Algebraic description of dynamic diffraction by ideal polyatomic crystals

V. K. Ignatovich

Joint Institute for Nuclear Research, Dubna
(Submitted 5 October 1989)
Zh. Eksp. Teor. Fiz. **97**, 1616–1625 (May 1990)

Neutron scattering by ideal polyatomic crystals with an arbitrary unit cell is described by means of recurrence relations.

1. INTRODUCTION

The expressions for the reflection and transmission amplitudes in the case of an arbitrary one-dimensional periodic potential are obtained in Ref. 1 on the assumption that the reflection r and transmission t amplitudes of a single period are known. It follows from these expressions that the reflection R_N and transmission T_N amplitudes of a periodic chain of length $L = Nl$, where l is the period and N is the number of periods in a chain, are

$$T_N=(1-R^2)\exp(iqL)\,[1-R\exp(iqL)R\exp(iqL)]^{-1}, \quad (1)$$

$$R_N=[R-\exp(iqL)R\exp(iqL)]\times[1-R\exp(iqL)R\exp(iqL)]^{-1}. \quad (2)$$

Here, R is the amplitude of reflection from a semiinfinite chain and q is the Bloch wave number. The following equations are obtained for R and q in Ref. 1:

$$R=r+tR(1-rR)^{-1}t, \quad (3)$$

$$\exp(iql)=(1-rR)^{-1}t. \quad (4)$$

Equation (3) has a very simple solution for the scattering of scalar particles.[1] However, in the case of spinor or other particles all the amplitudes and the number q are matrices and Eq. (3) is a system of equations which cannot always be solved analytically (in the spinor case this solution is possible in its general form).

Equations (1)–(4) are generalized in Ref. 2 to the three-dimensional case. The diffraction of neutrons by a three-dimensional ideal monatomic crystal with a tetragonal unit cell, in which one of the axes is perpendicular to the plane of the entry surface, is considered in Ref. 2. A crystal is assumed to be divided into separate crystalline monolayers of thickness equal to one unit cell, parallel to the entry surface plane assumed to be infinite. The reflection r and transmission t amplitudes of each layer are infinite-dimensional matrices. The matrix elements r_{ij} and t_{ij} represent the reflection and transmission amplitudes of a single monolayer when the component of the wave vector $\mathbf{k}_{\|}$, parallel to the entry surface plane, changes from $\mathbf{k}_{0\|}+\tau_j$ to $\mathbf{k}_{0\|}+\tau_i$, where $\mathbf{k}_{0\|}$ is the component of the wave vector of the primary neutron parallel to the monolayer and $\boldsymbol{\tau}_i$ is the reciprocal lattice vector inside the crystal plane parallel to the entry face.

It is shown in Ref. 2 that

$$r_{ij}=-2\pi i b e_i e_j/k_{\perp i}, \quad (5)$$

$$t_{ij}=e_i^2\delta_{ij}+r_{ij}, \quad (6)$$

where b is the amplitude for coherent scattering of this neutron by a nucleus,

$$k_{\perp i}^2=k_0^2-(\mathbf{k}_{0\|}+\boldsymbol{\tau}_i)^2,$$

and a new quantity is introduced:

$$e_i=\exp(ik_{\perp i}l/2). \quad (7)$$

The matrix element R_{ij} of the reflection amplitude of a crystal semiinfinite along the normal to its entry surface is then

$$R_{ij}=s_i r_{ij} s_j/(1-e_i e_j), \quad (8)$$

which is very similar to Eq. (5) where the additional coefficients s_i satisfy an infinite system of equations

$$s_i=1+s_i\sum_j r_{ij}s_j/(1-e_i e_j). \quad (9)$$

This system is readily terminated since the factors e_i fall exponentially beginning from a certain number i, which gives rise to a finite system of equations that is readily solved. In those case when the denominators in Eq. (9) are small, the Bragg conditions are obeyed and the equations become particularly simple. However, if the denominators are not small, the coefficients s_i are close to unity because of the smallness of the amplitudes b (which is typical of neutron physics).

The present paper generalizes the above expressions to the case of a polyatomic crystal with an arbitrary unit cell when the expressions (5) and (6) become more complex. The solution analogous to Eqs. (8) and (9) will be found.

The problem will be solved using the recurrence relationships, i.e., a crystal will be assumed to be divided by infinitesimally narrow (thin) vacuum spacers into separate layers parallel to the entry surface. The wave field in one interval between the crystal periods is expressed in terms of the wave field in the next interval. This method is quite effective and it can be used to solve many problems in mathematical physics. In particular, it is shown in Ref. 3 that the method of recurrence relationships provides a new approach to the numerical solution of the Schrödinger equation with an arbitrary potential. This method is used in Ref. 4 to solve the diffusion problem.

The method of recurrence relationships has been known for a long time. It was used by Darwin[5,6] back in 1914 to describe the diffraction by a layer system and was called the invariance principle by Ambartsumyan[7] and Chandrasekhar[8] in the 1940s in studies of the diffusion of light. Engibaryan and Mnatsakanyan[9] formulated in 1974 a system of equations which makes it possible to describe the reflection and transmission of arbitrary radiation by a medium of finite thickness in terms of the reflection from a semiinfinite medi-

 0038-5646/90/050913-05$03.00

um. However, this system of equations was not solved by the authors. This is clearly the reason why subsequently the scattering by a layer of finite thickness has been described using integrodifferential equations,[10,11] also formulated in Refs. 7–9. In the derivation of these equations the scattering by a monolayer is assumed to be infinitely weak and is treated only in the first order of perturbation theory.[9,11] In this approach one immediately loses sight of the fact that the scattering by a semiinfinite medium can be described identically [Eqs. (3) and (4)] in terms of the parameters of elementary layers and also in terms of parameters of layers of finite thickness. The equations not solved in Ref. 9 can be solved only if we avoid the differential approach[1], as demonstrated by Eqs. (1) and (2).

In Sec. 2 we obtain the scattering matrices r and t for a layer parallel to the entry surface and of thickness equal to one period of a crystal. For simplicity, we shall use perturbation theory, which is quite satisfactory in the case of a single layer. In Sec. 3 we derive the equations for R and find their solution. We consider some special cases in Sec. 4. Among them one important result on the n–e interaction is of special interest.[12,13]

2. SCATTERING OF NEUTRONS BY A MONOLAYER

We consider a layer parallel to the entry surface (xy plane) and assume that one unit cell can be fitted within its thickness. We assume that this layer is located in vacuum. The r and t matrices can be found from perturbation theory. The incident neutron is described by a plane wave

$$\vec{\psi}_0(\mathbf{r})=\exp(i\vec{\mathbf{k}}_0\mathbf{r}), \tag{10}$$

where the arrow does not indicate that the quantity is a vector, but simply shows that the wave is incident on the layer from the left. The scattered neutron is described

$$\overrightarrow{\overleftarrow{\psi}}(\mathbf{r})=-\sum_{i}\sum_{\alpha} b_\alpha\psi_{\alpha i}\eta(\mathbf{r}-\mathbf{r}_{\alpha i}), \tag{11}$$

where $\mathbf{r}_{\alpha i}$ is the coordinate of a nucleus α in a cell i; b_α is the coherent amplitude of the scattering by this nucleus; $\psi_{\alpha i}$ is the amplitude of the resultant wave incident on the nucleus;

$$\eta(\mathbf{r})=\exp(|\mathbf{r}|)/|\mathbf{r}|.$$

From now on the scattered waves traveling to the right, i.e., those that have traversed the layer must be considered separately from the waves traveling to the left, i.e., those reflected from the layer. We distinguish these two types of wave by the direction of the arrows above ψ. Applying perturbation theory, we obtain $\psi_{\alpha i}=\psi_0(\mathbf{r}_{\alpha i})$.

We can use the representation

$$\eta(\mathbf{r})=\int d^3p\exp(i\mathbf{pr})/2\pi^2(\mathbf{p}^2-\mathbf{k}^2-i\varepsilon)=i\int d^2p_\parallel \times\exp(i\mathbf{p}_\parallel\mathbf{r}_\parallel+ip_\perp|z|)/2\pi p_\perp,\quad p_\perp=(\mathbf{k}^2-\mathbf{p}_\parallel^2)^{1/2} \tag{12}$$

and the summation rule

$$\sum_{n=-\infty}^{\infty} f(n)=\sum_{m=-\infty}^{\infty}\int \exp(2\pi imx)f(x)\,dx. \tag{13}$$

Then,

$$\overrightarrow{\overleftarrow{\psi}}=-2\pi iN_2\sum_{\tau}\exp(i\vec{\mathbf{k}}_\tau\mathbf{r})\sum_{\alpha}(b_\alpha/k_{\tau\perp})\exp[i(\vec{\mathbf{k}}_0-\vec{\mathbf{k}}_\tau)\mathbf{r}_\alpha], \tag{14}$$

where $N_2=1/|[\mathbf{d}_1\mathbf{d}_2]|$ is the two-dimensional intensity of the unit cells in the layer, $d_{1,2}$ are the two-dimensional lattice periods,

$$\vec{\mathbf{k}}_\tau=(\mathbf{k}_{\tau\parallel},+k_{\tau\perp}),\quad \mathbf{k}_{\tau\parallel}=\mathbf{k}_{0\parallel}+\boldsymbol{\tau}_\parallel,\quad k_{\tau\perp}=(k_0^2-k_{\tau\parallel}^2)^{1/2}, \tag{15}$$

and $\boldsymbol{\tau}_\parallel$ are the vectors of the reciprocal two-dimensional lattice. The symbol $\parallel$ represents the components of the vector parallel to the layer, whereas $\perp$ is used for the components perpendicular to the layer.

It is convenient to introduce the total scattering amplitude of a unit cell

$$b_c=\sum_\alpha b_\alpha$$

and to express all the lengths in units of $\lambda=1/2\pi N_2 b_c$. (In the neutron scattering case the value of λ is $\approx 10^{-4}$ cm.) Then, Eq. (14) can be written in the following simple form:

$$\overrightarrow{\overleftarrow{\psi}}=\sum_{\tau}(-i/k_{\tau\perp})\exp(i\vec{\mathbf{k}}_\tau\mathbf{r})\sum_{\alpha} b_\alpha\exp[i(\vec{\mathbf{k}}_0-\vec{\mathbf{k}}_\tau)\mathbf{r}_\alpha], \tag{16}$$

where b_α is the scattering amplitude reduced to the total scattering amplitude of a unit cell b_c.

We introduce

$$|\vec{\tau}\rangle_l=\exp(i\vec{\mathbf{k}}_\tau\mathbf{r}),\quad |\vec{\tau}\rangle_r=\exp[i\vec{\mathbf{k}}_\tau(\mathbf{r}-\mathbf{l})],\quad \vec{\psi}_0=|\vec{0}\rangle_l, \tag{17}$$

where the indices l and r represent the spaces to the left and right of the layer, respectively. Then, the wave functions of the neutron reflected by the layer and transmitted by it are

$$\overleftarrow{\psi}=|\overleftarrow{\tau}\rangle_l\vec{r}_l\langle\vec{\tau}|\vec{\psi}_0,\quad \vec{\psi}=|\vec{\tau}\rangle_r\vec{t}_l\langle\vec{\tau}|\vec{\psi}_0. \tag{18}$$

The arrows above the matrices r and t indicate the direction of propagation of the incident wave. Since a unit cell may be asymmetric, the scattering depends on this direction.

Comparing Eqs. (18) and (16), we readily find the main elements from which the matrices r and t are constructed. These elements are the factor $K_\tau=1/k_{\tau\perp}$ and the form factor

$$\vec{F}^{\tau'\tau}_{t,r}=\sum_\alpha b_\alpha\exp[i(\vec{\mathbf{k}}_\tau-\vec{\mathbf{k}}_{\tau'})\mathbf{r}_\alpha]. \tag{19}$$

Using them we can express the matrices $\vec{r}$ and $\vec{t}$ as follows:

$$\vec{r}=-i\mathcal{K}\vec{\mathcal{F}}_r,\quad \vec{t}=\vec{\mathcal{E}}(1-i\mathcal{K}\vec{\mathcal{F}}_t), \tag{20}$$

where the matrix $\vec{\mathcal{F}}$ consists of the matrix elements of Eq. (19), whereas the matrices $\mathcal{K}$ and $\overrightarrow{\overleftarrow{\mathcal{E}}}$ are diagonal and contain the matrix elements K_τ and

$$\vec{E}_\tau=\exp(i\vec{\mathbf{k}}_\tau\mathbf{l}), \tag{21}$$

respectively.

We can find the reflection and transmission on the right if $\vec{\mathbf{k}}$ in Eq. (19) is replaced with $\overleftarrow{\mathbf{k}}_\tau$ and $\mathbf{r}_\alpha$ with $\mathbf{r}_\alpha-\mathbf{l}$, i.e., in the case when a plane wave is incident on a monolayer from the right, the form factor of Eq. (19) should be replaced by

$$\overleftarrow{F}^{\tau'\tau}_{t,r}=\sum_\alpha b_\alpha\exp[i(\overleftarrow{\mathbf{k}}_\tau-\overleftarrow{\mathbf{k}}_{\tau'})(\mathbf{r}_\alpha-\mathbf{l})]. \tag{22}$$

The expressions in Eq. (20) now become

$$\overleftarrow{r} = -i\mathcal{K}\overleftarrow{\mathcal{F}}_r, \quad \overleftarrow{t} = \overleftarrow{\mathcal{E}}^{-1}(1 - i\mathcal{K}\overleftarrow{\mathcal{F}}_t). \tag{23}$$

It is convenient to introduce

$$\overrightarrow{e}_{\tau\alpha} = \exp(i\overrightarrow{\mathbf{k}}_\tau \mathbf{r}_\alpha), \tag{24}$$

so that Eqs. (20) and (23) become

$$\overrightarrow{r} = -i\mathcal{K}\overleftarrow{e}^{-1}\mathcal{B}\cdot\mathcal{N}\overrightarrow{e}, \quad \overrightarrow{t} = \overrightarrow{\mathcal{E}}(1 - i\mathcal{K}\overleftarrow{e}^{-1}\mathcal{B}\cdot\mathcal{N}\overrightarrow{e}), \tag{25}$$

$$\overleftarrow{r} = -i\mathcal{K}\overrightarrow{\mathcal{E}}\overrightarrow{e}^{-1}\mathcal{B}\cdot\mathcal{N}\overleftarrow{e}\overleftarrow{\mathcal{E}}^{-1}, \quad \overleftarrow{t} = (1 - i\mathcal{K}\overleftarrow{e}^{-1}\mathcal{B}\cdot\mathcal{N}\overleftarrow{e})\overleftarrow{\mathcal{E}}^{-1}, \tag{26}$$

where the matrix $\mathcal{B}$ is diagonal and its elements are the amplitudes b_α; this matrix acts only in the space of the parameters α. The matrix $\mathcal{N}$ acts in the space of the parameters τ and has all the elements equal to 1, whereas the matrix e is diagonal both in the space τ and in the space α, and contains the matrix elements defined by Eq. (24).

3. REFLECTION FROM A HALF-SPACE

The equations for the matrix $\overrightarrow{R}$ representing the reflection by a half-space and for the Bloch wave vector $\vec{q}$, representing the propagation of a wave inside a crystal from its entry surface (the arrow indicates the direction of propagation, which in this case is from left to right) are fully analogous to Eqs. (3) and (4) given above (see Ref. 1):

$$\overrightarrow{R} = \overrightarrow{r} + \overleftarrow{t}\overrightarrow{R}(1 - \overleftarrow{r}\overrightarrow{R})^{-1}\overrightarrow{t}, \tag{27}$$

$$\exp(i\vec{\mathbf{q}}\mathbf{l}) = (1 - \overleftarrow{\mathbf{r}}\overrightarrow{R})^{-1}\overrightarrow{t}. \tag{28}$$

We rewrite Eq. (27) in the form

$$(\overrightarrow{R} - \overrightarrow{r})\overrightarrow{t}^{-1}(1 - \overleftarrow{r}\overrightarrow{R}) = \overleftarrow{t}\overrightarrow{R}. \tag{29}$$

It follows from Eq. (25) that the matrix $\overrightarrow{t}^{-1}$ is

$$\overrightarrow{t}^{-1} = (1 + i\mathcal{K}\overrightarrow{e}^{-1}\mathcal{G}\cdot\mathcal{N}\overrightarrow{e})\overrightarrow{\mathcal{E}}^{-1}, \tag{30}$$

where the matrix $\mathcal{G}$ is found from the condition $t^{-1}t = 1$:

$$\mathcal{G} = \mathcal{B}/(1 - i\mathcal{Q}\mathcal{B}), \tag{31}$$

and the matrix $\mathcal{Q}$ consists of the elements

$$\mathcal{Q}_{\alpha\alpha'} = \sum_\tau \overrightarrow{e}_{\tau\alpha}\overrightarrow{e}^{-1}_{\tau\alpha'}/k_{\tau\perp}. \tag{32}$$

The matrices $\mathcal{G}$ and $\mathcal{Q}$ are defined only in the space of the parameters α. In this space they are nondiagonal.

We seek the solution of Eq. (29) in the form $\overrightarrow{R} = \mathcal{K}\overrightarrow{\mathcal{R}}$. We shall substitute this solution and also Eqs. (25), (26), and (30) into Eq. (29). Since

$$\mathcal{N}\mathcal{A}\mathcal{N} = \mathcal{N}\sum_{\tau\tau'}\mathcal{A}_{\tau\tau'}$$

is true for any matrix $\mathcal{A}$, we can readily show that

$$\overrightarrow{r}\overrightarrow{t}^{-1} = -i\mathcal{K}\overleftarrow{e}^{-1}\mathcal{G}\cdot\mathcal{N}\overrightarrow{e}\overrightarrow{\mathcal{E}}^{-1}, \tag{33}$$

$$\overrightarrow{t}^{-1}\overleftarrow{r} = -i\mathcal{K}\overrightarrow{e}^{-1}\mathcal{G}\cdot\mathcal{N}\overleftarrow{e}\overleftarrow{\mathcal{E}}^{-1}, \tag{34}$$

$$\overrightarrow{r}\overrightarrow{t}^{-1}\overleftarrow{r} = -i\mathcal{K}\overleftarrow{e}^{-1}(\mathcal{B} - \mathcal{G})\cdot\mathcal{N}\overleftarrow{e}\overleftarrow{\mathcal{E}}^{-1}. \tag{35}$$

Then, Eq. (29) after division by $\mathcal{K}$ on the left and multiplication by $\mathcal{E} \equiv \overrightarrow{\mathcal{E}}$ on the right becomes

$$\mathcal{R} - \overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}} = -i(\mathcal{R}\mathcal{K}\overrightarrow{e}^{-1} + \overleftarrow{e}^{-1})\mathcal{G}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}), \tag{36}$$

and it can be rewritten in the form

$$(\mathcal{R} - \overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}})[1 + i\mathcal{K}\overrightarrow{e}^{-1}\mathcal{G}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}})]$$
$$= -i(\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}\mathcal{K}\overrightarrow{e}^{-1} + \overleftarrow{e}^{-1})\mathcal{G}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}),$$

which leads to

$$(R - \overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}) = -i(\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}\mathcal{K}\overrightarrow{e}^{-1} + \overleftarrow{e}^{-1})\mathcal{G}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}})$$
$$\times[1 + i\mathcal{K}\overrightarrow{e}^{-1}\mathcal{G}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}})]^{-1}$$
$$= -i(\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}\mathcal{K}\overrightarrow{e}^{-1} + \overleftarrow{e}^{-1})\mathcal{S}\cdot\mathcal{N}(\overrightarrow{e} + \overleftarrow{e}\mathcal{K}\overleftarrow{\mathcal{E}}^{-1}\mathcal{R}\overrightarrow{\mathcal{E}}), \tag{37}$$

where the matrix $\mathcal{S}$ acts in the space of the indices α and is described by the equation

$$\mathcal{S} - \mathcal{G} = -i\mathcal{S}\mathcal{T}\mathcal{G} = -i\mathcal{G}\mathcal{T}\mathcal{S}, \quad \mathcal{S} = (1 + i\mathcal{G}\mathcal{T})^{-1}\mathcal{G} = \mathcal{G}(1 + i\mathcal{T}\mathcal{G})^{-1}, \tag{38}$$

whereas the matrix $\mathcal{T}$ also acts in the space of the indices α and consists of the elements

$$\mathcal{T}_{\alpha\alpha'} = \sum_{\tau\tau'}(\overrightarrow{e}_{\tau\alpha}\delta_{\tau\tau'} + \overleftarrow{e}_{\tau\alpha}\mathcal{K}_\tau\overleftarrow{\mathcal{E}}^{-1}_\tau\mathcal{R}_{\tau\tau'}\overrightarrow{\mathcal{E}}_{\tau'})\mathcal{K}_{\tau'}\overrightarrow{e}^{-1}_{\tau'\alpha'}. \tag{39}$$

It can be written in the form $\mathcal{T} = \mathcal{D} + \mathcal{Q}_r$, where the matrix $\mathcal{Q}$ is defined by Eq. (32) and the matrix $\mathcal{D}$ consists of the elements

$$\mathcal{D}_{\alpha\alpha'} = \sum_{\tau\tau'}\overleftarrow{e}_{\tau\alpha}\mathcal{K}_\tau\overleftarrow{\mathcal{E}}^{-1}_\tau\mathcal{R}_{\tau\tau'}\overrightarrow{\mathcal{E}}_{\tau'}\mathcal{K}_{\tau'}\overrightarrow{e}^{-1}_{\tau'\alpha'}. \tag{40}$$

However, since $\mathcal{G}(1 + i\mathcal{Q}\mathcal{G})^{-1} = \mathcal{B}$, as deduced from Eq. (31), we find that

$$\mathcal{S} = \mathcal{B}(1 + i\mathcal{D}\mathcal{B})^{-1}. \tag{41}$$

Usually the scattering by a monolayer is weak, so that the elements of the matrix $\mathcal{D}\mathcal{B}$ are small and we can assume that $\mathcal{S} = \mathcal{B}$.

It follows from Eq. (37) and (41) that the matrix elements can again be represented in a form similar to Eq. (8). However, in the case of an arbitrary cell these elements are generally asymmetric so that it is more convenient to solve Eq. (37) directly for the matrix elements $\mathcal{R}_{\tau\tau'}$:

$$\mathcal{R}_{\tau\tau'} = -i\sum_\alpha\left\{\left[\sum_{\tau''}(\overleftarrow{\mathcal{E}}^{-1}_\tau\mathcal{R}_{\tau\tau''}\overrightarrow{\mathcal{E}}_{\tau''}\mathcal{K}_{\tau''}\overleftarrow{e}^{-1}_{\alpha\tau''}) + \overleftarrow{e}^{-1}_{\alpha\tau}\right]b_\alpha \times\left[\overrightarrow{e}_{\alpha\tau'} + \sum_{\tau''}(\overleftarrow{e}_{\alpha\tau''}\mathcal{K}_{\tau''}\overleftarrow{\mathcal{E}}^{-1}_{\tau''}\mathcal{R}_{\tau''\tau'}\overrightarrow{\mathcal{E}}_{\tau'})\right]\right\}\Big/(1 - \overleftarrow{\mathcal{E}}^{-1}_\tau\overrightarrow{\mathcal{E}}_{\tau'}). \tag{42}$$

All the terms on the right-hand side of Eq. (42) are small with the exception of those cases when the denominators are small. In fact, only the "resonance" terms characterized by small denominators are important. There are only a few resonance terms, so that the system of equations is finite and readily soluble to the desired accuracy by modern computers. The nonresonance terms are readily calculated employing perturbation theory. In the first approximation, we can assume that these terms are

$$\mathcal{R}_{\tau\tau'} = -i\sum_\alpha\overleftarrow{e}^{-1}_{\alpha\tau}b_\alpha\overrightarrow{e}_{\alpha\tau'}/\{1 - \exp[il_\perp(k_{\tau\perp} + k_{\tau'\perp})]\}. \tag{43}$$

If the product $\mathscr{D}\mathscr{B}$ in Eq. (41) cannot be ignored (which is true of the tight-binding case), then Eq. (42) becomes somewhat more complex, but it is still fully soluble by modern computers to any desired accuracy.

4. EXAMPLES

1. The solution of Eq. (42) is obtained most simply in the presence of just one resonance term. This corresponds to the two-wave approximation in the conventional theory of diffraction. One matrix element $x = \mathscr{R}_{\tau\tau'}$ is then important. If the amplitudes b_α are scalars, then x satisfies the quadratic equation

$$i(1-e)x=f+ex(1/k_{2\perp}+1/k_{1\perp})+f^*(ex)^2/k_{1\perp}k_{2\perp}, \qquad (44)$$

where

$$f=\sum b_\alpha \exp[i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}_\alpha], \quad f^*=\sum b_\alpha \exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}_\alpha],$$
$$\mathbf{k}_1=\vec{\mathbf{k}}_{\tau'}, \quad \mathbf{k}_2=\overleftarrow{\mathbf{k}}_{\tau}, \quad e=\exp[i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{l}]. \qquad (45)$$

The solution of Eq. (42) can be represented in the form

$$x=-(k_{1\perp}k_{2\perp})^{1/2}\exp(i\varphi)\,[(F_1^+)^{1/2}-(F_1^-)^{1/2}]/[(F_1^+)^{1/2}+(F_1^-)^{1/2}], \qquad (46)$$

where

$$\exp(i\varphi)=\exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{l}]\,(f/f^*)^{1/2}, \qquad (47)$$

$$F_1^{\pm}=k_{1\perp}+k_{2\perp}+ik_{1\perp}k_{2\perp}\{1-\exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{l}]\}$$
$$\pm 2|f|(k_{1\perp}k_{2\perp})^{1/2}. \qquad (48)$$

We can readily see that if the element $\mathscr{R}_{\tau'\tau}$, also exhibits a resonance, the expression for this element is found to be of the same type as that given by Eq. (46), but in Eqs. (47) and (48) we have to make the substitution $(\mathbf{k}_1-\mathbf{k}_2)_\parallel \mathbf{l} \to -(\mathbf{k}_1-\mathbf{k}_2)_\parallel \mathbf{l}$.

For $\tau=\tau'$, we are dealing with purely specular reflection and the amplitude of this reflection $R = x/k_{2\perp}$ is described—as demonstrated by Eq. (46)—by the expression

$$R=-\exp[-2ik_{1\perp}l_\perp]\,(f/f^*)^{1/2}$$
$$\times[(F_2^+)^{1/2}-(F_2^-)^{1/2}]/[(F_2^+)^{1/2}+(F_2^-)^{1/2}], \qquad (49)$$

where

$$F_2^{\pm}=1\pm|f|+ik_{1\perp}[1-\exp(-2ik_{1\perp}l_\perp)]/2. \qquad (50)$$

Since in the case of a "resonance" we characteristically have $2k_{1\perp}l_\perp \approx 2\pi n$, it follows that on the assumption that $k_0=\pi n/l_\perp$, we can use an approximate equation

$$ik_{1\perp}[1-\exp(-2ik_{1\perp}l_\perp)]$$
$$\approx i[k_{1\perp}+k_0)/2]2i(k_{1\perp}-k_0)l_\perp=-(k_{1\perp}^2-k_0^2)l_\perp, \qquad (51)$$

and, recalling that all the lengths are expressed in units of $1/2\pi N_2 b_c$, we obtain the amplitude of the specular (Bragg) reflection in the form

$$R=\exp(i\varphi)\,[(E-E_0)^{1/2}-(E-E_0-2u_0|f|)^{1/2}]/$$
$$[(E-E_0)^{1/2}+(E-E_0-2u_0|f|)^{1/2}], \qquad (52)$$

where dimensional quantities are used and the following notation is employed

$$E=k_{1\perp}^2, \quad E_0=k_0^2+u_0(1-|f|), \quad u_0=4\pi N_0 b_c, \quad N_0=N_2/l_\perp. \qquad (53)$$

If $k_{1\perp}l_\perp \ll 1$, we obtain the familiar expression describing specular reflection of slow electrons:

$$R=[k_{1\perp}-(k_{1\perp}^2-u_0)^{1/2}]/[k_{1\perp}+(k_{1\perp}^2-u_0)^{1/2}]. \qquad (54)$$

2. We now consider the scattering of a neutron by a magnetic crystal (allowing for the nuclear and electron magnetism). At each point inside such a crystal there is a field $\mathbf{H}(\mathbf{r})$ and the amplitude of the magnetic scattering by a unit volume d^3r is $B^i=\mu\boldsymbol{\sigma}\mathbf{H}(\mathbf{r}_i)d^3r_i$, i.e., it is a spinor. Moreover, each matrix element $\mathscr{R}_{\tau\tau'}$ is also a spinor. In the presence of just one resonance term we again have a second-order equation, but the sequence of the factors in this equation has to be maintained strictly.

If the field $\mathbf{H}$ inside the unit cell is homogeneous, then the direction of this field can be selected as the spin quantization axis and we can separate the equation for the spin matrix $R_{\tau\tau'}$ into two scalar equations representing the two polarizations of a neutron parallel and antiparallel to the field $\mathbf{H}$. Bearing in mind that, in addition to the magnetic scattering process, there is also the purely nuclear scattering, we can obtain the solution for the diffraction of a spinor neutron in the same form as in the case of a scalar neutron, but the coherent scattering amplitude of the cell b_c for two different polarizations should now be the sum or difference between the nuclear and magnetic amplitudes.

In the presence of an inhomogeneous field, we can assume for the sake of simplicity that

$$\int \mathbf{H}(\mathbf{r}_i)\,d^3r_i=0, \qquad (55)$$

i.e., the magnetic field averaged over the cell is zero, so that the equation for x allowing for the magnetic scattering process is

$$i(1-e)x=f+\mathbf{h}\boldsymbol{\sigma}+ex(1/k_{2\perp}+1/k_{1\perp})+x(f^*+\mathbf{h}^*\boldsymbol{\sigma})xe^2/k_{1\perp}k_{2\perp}, \qquad (56)$$

where

$$\mathbf{h}=\int \mathbf{H}(\mathbf{r}_i)\exp[i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}_i]\,d^3r_i,$$
$$\mathbf{h}^*=\int \mathbf{H}(\mathbf{r}_i)\exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}_i]\,d^3r_i. \qquad (57)$$

Multiplying both sides of Eq. (52) on the left by $(f^*\mathbf{h}^*\boldsymbol{\sigma})$ and denoting the product $(f^*+\mathbf{h}^*\boldsymbol{\sigma})x$ by y, we obtain the readily soluble equation for y:

$$i(1-e)y=Q^2+ey(1/k_{2\perp}+1/k_{1\perp})+(ey)^2/k_{1\perp}k_{2\perp}, \qquad (58)$$

where

$$Q^2=(f^*+\mathbf{h}^*\boldsymbol{\sigma})(f+\mathbf{h}\boldsymbol{\sigma}). \qquad (59)$$

It follows from Eqs. (56)–(58) that the spinor scattering amplitude R reduces to

$$R=-\exp[i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{l}]\,(f^*+\mathbf{h}^*\boldsymbol{\sigma})^{-1}Q(k_{1\perp}/k_{2\perp})^{1/2}$$
$$\times[(F_3^+)^{1/2}-(F_3^-)^{1/2}]/[(F_3^+)^{1/2}+(F_3^-)^{1/2}], \qquad (60)$$

where

$$F_3^{\pm}=k_{1\perp}+k_{2\perp}+ik_{1\perp}k_{2\perp}\{1-\exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{l}]\}\pm 2Q(k_{1\perp}k_{2\perp})^{1/2}, \quad (61)$$

$$Q^2=|f|^2+|\mathbf{h}|^2+\{2\,\mathrm{Re}\,(f\mathbf{h})-\mathrm{Im}\,([\mathbf{h}^*\mathbf{h}])\}\boldsymbol{\sigma}\equiv\alpha+\boldsymbol{\beta}\boldsymbol{\sigma}, \quad (62)$$

$$Q=\{[\alpha+(\alpha^2-\beta^2)^{1/2}]^{1/2}+(\beta/\beta)\sigma[\alpha-(\alpha^2-\beta^2)^{1/2}]^{1/2}\}/2^{1/2}. \quad (63)$$

Note that although the average field vanishes, magnetic scattering still takes place. In particular, neutron reflection may polarize an unpolarized beam and depolarize a polarized one. However, if we ignore the polarizations, we still must bear in mind that the magnetic form factor influences the overall scattering process. It must be allowed for in, for example, determination of the n–e scattering amplitude.[12,13] This magnetic form factor may explain also the anomalies of the scattering of slow neutrons by tungsten.

In fact, if the average field vanishes, i.e., when the condition (55) is satisfied but the form factor of this field given by Eq. (57) differs from zero, the intensity of the diffraction peaks (hkl) for an unpolarized neutron beam considered in the kinematic approximation can be written in the form[13]

$$I_{(hkl)}=K[(a+Zf_{(hkl)}a_{ne})^2+(1-f_{(hkl)})^2\gamma^2\,\mathrm{ctg}^2\,\vartheta_{(hkl)} +a^2|\mathbf{h}_{(hkl)}|^2]A_{(hkl)}\exp(-2W_{(hkl)})/\sin 2\vartheta_{(hkl)}, \quad (64)$$

where K is a coefficient constant for all the reflections; a is the coherent scattering length of a tungsten nucleus; Z is the number of electrons in an atom; $f_{(hkl)}$ is the atomic electric form factor of tungsten; a_{ne} is the scattering length due to the n–e interaction; $A_{(hkl)}$ is the absorption factor; $\vartheta_{(hkl)}$ is the Bragg angle; $\exp(-W_{(hkl)})$ is the Debye–Waller factor where $W=B(\sin\vartheta/\lambda)^2$, and λ is the neutron wavelength; $\gamma^2\,\mathrm{ctg}^2\,\vartheta$, where $\gamma=(\mu_n\hbar/2Mc)(Ze^2/\hbar c)$ allows for the Schwinger scattering; and $|\mathbf{h}|$ is the magnetic scattering form factor reduced to the coherent amplitude a. Comparing Eq. (64) above with Eq. (2) in Ref. 12, we can see that $a|\mathbf{h}|$ acts as the anomalous amplitude p introduced in Ref. 13 to account for the anomalous scattering by tungsten.

Naturally, the above results do not exclude the possibility that the anomalous amplitude p may be partly associated with the magnetic variation representing inclusions of foreign magnetic atoms in the tungsten matrix. The magnetic scattering effect discussed above can be distinguished by investigating the diffraction of polarized neutrons. In the case of a thick crystal when the polarization of the reflected neutrons is of no interest, the reflection coefficient deduced from Eq. (60) is

$$|R|^2k_{2\perp}/k_{1\perp}=|[(F_3^+)^{1/2}-(F_3^-)^{1/2}]/[(F_3^+)^{1/2}+(F_3^-)^{1/2}]|^2. \quad (65)$$

This reflection coefficient may differ considerably for neutrons polarized parallel and antiparallel to the vector $\boldsymbol{\beta}$, as defined by Eq. (62). Naturally, a similar dependence of the intensity of reflection on the polarization of the incident neutrons can be derived also for the case of a thin crystal. Unfortunately, the direction of the vector $\boldsymbol{\beta}$ must also be found experimentally.

It should be noted that the form factor $|\mathbf{h}|$ generally varies nonmonotonically with transferred momentum. This can account, in particular, for the anomalous increase in the amplitude of some of the reflections reported in Ref. 14.

The scattering discussed here is not paramagnetic. It may be due to different deformations of the electron shells with opposite spins. Determination of this deformation with the aid of neutrons would be very useful in studies of the behavior of atomic electrons in solids.

5. CONCLUSIONS

We considered the simplest cases as examples because investigation of these cases would not require the use of computers. However, if computers are used, we can deduce immediately the reflection spectrum for a given structure of a single crystal both for x rays and for neutrons. Moreover, we can find not only the positions of the peaks, which can be deduced from the simplest considerations without invoking the procedures described above, but also the structure of each peak. This is particularly important because if the resolution is sufficiently high, we can then determine the crystal structure from a single peak without any need for a Fourier analysis of the spectrum.

The problem of the scattering by point scatterers was solved earlier. By way of example, we can cite the work reported in Refs. 15–18. However, the methods employed in these investigations are not physically clear and are too mathematical, so that the solutions were obtained in a form difficult to interpret physically.

A multilayer description of the crystal is encountered quite frequently in the literature.[18,19] However, in such cases no allowance is made for the diffraction by one layer, since this diffraction is allowed for by specifying the required combination of the wave fields which are then reflected between the layers as a whole. In either case it is not possible to describe consistently the Laue diffraction process.

The method used above is physically clear, completely closed, provides a unified description of the Bragg and Laue diffraction cases, and can be employed in calculations of any number of reflections with any degree of accuracy.

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Translated by A. Tybulewicz