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1991 J. Phys.: Condens. Matter 3 5263

(http://iopscience.iop.org/0953-8984/3/28/002)

J. Phys.: Condens. Matter 3 (1991) 5263–5270. Printed in the UK

Total reflection at grazing incidence as a special case of the Bragg reflection in Ewald's extended theory

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Received 11 January 1991, in final form 18 March 1991

Abstract. The quantum mechanical version of Ewald's extended dynamical theory of diffraction is used for the study of the transmission and reflection of neutrons by a crystal. It is shown that the total reflection of neutrons at grazing incidence on a crystal is formally equivalent to the total reflection at the Bragg reflection position. Ewald's quantum mechanical and Fresnel's classical formulae for reflection and transmission at grazing incidence are compared.

1. Introduction

As the refraction index of neutrons in crystals is smaller than unity, total reflection at grazing angle of incidence occurs. This effect is usually explained in a similar way as in classical optics, by applying the Fresnel formulae to the de Broglie waves (Sears 1989). Of course, if the wavelength of neutrons is of the same order as the lattice constant of the crystal, the use of Fresnel's formulae (which, strictly speaking, are valid for continuous isotropic media only) is clearly an approximation (Litzman and Rózsa 1983, Litzman and Šebelová 1985), the validity of which should be verified within some microscopic theory. A more precise method considering at grazing incidence the discrete structure of the crystal was applied by Vineyard (1982), who used the distorted-wave approximation and by Dietrich and Wagner (1984) who used the Green function for the half-space together with a modified first Born approximation. In both papers the reflection of the electromagnetic waves is studied; this is formally more complicated than the reflection of neutrons considered in this paper. The paper by Smirnov (1977), who studied the total reflection on an amorphous film using a method similar to Darwin's dynamical theory, should be mentioned too.

Our approach is quite different. We shall use the quantum mechanical version of Ewald's dynamical theory of diffraction and show that the total reflection at grazing incidence on an ideal crystal can be understood as a special case of the Bragg reflection.

The detailed proof of this assertion is given below, but it is quite evident, considering the reflection of neutrons on a semi-infinite simple cubic lattice with lattice vectors $a\boldsymbol{e}_x$, $a\boldsymbol{e}_y$, $a\boldsymbol{e}_z$. Let us suppose that the surface plane of the crystal is the plane of the vectors $\boldsymbol{e}_x$, $\boldsymbol{e}_y$; further $\boldsymbol{e}_z$ points into the crystal, and the wavevector of the incident beam is $\boldsymbol{k}$, where $k_z > 0$. From simple symmetry considerations it follows that the wavevectors of the reflected beams are

$$K_{pq}^- = (k_x + p2\pi/a)e_x + (k_y + q2\pi/a)e_y - K_{pqz}e_z \qquad p, q \text{ integers} \tag{1.1}$$

where

$$K_{pqz} = +[k^2 - (k_x + p2\pi/a)^2 - (k_y + q2\pi/a)^2]^{1/2}.$$

In regard to the results of the dynamical theory of diffraction, the reflected beam is strong if the vectors k and K_{pq}^- satisfy approximately the Bragg diffraction condition which, in our simple case can be written as

$$K_{pqz} + k_z = n2\pi/a + \varepsilon/a \qquad |\varepsilon| \ll 1. \tag{1.2}$$

For a specularly reflected beam, $p = q = 0$, i.e. $K_{00z} = k_z$, and equation (1.2) reads

$$2k_z = n2\pi/a + \varepsilon/a. \tag{1.3}$$

At grazing incidence $ak_z \ll 1$. Thus, (1.3) can be satisfied for $n = 0$. It will be shown in section 3 that the reflected beam is "strong" (i.e. that total reflection at grazing incidence occurs) if the index of refraction is smaller than unity.

In the following we shall study the reflection of neutrons at grazing incidence on a crystal of finite thickness. The handling of this problem from the point of view of the dynamical theory of diffraction seems to us to be important, considering the number of many papers in which a more general case is studied, i.e. the Bragg scattering excited under the conditions of total external reflection (Afanas'ev and Melkonyan 1983, Zeilinger and Beatty 1983).

2. Extended dynamical theory of diffraction in Ewald's picture

In the following we shall deal with the scattering of neutrons on crystals, using the quantum mechanical generalization of Ewald's dynamical theory of diffraction (Dederichs 1972, Sears 1989). Let us recall briefly the main results of our previous papers on the dynamical theory of diffraction of particles on a periodic system of point scatterers (Fermi δ potentials) (Litzman 1986, Litzman and Dub 1990). We shall deal with the diffraction of the plane wave $f\exp(ik \cdot r)$ on a simple lattice forming a crystal of finite thickness (figure 1):

$$\begin{aligned} &R_m = m_1a_1 + m_2a_2 + m_3a_3 \qquad m = (m_1, m_2, m_3) \\ &\rho^{-1} = |a_1 \times a_2|a_{3z} \qquad a_{3z} > 0 \\ &m_1, m_2 = 0, \pm1, \pm2, \ldots, \pm\infty \qquad m_3 = 0, 1, 2, \ldots, N. \end{aligned} \tag{2.1}$$

The origin of the orthogonal coordinate system is at the lattice point (0, 0, 0), the plane Oxy coincides with the crystal surface plane (a_1, a_2). The axis Oz (unit vector e_3) and the vector $a_1 \times a_2$ point into the crystal. The lattice (g_1, g_2, g_3) is reciprocal to the three-dimensional lattice (a_1, a_2, a_3), i.e. $g_i \cdot a_j = 2\pi\delta_{ij}$, $i, j = 1, 2, 3$, whereas the lattice (b_1, b_2) is reciprocal to the two-dimensional lattice (a_1, a_2), i.e. $b_i \cdot a_j = 2\pi\delta_{ij}$, $b_i \perp e_3$, i,

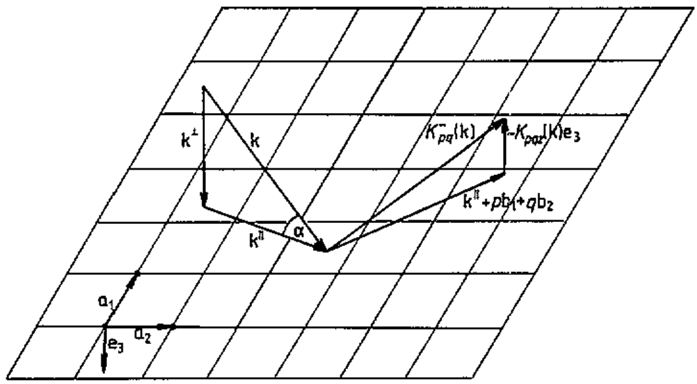

Figure 1. The scattering geometry. The two-dimensional crystal lattice $(\boldsymbol{a}_1, \boldsymbol{a}_2) \perp \boldsymbol{e}_3$ forms the surface of the crystal. $\boldsymbol{k} = \boldsymbol{k}^{\perp} + \boldsymbol{k}^{\parallel}$ is the wavevector of the incident beam; $\pi/2 - \alpha$ is the angle of incidence. $\boldsymbol{K}^{-}_{pq}(\boldsymbol{k}) = \boldsymbol{k}^{\parallel} + p\boldsymbol{b}_1 + q\boldsymbol{b}_2 - \boldsymbol{e}_3 K_{pqz}(\boldsymbol{k})$ is the wavevector of the reflected wave, where (p, q) are integers, $(\boldsymbol{b}_1, \boldsymbol{b}_2) \perp \boldsymbol{e}_3$ is the reciprocal lattice and $K_{pqz}(\boldsymbol{k}) = [k^2 - (\boldsymbol{k}^{\parallel} + p\boldsymbol{b}_1 + q\boldsymbol{b}_2)^2]^{1/2}$.

$j = 1, 2$. Further, $\boldsymbol{c}^{\parallel}$ and $\boldsymbol{c}^{\perp}$ denote the components of the vector $\boldsymbol{c} = \boldsymbol{c}^{\parallel} + \boldsymbol{c}^{\perp}$ parallel and perpendicular to the crystal surface, respectively. Then

$$\boldsymbol{b}_1 = \boldsymbol{g}_1^{\parallel} \qquad \boldsymbol{b}_2 = \boldsymbol{g}_2^{\parallel} \qquad \boldsymbol{g}_3^{\parallel} = 0.$$

Let $\boldsymbol{k}$ be the wavevector of the incident wave; $k_z > 0$. We assign to this vector $\boldsymbol{k}$ and to each (p, q), where p, q are integers, three other vectors $\boldsymbol{k}^{\parallel}_{pq}$ and $\boldsymbol{K}^{\pm}_{pq}(\boldsymbol{k})$, as follows:

$$\begin{aligned} \boldsymbol{k}^{\parallel}_{pq} &= \boldsymbol{k}^{\parallel} + p\boldsymbol{b}_1 + q\boldsymbol{b}_2 \\ \boldsymbol{K}^{\pm}_{pq}(\boldsymbol{k}) &= \boldsymbol{k}^{\parallel}_{pq} \pm \boldsymbol{e}_3 K_{pqz}(\boldsymbol{k}) \end{aligned} \tag{2.2a}$$

where

$$K_{pqz}(\boldsymbol{k}) = +[k^2 - (\boldsymbol{k}^{\parallel}_{pq})^2]^{1/2}.$$

This means that

$$|\boldsymbol{K}^{\pm}_{pq}(\boldsymbol{k})| = k.$$

For $(p, q) = (0, 0)$, it holds that $\boldsymbol{K}^{+}_{00}(\boldsymbol{k}) = \boldsymbol{k}$ and $K_{00z}(\boldsymbol{k}) = k_z$. Further, we define $\theta^{\pm}_{pq}$ as

$$\theta^{\pm}_{pq}(\boldsymbol{k}) = \boldsymbol{a}_3 \boldsymbol{K}^{\pm}_{pq}(\boldsymbol{k}) = \boldsymbol{a}_3^{\parallel} \boldsymbol{k}^{\parallel}_{pq} \pm a_{3z} K_{pqz}(\boldsymbol{k}). \tag{2.2b}$$

The wavefunction $\Psi(\boldsymbol{r})$ describing the diffraction of particles on a simple perfect lattice formed by δ potentials is (Litzman 1986, Litzman and Dub 1990)

$$\Psi(\boldsymbol{r}) = f \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) - \sum_n Q \frac{\exp(\mathrm{i}k|\boldsymbol{r} - \boldsymbol{R}_n|)}{|\boldsymbol{r} - \boldsymbol{R}_n|} \varphi^n(\boldsymbol{R}_n) \tag{2.3}$$

which is a superposition of the incident plane wave $f \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})$ and of the spherical waves excited by the point scatterers forming the crystal (2.1). The diffraction amplitude of the nth atom is $Q\varphi^n(\boldsymbol{R}_n)$, where $Q = Q_0/(1 + \mathrm{i}kQ_0)$ is the diffraction length of the scatterers (Q_0 is real). The "effective field" $\varphi^n(\boldsymbol{R}_n)$ incident on the nth atom must satisfy the equation

$$\varphi^n(\boldsymbol{R}_n) = f\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n) = \sum_{m\neq n}{}' Q\,\frac{\exp(\mathrm{i}k|\boldsymbol{R}_m-\boldsymbol{R}_n|)}{|\boldsymbol{R}_m-\boldsymbol{R}_n|}\,\varphi^m(\boldsymbol{R}_m). \tag{2.4}$$

Since the translational symmetry of our problem in the directions of the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ is conserved, it is clear that the wavevectors of the reflected particles are the vectors $\boldsymbol{K}^-_{pq}$ and the wavevectors of the transmitted particles are the vectors $\boldsymbol{K}^+_{pq}$ (2.2a) only.

From equations (29) and (30) of Litzman (1986), we found the solution of equations (2.3) and (2.4) to be in the form

$$\Psi(\boldsymbol{r}) = f\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) + \sum_{pq}\frac{1}{K_{pqz}}R_r(\theta^-_{pq})\exp(\mathrm{i}\theta^-_{pq})\exp(\mathrm{i}\boldsymbol{K}^-_{pq}\cdot\boldsymbol{r}) = u_{\mathrm{inc}} + \sum_{pq}u^r_{pq} \tag{2.5}$$

for $z<0$, and

$$\Psi(\boldsymbol{r}) = -\sum_{pq}\frac{1}{K_{pqz}}R_t(\theta^+_{pq})\exp(-\mathrm{i}N\theta^+_{pq})\exp(\mathrm{i}\boldsymbol{K}^+_{pq}\cdot\boldsymbol{r}) = \sum_{pq}u^t_{pq} \tag{2.6}$$

for $z > Na_{3z}$ where the coefficients $R_r(\theta^-_{pq})$ and $R_t(\theta^+_{pq})$ are given by equations (38) and (39) of Litzman (1986). In order to use these formulae we need the quantities ψ_j which are the solutions of the "dispersion relation" given as equation (57) of Litzman (1986):

$$1 + QS'(k^{\|}) - \sum_{pq} b_{pq}\left(\frac{\exp(\mathrm{i}\theta^+_{pq})}{\exp(\mathrm{i}\psi)-\exp(\mathrm{i}\theta^+_{pq})} + \frac{\exp(-\mathrm{i}\theta^-_{pq})}{\exp(-\mathrm{i}\psi)-\exp(-\mathrm{i}\theta^-_{pq})}\right) = 0 \tag{2.7}$$

in which $S'(k^{\|})$ is the two-dimensional lattice sum (Litzman 1986, appendix) and

$$b_{pq} = -2\pi\mathrm{i}Q/|\boldsymbol{a}_1\times\boldsymbol{a}_2|K_{pqz}. \tag{2.8}$$

The poles $\theta^{\mp}_{pq}$ of the expression on the left-hand side of (2.7) have an important physical meaning. As shown by Litzman and Dub (1990, appendix I), the condition for the confluence of two poles in (2.7)

$$\theta^+_{00} = \theta^-_{pq} + j2\pi \qquad j\ \text{integer} \tag{2.9a}$$

is equivalent to

$$\boldsymbol{K}^-_{pq} = \boldsymbol{k} + p\boldsymbol{g}_1 + q\boldsymbol{g}_2 - j\boldsymbol{g}_3 \qquad (\boldsymbol{K}^-_{pq})^2 = \boldsymbol{k}^2. \tag{2.9b}$$

Thus (2.9a) means that the incident vector $\boldsymbol{k}$ satisfies the Bragg condition for the reflection in the direction of the vector $\boldsymbol{K}^-_{pq}$.

Let us assume that

$$\theta^+_{00} = \theta^-_{rs} + j2\pi + \eta \qquad |\eta| \ll 1 \tag{2.9c}$$

holds. Using for the evaluation of the coefficients $R_r(\theta^-_{rs})$ and $R_t(\theta^+_{00})$ a similar procedure as in the work by Litzman and Rózsa (1990) we get for the reflected wave in the direction of K^-_{rs} (see (2.5))

$$u^r_{rs} = (1/K_{rsz})R_r(\theta^-_{rs})\exp(\mathrm{i}\theta^-_{rs})\exp(\mathrm{i}\boldsymbol{K}^-_{rs}\cdot\boldsymbol{r}) = f(k_z/K_{rsz})^{1/2}\,\mathrm{sgn}\,Q_0\exp(\mathrm{i}\eta/2)$$
$$\times\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_3)\exp[\mathrm{i}\boldsymbol{K}^-_{rs}\cdot(\boldsymbol{r}+\boldsymbol{a}_3)]/[Y-(Y^2-1)^{1/2}\coth\Psi] \quad z<0 \tag{2.10}$$

and for the transmitted wave (see (2.6))

$$u^t_{00} = -(1/k_z)R_t(\theta^+_{00})\exp(-\mathrm{i}N\theta^+_{00})\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$$
$$= (-f/\sinh\Psi)\{(Y^2-1)^{1/2}(x_1x_2)^{(N+1)/2}/[Y-(Y^2-1)^{1/2}\,\mathrm{coh}\,\Psi]\}$$
$$\times\exp\{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}-(N+1)\boldsymbol{a}_3]\} \qquad z > Na_{3z}. \tag{2.11}$$

The parameters used in (2.10) and (2.11) have the following meaning (Litzman and Dub 1990):

$$Y = [(\beta_{00} + \beta_{rs})/2(\beta_{00}\beta_{rs})^{1/2}]\cos(\eta/2) + [1/(\beta_{00}\beta_{rs})^{1/2}]\, H_{rs}\sin(\eta/2) \tag{2.12}$$

$$\exp\Psi = (x_1/x_2)^{(N+1)/2} \tag{2.13}$$

$$x_1/x_2 = 1 + [\![2/\{H_{rs}^2 + [(\beta_{00} - \beta_{rs})/2]^2\}]\!][\![\beta_{00}\beta_{rs}(1 - Y^2) + \sqrt{\beta_{00}\beta_{rs}}\,\{H_{rs}\cos(\eta/2) - [(\beta_{00} + \beta_{rs})/2]\sin(\eta/2)\}\sqrt{1 - Y^2}]\!] \tag{2.14a}$$

$$x_1 x_2 = \exp[\mathrm{i}(2\theta_{00}^{+} - \eta)][H_{rs} + \mathrm{i}(\beta_{00} - \beta_{rs})/2][H_{rs} - \mathrm{i}(\beta_{00} - \beta_{rs})/2]^{-1} \tag{2.14b}$$

$$\beta_{pq} = -2\pi Q_0/|\boldsymbol{a}_1 \times \boldsymbol{a}_2| K_{pqz} = -2\pi Q_0 \rho a_{3z}/K_{pqz}. \tag{2.15}$$

Here H_{rs} (Litzman and Dub 1990) is real, $H_{rs} = 1 + O(Q_0/a)$ and a is the lattice constant.

3. Grazing incidence

At grazing incidence,

$$a_{3z}k_z \simeq -a_{3z}k_z$$

i.e. according to (2.2*b*)

$$\theta_{00}^{+}(\boldsymbol{k}) = \theta_{00}^{-}(\boldsymbol{k}) + \eta \tag{3.1}$$

which means that the grazing incidence can be understood as a special case of the Bragg reflection (2.9*c*) whereby in the dispersion relation (2.7) the poles θ_{00}^{+} and θ_{00}^{-} nearly coincide. Thus, to get the reflected and transmitted waves at grazing incidence, we put in the expressions (2.10)–(2.12), (2.14) and (2.15)

$$r, s = 0, 0 \qquad \eta = \theta_{00}^{+} - \theta_{00}^{-} = 2a_{3z}k_z = 2a_{3z}k\sin\alpha \tag{3.2}$$

$$\beta_{00} = -4x/\eta \qquad x = \pi Q_0 a_{3z}/|\boldsymbol{a}_1 \times \boldsymbol{a}_2| = Q_0/a \tag{3.3}$$

where α is the grazing incidence angle and a the lattice constant. By this means we obtain

$$u_{00}^{r} = \{f\,\mathrm{sgn}\,Q_0\exp(-\mathrm{i}a_{3z}k_z)/[Y - (Y^2 - 1)^{1/2}\coth\Psi]\} \times \exp(\mathrm{i}\boldsymbol{K}_{00}^{-}\boldsymbol{r}) \qquad z < 0 \tag{3.4}$$

$$u_{00}^{t} = (-f/\sinh\Psi)\{(Y^2 - 1)^{1/2}\exp[-\mathrm{i}a_{3z}(N+1)k_z]/[Y - (Y^2 - 1)^{1/2}\coth\Psi]\} \times \exp(\mathrm{i}\boldsymbol{k}\boldsymbol{r}) \qquad z > Na_{3z} \tag{3.5}$$

where

$$Y = -\mathrm{sgn}\,Q_0\cos(\eta/2) + [H_{00}\eta\sin(\eta/2)]/4|x| \tag{3.6}$$

$$\Psi = [(N+1)/2]\ln(x_1/x_2) = [(N+1)/2]\ln\{1 + (8|x|/\eta H_{00})\sqrt{1 - Y^2} \times [\cos(\eta/2) + (4|x|/\eta H_{00})\sqrt{1 - Y^2} + (4x/\eta H_{00})\sin(\eta/2)]\}. \tag{3.7}$$

Following Litzman and Dub (1990), $H_{00} = 1 + Q_0/a$ and further it can be shown that $(4|x|/H_{00}\eta)^{-1}\sqrt{1 - Y^2} = 0(|x|^{1/2})$.

Let us compare our results (3.4)–(3.7) with those offered by the procedure in which the crystal is supposed to be a continuous medium described by the potential (Sears 1989)

$$v_0 = (2\pi\hbar^2/m)\rho Q_0 \tag{3.8}$$

or the refraction index

$$n = (1 - v_0/E)^{1/2}. \tag{3.9}$$

In this case we have to solve the Schrödinger equation

$$\begin{aligned} -(\hbar^2/2m)\,\Delta u &= Eu \qquad z<0, z>d \\ -(\hbar^2/2m)\,\Delta u + v_0 u &= Eu \qquad d<z<0. \end{aligned} \tag{3.10}$$

The solution reads

$$\begin{aligned} u &= f\exp[\mathrm{i}(xk_x + zk_z)] + A\exp[\mathrm{i}(xk_x - zk_z)] && z<0 \\ u &= B\exp[\mathrm{i}(x\kappa_x + z\kappa_z)] + C\exp[\mathrm{i}(x\kappa_x - z\kappa_z)] && 0>z>d \\ u &= D\exp[\mathrm{i}(xk_x + zk_z)] && z<d \end{aligned} \tag{3.11}$$

where

$$k^2 = (2m/\hbar^2)E \qquad \kappa^2 = k^2 - (2m/h^2)v_0. \tag{3.12}$$

Requiring that $u(r)$ and grad $u(r)$ be continuous at the boundaries we get

$$k_x = \kappa_x$$

i.e.

$$\kappa_z = (k_z^2 - 4\pi Q_0\rho)^{1/2} \qquad \operatorname{sgn}(k_z^2 - \kappa_z^2) = \operatorname{sgn} Q_0 \tag{3.13}$$

together with a system of four linear algebraic equations for the amplitudes A, B, C, D in (3.11) which will not be given here. By a standard procedure we get for the reflected wave

$$u_{00}^{\mathrm{r}} = \{f\exp[\mathrm{i}(xk_x - zk_z)]\}/[y - \operatorname{sgn}(k_z^2 - \kappa_z^2)(y^2-1)^{1/2}\coth\psi] \tag{3.14}$$

and for the transmitted wave

$$\begin{aligned} u_{00}^{\mathrm{t}} = (-f/\sinh\psi)\{(y^2-1)^{1/2}\exp(-\mathrm{i}dk_z)\exp[\mathrm{i}(xk_x + zk_z)]\}/[y\operatorname{sgn}(k_z^2 - \kappa_z^2) \\ - (y^2-1)^{1/2}\coth\psi]. \end{aligned} \tag{3.15}$$

We have introduced

$$y = -1 + k_z^2(2\pi Q_0\rho)^{-1} = -1 + \eta^2/8x \tag{3.16}$$

$$\psi = \mathrm{i}d\kappa_z = \mathrm{i}(d/a_{3z})(4|x|/\eta)\sqrt{y^2-1}. \tag{3.17}$$

We can see that the quantum mechanical Ewald formulae (3.4) and (3.5) have the same form as the Fresnel formulae (3.14) and (3.15); the physical meanings of the parameters Y (3.6), Ψ (3.7) and y (3.16) and ψ (3.17) are of course different. The differences are of the order of η^2 and $|x|^{1/2}$.

Comparing (3.7) with (3.17) we can see that the thickness of the crystal containing $N+1$ rows should be taken as

$$d = (N+1)a_{3z} \tag{3.18}$$

(rather than Na_{3z}). This also explains the phase factor $\exp(-ia_{3z}K_z)$ in (3.4).

Analysing the solution (3.11) for a semi-infinite crystal we find that in a semi-infinite crystal without absorption we must put $\coth\psi = \coth\Psi = -1$ in (3.4) and (3.14). Then these equations yield

$$|u_{00}^{\zeta}|^2 = |f|^2 \qquad \text{for } |Y|, |y| < 1. \tag{3.19}$$

Thus the condition for the specularly reflected wave u_{00}^{ζ} in the superposition (2.5) to be strong is $|Y| < 1$. It follows from (3.6) that in this case the inequality $\operatorname{sgn} Q_0 > 0$ must hold, i.e. the refraction index n (3.9) is smaller than unity.

The conditions for the limits of the total grazing reflection angles α are (see (3.6) and (3.16))

$$\begin{aligned} &Y = 1, \text{ i.e. } (a_{3z}k\sin\alpha)^2 = 4|x|[1 + \mathrm{O}(x) + \mathrm{O}(Q_0/a)] \\ &y = 1, \text{ i.e. } (a_{3z}k\sin\alpha)^2 = 4|x|. \end{aligned} \tag{3.20}$$

4. Concluding remarks

Using Ewald's quantum mechanical conception of the dynamical theory of diffraction (Litzman 1986, Litzman and Dub 1990), we can see that the beam incident at a very small grazing angle satisfies the Bragg reflection condition. Thus the intensities of the reflected and transmitted rays can be evaluated using the general formulae of the dynamical theory of diffraction for the Bragg reflection. The reflection curves given by the Fresnel formula (3.14) and by the Ewald dynamical theory of diffraction (3.4) for the semi-infinite crystal ($\coth\psi = \coth\Psi = -1$) are presented in figure 2 for $x = 10^{-4}$ and the bounds of the intervals $\langle\eta_E, \eta_F\rangle$ for $x = 10^{-3}$, 10^{-4} and 10^{-5} are evaluated as well. (For Si, $x \simeq Q_0/a \simeq 10^{-5}$.) In a crystal with absorption, Q_0 is complex and the deformation of the shapes of the reflection curves similar to the well known deformation of the rocking curves of the x-rays (of course without a shift) is to be expected, but the influence of absorption is generally much less important for neutrons than for x-rays (Rauch and Petraschek 1978).

The corrections introduced by the dynamical theory of diffraction into the standard Fresnel formulae of neutron optics (Sears 1989) are small. However, it is not clear how the above-used Ewald method influences the results of the commonly used Laue theory in a more general case, when the grazing incident beam satisfies simultaneously the Bragg reflection condition for planes nearly perpendicular to the crystal surface (Afanas'ev and Melkonyan 1983, Bernhard *et al* 1987, Hashizume and Sakata 1989, Jach *et al* 1989, Rhan and Pietsch 1990, Rieutord 1990, Zeilinger and Beatty 1983). In this case, not two but three or more poles of the dispersion equation (2.7) coincide but equations (2.5) and (2.6) do not change. Then (Litzman 1991) there is a substantial difference between Ewald's and Laue's conceptions of the conventional and extended dynamical theory of diffraction.

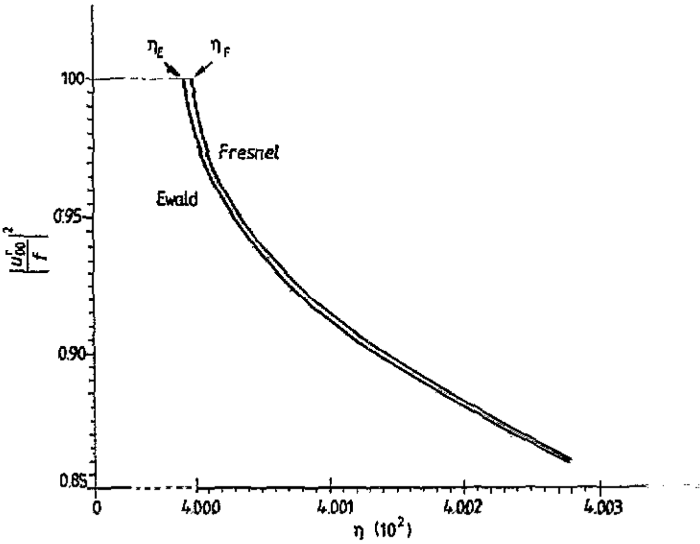

Figure 2. Reflection curves given by the Fresnel formula (3.14) and by the Ewald dynamical theory of diffraction (3.4) for the semi-infinite crystal: $x = \pi Q_0 a_{3z}|\boldsymbol{a}_1 \times \boldsymbol{a}_2|^{-1} = 10^{-4}$; $\eta = 2a_{3z}k \sin\alpha$. Numerical values of the bounds of the interval $\langle \eta_E, \eta_F \rangle$ for some values of the parameter x: $x = 10^{-3}, \langle 0.1264700, 0.1264911\rangle$; $x = 10^{-4}, \langle 0.0399993, 0.0400000\rangle$; $x = 10^{-5}$, $\langle 0.0126490, 0.0126491\rangle$.

Acknowledgment

The author thanks Dr J Marek for some helpful numerical computations.

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