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A simple view of the spherical wave in dynamical theory

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Abstract

The results of the Kato spherical-wave approach to the dynamical theory for perfect crystals are obtained by a simple and straightforward method based on the multiple-scattering expansion.

1. Introduction

The present paper is mainly of pedagogical interest, since the final formulae are those of the spherical-wave theory of Kato (1961) in the case of perfect crystals. There are two usual methods to derive the intensity distribution of the spherical wave: the first one, formulated by Kato (1961), uses the Fourier expansion of the spherical wave in plane waves and the usual results of the plane-wave dynamical theory; the second one is based on the solution of the Takagi equations (Takagi, 1962, 1969) using the concept of the Riemann function for second-order differential equations (Authier & Simon, 1968; Takagi, 1969). The method of the present paper is independent of the plane-wave theory, is free of mathematical complexity and has a clear physical meaning; this method is based on the phenomenon of multiple scattering from the incident direction to the Bragg direction and *vice versa*. Starting from the Takagi–Taupin equations written as integral equations, we obtain iteratively the successive terms of the multiple-scattering expansion. The sum of terms of scattering order 0, 2, 4, ... represents the amplitude of the forward wave, including the wave refracted without Bragg reflection (the term of order 0); the sum of terms of scattering order 1, 3, 5, ... represents the amplitude of the Bragg wave. This iteration process is carried out in the Laue case and in the Bragg case for a thick crystal with a planar surface.

Let us first define our utilization of the Takagi theory. According to Takagi (1962), in the case of a Bragg reflection of scattering vector $\mathbf{h}$, the incident wave and the wave in the crystal are presupposed to be of the following form:

$$\psi_{\rm inc} = \exp(i\mathbf{k}_o \cdot \mathbf{r})D_{\rm inc}(\mathbf{r})$$

and

$$\psi_{\rm cryst} = \exp(i\mathbf{K}_o \cdot \mathbf{r})D_o(\mathbf{r}) + \exp(i\mathbf{K}_h \cdot \mathbf{r})D_h(\mathbf{r}),$$

where $|\mathbf{k}_o| = k = 2\pi/\lambda$ and $\mathbf{K}_h = \mathbf{K}_o + \mathbf{h}$; the modulated amplitudes (the D functions) are supposed to have slow variations, as compared to the exponential terms. There is some arbitrariness in the choice of the vectors $\mathbf{k}_o$ and $\mathbf{K}_o$. We choose $\mathbf{k}_o$ as the wavevector of the incident wave in vacuum such that the Bragg condition is exactly fulfilled in the crystal; in the case of an incident plane wave, the departure from the exact Bragg position would then appear in $D_{\rm inc}(\mathbf{r})$. We choose $\mathbf{K}_o$ as the corresponding refracted wavevector. In the case of an absorbing crystal, $\mathbf{K}_o$ (and $\mathbf{K}_h$) has an imaginary part perpendicular to the crystal surface; the real parts of $\mathbf{K}_o$ and $\mathbf{K}_h$ have the same length; the amplitudes $D_o(\mathbf{r})$ and $D_h(\mathbf{r})$, using oblique coordinates (s_o, s_h) along the directions of the real parts of $\mathbf{K}_o$ and $\mathbf{K}_h$, are then shown to satisfy the partial differential equations

$$\partial D_o/\partial s_o = i(\pi/\lambda)\chi_{-h}D_h(s_o, s_h) \qquad (1a)$$

$$\partial D_o/\partial s_h = i(\pi/\lambda)\chi_h D_o(s_o, s_h), \qquad (1b)$$

in which χ_h and χ_{-h} are the Fourier components of the crystal susceptibility. The incident wave must be taken into account in the boundary conditions. This can be performed by means of integral equations, as explained by Bremer (1984). The integral-equations method is particularly well suited to the calculation of the multiple-scattering expansion in the case of the spherical wave defined by Kato, corresponding to an incident wave limited by an infinitely narrow slit on the entrance surface of the crystal. The wave function of the incident wave is then $\exp(i\mathbf{k}_o \cdot \mathbf{r})\delta(s_h)$ and the wave function of the wave refracted in the crystal without Bragg reflection is $\exp(i\mathbf{K}_o \cdot \mathbf{r})\delta(s_h)$. In these expressions, $\delta(s_h)$ is a Dirac distribution which represents, as is usual in optics, a point source located on the entrance surface of the crystal. The experimental set-up corresponds to a narrow slit with a spatially incoherent illumination. The different points of the slit produce identical but laterally displaced intensity profiles in the recording plane; the maximum displacement is equal to the width of the slit and may be neglected if the slit is sufficiently narrow.

2. Multiple-scattering expansion in the Laue case

Let us choose as the origin of the coordinates the point of incidence of the infinitely narrow incident wave on the crystal (see Fig. 1). As pointed out at the end of the previous section, the modulated amplitude of the wave refracted in the crystal without Bragg reflection is taken as $D_o(s_o, s_h) = \delta(s_h)$. Equations (1$a$) and (1$b$) can then be written as the integral equations

$$D_o(s_o, s_h) = \delta(s_h) + i(\pi/\lambda)\chi_{-h}\int\limits_0^{s_o} {\rm d}\,s'_o\, D_h(s'_o, s_h) \qquad (2a)$$

$$D_h(s_o, s_h) = i(\pi/\lambda)\chi_h \int\limits_0^{s_h} {\rm d}\,s'_h\, D_o(s_o, s'_h). \qquad (2b)$$

The amplitudes $D_o(s_o, s_h)$ and $D_h(s_o, s_h)$ are obviously equal to zero outside the region of influence that corresponds to positive values of s_o and s_h; in fact, in equations (2a) and (2b), it is supposed that $s_o, s_h > 0$. From these integral equations, it is easy to calculate the multiple-scattering expansion in which the terms of even order belong to $D_o(s_o, s_h)$ and the terms of odd order belong to $D_h(s_o, s_h)$. The zero-order term of this expansion is present in equation (2a) as $D_o^{(0)} = \delta(s_h)$; the first-order term, obtained by replacing $D_o(s_o, s'_h)$ by $\delta(s'_h)$ in (2b), is

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$D_h^{(1)} = i(\pi/\lambda)\chi_h$; the second-order term obtained by replacing $D_h(s'_o, s_h)$ by $D_h^{(1)}$ in the integral of (2a) is $D_o^{(2)} = -(\pi/\lambda)^2 \chi_h \chi_{-h} s_o$; the successive terms, up to any order, are obtained iteratively by the following sequence of integrations:

$$D_h^{(2n+1)}(s_o, s_h) = i(\pi/\lambda)\chi_h \int_0^{s_h} \mathrm{d}\, s'_h \, D_o^{(2n)}(s_o, s'_h)$$
$$D_o^{(2n+2)}(s_o, s_h) = i(\pi/\lambda)\chi_{-h} \int_0^{s_o} \mathrm{d}\, s'_o \, D_h^{(2n+1)}(s'_o, s_h).$$

The general terms thus obtained are

$$D_h^{(2n+1)}(s_o, s_h) = i(\pi/\lambda)^{(2n+1)} \chi_h (-)^n (\chi_h s_h)^n (\chi_{-h} s_o)^n / n! n!$$
$$D_o^{(2n+2)}(s_o, s_h) = -(\pi/\lambda)^{(2n+2)} \chi_h (-)^n (\chi_{-h} s_o)^{n+1} \times (\chi_h s_h)^n / (n+1)! n!$$

It is convenient to define the interaction length $L = (\lambda/\pi)(\chi_h \chi_{-h})^{-1/2}$. We can then write

$$D_o(s_o, s_h) = \delta(s_h) - L^{-1}(s_o/s_h)^{1/2} \times \sum_{n=0}^{\infty} \{(-)^n [(s_o s_h)^{1/2}/L]^{2n+1} / (n+1)! n!\}$$
$$D_h(s_o, s_h) = i(\pi/\lambda)\chi_h \sum_{n=0}^{\infty} (-s_o s_h / L^2)^n / n! n!,$$

in which, the well known formulae first obtained by Kato (1961),

$$D_o(s_o, s_h) = \delta(s_h) - L^{-2} s_o 2 J_1(X)/X$$
$$D_h(s_o, s_h) = i(\pi/\lambda)\chi_h J_0(X)$$

with

$$X = 2(s_o s_h)^{1/2}/L,$$

can be recognized, by recalling the familiar series expansion of Bessel functions. In the case of an absorbing crystal, L is a complex length since $(\chi_h \chi_{-h})$ is in general complex and we actually obtain Bessel functions with a complex argument.

3. Multiple-scattering expansion in the Bragg case

We consider the reflection of a spherical wave by an infinitely thick crystal in the Bragg case. In contrast to the Laue case, it is necessary to take into account the asymmetry factor $\gamma = |\gamma_h|/\gamma_o$, in which $\gamma_{o,h} = \cos(\mathbf{K}_{o,h}, \mathbf{n})$, $\mathbf{n}$ indicating the inward direction normal to the crystal surface. As shown in Fig. 2, the region of influence is $(s_o > 0, s_h > 0, s_o - \gamma s_h > 0)$. The integral equations are

$$D_o(s_o, s_h) = \delta(s_h) + i(\pi/\lambda)\chi_{-h} \int_{\gamma s_h}^{s_o} \mathrm{d}s'_o \, D_h(s'_o, s_h) \qquad (3a)$$

$$D_h(s_o, s_h) = i(\pi/\lambda)\chi_h \int_0^{s_h} \mathrm{d}s'_h \, D_o(s_o, s'_h). \qquad (3b)$$

The integration limits are such that $[D_o(s_o, s_h) - \delta(s_h)] = 0$ for $s_o = \gamma s_h$ (the crystal surface). The zero-order term of the multiple-scattering expansion is present in equation (3a) as $D_o^{(0)} = \delta(s_h)$; the first-order term obtained by replacing $D_o(s_o, s'_h)$ by $\delta(s'_h)$ in (3b) is $D_h^{(1)} = i(\pi/\lambda)\chi_h$; the second-order term is $D_o^{(2)} = -(\pi/\lambda)^2 \chi_h \chi_{-h}(s_o - \gamma s_h)$; the successive terms, up to any order, are obtained iteratively by the following sequence of integrations:

$$D_h^{(2n+1)}(s_o, s_h) = i(\pi/\lambda)\chi_h \int_0^{s_h} \mathrm{d}s'_h \, D_o^{(2n)}(s_o, s'_h)$$
$$D_o^{(2n+2)}(s_o, s_h) = i(\pi/\lambda)\chi_{-h} \int_{\gamma s_h}^{s_o} \mathrm{d}s'_o \, D_h^{(2n+1)}(s'_o, s_h),$$

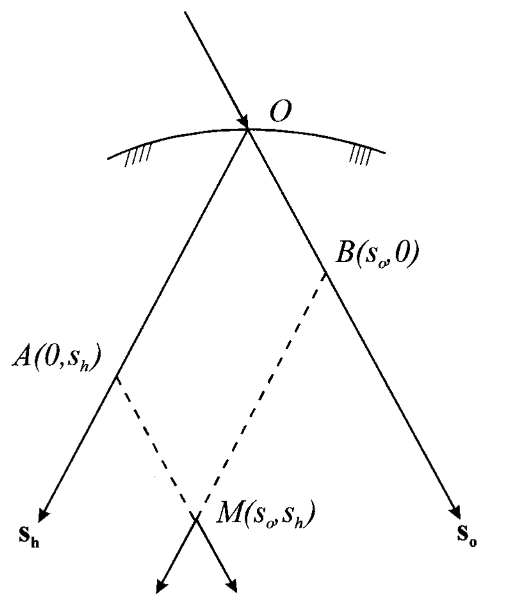

Fig. 1. The spherical-wave geometry in the Laue case. The oblique coordinates of the point M are $s_o = \overline{AM}$ and $s_h = \overline{BM}$. The integrations of formulae (2a) and (2b) are carried out along $\overline{AM}$ and $\overline{BM}$, respectively.

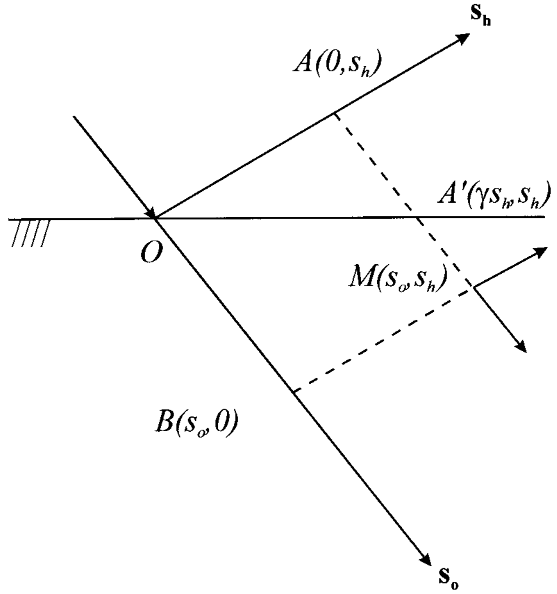

Fig. 2. The spherical-wave geometry in the Bragg case for a thick crystal. The integration of formula (3a) is carried out along $\overline{A'M}$, where the point A' is on the crystal surface; the integration of formula (3b) is carried out along $\overline{BM}$.

which are a little more complicated than in the Laue case. The general terms, for $n = 1, 2, \ldots,$ are

$$D_h^{(2n+1)}(s_o, s_h) = i(\pi/\lambda)^{(2n+1)}\chi_h(-\chi_h\chi_{-h})^n[(s_o s_h)^n/n!n! - \gamma s_o^{n-1}s_h^{n+1}/(n-1)!(n+1)!]$$

$$D_o^{(2n+2)}(s_o, s_h) = (\pi/\lambda)^{(2n+2)}(-\chi_h\chi_{-h})^{n+1} \times (s_o - \gamma s_h)(s_o s_h)^n/(n+1)!n!.$$

Using again the series expansion of Bessel functions, we obtain, again with $X = 2(s_o s_h)^{1/2}/L$,

$$D_o(s_o, s_h) = \delta(s_h) - L^{-2}(s_o - \gamma s_h)2J_1(X)/X$$
$$D_h(s_o, s_h) = i(\pi/\lambda)\chi_h[J_0(X) + \gamma(s_h/s_o)J_2(X)],$$

which are similar to formulae obtained by Uragami (1969) and by Afanas'ev & Kohn (1971).

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