$
$$\times\{\cosh[2(\tau_e/\Lambda)(T/\Lambda)] - 1\}$$
$$\times\exp[-2(\tau_e/\Lambda)(T/\Lambda)], \tag{29a}$$

$$R_g^i = (1-E^2)H_g\exp(-\mu_o T)(\tau_e/\Lambda)^{-1}$$
$$\times\sinh[2(\tau_e/\Lambda)(T/\Lambda)]$$
$$\times\exp[-2(\tau_e/\Lambda)(T/\Lambda)], \tag{29b}$$

where

$$\tau_e = E\Lambda + (1-E^2)\tau. \tag{30}$$

The calculations of $M_o^{(i)}$ and $M_g^{(i)}$ ($i=1$ and 2) are more complicated. Here, the outline is described. The convolutional integrals appearing in (19) can be written as follows with the use of (23) and (24):

$$L[k_g*l_o]_t = (2Z\tilde{L})^{-1}\{\tfrac{1}{2}(m_1-m_2) - \tfrac{1}{2}(n_1-n_2)\}, \tag{31a}$$

$$L[k_o*l_g]_t = (2Z\tilde{L})^{-1}\{\tfrac{1}{2}(n_1+n_2) - n_3\}, \tag{31b}$$

$$L[\bar{k}_o*l_o]_t = (2Z\tilde{L})^{-1}\{\tfrac{1}{2}(m_1+m_2) - m_3 - \tfrac{1}{2}(n_1+n_2)$$
$$+ n_3\}, \tag{31c}$$

$$L[k_g*l_g]_t = (2Z\tilde{L})^{-1}\{\tfrac{1}{2}(n_1-n_2)\}, \tag{31d}$$

where $\{m_j\}$ and $\{n_j\}$ are the integrals defined by

$$\{m_j\} = L\{\exp -X_j t\}*\{(2Zt)\exp -Mt\} \tag{32a}$$

$$= (L/Y_j)[(2Zt) - (2Z/Y_j)$$
$$\times(1-\exp -Y_j t)]\exp -Mt, \tag{32b}$$

$$\{n_j\} = L\{\exp -X_j t\}*\{W(2Zt)\exp -Mt\} \tag{33a}$$

$$= (L/Y_j)[W(2Zt) - 2Z\exp(-Y_j t)$$
$$\times\int_0^t J_0(2Zt')\exp(Y_j t')\,dt']\exp -Mt. \tag{33b}$$

Here,

$$X_j = \tilde{M}-\tilde{L},\ \tilde{M}+\tilde{L}\ \text{and}\ \tilde{M}, \tag{34a,b,c}$$

and

$$Y_j = X_j - M = -(1-E^2)L,\ (1-E^2)L + 4Z\ \text{and}\ 2Z \tag{35a,b,c}$$

for $j = 1$, 2 and 3, respectively. The integral involved in (33*b*) can be represented by a series of Bessel functions as in the case of the Waller integral (25*b*). The details are explained in Appendix *C*.

From (19) and (31), finally, the mixed components of the integrated intensity can be written as

$$M_o = M_o^{(1)} + M_o^{(2)} = \tfrac{1}{4}E(1-E^2)H_o\{\tfrac{1}{2}(m_1 - m_2) + n_2 - n_3\}, \quad (36a)$$

$$M_g = M_g^{(1)} + M_g^{(2)} = \tfrac{1}{4}E(1-E^2)H_g\{\tfrac{1}{2}(m_1 + m_2) - m_3 - n_2 + n_3\}. \quad (36b)$$

Fig. 2 shows the integrated intensity for $E = 0{\cdot}1$ and $\tau/\Lambda = 0{\cdot}1$ as an example of the case in which secondary extinction is predominant. When $E < 0{\cdot}1$, the coherent component R_g^c and the mixed component M_g are negligible. It is worth mentioning, however, that the asymptotic value of R_g^i is appreciably smaller than that in the conventional secondary-extinction theory [$E = 0$], because the effective coherent length τ_e is larger than τ.

Fig. 3 shows the case of $E = 0{\cdot}9$ and $\tau/\Lambda = 0{\cdot}1$, which is an example of the case in which primary extinction is predominant. Firstly, the spacing of the *Pendellösung* fringes is elongated by the factor $(1/E)$. Next, the intensity R_g^c attenuates due to the transformation to the mixed component M_o.

A more significant point is that the mixed component M_g is appreciably large for a crystal thicker than a few *Pendellösung* fringes. This is because the coherent component R_o^c is very large for thick crystals and transformed to M_g unless E is very close to unity or τ/Λ is very small. Although the detailed analysis is required, the observation of Wada & Kato (1976) that the background of the traverse topograph of the nearly perfect crystal is unexpectedly large can be partly explained from this consideration. In fact, M_o and M_g are gradually increasing even for $E = 0{\cdot}1$, as shown in Fig. 2(*a*) and (*b*). In this particular case, however, the amounts are practically negligible, because the coherent source R_o^c is small for a finite crystal thickness.

5. Discussion and summary

In this series of papers, it is intended to study systematically diffraction phenomena in crystals having

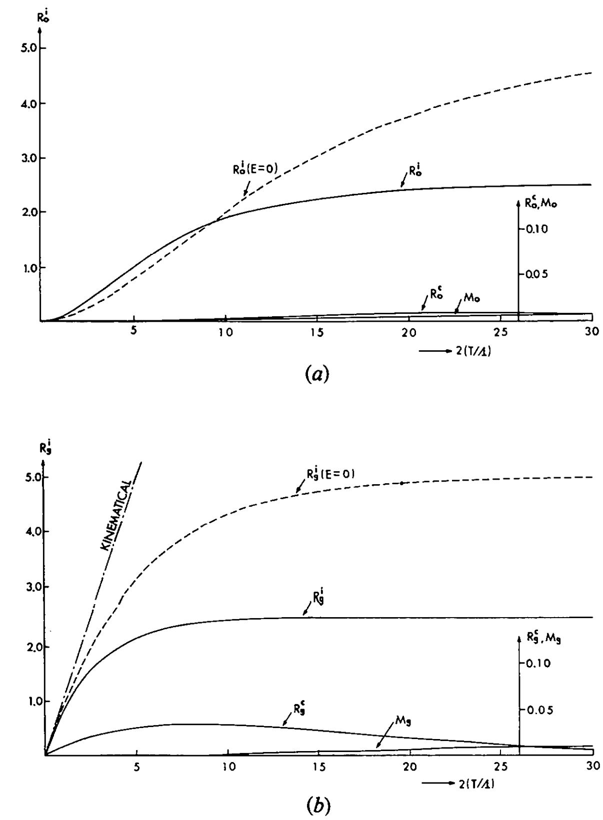

Fig. 2. The integrated intensities [*cf.* equations (26), (29) and (36)] in the case of $E = 0{\cdot}1$ and $\tau/\Lambda = 0{\cdot}1$ on the scale of $H_o \exp(-\mu_o T)$ and $H_g \exp(-\mu_o T)$ for the transmission (*a*) and the Bragg-reflection cases (*b*).

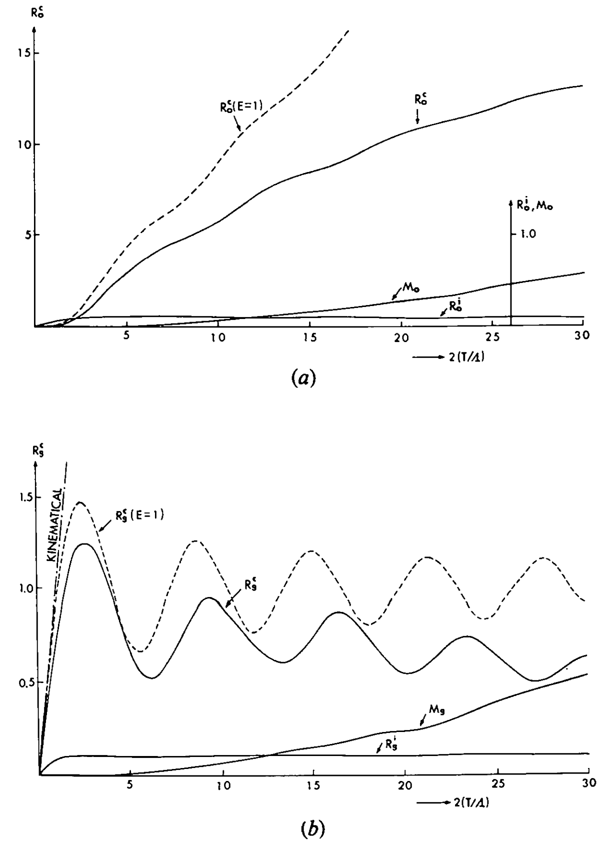

Fig. 3. The integrated intensities in the case of $E = 0{\cdot}9$ and $\tau/\Lambda = 0{\cdot}1$ on the same scale as in Fig. 2. (*a*) Transmission. (*b*) Bragg reflection.

a wide range of crystal perfection. The experimental objects are the topographic observations on the one hand and the extinction phenomena of the integrated intensity on the other.

(a) *Section topographs*

The nearly perfect crystals including invisible defects and the imperfect crystals in which the defects are not individually distinguishable can be dealt with by the present theory (§ 3). We shall, however, leave the detailed discussion for a future paper because one needs the numerical analysis of the mixed components $I_o^{(i)}$ and $I_g^{(i)}$ (i = 1 and 2) based on (9) and (10). Nevertheless, the physics underlying these analytical expressions is clear, as stated at the end of § 3. Also, when the mixed components are negligibly small ($E \lesssim 0{\cdot}1$), $I_o^{(3)}$ and $I_g^{(3)}$ are sufficient to describe the section topographs.

(b) *Traverse topographs and extinction phenomena*

In this paper, to avoid mathematical complexity, only the symmetrical Laue case for parallel-sided crystals was treated. Some numerical results which were obtainable by a hand calculator and a table of Bessel functions were given in § 4. Again, we shall leave the other cases to the future studies. Here, two extreme cases are discussed in connection with the conventional extinction theories.

(i) *Nearly perfect crystals* ($E \gtrsim 0{\cdot}9$). *Pendellösung* fringes are visible in R_g^c. The contrast, however, will be disturbed by the presence of the mixed component M_g. Only when $\Lambda \gg \tau$ does the conventional dynamical theory (primary-extinction theory) hold provided that the structure factor is corrected by the 'static' Debye–Waller factor E. Incidentally, in the case of $E \gg \tau/\Lambda$, the physical meaning of τ is the size of modulation from the averaged perfect lattice. The crystal looks more perfect as τ decreases.

(ii) *Reasonably imperfect crystals* ($E \lesssim 0{\cdot}1$). The general trend of the integrated intensity is predictable by the scheme of secondary extinction, provided τ_e is used instead of τ [equations (29)]. The intensity value, however, depends upon the size of τ/Λ for a fixed E. Only when $\tau/\Lambda \gg E$ is the conventional secondary extinction theory applicable. In this case, the physical meaning of τ is the size of the crystallites. In contrast to the previous case ($E \gg \tau/\Lambda$), as τ increases, the crystal becomes more perfect.

Next, we shall discuss a few feasible improvements of the present theory.

(*a*) *Borrmann absorption*. As mentioned in the footnote of Appendix *B*, Borrmann absorption has been neglected in the calculations of the integrated intensity. In nearly perfect crystals, however, the exact expression (Kato, 1968) for R_g^c or a practically useful one (Kato, 1954) is available for a crystal having Borrmann absorption.

(*b*) *The use of the correlation length* τ_2. This problem has been raised already in § 5(*b*) of Kato (1980*b*). The definition of τ_2 was given by equation (II.2).* It has to be used in the calculation of the beam intensity, which is associated with a set of optical routes R and R' including no isolated kink point such as a, b, a' and b' in Fig. 3 of paper 1. The expression for the intensity can be written as $I_o^{(3)}(\tau_2')$ and $I_g^{(3)}(\tau_2')$, where $\tau_2' = (1 - E^2)\tau_2$ and τ in (9*c*) and (10*c*) is replaced by τ_2. Since, however, the intensity for such a set of routes is already included in (9*c*) and (10*c*) as the forms of $I_o^{(3)}(\tau')$ and $I_g^{(3)}(\tau')$, τ' being $(1 - E^2)\tau$, one needs to subtract them from the respective expressions. Thus, the correct intensities must be

$$I_o^{(3)} = I_o^{(3)}(\tau_e) + I_o^{(3)}(\tau_2') - I_o^{(3)}(\tau'), \qquad (37a)$$

$$I_g^{(3)} = I_g^{(3)}(\tau_e) + I_g^{(3)}(\tau_2') - I_g^{(3)}(\tau'). \qquad (37b)$$

When E tends to zero, the first and third terms on the right sides cancel out in each equation so that the results are identical to those obtained in II. Also, when E tends to one, the contribution of $I_o^{(3)}$ to the total intensity is negligible.

Further, one can improve the mixed components $I_o^{(i)}$ and $I_g^{(i)}$ (i = 1 and 2) by taking similar expressions to (37) for the first functions of the convolutional forms of (9*a*) and (9*b*) and (10*a*) and (10*b*). The expressions, however, are too complex in practice.

For the expressions of the integrated intensities also, similar arguments can be applied. The simplest improvement is expected by taking

$$R_o^i = R_o^i(\tau_e) + R_o^i(\tau_2') - R_o^i(\tau'), \qquad (38a)$$

$$R_g^i = R_g^i(\tau_e) + R_g^i(\tau_2') - R_g^i(\tau'), \qquad (38b)$$

instead of expressions (15*a*) and (15*b*), respectively.

It is desirable to compare the present results with experiment. The most feasible experiment is the study of the wavelength dependence of the integrated intensities under the same diffraction conditions.

APPENDIX *A*

The Laplace inverse transform of *G*(*p*,*q*) and the related functions

(1) $G(p,q)$ [*definition: equation* (6)]

We shall calculate the function

$$G(s_o,s_g) = \left(\frac{1}{2\pi i}\right)^2 \int_{\gamma-i\infty}^{\gamma+i\infty}\int \frac{\exp[ps_o + qs_g]}{(p + \tilde{\mu}_e)(q + \tilde{\mu}_e) - \tilde{\sigma}^2}\,\mathrm{d}p\,\mathrm{d}q. \qquad (A.1)$$

* The function $f(z)$, however, should be replaced by $g(z)$.

The first-order pole in the p complex plane is located at

$$p = -\tilde{\mu}_e + \tilde{\sigma}^2/(q + \tilde{\mu}_e).$$

Taking the integral contour surrounding this pole, we have

$$\begin{aligned} G(s_o,s_g) &= \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} (q+\tilde{\mu}_e)^{-1} \exp\left[\frac{\tilde{\sigma}^2 s_o}{q+\tilde{\mu}_e} + qs_g\right] \mathrm{d}q \\ &\quad \times \exp -\tilde{\mu}_e s_o \quad (s_o > 0) \\ &= \frac{1}{2\pi i}\int_{\gamma+\mu_e-i\infty}^{\gamma+\mu_e+i\infty} \frac{1}{q'} \exp\left[\frac{\tilde{\sigma}^2 s_o}{q'} + q' s_g\right] \mathrm{d}q' \\ &\quad \times \exp -\tilde{\mu}_e(s_o+s_g) \\ &= I_o(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o+s_g) \quad (s_o,s_g > 0). \end{aligned} \qquad (A.2)$$

(2) $G_1(p,q) = (q - \tilde{\mu}_e)G(p,q)$

$$G_1(s_o,s_g) = \left(\frac{1}{2\pi i}\right)^2 \int\int_{\gamma-i\infty}^{\gamma+i\infty} (q+\tilde{\mu}_e) \times \frac{\exp[ps_o + qs_g]}{(p+\tilde{\mu}_e)(q+\tilde{\mu}_e) - \tilde{\sigma}^2} \mathrm{d}p\,\mathrm{d}q \qquad (A.3)$$

$$\begin{aligned} &= \frac{1}{2\pi i}\int_{\gamma+\mu_e-i\infty}^{\gamma+\mu_e+i\infty} \exp\left[\frac{\tilde{\sigma}^2 s_o}{q'} + q's_g\right] \mathrm{d}q' \\ &\quad \times \exp -\tilde{\mu}_e(s_o+s_g) \quad (s_o > 0) \\ &= \tilde{\sigma}\sqrt{\frac{s_o}{s_g}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \\ &\quad \times \exp -\tilde{\mu}_e(s_o+s_g) \quad (s_o,s_g > 0). \end{aligned} \qquad (A.4)$$

In this case, the integral includes $\delta(s_g)$, but it can be omitted for $s_g > 0$.

(3) $G_2(p,q) = (p + \tilde{\mu}_e)G(p,q)$

$$G_2(s_o,s_g) = \left(\frac{1}{2\pi i}\right)^2 \int\int_{\gamma-i\infty}^{\gamma+i\infty} (p+\tilde{\mu}_e) \times \frac{\exp[ps_o + qs_g]}{(p+\tilde{\mu}_e)(q+\tilde{\mu}_e) - \tilde{\sigma}^2} \mathrm{d}p\,\mathrm{d}q. \qquad (A.5)$$

If p and q and s_o and s_g are interchanged, the function is identical to case (2). Therefore,

$$G_2(s_o,s_g) = \tilde{\sigma}\sqrt{\frac{s_g}{s_o}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \exp -\tilde{\mu}_e(s_o+s_g). \qquad (A.6)$$

(4) $G_3(p,q) = (p + \tilde{\mu}_e)^{-1} G(p,q)$

$$G_3(s_o,s_g) = \left(\frac{1}{2\pi i}\right)^2 \int\int_{\gamma-i\infty}^{\gamma+i\infty} (p+\tilde{\mu}_e)^{-1} \times \frac{\exp[ps_o + qs_g]}{(p+\tilde{\mu}_e)(q+\tilde{\mu}_e) - \tilde{\sigma}^2} \mathrm{d}p\,\mathrm{d}q. \qquad (A.7)$$

Firstly, we calculate the contour integral in q space. Then, we have

$$\begin{aligned} G_3(s_o,s_g) &= \left(\frac{1}{2\pi i}\right) \int_{\gamma-i\infty}^{\gamma+i\infty} (p+\tilde{\mu}_e)^{-2} \\ &\quad \times \exp\left[ps_o + \frac{\tilde{\sigma}^2 s_g}{p+\tilde{\mu}_e}\right] \mathrm{d}p \\ &\quad \times \exp -\tilde{\mu}_e s_g \quad (s_g > 0) \\ &= \tilde{\sigma}^{-1}\sqrt{\frac{s_o}{s_g}}\, I_1(2\tilde{\sigma}\sqrt{s_o s_g}) \\ &\quad \times \exp -\tilde{\mu}_e(s_o+s_g) \quad (s_o,s_g > 0). \end{aligned} \qquad (A.8)$$

APPENDIX *B*

Integrals required for the integrated intensity

(a) The definitions

In terms of the normalized variable ζ defined by equation (IV.14), we shall define the following integrals.

$$u_o = \frac{1}{2}\int_{-1}^{1} \left[\frac{1-\zeta}{1+\zeta}\right]^{1/2} I_1(\tilde{L}t\sqrt{1-\zeta^2}) \exp(\tilde{N}t\zeta)\,\mathrm{d}\zeta$$

[*cf.* (15*a*)], (*B*.1*a*)

$$\bar{u}_o = \frac{1}{2}\int_{-1}^{1} \left[\frac{1+\zeta}{1-\zeta}\right]^{1/2} I_1(\tilde{L}t\sqrt{1-\zeta^2}) \exp(\tilde{N}t\zeta)\,\mathrm{d}\zeta, \qquad (B.1b)$$

$$u_g = \tfrac{1}{2}\int_{-1}^{1} I_o(\tilde{L}t\sqrt{1-\zeta^2}) \exp(\tilde{N}t\zeta)\,\mathrm{d}\zeta \quad [cf.\ (15b)], \qquad (B.1c)$$

$$w_o = \frac{1}{2}\int_{-1}^{1} \frac{1-\zeta}{1+\zeta} |J_1(Zt\sqrt{1-\zeta^2})|^2 \exp(Nt\zeta)\,\mathrm{d}\zeta$$

[*cf.* (11*a*)], (*B*.1*d*)

$$w_g = \tfrac{1}{2}\int_{-1}^{1} |J_o(Zt\sqrt{1-\zeta^2})|^2 \exp(Nt\zeta)\,\mathrm{d}\zeta$$

[*cf.* (11*b*)]. (*B*.1*e*)

For representing the mixed components of the integrated intensity (19), we shall also define the following functions.

$$(k_o,\bar{k}_o,k_g) = (u_o,\bar{u}_o,u_g)t \exp -\tilde{M}t, \qquad (B.2a)$$

$$(l_o,l_g) = (w_o,w_g)t \exp -Mt. \qquad (B.2b)$$

Most of these have been obtained in the previous papers [u_o and u_g: Kato (1980*a*); w_g: Kato (1968)]. $\bar{u}_o$ is derived from u_o simply by changing the sign of $\tilde{N}$. For this reason, only w_o is discussed in detail, but w_g is also treated for showing the relations between w_o and w_g. Here, however, only the case of real Z is explained, because the case of complex Z is very complicated.†

(b) The calculation of w_g and l_g

Using the Neumann's integral representation [equation (11.4.7) in Abramowitz & Stegun, 1964],

$$\{J_m(\rho)\}^2 = \frac{1}{\pi}\int_0^{\pi} J_{2m}(2\rho \sin \varphi)\, d\varphi, \qquad (B.3)$$

one can write

$$w_g(t) = \frac{1}{\pi}\int_0^{\pi} w_g(\varphi)\, d\varphi, \qquad (B.4)$$

where

$$w_g(\varphi) = \tfrac{1}{2}\int_{-1}^{1} J_0(x\sqrt{1-\zeta^2}) \exp(y\zeta)\, d\zeta \qquad (B.5)$$

and

$$x = 2Zt \sin \varphi, \quad y = Nt. \qquad (B.6a,b)$$

The function $w_g(\varphi)$ is well known and given by

$$w_g(\varphi) = \sinh X/X, \qquad (B.7)$$

where

$$X = (y^2 - x^2)^{1/2}. \qquad (B.8)$$

By inserting (B.7) into (B.4), $w_g(t)$ can be obtained. Here, for convenience, we shall calculate first $l_g(t)$ defined by ($B.2b$); namely

$$l_g(t) = \frac{1}{\pi}\int_0^{\pi} \sinh [N^2 - 4Z^2 \sin^2 \varphi]^{1/2}\, t \times [N^2 - 4Z^2 \sin^2 \varphi]^{-1/2}\, d\varphi \exp(-Mt). \qquad (B.9)$$

Taking the Laplace transform of this expression, we have

$$l_g(p) = \frac{1}{\pi}\int_0^{\pi} [(p+M)^2 - (N^2 - 4Z^2 \sin^2 \varphi)]^{-1}\, d\varphi = \{(p+M)^2 - N^2\}^{-1/2}\{(p+M)^2 + (4Z^2 - N^2)\}^{-1/2}. \qquad (B.10)$$

Thus, using the Laplace inverse transform and the convolutional theorem, we have

$$l_g(t) = \{I_0(Nt)*J_0[(4Z^2 - N^2)^{1/2}\, t]\} \exp(-Mt), \qquad (B.11)$$

where * implies the convolutional integration, and I_0 and J_0 are the modified and ordinary Bessel functions of the zeroth order, respectively. The function $w_g(t)$ is given immediately as

$$w_g(t) = \frac{1}{t}\{I_0(Nt)*J_0[(4Z^2 - N^2)^{1/2}\, t]\}. \qquad (B.12)$$

(c) w_o and l_o

Similarly to (B.4) and (B.5), we have

$$w_o(t) = \frac{1}{\pi}\int_0^{\pi} w_o(\varphi)\, d\varphi, \qquad (B.13)$$

where

$$w_o(\varphi) = \frac{1}{2}\int_{-1}^{1} \left[\frac{1-\zeta}{1+\zeta}\right] J_2(x\sqrt{1-\zeta^2}) \exp(y\zeta)\, d\zeta. \qquad (B.14)$$

If one defines the function

$$v_o(\varphi) = \frac{1}{2}\int_{-1}^{1} \sum_{n=0}^{\infty} \frac{(-1)^n (1-\zeta^2)^n}{n!(n+2)!} \left(\frac{x}{2}\right)^{2n+2} \exp(y\zeta)\, d\zeta, \qquad (B.15)$$

it is easily shown from the series expansion of $J_2(x\sqrt{1-\zeta^2})$ that

$$w_o(\varphi) = 1 - 2\frac{\partial v_o}{\partial y} + \frac{\partial^2 v_o}{\partial y^2}. \qquad (B.16)$$

Also, comparing (B.15) with (B.5) [*cf.* the power series of $J_0(x\sqrt{1-\zeta^2})$], we have

$$4\frac{\partial}{\partial(x^2)}\frac{\partial}{\partial(x^2)}[x^2 v_o] = w_g(\varphi) = \sinh X/X. \qquad (B.17)$$

Integrating this with the conditions

$$x^2 v_o = 0, \quad \frac{\partial}{\partial(x^2)}[x^2 v_o] = 0$$

at $x^2 = 0$, we obtain

$$v_o(\varphi) = (1/x^2)[X \sinh X - \cosh X - y \sinh y + \cosh y] + \tfrac{1}{2}\cosh y. \qquad (B.18)$$

Then, by the use of (B.16), we have

$$w_o(\varphi) = [e^{-y} - \sinh X/X] + (2/x^2)[y^2 \sinh X/X - y \cosh X + ye^{-y}]. \qquad (B.19)$$

As in the case of $w_g(t)$, we shall first calculate $l_o(t)$ defined by ($B.2b$). The Laplace transform of $l_o(t)$ is given by

$$l_o(p) = (p+M+N)^{-2} - [(p+M)^2 - N^2]^{-1/2} \times [(p+M)^2 + 4Z^2 - N^2]^{-1/2} + 2N(p+M+N)^{-1}[(p+M)^2 - N^2]^{-1/2} \times [(p+M)^2 + 4Z^2 - N^2]^{-1/2}. \qquad (B.20)$$

† This implies neglecting Borrmann anomalous transmission. Kato (1968) treated the integral w_g for complex Z.

Therefore, we have

$$l_o(t) = \{t \exp(-Nt) - I_0(Nt) * J_0[(4Z^2 - N^2)^{1/2}t] + 2N[\exp(-Nt)] * I_0(Nt) * J_0[(4Z^2 - N^2)^{1/2}t]\} \exp(-Mt). \quad (B.21)$$

Finally, we obtain

$$w_o(t) = \exp(-Nt) - \frac{1}{t}\{I_0(Nt) * J_0[(4Z^2 - N^2)^{1/2}t]\} + \frac{2N}{t}\{[\exp(-Nt)] * I_0(Nt) * J_0[(4Z^2 - N^2)^{1/2}t]\}. \quad (B.22)$$

APPENDIX *C*

$$J(\rho;\eta) = \exp -\eta\rho \int_0^{\varrho} J_0(\rho) \exp \eta\rho \, d\rho.$$

Here, the parameter η is assumed to be real. Using the integral representation

$$J_0(\rho) = \frac{1}{\pi}\int_0^{\pi} \exp i(\rho \cos\theta) \, d\theta, \quad (C.1)$$

we have

$$J(\rho;\eta) = K(\rho;\eta) - K(0;\eta) \exp -\eta\rho, \quad (C.2)$$

where

$$K(\rho;\eta) = \frac{1}{\pi}\int_0^{\pi} \frac{\exp i(\rho\cos\theta)}{\eta + i\cos\theta} \, d\theta. \quad (C.3)$$

If we use the relationship

$$\exp[i(\rho\cos\theta)] = J_0(\rho) + 2\sum_{k=1}^{\infty} (i)^k J_k(\rho)\cos(k\theta), \quad (C.4)$$

it follows that

$$K(\rho;\eta) = J_0(\rho)L_0(\eta) + 2\sum_{k=1}^{\infty} (i)^k J_k(\rho)L_k(\eta), \quad (C.5)$$

where

$$L_k(\eta) = \frac{1}{\pi}\int_0^{\pi} \frac{\cos(k\theta)}{\eta + i\cos\theta} \, d\theta. \quad (C.6)$$

Thus, the problem is reduced to the integration of $L_k(\eta)$. The two cases have to be treated separately.

(i) $\eta > 0$.

$$L_k(\eta) = (-i)^k (\eta^2 + 1)^{-1/2} [(\eta^2 + 1)^{1/2} - \eta]^k. \quad (C.7a)$$

(ii) $\eta < 0$. Using the relationship $L_k(-\eta) = -\{L_k(|\eta|)\}^*$, we obtain

$$L_k(\eta) = -(i)^k (\eta^2 + 1)^{-1/2} [(\eta^2 + 1)^{1/2} - |\eta|]^k. \quad (C.7b)$$

Inserting these into (5) and (2), we have

(i) $\eta > 0$.

$|\eta|]^k.$

$$J(\rho;\eta) = [\eta^2 + 1]^{-1/2}\{J_0(\rho) + 2\sum_{k=1}^{\infty} [(\eta^2 + 1)^{1/2} - \eta]^k J_k(\rho)\} - [\eta^2 + 1]^{-1/2} \exp(-\eta\rho). \quad (C.8a)$$

(ii) $\eta < 0$.

$$J(\rho;\eta) = -[\eta^2 + 1]^{-1/2}\{J_0(\rho) + 2\sum_{k=1}^{\infty} (-1)^k [(\eta^2 + 1)^{1/2} - |\eta|]^k J_k(\rho)\} + [\eta^2 + 1]^{-1/2} \exp(|\eta|\rho). \quad (C.8b)$$

Incidentally, the case of $\eta = 0$ is immediately obtained from the definition of $J(\rho;\eta)$ as follows

$$J(\rho;0) = \int_0^{\varrho} J_0(\rho) \, d\rho = 2\sum_{k=0}^{\infty} J_{2k+1}(\rho) \, d\rho. \quad (C.9)$$

This result is also derived from (*C*.8) from the relationship

$$J_0(\rho) + 2\sum_{k=1}^{\infty} J_{2k}(\rho) = 1$$

[Abramowitz & Stegun (1964); equation (9.1.46)].

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