A Theoretical Approach to Dynamical Diffraction of X-rays in the Laue Case with the Green's Function Method

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X-ray dynamical diffraction for the Laue case is treated theoretically as an application of the theory for a largely distorted crystal using the Green's function method given by the previous report. In the Laue case, the transmitted and the diffracted waves in the crystal are expressed as the integrals with the kernels of the transmitted and diffracted wave components of the Green's function over the crystal surface. In the case of a perfect crystal, the Green's function components are analytically obtained and the waves in the crystal are expressed using the analytical forms of the Green's function. The result shows the analytical forms of the waves are essentially three-dimensional with a divergent wave image like a spherical wave, which are different from those given by Takagi's theory, and, however, are reducible to those.

Key Words : X-rays, Dynamical Diffraction, Laue Case, Maxwell's Equation, Green's Function

1. Introduction

Historically, dynamical diffraction theories of X-rays using the Green's function were first developed based on quantum mechanics in 1960's[(1)-(3)]. Later the fundamental solution of the Green's function of the classical Maxwell's equation was shown analytically in 1970's [(4)], which brought useful results for dynamical diffraction studies. However, the theoretical treatment was developed based on the equation of Helmholtz type deduced from Maxwell's equation, although the Maxwell's equation is originally non-Helmholtz type. Recently, the present author gave a new dynamical theory for a largely distorted crystal based on the Maxwell's equation of non-Helmholtz type, for which a Green's function of tensor type was introduced to describe the wave field in the crystal[(5),(6)]. In this paper, dynamical diffraction in the Laue case is theoretically treated with the Green's function, based on the dynamical theory. The wave filed in the crystal in the Laue case is directly represented using the surface integrals with the Green's function. When the crystal is perfect, the Green's function is analytically obtained in 3-dimensional form. This becomes an extension of Takagi's theory [(7)] which treats two-dimensional diffraction process.

2. Fundamental Equation

In dynamical diffraction of X-rays in a perfect or distorted crystal, X-ray wave field excited in the crystal is described by Maxwell's equation with the dielectric constant periodical or quasi-periodical over the crystal lattice. When a beam of X-rays monochromatic with the angular frequency ω is incident on the crystal and then excites an X-ray wave filed with the same angular frequency in the crystal, the crystal wave filed may be expressed with the electric field, $\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{r})\exp(-i\omega t)$, then the behavior of the crystal wave field is described by the following Maxwell's equation:

$$-\mathrm{rot}\,\mathrm{rot}\,\boldsymbol{E}(\boldsymbol{r}) + k^2\boldsymbol{E}(\boldsymbol{r}) + k^2\chi(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) = 0\,, \tag{1}$$

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where k is 2π times the wavenumber of the X-rays, $k=\omega/c$, c the light velocity, and χ the polarizability of the crystal generally being a function of position. In general, when a crystal lattice is distorted and the lattice displacement is given by a function of position, $\boldsymbol{u}(\boldsymbol{r})$, at arbitrary position point $\boldsymbol{r}$, the polarizability of the distorted crystal is given by

$$\chi(\boldsymbol{r})=\sum_{g}\chi_g\exp\{i\boldsymbol{g}\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\ , \tag{2}$$

$\boldsymbol{g}$ being the reciprocal lattice vector.

In the previous report[5], in order to treat a general case of one or more strong diffracted crystal waves, the waves in a distorted crystal were expressed by a sum of modulated waves

$$\boldsymbol{E}(\boldsymbol{r})=\sum_{g}\boldsymbol{E}_g(\boldsymbol{r})\ ,\quad \boldsymbol{E}_g(\boldsymbol{r})=\boldsymbol{\varphi}_g(\boldsymbol{r})\exp(i\boldsymbol{k}_g\cdot\boldsymbol{r})\ ,\ \ \boldsymbol{k}_g=\boldsymbol{k}_0+\boldsymbol{g}\ , \tag{3}$$

where $\boldsymbol{k}_0$ is the wave vector of the transmitted wave. Each amplitude function $\boldsymbol{\varphi}_g(\boldsymbol{r})$ in eq. (3) and each $\chi_g\exp\{-i\boldsymbol{g}\cdot\boldsymbol{u}(\boldsymbol{r})\}$ in eq. (2) are assumed to be slowly varying so that their high frequency Fourier coefficients higher than a given level are neglected.

$$\boldsymbol{E}_g(\boldsymbol{\kappa})=0\ ,\ \ \chi_g(\boldsymbol{\kappa})=0\ ,\qquad |\boldsymbol{\kappa}|>\kappa_0\ , \tag{4}$$

where $\kappa_0=2\pi/(3a_{max})$, a_{max} being the longest side length of the three sides constituting the unit cell of the crystal, and $\boldsymbol{E}_g(\boldsymbol{\kappa})$ is the Fourier coefficient of $\boldsymbol{\varphi}_g(\boldsymbol{r})$ defined by

$$\boldsymbol{\varphi}_g(\boldsymbol{r})=\int_{V_c^*}\boldsymbol{E}_g(\boldsymbol{\kappa})\exp\{i\boldsymbol{\kappa}\cdot\boldsymbol{r}\}\frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\ , \tag{5}$$

where V_c^* is the unit cell region of the reciprocal crystal lattice, and $\chi_g(\boldsymbol{\kappa})$ is the Fourier coefficient of the reciprocal lattice component of $\chi(\boldsymbol{r})$ defined by

$$\chi_g\exp\{-i\boldsymbol{g}\cdot\boldsymbol{u}(\boldsymbol{r})\}=\int\chi_g(\boldsymbol{\kappa})\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{r})\frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\ . \tag{6}$$

Assuming eq. (4), Maxwell's equation (1) derives a set of equations for the crystal waves [5]

$$(-\mathrm{rot\ rot}+k^2)\boldsymbol{E}_g(\boldsymbol{r})+k^2\sum_{g'}\chi_{g-g'}\exp\{i(\boldsymbol{g}-\boldsymbol{g}')\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{E}_{g'}(\boldsymbol{r})\ =0\ . \tag{7}$$

This is the fundamental equation to determine the wave field of the crystal. When the crystal wave is divided into the transverse component $\boldsymbol{E}^{(t)}$ and the longitudinal components $\boldsymbol{E}^{(l)}$ by

$$\boldsymbol{E}_g(\boldsymbol{r})=\boldsymbol{E}_g^{(t)}(\boldsymbol{r})+\boldsymbol{E}_g^{(l)}(\boldsymbol{r})\ ,\qquad \mathrm{div}\,\boldsymbol{E}_g^{(t)}(\boldsymbol{r})=0\ ,\ \mathrm{rot}\,\boldsymbol{E}_g^{(l)}(\boldsymbol{r})=0\ , \tag{8}$$

then, with respect to the left second term in eq. (7), the longitudinal components of the waves may be neglected [5] so that eq. (7) becomes

$$\boldsymbol{\nabla}^2\boldsymbol{E}_g^{(t)}(\boldsymbol{r})+k^2\boldsymbol{E}_g(\boldsymbol{r})+k^2\sum_{g'}\chi_{g-g'}(\boldsymbol{r})\exp\{i(\boldsymbol{g}-\boldsymbol{g}')\cdot\boldsymbol{r}\}\boldsymbol{E}_{g'}^{(t)}(\boldsymbol{r})=0\ . \tag{9}$$

From eq. (9) may be derived the equation for the Fourier coefficient of $\boldsymbol{E}_g(\boldsymbol{r})$. Using $\boldsymbol{E}_g(\boldsymbol{\kappa})$ defined by eq. (5), the Fourier expansion of $\boldsymbol{E}_g(\boldsymbol{r})$ is given by

$$\boldsymbol{E}_g(\boldsymbol{r})=\int_{V_c^*}\boldsymbol{E}_g(\boldsymbol{\kappa})\exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r}\}\frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\ ,\qquad \boldsymbol{K}_g=\boldsymbol{k}_g+\ \boldsymbol{\kappa}\ . \tag{10}$$

When $\boldsymbol{E}_g(\boldsymbol{\kappa})$ is expressed as a sum of the components of three independent polarizations, it may be shown as

$$\boldsymbol{E}_g(\boldsymbol{\kappa}) = E_g^1(\boldsymbol{\kappa})|e_g^1(\boldsymbol{\kappa})\rangle + E_g^2(\boldsymbol{\kappa})|e_g^2(\boldsymbol{\kappa})\rangle + E_g^3(\boldsymbol{\kappa})|e_g^3(\boldsymbol{\kappa})\rangle\,, \tag{11}$$

where $|e_g^1(\boldsymbol{\kappa})\rangle$ and $|e_g^2(\boldsymbol{\kappa})\rangle$ are two independent polarization vectors perpendicular to $\boldsymbol{K}_g$, *i.e*, polarization vectors for the transverse wave components of $\boldsymbol{E}_g$, and $|\boldsymbol{e}_g^3(\boldsymbol{\kappa})\rangle$ is the longitudinal polarization vector parallel to $\boldsymbol{K}_g$, represented as column vectors using the bra-ket notation. Then the Fourier expansions of the transverse waves are expressed as

$$\boldsymbol{E}_g^{(t)}(\boldsymbol{r}) = \sum_{\mu=1}^{2} \int_{V_c^*} E_g^\mu(\boldsymbol{\kappa}) \exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r}\}\frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\;. \tag{12}$$

Also, the electric field vector itself is represented as a column vector. Using eqs. (6), (10), (11) and (12), equation (9) gives the following equations for the Fourier coefficients of the transverse waves:

$$\{k^2(1+\chi_0) - {\boldsymbol{K}_g}^2\}E_g^\mu(\boldsymbol{\kappa}) + k^2\sum_{g'\neq g}\sum_{\mu'=1}^{2}\int_{|\boldsymbol{\kappa}'|<\kappa_0} \chi_{g-g'}(\boldsymbol{\kappa}')C_{gg'}^{\mu\mu'}(\boldsymbol{\kappa},\boldsymbol{\kappa}')E_{g'}^{\mu'}(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3} = 0\,, \tag{13}$$

where $\mu = 1, 2$ and $C_{gg'}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}') = \langle e_g^\mu(\boldsymbol{\kappa})|e_{g'}^\nu(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\rangle$ being the inner product of the two vectors. The transverse waves can be determined by eq. (13), because the longitudinal waves are not included in the equation. Similarly equation (9) gives the determination equations of the longitudinal waves[5]. However, in general, the longitudinal waves are negligible, that is, their magnitudes are in the order of the crystal polarizability χ, $10^{-4\sim-5}$, compared with those of the transverse waves.

3. Green's Function

Based on equation (1), a Green's function in 3-dimensional tensor form is defined by

$$-\mathrm{rot}\,\mathrm{rot}\,\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}') + k^2\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}') + k^2\chi(\boldsymbol{r})\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}') = -\delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathbf{I}^{(3)}\,, \tag{14}$$

where $\delta(\boldsymbol{r}-\boldsymbol{r}')$ is the Dirac's delta function and $\mathbf{I}^{(3)}$ is the 3-dimensional unit matrix tensor.

The following relationship is established between the Green's function and the wave field in a crystal [6]:

$$\boldsymbol{E}(\boldsymbol{r}) = \int_S\left\{\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}')\frac{\partial}{\partial n'}\,\boldsymbol{E}(\boldsymbol{r}') - \left(\frac{\partial}{\partial n'}\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}')\right)\boldsymbol{E}(\boldsymbol{r}') + (\boldsymbol{E}(\boldsymbol{r}')\cdot\boldsymbol{n}')\,\mathrm{div}\,\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}') - \left(\mathrm{div}\,\boldsymbol{E}(\boldsymbol{r}')\right)\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}'\right\}\mathrm{d}S'\,, \tag{15}$$

where S is the crystal surface, $\boldsymbol{n}'$ the unit vector normal to the crystal surface toward the outer direction, $\mathrm{div}\,\boldsymbol{G}$ a column vector with the i-th component (i = 1, 2, 3) being the divergence of the i-th row vector of $\boldsymbol{G}$.

The Green's function, as seen from the definition equation (14), satisfies exactly the same equation (1) as the crystal wave field does in all points except the point $\boldsymbol{r}=\boldsymbol{r}'$. As seen from eq. (15), if the amplitudes of the crystal waves are slowly varying, the Green's function itself should be represented as a sum of slowly varying modulated waves given by

$$\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}') = \sum_{g,g'}\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}')\;,\qquad \boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}') = \boldsymbol{\psi}_{gg'}(\boldsymbol{r},\boldsymbol{r}')\exp\{i\boldsymbol{k}_g\cdot\boldsymbol{r} - i\,\boldsymbol{k}_{g'}\cdot\boldsymbol{r}'\}\;, \tag{16}$$

where $\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}')$ is the $(\boldsymbol{g},\boldsymbol{g}')$-th diffracted wave component with the slowly varying amplitude $\boldsymbol{\psi}_{gg'}(\boldsymbol{r},\boldsymbol{r}')$, both of which are 3×3 matrix tensors. $\boldsymbol{\psi}_{gg'}(\boldsymbol{r},\boldsymbol{r}')$ should be assumed to be slowly varying for each of the main and vice variables, $\boldsymbol{r}$ and $\boldsymbol{r}'$, in the same meaning as for the crystal waves, because the reciprocal relationship $\boldsymbol{G}(\boldsymbol{r}',\boldsymbol{r}) = \boldsymbol{G}^T(\boldsymbol{r},\boldsymbol{r}')$ holds.

On this assumption, equation (14) gives the fundamental equations to determine the component waves of the Green's function[6],

$$(-\mathrm{rot}\,\mathrm{rot} + k^2)\,\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}') + k^2\sum_{g''}\chi_{g-g''}\exp\{i(\boldsymbol{g}-\boldsymbol{g}'')\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{G}_{g''g'}(\boldsymbol{r},\boldsymbol{r}') = -\Delta_{gg'}(\boldsymbol{r},\boldsymbol{r}')\;, \tag{17}$$

where

$$\Delta_{gg'}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu,\nu=1}^{3} \iint_{V_c^*} \delta_{\mu\nu}\, \delta_{gg'} \delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}') \exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r} - i\,\boldsymbol{K}'_{g'}\boldsymbol{r}'\} |e_g^{\mu}(\boldsymbol{\kappa})\rangle\langle e_{g'}^{\nu}(\boldsymbol{\kappa}')|\, \mathrm{d}\boldsymbol{\kappa}\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3}\ . \tag{18}$$

If the Green's function is divided into the transverse component $\boldsymbol{G}^{(t)}$ and the longitudinal wave component $\boldsymbol{G}^{(l)}$ given by

$$\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}') = \boldsymbol{G}_{gg'}^{(t)}(\boldsymbol{r},\boldsymbol{r}') + \boldsymbol{G}_{gg'}^{(l)}(\boldsymbol{r},\boldsymbol{r}')\ , \qquad \mathrm{div}_r\, \boldsymbol{G}_{gg'}^{(t)} = 0\ , \quad \mathrm{rot}_r\, \boldsymbol{G}_{gg'}^{(l)} = 0\ , \tag{19}$$

and the longitudinal waves of $\boldsymbol{G}$ is neglected in the left second term in eq. (17), then equation (17) becomes

$$\boldsymbol{\nabla}^2 \boldsymbol{G}_{gg'}^{(t)}(\boldsymbol{r},\boldsymbol{r}') + k^2 \boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}') + k^2 \sum_{g"} \chi_{g-g"} \exp\{i(\boldsymbol{g}-\boldsymbol{g}")\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\} \boldsymbol{G}_{g"g'}^{(t)}(\boldsymbol{r},\boldsymbol{r}') = -\Delta_{gg'}(\boldsymbol{r},\boldsymbol{r}')\ . \tag{20}$$

This equation is transformed to that for the Fourier coefficients of the Green's function. When the Fourier expansions of the wave components $\boldsymbol{G}_{gg'}$ and $\boldsymbol{G}_{gg'}^{(t)}$ are given by

$$\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu,\nu=1}^{3} \iint_{V_c^*} G_{gg'}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\ \exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r} - i\,\boldsymbol{K}'_{g'}\cdot\boldsymbol{r}'\} |e_g^{\mu}(\boldsymbol{\kappa})\rangle\langle e_{g'}^{\nu}(\boldsymbol{\kappa}')| \frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3}\ , \tag{21}$$

and

$$\boldsymbol{G}_{gg'}^{(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{2}\sum_{\nu=1}^{3} \iint_{V_c^*} G_{gg'}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\ \exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r} - i\,\boldsymbol{K}'_{g'}\cdot\boldsymbol{r}'\} |e_g^{\mu}(\boldsymbol{\kappa})\rangle\langle e_{g'}^{\nu}(\boldsymbol{\kappa}')| \frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3}\ , \tag{22}$$

with $\boldsymbol{K}_g = \boldsymbol{k}_g + \boldsymbol{\kappa},\ \boldsymbol{K}'_{g'} = \boldsymbol{k}_{g'} + \boldsymbol{\kappa}'$, then using eqs. (6) and (18) equation (20) gives

$$\begin{aligned}&\{k^2(1+\chi_0) - \boldsymbol{K}_g^2\} G_{gg'}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}') + k^2 \sum_{g"\neq g}\sum_{\mu'=1}^{2} \int_{|\boldsymbol{\kappa}"|<\kappa_0} C_{gg"}^{\mu\mu'}(\boldsymbol{\kappa},\boldsymbol{\kappa}")\chi_{g-g"}(\boldsymbol{\kappa}")\ G_{g"g'}^{\mu'\nu}(\boldsymbol{\kappa}-\boldsymbol{\kappa}",\boldsymbol{\kappa}')\frac{\mathrm{d}\boldsymbol{\kappa}"}{(2\pi)^3} \\ &\quad = -(2\pi)^3 \delta_{gg'}\delta_{\mu\nu}\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\ ,\quad \mu = 1,2\ ,\quad \nu = 1,2,3\ .\end{aligned} \tag{23}$$

All of the Fourier coefficients of the component waves of the Green's function to be determined by eq. (23) give enough information to calculate $\boldsymbol{G}_{gg'}^{(t)}$. Similarly, the remained coefficients of $\mu = 3$ and $\nu = 1,2,3$ are the longitudinal components and negligible as indicated in the previous paper[6].

As mentioned in section 2, the longitudinal component waves are negligible. Ishida[6] showed that on the assumption of slow varying equation (15) is reduced to

$$\boldsymbol{E}_g(\boldsymbol{r}) = \sum_{g'}\int_S \left\{\boldsymbol{G}_{gg'}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')\frac{\partial \boldsymbol{E}_{g'}^{(e)}(\boldsymbol{r}')}{\partial n'} - \frac{\partial \boldsymbol{G}_{gg'}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')}{\partial n'}\boldsymbol{E}_{g'}^{(e)}(\boldsymbol{r}')\right\} dS'\ , \tag{24}$$

where $\boldsymbol{E}^{(e)}(\boldsymbol{r})$ is a wave in vacuum, consisting of the incident wave and diffracted waves with the amplitudes being slowly varying given by

$$\boldsymbol{E}^{(e)}(\boldsymbol{r}) = \sum_{g} \boldsymbol{E}_g^{(e)}(\boldsymbol{r})\ , \quad \boldsymbol{E}_g^{(e)}(\boldsymbol{r}) = \boldsymbol{\Phi}_g^{(e)}(\boldsymbol{r})\exp\{i\boldsymbol{k}_g\cdot\boldsymbol{r}\}\ , \quad \mathrm{div}\boldsymbol{E}_g^{(e)}(\boldsymbol{r}) = 0\ . \tag{25}$$

The vacuum waves are connected to the crystal waves by the boundary conditions given by the continuity of the wave function itself and its derivative normal to the crystal surface. $\boldsymbol{G}_{gg'}^{F(t)}$ is referred as "Forward propagation Green's function"[6], which is defined, using the pure transverse part of the Fourier coefficients of the amplitude function of $\boldsymbol{G}_{gg'}(\boldsymbol{r},\boldsymbol{r}')$,

$$\boldsymbol{G}_{gg'}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu,\nu=1}^{2} \iint_{V_c^*(\eta_{gg'}>0)} G_{gg'}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\exp\{i\boldsymbol{K}_g\cdot\boldsymbol{r} - i\,\boldsymbol{K}'_{g'}\cdot\boldsymbol{r}'\} |e_g^{\mu}(\boldsymbol{\kappa})\rangle\langle e_{g'}^{\nu}(\boldsymbol{\kappa}')| \frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3}\ , \tag{26}$$

where $\eta_{gg'} > 0$ means

$$\eta_{gg'} = (\boldsymbol{K}_g + \boldsymbol{K}'_{g'}) \cdot (\boldsymbol{r} - \boldsymbol{r}') > 0 \ , \tag{27}$$

which limits the integral volume of V_c^*. The use of equation (26) is much more useful, which enables us to express directly the crystal waves in the Laue case and in the cases where all strong diffracted waves emerges from the back surface of the crystal. In such cases, the integral over the back crystal surface can be neglected [6] and the boundary conditions

$$\boldsymbol{E}_0 = \boldsymbol{E}_0^{(e)} , \ \frac{\partial \boldsymbol{E}_0}{\partial n} = \frac{\partial \boldsymbol{E}_0^{(e)}}{\partial n} \ , \ \boldsymbol{E}_g = \boldsymbol{E}_g^{(e)} = \frac{\partial \boldsymbol{E}_g}{\partial n} = \frac{\partial \boldsymbol{E}_g^{(e)}}{\partial n} = 0 \ , \ \boldsymbol{g} \neq \boldsymbol{0} \ , \tag{28}$$

on the entrance surface of the crystal are given . Then, equation (24) becomes

$$\boldsymbol{E}_g(\boldsymbol{r}) = \int_{\Gamma_1} \left\{ \boldsymbol{G}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') \frac{\partial \boldsymbol{E}_0^{(e)}(\boldsymbol{r}')}{\partial n'} - \frac{\partial \boldsymbol{G}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')}{\partial n'} \boldsymbol{E}_0^{(e)}(\boldsymbol{r}') \right\} dS' \ , \tag{29}$$

where Γ_1 is the entrance surface of the crystal. [6] This means that the crystal waves are given directly by the integrals of the incident wave with the kernel of the Green's function over the entrance surface.

4. Two-Wave Approximation for the Laue case

In the case of two strong waves, that is, in the case where the transmitted and only one diffracted waves have appreciable amplitudes, the fundamental equations are given from eq. (7) by

$$\left.\begin{aligned} &\{-\mathrm{rot\ rot} + k^2(1+\chi_0)\}\boldsymbol{E}_0(\boldsymbol{r}) + k^2\chi_{-h}\exp\{-i\boldsymbol{h}\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{E}_h(\boldsymbol{r}) = 0 \ , \\ &\{-\mathrm{rot\ rot} + k^2(1+\chi_0)\}\boldsymbol{E}_h(\boldsymbol{r}) + k^2\chi_{h}\exp\{i\boldsymbol{h}\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{E}_0(\boldsymbol{r}) = 0 \ , \end{aligned}\right\} \tag{30}$$

or using the transverse wave approximation (9) by

$$\left.\begin{aligned} &\boldsymbol{\nabla}^2\boldsymbol{E}_0^{(t)}(\boldsymbol{r}) + k^2\boldsymbol{E}_0(\boldsymbol{r}) + k^2\chi_0\boldsymbol{E}_0^{(t)}(\boldsymbol{r}) + k^2\chi_{-h}\exp\{-i\boldsymbol{h}\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{E}_h^{(t)}(\boldsymbol{r}) = 0 \ , \\ &\boldsymbol{\nabla}^2\boldsymbol{E}_h^{(t)}(\boldsymbol{r}) + k^2\boldsymbol{E}_h(\boldsymbol{r}) + k^2\chi_0\boldsymbol{E}_h^{(t)}(\boldsymbol{r}) + k^2\chi_{h}\exp\{i\boldsymbol{h}\cdot(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))\}\boldsymbol{E}_0^{(t)}(\boldsymbol{r}) = 0 \ , \end{aligned}\right\} \tag{31}$$

where $\boldsymbol{E}_0$ and $\boldsymbol{E}_h$ are the transmitted ant diffracted waves, respectively. When expressing with the Fourier coefficients of the waves, the fundamental equations (13) become

$$\left.\begin{aligned} &\{k^2(1+\chi_0) - \boldsymbol{K}_0{}^2\}E_0^{\mu}(\boldsymbol{\kappa}) + k^2\sum_{\nu=1,2}\int_{|\boldsymbol{\kappa}'|<\boldsymbol{\kappa}_0} C_{0h}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\chi_{-h}(\boldsymbol{\kappa}')E_h^{\nu}(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\frac{d\boldsymbol{\kappa}'}{(2\pi)^3} = 0 \ , \\ &\{k^2(1+\chi_0) - \boldsymbol{K}_h{}^2\}E_h^{\mu}(\boldsymbol{\kappa}) + k^2\sum_{\nu=1,2}\int_{|\boldsymbol{\kappa}'|<\boldsymbol{\kappa}_0} C_{h0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\chi_{h}(\boldsymbol{\kappa}')E_0^{\nu}(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\frac{d\boldsymbol{\kappa}'}{(2\pi)^3} = 0 \ . \end{aligned}\right\} \tag{32}$$

To get the solution of the equations, eq. (29) is available, because the boundary conditions may be given by eq. (28), *i.e.*,

$$\boldsymbol{E}_0(\boldsymbol{r}) = \int_{\Gamma_1} \left\{ \boldsymbol{G}_{00}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') \frac{\partial \boldsymbol{E}_0^{(e)}(\boldsymbol{r}')}{\partial n'} - \frac{\partial \boldsymbol{G}_{00}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')}{\partial n'} \boldsymbol{E}_0^{(e)}(\boldsymbol{r}') \right\} dS' \ , \tag{33}$$

and

$$\boldsymbol{E}_h(\boldsymbol{r}) = \int_{\Gamma_1} \left\{ \boldsymbol{G}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') \frac{\partial \boldsymbol{E}_0^{(e)}(\boldsymbol{r}')}{\partial n'} - \frac{\partial \boldsymbol{G}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')}{\partial n'} \boldsymbol{E}_0^{(e)}(\boldsymbol{r}') \right\} dS' \ . \tag{34}$$

Therefore, it is enough the use of the two components of the Green's function, $\boldsymbol{G}_{00}^{F(t)}$ and $\boldsymbol{G}_{h0}^{F(t)}$ to give the solution. The Fourier coefficients of the two component are determined as derived from eq. (23) by

$$\left.\begin{aligned}
&\{k^2(1+\chi_0)-\boldsymbol{K}_0{}^2\}G_{00}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')+k^2\sum_{\mu'=1}^{2}\int_{|\boldsymbol{\kappa}"|<\boldsymbol{\kappa}_0} C_{0h}^{\mu\mu'}(\boldsymbol{\kappa},\boldsymbol{\kappa}")\chi_{-h}(\boldsymbol{\kappa}")\,G_{h0}^{\mu'\nu}(\boldsymbol{\kappa}-\boldsymbol{\kappa}",\boldsymbol{\kappa}')\frac{d\boldsymbol{\kappa}"}{(2\pi)^3}\\
&=-(2\pi)^3\delta_{\mu\nu}\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\ ,\\
&\{k^2(1+\chi_0)-\boldsymbol{K}_h{}^2\}G_{h0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')+k^2\sum_{\mu'=1}^{2}\int_{|\boldsymbol{\kappa}"|<\boldsymbol{\kappa}_0} C_{h0}^{\mu\mu'}(\boldsymbol{\kappa},\boldsymbol{\kappa}")\chi_{h}(\boldsymbol{\kappa}")\,G_{\mathbf{00}}^{\mu'\nu}(\boldsymbol{\kappa}-\boldsymbol{\kappa}",\boldsymbol{\kappa}')\frac{d\boldsymbol{\kappa}"}{(2\pi)^3}=0\ .
\end{aligned}\right\}\tag{35}$$

Equations (33) and (34) gives general expressions of the two waves for the Laue case, where the incident wave with any waveform may be available as long as the assumption of slow varying is kept. If the modulated amplitude functions as defined in eqs. (3), (16) and (25) are used, then equations (33) and (34) may be rewritten as

$$\boldsymbol{\varphi}_g(\boldsymbol{r})=\int_{\Gamma_1}\left\{\boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')\frac{\partial\boldsymbol{\Phi}_0^{(e)}(\boldsymbol{r}')}{\partial n'}-\frac{\partial\boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')}{\partial n'}\boldsymbol{\Phi}_0^{(e)}(\boldsymbol{r}')-2ik_{0z}\boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{\Phi}_0^{(e)}(\boldsymbol{r}')\right\}dS'\ ,\tag{36}$$

Here, $\boldsymbol{g}=\mathbf{0},\boldsymbol{h}$, k_{0z} is the component of the wave vector $\boldsymbol{k}_0$ of the incident wave normal to the crystal surface toward the inner direction, and $\boldsymbol{\psi}_{g0}^{F(t)}$ is the amplitude function of $\boldsymbol{G}_{g0}^{F(t)}$, using eqs. (16) and (26), expressed by

$$\boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')=\sum_{\mu,\nu=1}^{2}\iint_{V_c^*(\eta_{g0}>0)} G_{g0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\exp\{i\boldsymbol{\kappa}\cdot\boldsymbol{r}-i\,\boldsymbol{\kappa}'\cdot\boldsymbol{r}'\}|e_g^{\mu}(\boldsymbol{\kappa})\rangle\langle e_0^{\nu}(\boldsymbol{\kappa}')|\frac{\mathrm{d}\boldsymbol{\kappa}}{(2\pi)^3}\frac{\mathrm{d}\boldsymbol{\kappa}'}{(2\pi)^3}\ .\tag{37}$$

If the variations of the amplitudes $\boldsymbol{\Phi}_0^{(e)}$ and $\boldsymbol{\psi}_{g0}^{F(t)}$ are negligibly small compared with k_{0z} so that the first and second terms may be omitted and only the third term is retained in the integral in eq. (36), then

$$\boldsymbol{\varphi}_g(\boldsymbol{r})=\ -2i\int_{\Gamma_1}k_{0z}\boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{\Phi}_0^{(e)}(\boldsymbol{r}')dS',\quad \boldsymbol{g}=\mathbf{0},\boldsymbol{h}\ .\tag{38}$$

This equation leads to the result given by another theory, as discussed in section 6.

5. Perfect Crystal

In the case of a perfect crystal, *i.e.*, in the case where a crystal is undistorted so that the lattice displacement vector $\boldsymbol{u}(\boldsymbol{r})$ equals to 0, the Fourier component of the crystal polarizability $\chi_g(\boldsymbol{\kappa})$ equals to$(2\pi)^3\chi_g\delta(\boldsymbol{\kappa})$. Here, the polarization vectors $\boldsymbol{e}_0^1(\boldsymbol{\kappa})$ and $\boldsymbol{e}_h^1(\boldsymbol{\kappa})$ are chosen as σ-polarization, and $\boldsymbol{e}_0^2(\boldsymbol{\kappa})$ and $\boldsymbol{e}_h^2(\boldsymbol{\kappa})$ to π-polarization. Then, $C_{h0}^{11}(\boldsymbol{\kappa},0)=C_{0h}^{11}(\boldsymbol{\kappa},0)=1$, $C_{h0}^{22}(\boldsymbol{\kappa},0)=C_{0h}^{22}(\boldsymbol{\kappa},0)=\cos 2\theta_h(\boldsymbol{\kappa})$ with $2\theta_h(\boldsymbol{\kappa})$ being the angle between the directions of $\boldsymbol{K}_0$ and $\boldsymbol{K}_h$, and $C_{h0}^{12}(\boldsymbol{\kappa},0)=C_{0h}^{12}(\boldsymbol{\kappa},0)=C_{h0}^{21}(\boldsymbol{\kappa},0)=C_{0h}^{21}(\boldsymbol{\kappa},0)=0$ so that equations (32) are reduced to the well-known determination equation for the transmitted and diffracted waves [(8) (9)].

$$\left.\begin{aligned}
&\{k^2(1+\chi_0)-\boldsymbol{K}_0{}^2\}E_0^{\mu}(\boldsymbol{\kappa})+k^2C_\mu\,\chi_{-h}E_h^{\mu}(\boldsymbol{\kappa})\ =0\ ,\\
&\{k^2(1+\chi_0)-\boldsymbol{K}_h{}^2\}E_h^{\mu}(\boldsymbol{\kappa})+k^2\,C_\mu\chi_{\boldsymbol{h}}E_0^{\mu}(\boldsymbol{\kappa})\ =0\ ,
\end{aligned}\right\}\quad \mu=1,2\ ,\tag{39}$$

where C_μ is the polarization factor given by $C_1=1$ for σ-polarization and $C_2=\cos 2\theta_h(\boldsymbol{\kappa})$ for π-polarization. Similarly, for the Green's function equations (35) become

$$\left.\begin{aligned}
&\{k^2(1+\chi_0)-\boldsymbol{K}_0{}^2\}G_{00}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')+k^2C_\mu\,\chi_{-h}G_{h0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\ =-(2\pi)^3\delta_{\mu\nu}\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\ ,\\
&\{k^2(1+\chi_0)-\boldsymbol{K}_h{}^2\}G_{h0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')+k^2\,C_\mu\chi_hG_{00}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\ =0\ ,
\end{aligned}\right\}\quad \mu,\nu=1,2\ .\tag{40}$$

Equation (40) is a set of linear equations with unknown G_{00} and G_{h0}, and the solution may be given by

$$G_{g0}^{\mu\nu}(\boldsymbol{\kappa},\boldsymbol{\kappa}') = (2\pi)^3\delta_{\mu\nu}\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')G_{g0}^{\mu}(\boldsymbol{\kappa}) \ , \quad \boldsymbol{g} = \boldsymbol{0},\boldsymbol{h} \ . \tag{41}$$

Here, using $\boldsymbol{K} = \boldsymbol{k_0} + \boldsymbol{\kappa} = \boldsymbol{K_0}$,

$$G_{00}^{\mu}(\boldsymbol{\kappa}) = -\{k^2(1+\chi_0) - \boldsymbol{K}_h{}^2\}/D(\boldsymbol{K}) \equiv G_{00}^{\mu}(\boldsymbol{K}) \ , \tag{42}$$

$$G_{h0}^{\mu}(\boldsymbol{\kappa}) = k^2 C_\mu \chi_h/D(\boldsymbol{K}) \equiv G_{h0}^{\mu}(\boldsymbol{K}) \ , \tag{43}$$

with $D(\boldsymbol{K})$ being

$$D(\boldsymbol{K}) = \{k^2(1+\chi_0) - \boldsymbol{K}^2\}\{k^2(1+\chi_0) - \boldsymbol{K}_h{}^2\} - k^4 C_\mu^2\,\chi_{\boldsymbol{h}}\,\chi_{-\boldsymbol{h}}\,. \tag{44}$$

By substituting eqs. (41), (42) and (43) into eq. (26) and integrating it, $\boldsymbol{G}_{00}^{F(t)}$ and $\boldsymbol{G}_{h0}^{F(t)}$ can be obtained analytically. Here, we introduce an approximation to extend the integral range of eq. (26) from the reciprocal unit cell space to infinite space. Such approximation has no negative effect on the integrals (33) and (34), because the incident wave amplitudes are slowing varying within the present assumption given by eq. (4) and, therefore, the integrals are significant only around the region satisfying the condition (4). In addition, as seen from eqs. (42) and (43), since $G_{00}(\boldsymbol{\kappa})$ and $G_{h0}(\boldsymbol{\kappa})$ are the functions of $\boldsymbol{K}(= \boldsymbol{K}_0 = \boldsymbol{k}_0 + \boldsymbol{\kappa})$, let the integral variables change from $\boldsymbol{\kappa}$ to $\boldsymbol{K}$ and let $G_{00}(\boldsymbol{K})$ and $G_{h0}(\boldsymbol{K})$ be used instead of $G_{00}(\boldsymbol{\kappa})$ and $G_{h0}(\boldsymbol{\kappa})$. Then, equation (26) may be approximated by

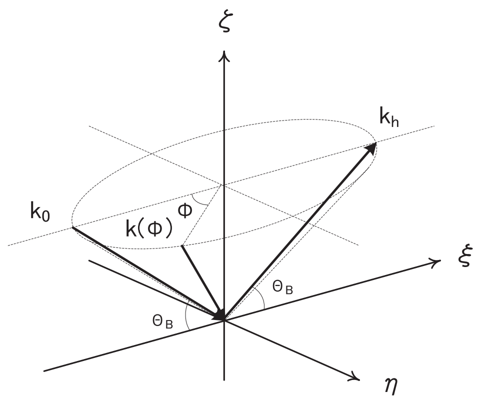

Fig. 1 $\xi\eta\zeta$-coordinate system.

$$\boldsymbol{G}_{g0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{2}\int_{\eta_g>0} G_{g0}^{\mu}(\boldsymbol{K})\exp\{i\boldsymbol{K}\cdot(\boldsymbol{r}-\boldsymbol{r}') + i\,\boldsymbol{g}\cdot\boldsymbol{r}\}|e_g^{\mu}(\boldsymbol{K})\rangle\langle e_0^{\mu}(\boldsymbol{K})|\frac{\mathrm{d}\boldsymbol{K}}{(2\pi)^3} \ , \qquad \boldsymbol{g} = \boldsymbol{0},\boldsymbol{h} \ , \tag{45}$$

where the integral is over the total space constrained by a condition $\eta_g = (2\boldsymbol{K}+\boldsymbol{g})\cdot(\boldsymbol{r}-\boldsymbol{r}') > 0$. The notation of the polarization vector is changed from $\boldsymbol{e}^{\mu}(\boldsymbol{\kappa})$ to $\boldsymbol{e}^{\mu}(\boldsymbol{K})$. For convenience, when integrating eq. (45), $G_{00}(\boldsymbol{K})$ is divided by modifying eq. (42) into two terms in order to calculate them separately, as follows:

$$G_{00}^{\mu}(\boldsymbol{K}) = \frac{1}{\boldsymbol{K}^2 - k^2(1+\chi_0)} + \frac{1}{\boldsymbol{K}^2 - k^2(1+\chi_0)}\cdot\frac{k^4 C_\mu^2\,\chi_{\boldsymbol{h}}\,\chi_{-\boldsymbol{h}}}{D(\boldsymbol{K})} \ . \tag{46}$$

When substituting eqs. (46) and (43) to eq. (45) and integrating eq. (45) , the result becomes as follows (see Appendix A):

$$\boldsymbol{G}_{00}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = G_0(\boldsymbol{r}-\boldsymbol{r}')\mathbf{I}^{(3)} + \sum_{\mu=1}^{2} e^{-i\frac{\pi}{4}}\sqrt{\frac{k\cos\theta_B}{2\pi\rho(\boldsymbol{r}-\boldsymbol{r}')}}W_{00}^{\mu}\big(s_0(\boldsymbol{r}-\boldsymbol{r}'),s_h(\boldsymbol{r}-\boldsymbol{r}')\big)\exp\{ik\cos\theta_B \times\rho(\boldsymbol{r}-\boldsymbol{r}') - ik\sin\theta_B\,(\zeta-\zeta')\}\,|e_0^{\mu}(\boldsymbol{k}(\phi))\rangle\langle e_0^{\mu}(\boldsymbol{k}(\phi))| \ , \tag{47}$$

and

$$\boldsymbol{G}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{2} e^{-i\frac{\pi}{4}}\sqrt{\frac{k\cos\theta_B}{2\pi\rho(\boldsymbol{r}-\boldsymbol{r}')}}W_{h0}^{\mu}\big(s_0(\boldsymbol{r}-\boldsymbol{r}'),s_h(\boldsymbol{r}-\boldsymbol{r}')\big)\exp\{ik\cos\theta_B\cdot\rho(\boldsymbol{r}-\boldsymbol{r}') - ik\sin\theta_B\,(\zeta-\zeta') + i\,\boldsymbol{h}\cdot\boldsymbol{r}\}\,|e_h^{\mu}(\boldsymbol{k}(\phi_0))\rangle\langle e_0^{\mu}(\boldsymbol{k}(\phi_0))| \ , \tag{48}$$

where

$$G_0(\boldsymbol{r}-\boldsymbol{r}') = \frac{e^{ik(1+\chi_0)^{1/2}|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \quad . \tag{49}$$

The 3×3 unit matrix tensor $\mathbf{I}^{(3)}$ has the property of $\mathbf{I}^{(3)} = \sum_{i=1}^{3}|e_0^i(\boldsymbol{K})\rangle\langle e_0^i(\boldsymbol{K})|$ for any wave vector $\boldsymbol{K}$. And,

$$W_{00}^{\mu}(s_0,s_h) = -i\frac{C(\chi_h\chi_{-h})^{\frac{1}{2}}}{4\sin 2\theta_B}\sqrt{\frac{s_0}{s_h}}J_1\left(\beta\sqrt{s_0 s_h}\right)\cdot e^{\frac{ik\chi_0(s_0+s_h)}{2}} , \qquad s_0>0,\ s_h>0 , \tag{50}$$

$$W_{h0}^{\mu}(s_0,s_h) = -\frac{C\chi_h}{4\sin 2\theta_B}J_0\left(\beta\sqrt{s_0 s_h}\right)\cdot e^{\frac{ik\chi_0(s_0+s_h)}{2}} , \qquad s_0>0,\ s_h>0 . \tag{51}$$

Here, J_0 and J_1 are the Bessel functions of 0-th and 1-st order, respectively, and $\beta = kC(\chi_h\chi_{-h})^{\frac{1}{2}}$. If $s_0<0$ or $s_h<0$, then $W_{00}^{\mu}(s_0,s_h) = W_{h0}^{\mu}(s_0,s_h) = 0$. Furthermore, θ_B is the Bragg angle given by $2d\sin\theta_B = \lambda$, C the polarization factor given by $C = 1, \cos 2\theta_B$ $(\mu = 1,2)$. As shown in Fig.1, when we use an orthogonal coordinate system (ξ,η,ζ) where ζ- axis is taken along the reciprocal lattice vector $\boldsymbol{h}$, and $\xi-\zeta$ plane is a plane made by $\boldsymbol{k}_0$ and $\boldsymbol{k}_h$, the coordinates of points $\boldsymbol{r}$ and $\boldsymbol{r}'$ are expressed as $\boldsymbol{r} = (\xi,\eta,\zeta)$ and $\boldsymbol{r}' = (\xi',\eta',\zeta')$. Then, the factor $\rho(\boldsymbol{r}-\boldsymbol{r}')$ in eqs. (47) and (48) is given by

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \sqrt{(\xi-\xi')^2+(\eta-\eta')^2} , \tag{52}$$

and $s_0(\boldsymbol{r})$ and $s_h(\boldsymbol{r})$ is given by

$$s_0(\boldsymbol{r}) = \frac{\rho(\boldsymbol{r})}{2\cos\theta_B} - \frac{\zeta}{2\sin\theta_B} , \quad s_h(\boldsymbol{r}) = \frac{\rho(\boldsymbol{r})}{2\cos\theta_B} + \frac{\zeta}{2\sin\theta_B} . \tag{53}$$

Also, $\boldsymbol{k}(\phi_0)$ is defined, in the $\xi\eta\zeta$ coordinate system, using the following vector

$$\boldsymbol{k}(\phi) = (k\cos\theta_B\cos\phi, k\cos\theta_B\sin\phi, -k\sin\theta_B) , \tag{54}$$

where ϕ_0 is given, using the coordinates of $\boldsymbol{r}-\boldsymbol{r}'$, by $\tan\phi_0 = (\eta-\eta')/(\xi-\xi')$.

By substituting eqs. (47) and (48) into eqs. (33) and (34), the two crystal waves are expressed analytically. When the expressions of the wave amplitudes are desired, equation (36) is available. In this case, let the wave vector $\boldsymbol{k}_0$ referred in eq. (3) to be

$$\boldsymbol{k}_0 = \boldsymbol{k}(\phi=0) = (k\cos\theta_B, 0, -k\sin\theta_B) , \tag{55}$$

as shown in Fig.1. Then, the amplitude functions $\boldsymbol{\psi}_{00}^{F(t)}$ and $\boldsymbol{\psi}_{h0}^{F(t)}$ are given using eqs. (47) , (48) and (16) by

$$\begin{aligned}\boldsymbol{\psi}_{00}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = G_0(\boldsymbol{r}-\boldsymbol{r}')e^{-i\boldsymbol{k}_0\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathbf{I}^{(3)} + \sum_{\mu=1}^{2} e^{-i\frac{\pi}{4}}\sqrt{\frac{k\cos\theta_B}{2\pi\rho(\boldsymbol{r}-\boldsymbol{r}')}}W_{00}^{\mu}\big(s_0(\boldsymbol{r}-\boldsymbol{r}'), s_h(\boldsymbol{r}\\ -\boldsymbol{r}')\big)\exp\{ik\cos\theta_B\cdot(\rho(\boldsymbol{r}-\boldsymbol{r}')-(\xi-\xi'))\}\,|e_0^{\mu}(\boldsymbol{k}(\phi))\rangle\langle e_0^{\mu}(\boldsymbol{k}(\phi))| ,\end{aligned} \tag{56}$$

$$\begin{aligned}\boldsymbol{\psi}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{2} e^{-i\frac{\pi}{4}}\sqrt{\frac{k\cos\theta_B}{2\pi\rho(\boldsymbol{r}-\boldsymbol{r}')}}W_{h0}^{\mu}\big(s_0(\boldsymbol{r}-\boldsymbol{r}'), s_h(\boldsymbol{r}-\boldsymbol{r}')\big)\exp\{ik\cos\theta_B\\ \times(\rho(\boldsymbol{r}-\boldsymbol{r}')-(\xi-\xi'))\}\,|e_h^{\mu}(\boldsymbol{k}(\phi))\rangle\langle e_0^{\mu}(\boldsymbol{k}(\phi))| .\end{aligned} \tag{57}$$

Substituting eqs. (56) and (57) into eq. (36), the waves are obtained analytically in the case of a perfect crystal.

6. Comparison With Other Theory

To investigate the validity for the result given in the former section, we compare the present results with those given by Takagi's theory. Let us assume that the incident wave amplitude $\boldsymbol{\Phi}_0^{(e)}$ is much smaller compared with the wave vector. Then, the crystal waves may be calculated by eq. (38). The crystal surface is assumed to be flat so that k_{0z} is constant. If the distribution of $\boldsymbol{\Phi}_0^{(e)}$ is homogeneous toward the η-direction perpendicular to the incident plane made by $\boldsymbol{k}_0$ and $\boldsymbol{k}_h$ as shown in Fig.2, instead of $\boldsymbol{\psi}_{00}^{F(t)}$ and $\boldsymbol{\psi}_{h0}^{F(t)}$ the next functions given by

$$\boldsymbol{v}_{g0}^{F(t)}(\boldsymbol{\xi},\boldsymbol{\xi}') = \int_{\Gamma_\eta} \boldsymbol{\psi}_{g0}^{F(t)}(\boldsymbol{\xi},\boldsymbol{r}')d\eta' , \quad \boldsymbol{g} = \boldsymbol{0},\boldsymbol{h} , \tag{58}$$

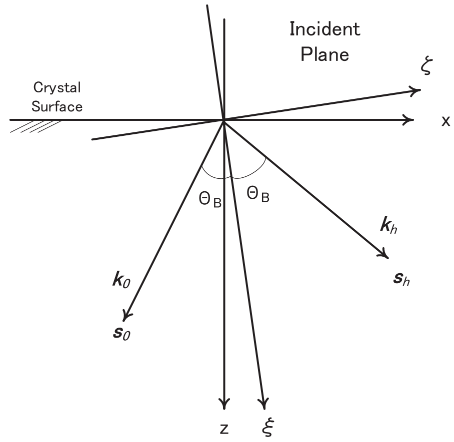

Fig. 2 The relation between the rectangular ξ-ζ, x-z coordinate systems and oblique s_o-s_h coordinate system.

may be used, and then eq. (38) becomes

$$\boldsymbol{\varphi}_g(\boldsymbol{\xi}) = -2i \int_{\Gamma_x} k_{0z}\boldsymbol{v}_{g0}^{F(t)}(\boldsymbol{\xi},x')\boldsymbol{\Phi}_0^{(e)}(x')dx' , \tag{59}$$

where $\boldsymbol{\xi}$ and $\boldsymbol{\xi}'$ are points in $\xi-\zeta$ plane represented as $\boldsymbol{\xi} = (\xi,\zeta)$ and $\boldsymbol{\xi}' = (\xi',\zeta')$, and $\boldsymbol{r}' = (\xi',\eta',\zeta')$. Γ_x and Γ_η show the integral ranges for x and η, respectively.

If we suppose that the crystal surface is infinitely extended to η-direction, then the integrals (58) become

$$\boldsymbol{v}_{00}^{F(t)}(\boldsymbol{\xi},\boldsymbol{\xi}') = \frac{i\delta\big(s_h(\boldsymbol{\xi}-\boldsymbol{\xi}')\big)}{2k\sin 2\theta_B} e^{ik\chi_0 s_0(\boldsymbol{\xi}-\boldsymbol{\xi}')/2}\cdot \mathbf{I}^{(3)} + \sum_{\mu=1}^{2} W_{00}^{\mu}\big(s_0(\boldsymbol{\xi}-\boldsymbol{\xi}'),s_h(\boldsymbol{\xi}-\boldsymbol{\xi}')\big)\,|e_0^{\mu}(\boldsymbol{k}_0)\rangle\langle e_0^{\mu}(\boldsymbol{k}_0)| , \tag{60}$$

$$\boldsymbol{v}_{h0}^{F(t)}(\boldsymbol{\xi},\boldsymbol{\xi}') = \sum_{\mu=1}^{2} W_{h0}^{\mu}\big(s_0(\boldsymbol{\xi}-\boldsymbol{\xi}'),s_h(\boldsymbol{\xi}-\boldsymbol{\xi}')\big)\,|e_h^{\mu}(\boldsymbol{k}_0)\rangle\langle e_0^{\mu}(\boldsymbol{k}_0)| , \tag{61}$$

using eqs. (56) and (57), where

$$s_0(\boldsymbol{\xi}) = \frac{\xi}{2\cos\theta_B} - \frac{\zeta}{2\sin\theta_B} , \quad s_h(\boldsymbol{\xi}) = \frac{\xi}{2\cos\theta_B} + \frac{\zeta}{2\sin\theta_B} . \tag{62}$$

The first term on the right-hand side of eq. (60) can be obtained, using the Fourier expansion of the function G_0 where the Fourier coefficient $1/\{\boldsymbol{K}^2 - k^2(1+\chi_0)\}$ is approximated by $1/(2\boldsymbol{k}_0\cdot\boldsymbol{\delta k} - k^2\chi_0)$ with $\boldsymbol{\delta k} = \boldsymbol{K} - \boldsymbol{k}_0$ in the first order around $\boldsymbol{K} = \boldsymbol{k}_0$. The second term on the right-hand side of eq. (60) and the right-hand side of eq. (61) can be obtained by integrating with the saddle point method, substituting the second term on the right-hand side of eq. (56) and the right-hand side of eq. (57) into eq. (58).

According to eq. (59), when the incident wave is singly polarized and its amplitude width is very narrow, namely,

$$\boldsymbol{\Phi}_0^{(e)}(x) = \delta(x)\,|e_0^{\mu_0}(\boldsymbol{k}_0)\rangle , \tag{63}$$

then the crystal waves are expressed as

$$\boldsymbol{\varphi}_g(\boldsymbol{\xi}) = -2ik_{0z}\boldsymbol{v}_{g0}^{F(t)}(\boldsymbol{\xi},0)\,|e_0^{\mu_0}(\boldsymbol{k}_0)\rangle , \quad \boldsymbol{g} = \boldsymbol{0},\boldsymbol{h} . \tag{64}$$

Alternatively, using eqs. (50), (51), (60), (61) and (64), they are expressed by

$$\boldsymbol{\varphi}_0(s_0, s_h) = \left\{ \frac{\gamma_0}{\sin 2\theta_B} \delta(s_h) e^{ik\chi_0 s_0/2} - \frac{kC(\chi_h \chi_{-h})^{\frac{1}{2}}}{2\sin 2\theta_B} \gamma_0 \sqrt{\frac{s_0}{s_h}} J_1\left(\beta\sqrt{s_0 s_h}\right) \cdot e^{\frac{ik\chi_0(s_0+s_h)}{2}} \right\} |e_0^{\mu_0}(\boldsymbol{k}_0)\rangle \ , \tag{65}$$

$$\boldsymbol{\varphi}_h(s_0, s_h) = i \frac{kC\chi_h}{2\sin 2\theta_B} \gamma_0 J_0\left(\beta\sqrt{s_0 s_h}\right) \cdot e^{\frac{ik\chi_0(s_0+s_h)}{2}} |e_h^{\mu_0}(\boldsymbol{k}_0)\rangle \ , \tag{66}$$

where $s_0 = s_0(\boldsymbol{\xi}), s_h = s_h(\boldsymbol{\xi})$ and $\gamma_0 = k_{0z}/k$.

Thus, the obtained results are comparable with those shown by the previous theory given by Takagi [7]. The expressions of the waves given by eqs. (65) and (66) are essentially the same as the fundamental solution of Takagi's equation [10]. Therefore, it may be concluded that the present theory becomes an extension of Takagi's theory.

7. Conclusion

Many experimental studies on X-ray dynamical diffraction have been performed using experimental arrangements for the two strong wave case of the transmitted and only one diffracted wave. In that sense, it is important to show in detail what useful results are derived in the case of the two-wave approximation, when investigating the effectiveness of dynamical diffraction theory. In this paper, we took up the Laue case, which is one of the typical cases of two-wave diffraction. There, it has been shown in detail how the wave field in a crystal is represented using the Green's function, especially in a general case of arbitrary incident wave with any amplitude function. If the crystals are perfect, it has been shown that the Green's function is analytically obtained and explicitly expressed with a spherical wave and Bessel functions. In a special case of the present theory, these results are reduced to those given by Takagi's theory, and, therefore, the present theory becomes an extension of Takagi's theory. In the two-beam approximation, besides the Laue case, there is another typical case called the Bragg case. Because the boundary conditions are different between the Laue case and Bragg case, the present results are not available for the Bragg case. A detailed investigation for the Bragg case will be reported in another paper [11].

Appendix

A. Derivation of eqs. (47) and (48)

At first, we will show the deviation of the right first term of eq. (47). When performing the Fourier integral of the first term on the right-hand side of (46) using eq. (45), the longitudinal tensor component $|e_0^3(\boldsymbol{K})\rangle\langle e_0^3(\boldsymbol{K})|$ may be added to the summation of $\sum_{\mu=1}^{2}|e_0^\mu(\boldsymbol{K})\rangle\langle e_0^\mu(\boldsymbol{K})|$ to use the relation $\sum_{\mu=1}^{3}|e_0^\mu(\boldsymbol{K})\rangle\langle e_0^\mu(\boldsymbol{K})| = \mathbf{I}^{(3)}$, because the vacuum wave is pure traverse and so the longitudinal component does not contribute at all to the integral of eq. (33). Then the integral becomes

$$\boldsymbol{G}_0(\boldsymbol{r},\boldsymbol{r}') = \int_{\boldsymbol{K}\cdot(\boldsymbol{r}-\boldsymbol{r}')>0} \frac{e^{i\boldsymbol{K}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\boldsymbol{K}^2 - k^2(1+\chi_0)} \sum_{\mu=1}^{3} |e_0^\mu(\boldsymbol{K})\rangle\langle e_0^\mu(\boldsymbol{K})| \frac{\mathrm{d}\boldsymbol{K}}{(2\pi)^3} \approx \frac{e^{ik(1+\chi_0)^{\frac{1}{2}}|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\mathbf{I}^{(3)} - \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\mathbf{I}^{(3)} \ .$$

Here, the second term on the right-hand side is neglected since it does not propagate as wave, and then the first term on the right-hand side of eq. (47) is derived.

Next, we explain about the derivation of eq. (48). According to eq. (45), $\boldsymbol{G}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}')$ may be calculated with

$$\boldsymbol{G}_{h0}^{F(t)}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\mu=1}^{2} \int_{\eta_h>0} G_{h0}^\mu(\boldsymbol{K}) \exp\{i\boldsymbol{K}\cdot(\boldsymbol{r}-\boldsymbol{r}') + i\,\boldsymbol{h}\cdot\boldsymbol{r}\} |e_h^\mu(\boldsymbol{K})\rangle\langle e_0^\mu(\boldsymbol{K})| \frac{\mathrm{d}\boldsymbol{K}}{(2\pi)^3} \ . \tag{A1}$$

In the $\xi\eta\zeta$ coordinate system, since the reciprocal lattice vector $\boldsymbol{h}$ is represented as $\boldsymbol{h} = (0, 0, 2k\sin\theta_B)$, $\boldsymbol{k}(\phi)$ defined by eq. (54) is a wave vector satisfying the Bragg's diffraction law, *i.e.*,$|\boldsymbol{k}(\phi)| = |\boldsymbol{k}(\phi)+\boldsymbol{h}| = k$. Here, let $\boldsymbol{K}$ to be $\boldsymbol{K} = \boldsymbol{k}(\phi) + \delta\boldsymbol{k}$, and $\delta\boldsymbol{k}$ to be represented as $\delta\boldsymbol{k} = (\delta k_\rho\cos\phi, \delta k_\rho\sin\phi, \delta k_\zeta)$ in the $\xi\eta\zeta$ coordinate system. Then, it is shown that $(2\boldsymbol{k}(\phi)+\boldsymbol{h})\cdot\delta\boldsymbol{k} = 2k\cos\theta_B\cdot\delta k_\rho \equiv k\tau_\rho$, and $\boldsymbol{h}\cdot\delta\boldsymbol{k} = 2k\sin\theta_B\cdot\delta k_\zeta \equiv k\tau_\zeta$. The Fourier component $G_{h0}^\mu(\boldsymbol{K})$ shown by eq. (43) has a significant value around $|\boldsymbol{K}|\sim|\boldsymbol{K}+\boldsymbol{h}|\sim k$. Around this area, $\delta\boldsymbol{k}$ may be supposed to be small amount compared with $\boldsymbol{K}$, and $C_\mu \sim C(= 1, \cos 2\theta_B$ for $\mu = 1,2)$. If we neglect higher orders of $\delta \boldsymbol{k}$, $\boldsymbol{K_0}^2 = \boldsymbol{K}^2 = k^2 + k(\tau_\rho - \tau_\zeta)$ and $\boldsymbol{K_h}^2 = k^2 + k(\tau_\rho + \tau_\zeta)$ so that equation (43) becomes

$$G^\mu_{h0}(\boldsymbol{K}) = \frac{C\chi_h}{(\tau_\rho - k\chi_0)^2 - \tau_\zeta{}^2 - \beta^2} \equiv G^\mu_{h0}(\tau_\rho, \tau_\zeta) \ , \tag{A2}$$

where $\beta = kC(\chi_h \chi_{-h})^{\frac{1}{2}}$.

On the other hand, the phase part of the integrand of the Fourier integral given by eq. (A1) is rewritten as

$$\boldsymbol{K} \cdot (\boldsymbol{r} - \boldsymbol{r}') = \boldsymbol{k}(\phi) \cdot (\boldsymbol{r} - \boldsymbol{r}') + \frac{\tau_\rho}{2\cos\theta_B}\{(\xi - \xi')\cos\phi + (\eta - \eta')\sin\phi\} + \frac{\tau_\zeta}{2\sin\theta_B}(\zeta - \zeta') \ . \tag{A3}$$

Furthermore, changing the integral variable as $\mathrm{d}\boldsymbol{K} \cong (k\cos\theta_B / 2\sin 2\theta_B) d\phi d\tau_\rho d\tau_\zeta$ and approximating $|e^\mu_h(\boldsymbol{K})\rangle\langle e^\mu_0(\boldsymbol{K})| \approx |e^\mu_h(\boldsymbol{k}(\phi))\rangle\langle e^\mu_0(\boldsymbol{k}(\phi))|$, the result of the integration of eq. (A1) becomes

$$\boldsymbol{G}^{F(t)}_{h0}(\boldsymbol{r}, \boldsymbol{r}') = \sum_{\mu=1}^{2} k\cos\theta_B \int_{\eta_h > 0} \frac{d\varphi}{2\pi} e^{ik(\varphi)\cdot(r-r') + ih\cdot r} |e^\mu_h(\boldsymbol{k}(\varphi))\rangle\langle e^\mu_0(\boldsymbol{k}(\varphi))| \, W^{(\mu)}_{h0}(s,t) \ , \tag{A4}$$

where

$$W^{(\mu)}_{h0}(s,t) = \frac{1}{2\sin 2\theta_B} \iint_{-\infty}^{\infty} G^\mu_{h0}(\tau_\rho, \tau_\zeta)\, e^{i\tau_\rho s + i\tau_\zeta t} \frac{d\tau_\rho d\tau_\zeta}{4\pi^2} \ , \tag{A5}$$

and

$$s = \frac{1}{2\cos\theta_B}\{(\xi - \xi')\cos\phi + (\eta - \eta')\sin\phi\} \ , \qquad t = \frac{1}{2\sin\theta_B}(\zeta - \zeta') \ . \tag{A6}$$

By substituting eq. (A2) into eq. (A5), the integration of eq. (A5) can exactly be performed. The result is shown by

$$W^\mu_{\boldsymbol{h0}}(s,t) = -\frac{C\chi_h}{4\sin 2\theta_B} J_0\left(\beta\sqrt{s^2 - t^2}\right) e^{ik\chi_0 s} \ , \tag{A7}$$

when $s > |t|$. If $s < |t|$, $W^{(\mu)}_{ho}(s,t) = 0$. Alternatively, introducing new variables given by

$$s_0 = s - t, \ s_h = s + t, \tag{A8}$$

equation (A7) is rewritten as the following equation , when $s_0 > 0$ and $s_h > 0$.

$$W^\mu_{\boldsymbol{h0}}(s_0, s_h) = -\frac{C\chi_h}{4\sin 2\theta_B} J_0\left(\beta\sqrt{s_0 s_h}\right) e^{\frac{ik\chi_0(s_0 + s_h)}{2}} \ . \tag{A9}$$

If $s_0 < 0$ or $s_h < 0$, $W^\mu_{h0}(s_0, s_h) = 0$. Finally, if integrate eq. (A4) with the saddle point method, equation (A4) is reduced to eq. (48). In this case, there are two saddle points $\phi = \phi_0$ and $\phi = \phi_0 + \pi$. But the latter saddle point is excluded, because the integral constraint condition, $\eta_h = (2\boldsymbol{K} + \boldsymbol{h}) \cdot (\boldsymbol{r} - \boldsymbol{r}') \approx (2\boldsymbol{k}(\phi) + \boldsymbol{h}) \cdot (\boldsymbol{r} - \boldsymbol{r}') > 0$, that is, $\cos(\phi - \phi_0) > 0$, as derived from $\boldsymbol{k}(\phi) \cdot (\boldsymbol{r} - \boldsymbol{r}') = k\cos\theta_B \cdot \rho(\boldsymbol{r} - \boldsymbol{r}') \cdot \cos(\phi - \phi_0) - k\sin\theta_B \cdot (\zeta - \zeta')$ and $\boldsymbol{h} = (0, 0, 2k\sin\theta_B)$. Similarly, the second term on the right-hand side of eq. (47) can be derived. If we refer the second term of eq. (46) as $G^{\mu(2)}_{00}(\boldsymbol{K})$, using eqs. (43) and (A2) it can be rewritten

$$G^{\mu(2)}_{00}(\boldsymbol{K}) = \frac{1}{\boldsymbol{K}^2 - k^2(1+\chi_0)} \cdot \frac{k^4 C^2_\mu \chi_{\boldsymbol{h}} \chi_{-\boldsymbol{h}}}{D(\boldsymbol{K})} = \frac{k^2 C_\mu \chi_{-\boldsymbol{h}}}{\boldsymbol{K}^2 - k^2(1+\chi_0)} G^\mu_{h0}(\boldsymbol{K}) \approx \frac{k\, C\chi_{-\boldsymbol{h}}}{(\tau_\rho - \tau_\zeta) - k\chi_0} G^\mu_{h0}(\tau_\rho, \tau_\zeta).$$

By integrating this term according to eq. (45), similar to derive from eq. (A1) to eq. (A4), the following result is derived:

$$\sum_{\mu=1}^{2}\int_{\eta_0>0} G_{00}^{\mu(2)}(\boldsymbol{K})\exp\{i\boldsymbol{K}\cdot(\boldsymbol{r}-\boldsymbol{r}')\}|e_0^{\mu}(\boldsymbol{K})\rangle\langle e_0^{\mu}(\boldsymbol{K})|\frac{\mathrm{d}\boldsymbol{K}}{(2\pi)^3}$$
$$=\sum_{\mu=1}^{2}k\cos\theta_B\int_{\eta_0>0}\frac{d\phi}{2\pi}e^{i\boldsymbol{k}(\phi)\cdot(\boldsymbol{r}-\boldsymbol{r}')}|e_0^{\mu}(\boldsymbol{k}(\phi))\rangle\langle e_0^{\mu}(\boldsymbol{k}(\phi))|W_{00}^{(\mu)}(s,t)\,. \tag{A10}$$

Here,

$$W_{00}^{(\mu)}(s,t)=\frac{k\,C\chi_{-\boldsymbol{h}}}{2\sin 2\theta_B}\iint_{-\infty}^{\infty}\frac{G_{h0}^{\mu}(\tau_\rho,\tau_\zeta)}{(\tau_\rho-\tau_\zeta)-k\chi_0}e^{i\tau_\rho s+i\tau_\zeta t}\frac{d\tau_\rho d\tau_\zeta}{4\pi^2}, \tag{A11}$$

The integration of eq. (A11) becomes

$$W_{00}^{(\mu)}(s,t)=-\frac{kC^2\chi_h\chi_{-\boldsymbol{h}}}{4\sin 2\theta_B}e^{ik\chi_0 s}\frac{i}{2}\int_0^{s_0}ds_0\,J_0\left(\beta\sqrt{s_0 s_h}\right)=-i\frac{C(\chi_h\chi_{-\boldsymbol{h}})^{1/2}}{4\sin 2\theta_B}e^{ik\chi_0 s}\sqrt{\frac{s_0}{s_h}}J_1\left(\beta\sqrt{s_0 s_h}\right)\,, \tag{A12}$$

when $s_0>0$ and $s_h>0$. If $s_0<0$ or $s_h<0$, $W_{00}^{(\mu)}=0$. Finally, if the right side of eq. (A10) is integrated with the saddle point method, then the second term on the right-hand side of eq. (47) can be derived.

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