Interference of inelastic scattering channels during motion of a fast particle in matter

É. A. Kantsyper

Tallin Electronics Institute
(Submitted 28 February 1992; resubmitted 15 June 1992)
Zh. Eksp. Teor. Fiz. **102**, 1259–1279 (October 1992)

A diagram technique is proposed for describing elastic and inelastic scattering of particles in matter. The technique is used to construct a theory of the interference of physically different inelastic scattering channels for a fast particle moving in matter. It is shown that the wave function of a particle undergoing inelastic scattering of particular physical nature must take into account the damping of the wave field of the particle both before and after the inelastic collision; in addition, all inelastic processes, including the process in question, contribute to the damping. It is determined that when the two-state approximation (employed in the classical theory of the optical potential) is used to describe the interference of inelastic collisions in matter, the quantum-mechanical reciprocity theorem is violated. As an illustration of the application of the formalism developed, competition with inelastic collisions is examined in detail when a fast electron undergoes diffraction channeling in a single crystal. It is found that when the inelastic scattering channel singled out corresponds to generation of a bulk plasmon, the competition between inelastic collisions is the determining physical mechanism responsible for the pronounced orientational dependence of the cross section of the corresponding inelastic process. Other possible manifestations of the interference of inelastic collisions of different physical nature are discussed.

1. INTRODUCTION

The interference of different scattering channels as a physical phenomena has been known for a long time. In spite of this, a satisfactory general theory has been constructed only in the case when a particular elastic scattering channel is affected by all other scattering channels (both inelastic and other elastic channels).[1)] Physically, an effect of this type results in ejection particles from the initial energy state and it changes the character of the initial spatial localization (coherence) of the particles through different elastic and inelastic collision events. Formally, this process is determined completely by the amplitude of elastic scattering of a particle at zero angle[1] and results in spatial damping of the wave function of the particle in the particular elastic scattering channel as the particle propagates in the scattering medium; in both the Schrödinger-equation formalism[2] and the quantum kinetic-equation formalism[3] this process corresponds to an effective complex scattering potential, called the optical potential.

The effect of elastic scattering channels on a particular inelastic channel can also, in principle, be given a general description.

The interaction of elastic and inelastic scattering channels is most clearly manifested in the case of scattering of particles in spatially nonuniform media. In this case, the interference of these scattering channels can become so important that it has to be treated systematically in order to explain the physics of phenomena such as the anomalous passage of particles in a crystal (the Borrmann effect),[4] to predict the appearance of bremmstrahlung of longitudinal electromagnetic waves, which is associated with excitation of delocalized electronic states by the charged particle,[5] and to show that this phenomena, which is of general physical interest, can in principle be observed directly.[6]

In this context the problem of the interaction of different inelastic scattering channels is less obvious. This is apparently due to two basic factors. First, inelastic scattering is more complicated than elastic scattering. Second, different inelastic scattering channels can have a significantly different physical nature, and this makes it extremely difficult to describe them together on the basis of a single microscopic theory. In this respect, it should be noted that we know of only one work (Ref. 7) in which the interaction of inelastic scattering channels of the same nature is taken into account systematically (the effect of the surface plasmon excitation channel on the channel associated with the bulk plasmon). It seems that the coupling of the inelastic scattering channels, as also the interaction of elastic and inelastic scattering channels, will be pronounced in spatially inhomogeneous media, for example, crystals. In this connection, as an application of the general theory developed below in Secs. 2–5, we examine in detail in Sec. 6 the competition between inelastic collisions of different physical nature when a fast charged particle in a single crystal experiences diffraction channeling.

2. SYSTEM OF COUPLED SCHRÖDINGER EQUATIONS FOR A PARTICLE UNDERGOING SCATTERING IN MATTER

The wave function $\Psi(\mathbf{r},\mathbf{R})$ of the particle-medium system satisfies the Schrödinger equation

$$\Delta\Psi(\mathbf{r},\mathbf{R})+\frac{2m}{\hbar^2}[E-\hat{H}(\mathbf{r},\mathbf{R})-\hat{H}_s(\mathbf{R})]\Psi(\mathbf{r},\mathbf{R})=0, \quad (1)$$

where $\mathbf{r}$ is the radius vector of the particle under consideration, $\mathbf{R}$ designates the set of radius vectors of the scattering centers of the medium, E is the energy of the system, $\hat{H}(\mathbf{r},\mathbf{R})$ is the Hamiltonian describing the interaction between the particle and the scattering medium, and $\hat{H}_s(\mathbf{R})$ is the interaction Hamiltonian for the particles of the medium themselves.

If the velocity v of a particle is much higher than the velocities v_s of the scattering centers of the medium,[2)] then

 0038-5646/92/100683-10$05.00

the total wave function $\Psi(\mathbf{r},\mathbf{R})$ can be expanded in a series in the complete set of wave functions $|\Phi_k(\mathbf{R})\rangle$ of the system of scattering centers:[1]

$$\Psi(\mathbf{r},\mathbf{R})=\sum_k \varphi_k(\mathbf{r})\,|\Phi_k(\mathbf{R})\rangle. \qquad (2)$$

Substituting Eq. (2) into Eq. (1) and expanding in the bra vectors $\langle\Phi_i|$ and $\langle\Phi_n|$ of the ground (i) and excited (n) states of the medium, respectively, we obtain a system of coupled equations for the wave functions $\varphi_k(\mathbf{r})$ of the scattered particle

$$\Delta\varphi_i(\mathbf{r})+\frac{2m}{\hbar^2}[E-\varepsilon_i-U_i(\mathbf{r})]\varphi_i(\mathbf{r})=\frac{2m}{\hbar^2}\sum_{k\neq i} H_{ik}(\mathbf{r})\varphi_k(\mathbf{r}),$$
$$\Delta\varphi_n(\mathbf{r})+\frac{2m}{\hbar^2}[E-\varepsilon_n-U_n(\mathbf{r})]\varphi_n(\mathbf{r})=\frac{2m}{\hbar^2}\sum_{k\neq n} H_{nk}(\mathbf{r})\varphi_k(\mathbf{r}). \qquad (3)$$

In Eq. (3) the matrix element $H_{mk}(\mathbf{r})$ is determined by the formula

$$H_{mk}(\mathbf{r})=\int d\mathbf{R}\,\Phi_m^*(\mathbf{R})\hat{H}(\mathbf{r},\mathbf{R})\Phi_k(\mathbf{R}), \qquad (4)$$

and the diagonal matrix element $H_{mm}(\mathbf{r})$ is denoted as $U_m(\mathbf{r})$; the quantities ε_i and ε_n are the energies of the particles of the medium in the ground and excited states. The wave function $\varphi_k(\mathbf{r})$ determines the probability amplitude for observing the scattered particle at the point $\mathbf{r}$ and the scattering medium in the state k.

For convenience, we now switch to the operator form of the system (3) of the coupled equations. We introduce the differential tensor operator $\hat{G}^{-1}(\mathbf{r})$, whose mk th element is determined by the relations

$$\hat{G}_{mk}^{-1}(\mathbf{r})=\hat{G}_m^{-1}(\mathbf{r})\delta_{mk},$$
$$\hat{G}_m^{-1}(\mathbf{r})=\hbar^2(\Delta+k_m^2)/2m-U_m(\mathbf{r}). \qquad (5)$$

The operator $\hat{G}^{-1}$ is the inverse of the integral tensor operator $\hat{G}$ with elements $\hat{G}_{mk}=\hat{G}_m\delta_{mk}$; here

$$\hat{G}_m f(\mathbf{r})=\int d\mathbf{r}'\mathscr{G}_m(\mathbf{r},\mathbf{r}',E-\varepsilon_m)f(\mathbf{r}'), \qquad (6)$$

where $\mathscr{G}_m(\mathbf{r},\mathbf{r}',E-\varepsilon_m)=\langle\mathbf{r}|\hat{G}_m|\mathbf{r}'\rangle$ is the Green's function of the scattered particle and is determined by the differential equation

$$\left[\Delta+k_m^2-\frac{2m}{\hbar^2}U_m(\mathbf{r})\right]\mathscr{G}_m(\mathbf{r},\mathbf{r}',E-\varepsilon_m)=\frac{2m}{\hbar^2}\delta(\mathbf{r}-\mathbf{r}'). \qquad (7)$$

In Eqs. (5) and (7) we have written $k_m^2=2m\hbar^{-2}(E-\varepsilon_m)$.

With the help of the definitions (5)–(7) the system (3) of coupled equations can be rewritten in a form convenient for further analysis:

$$\hat{G}_i^{-1}\varphi_i(\mathbf{r})=\sum_{k\neq i} H_{ik}(\mathbf{r})\varphi_k(\mathbf{r}),$$
$$\hat{G}_n^{-1}\varphi_n(\mathbf{r})=\sum_{k\neq n} H_{nk}(\mathbf{r})\varphi_k(\mathbf{r}). \qquad (8)$$

3. POLARIZATION SCATTERING OPERATOR

The system (8) of coupled equations makes it possible to perform a formal analysis of the effect of inelastic scattering channels on the channel coupled with an elastic channel without any additional assumptions. In order to avoid involved calculations, however, we shall examine this problem in the two-state approximation,[2] which makes it possible to obtain the actual result immediately.

The crux of the two-state approximation is the assumption that all quantum transitions of the system out of the ground state i into some excited state n proceed without additional intermediate excited states. The formal consequence of this approximation is the vanishing of the matrix elements H_{mk} of the particle-medium interaction operator one of whose indices is not equal to the index i of the ground state, (this property does not pertain to the diagonal matrix elements).

In the two-state approximation the system (8) of coupled equations acquires the form

$$\hat{G}_i^{-1}\varphi_i(\mathbf{r})=\sum_{k\neq i} H_{ik}(\mathbf{r})\varphi_k(\mathbf{r}),$$
$$\varphi_n(\mathbf{r})=\hat{G}_n H_{ni}(r)\varphi_i(\mathbf{r}). \qquad (9)$$

The question of justifying the two-state approximation, which actually reduces to truncating the infinite series in Eq. (8), remains open from a theoretical standpoint for a wide class of physical systems, because it requires estimation of the matrix elements of the interaction operator $\hat{H}$. It is obvious that this problem cannot be solved in its general form. At the same time, if the result of solving Eq. (8) in this approximation contradicts some general physical principles, then this approximation is unsatisfactory. In particular, we show in Sec. 5 that the two-state approximation cannot be used to describe the coupling of inelastic collisions in matter, since it leads to violation of the quantum-mechanical reciprocity theorem.

It follows from Eq. (9) that the wave function $\varphi_i(\mathbf{r})$ of a particle in the input channel satisfies the equation

$$\left[\hat{G}_i^{-1}-\left(\sum_{k\neq i} H_{ik}\hat{G}_k H_{ki}\right)\right]\varphi_i(\mathbf{r})=0, \qquad (10)$$

which is the Schrödinger equation with the effective nonlocal potential (see, for example, Ref. 8):

$$A_i(\mathbf{r},\mathbf{r}')=\langle\mathbf{r}|\hat{A}_i|\mathbf{r}'\rangle=\sum_{k\neq i} H_{ik}(\mathbf{r})\mathscr{G}_k(\mathbf{r},\mathbf{r}',E-\varepsilon_k)H_{ki}(\mathbf{r}'). \qquad (11)$$

The solution of Eq. (10) can be represented in the form of an infinite series

$$\varphi_i(\mathbf{r})=\varphi_i^0(\mathbf{r})+\hat{G}_i\left(\sum_{k\neq i} H_{ik}\hat{G}_k H_{ki}\right)\varphi_i^0(\mathbf{r})$$
$$+\hat{G}_i\left(\sum_{k\neq i} H_{ik}\hat{G}_k H_{ki}\right)\hat{G}_i\left(\sum_{m\neq i} H_{im}\hat{G}_m H_{mi}\right)\varphi_i^0(\mathbf{r})+\ldots, \qquad (12)$$

in which the function $\varphi_i^0(\mathbf{r})$ satisfies the equation

$$\hat{G}_i^{-1}\varphi_i^0(\mathbf{r})=0. \qquad (13)$$

We note that each term in Eq. (12) has a clear physical meaning, which makes it possible to represent the wave function $\varphi_i(\mathbf{r})$ of a particle in the ith scattering channel in the form of a set of diagrams. The first term corresponds to the wave field of the particle in the absence of any effect due to inelastic collisions. The second term,

$$\hat G_i \hat A_i \varphi_i^0 = \hat G_i \left(\sum_{k\neq i} H_{ik}\hat G_k H_{ki}\right)\varphi_i^0,$$

describes the particle moving in the elastic channel so that it undergoes two successive inelastic collisions whose overall effect is that the particle remains in the elastic channel. It is natural to call such generation-absorption collisions polarization collisions. The higher-order terms in Eq. (12) correspond to polarization collisions of higher orders. This interpretation of the expansion under consideration makes it possible to represent this expansion as an infinite set of diagrams (see Fig. 1a).[3] The large hatched arrow in the diagrams corresponds to the wave function φ_i of the particle in the elastic channel, taking into account the effect of inelastic collisions; the large unhatched arrow designates the wave function φ_i^0 of the particle in the absence of inelastic collisions. A thin solid line with an arrow corresponds to the Green's operator $\hat G$ of the fast particle, describing the evolution of the wave field of the particle between two successive collisions; a dashed line with an arrow directed away from a vertex corresponds to an inelastic collision accompanied by energy loss by the particle moving in the medium (depleting collision); correspondingly, a similar line with an arrow entering a vertex describes a collision accompanied by an increase in the energy of the fast particle (absorbing collision).

The infinite sequence of diagrams shown in Fig. 1a can be summed, as a result of which the wave function of the particle in the elastic channel will be determined by the diagram shown in Fig. 1b. The hatched half-circle in this diagram corresponds to an infinite sum of polarization loops (see Fig. 1c). The result of summation of the diagrams can be represented in the analytical form

$$\varphi_i(\mathbf r) = [\hat I + \hat G_i \hat\Sigma^i_{pol}]\varphi_i^0(\mathbf r). \tag{14}$$

Here $\hat I$ is the unit operator and the operator $\hat\Sigma^i_{\rm pol}$ represents the result of summing an infinite sequence of polarization loops (Fig. 1c).

On the other hand, it is well known (see, for example,

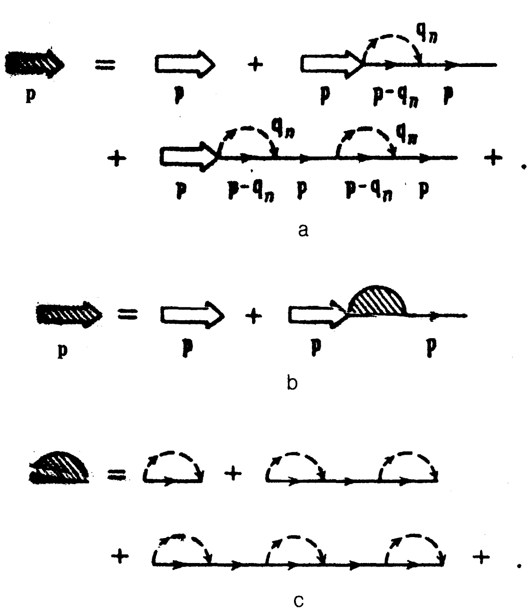

FIG. 1. Diagrammatic representation of the elastic scattering process; **p** is the momentum of the particle in the initial state and $\mathbf q_n$ is the momentum lost by the particle in an inelastic collision.

Refs. 2 and 8) that when polarization processes are included, the wave field of the fast particle decays in the matter:

$$\varphi_i(\mathbf r) = \hat{\mathscr R}_i \varphi_i^0(\mathbf r), \tag{15}$$

where

$$\hat{\mathscr R}_i = \hat I + \hat G_i \hat\Sigma^i_{pol} \tag{16}$$

is the polarization operator. In the language of differential equations for the wave field of the particle, this means that the function $\hat{\mathscr R}_i\varphi_i^0$, in contrast to the function φ_i^0, satisfies the Schrödinger equation with the effective nonlocal potential (11):

$$\hat G_i^{-1}(\hat{\mathscr R}_i\varphi_i^0) - \left(\sum_{k\neq i} H_{ik}\hat G_k H_{ki}\right)(\hat{\mathscr R}_i\varphi_i^0) = 0. \tag{17}$$

The boundary conditions for the function $\hat{\mathscr R}_i\varphi_i^0$ are identical to the boundary conditions for the function $\varphi_i^0(\mathbf r)$. Correspondingly, the equation for the Green's operator $\hat{\mathscr R}_i\hat G_i$ of the particle in the coordinate representation will also differ from the equation for $\langle \mathbf r|\hat G_i|\mathbf r'\rangle$ in having a nonlocal potential:

$$\hat G_i^{-1}(\mathbf r)\langle \mathbf r|\hat{\mathscr R}_i\hat G_i|\mathbf r'\rangle - \frac{2m}{\hbar^2}\int d\mathbf r'' A_i(\mathbf r,\mathbf r'')\langle \mathbf r''|\hat{\mathscr R}_i\hat G_i|\mathbf r'\rangle = \frac{2m}{\hbar^2}\delta(\mathbf r-\mathbf r'). \tag{18}$$

The boundary conditions for $\langle \mathbf r|\hat{\mathscr R}_i\hat G_i|\mathbf r'\rangle$ are identical to those for $\langle \mathbf r|\hat G_i|\mathbf r'\rangle$.

Thus we have determined the action of the polarization operator, associated with the summation of an infinite sequence of polarization diagrams, on the wave functions and the propagator.

4. INTERFERENCE OF INELASTIC SCATTERING CHANNELS OF ARBITRARY PHYSICAL NATURE

When a fast particle moves through a medium, different physical processes can occur. As a rule, besides the elastic scattering channel, several inelastic channels, differing substantially from one another, can play an important role.

Let the total Hamiltonian $\hat H(\mathbf r,\mathbf R)$ of the inelastic interaction of the particle with the medium be additive in all physical processes leading to inelastic scattering of the particle in the matter:

$$\hat H(\mathbf r,\mathbf R) = \hat H^d(\mathbf r,\mathbf R) + \hat H^{bg}(\mathbf r,\mathbf R). \tag{19}$$

In Eq. (19) the Hamiltonian $\hat H^d$ is responsible for inelastic collisions of the fast particle having a particular physical nature. Correspondingly, the remaining collisions, which are different from these collisions, are described by the Hamiltonian $\hat H^{bg}$. We term such collisions background collisions.

We now examine, using the diagrammatic technique constructed in the preceding section, the effect of the background inelastic scattering channels on the inelastic scattering channel which we have distinguished. Far from the energy threshold of $\hat H^d$ scattering, the energies of the particle before and after the collisions of the specified type are virtually identical. This fact makes it possible to describe the interaction of the inelastic scattering channels by means of simple polarization diagrams of the same type as were used in the description of the effect of inelastic scattering channels on the channel associated with elastic scattering.

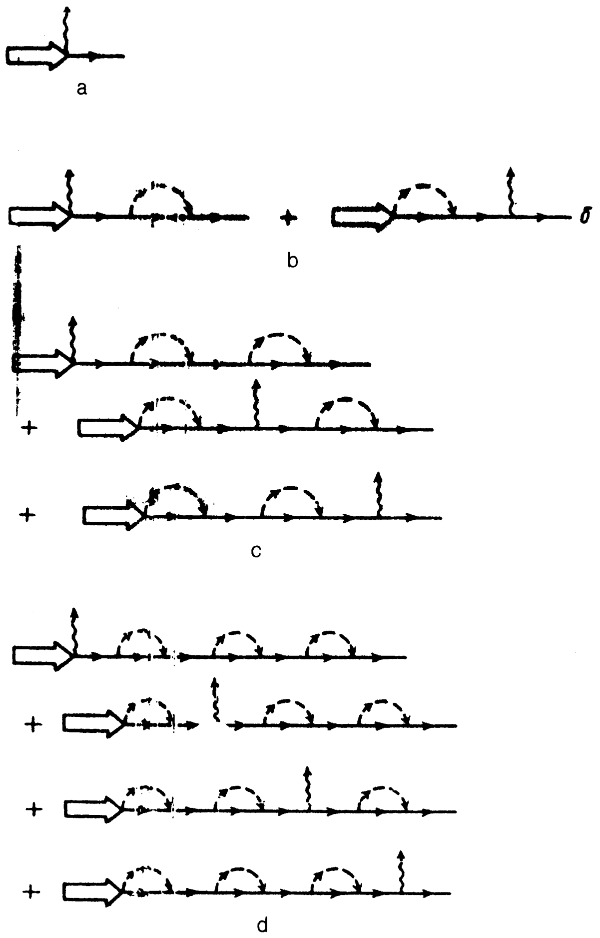

FIG. 2. Diagrammatic representation of the inelastic scattering process; diagrams of the zeroth (a), second (b), fourth (c), and sixth (d) orders in the background interaction.

We study first only effects which are first order in the specified interaction. The wave function $\varphi^{(1)}_{n,d}(\mathbf{r})$ (of first order in $\hat{H}^d$) of the particle which has experienced a single characteristic energy loss $\varepsilon^d_{\text{in}}$ can be represented, in the presence of background inelastic collisions, as an infinite sum of diagrams, some of which are shown in Fig. 2. In addition to the previously adopted graphical designations, a wavy line with an arrow emanating from a vertex corresponds to a collision of the specified nature $\hat{H}^d$, accompanied by energy loss $\varepsilon^d_{\text{in}}$; all polarization loops are due to background collisions.

The diagrams of the infinite series under consideration can be summed. For this, we divide all diagrams in Fig. 2 into four groups. The first group consists of a single diagram, shown in Fig. 2a. The second group contains all diagrams with polarization loops, whose extreme right-hand element is the element shown in Fig. 3a. To such diagrams there is associated a second diagram in Fig. 2b, the third diagram in Fig. 2c, the fourth diagram in Fig. 2d, etc. Their sum, together with the diagram of the first group, is shown in Fig. 4a.

The infinite sequence of diagrams with polarization

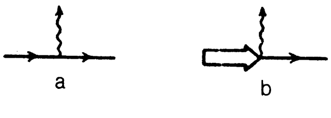

FIG. 3.

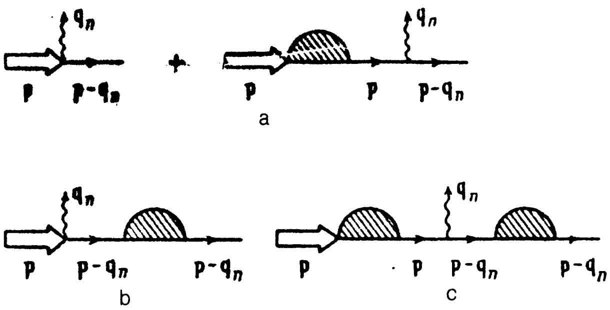

FIG. 4. Summation of diagrams in the theory of inelastic scattering; $\mathbf{p}$ is the momentum of the particle in the initial state and $\mathbf{q}_n$ is the momentum lost by the particle in an inelastic collision of the specified type.

loops, whose extreme left-hand element is the element shown in Fig. 3b, comprises the third group of diagrams. These diagrams consist of the first diagrams in Figs. 2b, c, d, etc. Their sum can be represented by the diagram shown in Fig. 4b. The remaining diagrams with polarization loops comprise the fourth group. Their sum, as one can easily see, is represented by the diagram shown in Fig. 4c. The hatched half-circle in Fig. 4 represents the result of the summation of an infinite sequence of background polarization loops (see Fig. 1c).

Following Fig. 4, we can write down the following expression for the desired wave function $\varphi^{(1)}_{n,d}(\mathbf{r})$:

$$\varphi^{(1)}_{n,d}(\mathbf{r})=\hat{G}_n H_{ni}{}^d\varphi_i{}^0(\mathbf{r})+\hat{G}_n H_{ni}{}^d\hat{G}_i\hat{\Sigma}_{bg}{}^i\varphi_i{}^0(\mathbf{r})$$
$$+\hat{G}_n\hat{\Sigma}_{bg}{}^n\hat{G}_n H_{ni}{}^d\varphi_i{}^0(\mathbf{r})+\hat{G}_n\hat{\Sigma}_{bg}{}^n\hat{G}_n H_{ni}{}^d\hat{G}_i\hat{\Sigma}_{bg}{}^i\varphi_i{}^0(\mathbf{r}).$$

After elementary transformations, we obtain

$$\varphi^{(1)}_{n,d}(\mathbf{r})=(\hat{\mathcal{R}}_n{}^{bg}\hat{G}_n)H_{ni}{}^d(\hat{\mathcal{R}}_i{}^{bg}\varphi_i{}^0). \quad (20)$$

Here the function $\hat{\mathcal{R}}^{bg}_i\varphi^0_i$ satisfies Eq. (17), in which the Hamiltonian $\hat{H}$ is replaced by the Hamiltonian $\hat{H}^{bg}$. Since we are not considering energy threshold effects, far from the energy threshold of the $\hat{H}^d$-scattering channel the energy $E_n=E-\varepsilon_n$ of the particle in the excited state is virtually identical to the energy $E_i=E-\varepsilon_i$ of the particle in the ground state and the propagator satisfies the equation [see Eqs. (11) and (18)]

$$G_n{}^{-1}(\mathbf{r})\langle\mathbf{r}|\hat{\mathcal{R}}_n{}^{bg}\hat{G}_n|\mathbf{r}'\rangle-\frac{2m}{\hbar^2}\int d\mathbf{r}''A_n{}^{bg}(\mathbf{r},\mathbf{r}'')$$
$$\times\langle\mathbf{r}''|\hat{\mathcal{R}}_n{}^{bg}\hat{G}_n|\mathbf{r}'\rangle=\frac{2m}{\hbar^2}\delta(\mathbf{r}-\mathbf{r}'). \quad (21)$$

The nonlocal potential in Eq. (21) is of a background nature and is determined by a formula related to Eq. (11). In order to derive its specific form, generally speaking, we must go beyond the two-state approximation.

Equation (20) means that in order to calculate the wave function of the particle which is first-order in the specified interaction we must take into account the damping of the wave function of the particle both in the initial and final states. The damping of the wave field of the particle in this case is entirely determined by background collisions.

The physics of the result obtained above is quite obvious. The result means that the particle, recorded in the final state as having lost some energy $\varepsilon^d_{\text{in}}$ as a result of a single $\hat{H}^d$ collision, could pass into the excited state n only if before doing so the particle either did not experience any inelastic collisions that would transfer the particle out of the ground state or if the background inelastic collisions were of a polarization character, as a result of which, after a series of background inelastic collisions, the particle once again ended up in the elastic channel. In addition, Eq. (20) takes into account the effect of ejection particles from the final state n as a result of background polarization processes. In this sense, the formula under discussion incorporates the effects of multiple inelastic scattering for background collisions. We note especially that the equal importance of damping for the initial and final states of the particle ensures that the quantum-mechanical reciprocity theorem is satisfied.

In the general case, besides background polarization collisions, polarization collisions of the specified nature will also play a definite role. It is obvious that they lead to the appearance of the $\hat{H}^d$ polarization loops in the diagrams shown in Figs. 2 and 4. It is easy to verify that the summation of these diagrams gives a formula of the type (20), in which the polarization operator $\hat{\mathscr{R}}^{bg}$ will be replaced by the operator $\hat{\mathscr{R}} = \hat{I} + \hat{G}(\hat{\Sigma}_{bg} + \hat{\Sigma}_d)$:

$$\varphi_{n,d}(\mathbf{r}) = (\hat{\mathscr{R}}_n \hat{G}_n) H^d_{ni} (\hat{\mathscr{R}}_i \varphi_i^0). \qquad (22)$$

Thus all possible polarization processes, including the specified polarization processes, will contribute to the effective nonlocal potential (and therefore also to the damping of the wave field in both the initial and final states). This result is less obvious than Eq. (20) and is correct if it is assumed that inelastic collisions of different nature are not correlated.

5. DISCUSSION OF THE TWO-STATE APPROXIMATION IN THE THEORY OF INELASTIC SCATTERING

In deriving the formulas (20) and (22), strictly speaking, we went beyond the two-state approximation, because, as we now show, in the two-state approximation the polarization operator $\hat{\mathscr{R}}_n$ $(n \neq i)$ is identical to the unit operator.

We start from Eqs. (9). If the interaction $\hat{H}^d$ which we have singled out is, in a certain sense, small, then the solution (9) can be expanded in a series in the multiplicity of $\hat{H}^d$ collisions:

$$\varphi_k(\mathbf{r}) = \sum_{\alpha=0}^{\infty} \varphi_k^{(\alpha)}(\mathbf{r}). \qquad (23)$$

The wave function $\varphi_k^{(\alpha)}$ describes a particle which has undergone α collisions of the nature singled out. At the same time, this function is already "summed" over all $\hat{H}^{bg}$ collisions. The latter fact means that when we consider a specific $\hat{H}^d$ collision, we take into account fully the effect of all inelastic scattering processes of the remaining (background) nature on this collision. Assuming the dependence of the Green's operator $\hat{G}$ on the Hamiltonian $\hat{H}$ is weak,[8] we obtain from Eqs. (9), (19), and (23) a system of coupled recurrence equations for the successive wave functions:

$$\varphi_i^{(\alpha)}(\mathbf{r}) = \hat{G}_i \Big[\sum_{k\neq i} H_{ik}{}^d \varphi_k^{(\alpha-1)}(\mathbf{r}) + \sum_{k\neq i} H_{ik}^{bg} \varphi_k^{(\alpha)}(\mathbf{r}) \Big],$$
$$\varphi_n^{(\alpha)}(\mathbf{r}) = \hat{G}_n [H_{ni}{}^d \varphi_i^{(\alpha-1)}(\mathbf{r}) + H_{ni}^{bg} \varphi_i^{(\alpha)}(\mathbf{r})]. \qquad (24)$$

In Eq. (24) the wave function $\varphi_i^{(\alpha)}$ describes the scattering of a particle which was initially in the ground state i and, having undergone α collisions of $\hat{H}^d$ nature, remained, as before, in the channel associated with elastic scattering. It is obvious that under the assumption that the collisions of different physical nature are uncorrelated,[4,8] the particle can remain in the input channel after α collisions only if α is an even number, and the collisions themselves are of a successive depleting-absorbing (polarization) character. This means that

$$\varphi_i^{(2\beta-1)}(\mathbf{r}) = 0. \qquad (25)$$

Now, it follows from Eq. (24) that

$$\varphi_i^{(2\beta)}(\mathbf{r}) = \hat{G}_i \Big[\sum_{k\neq i} H_{ik}{}^d \varphi_k^{(2\beta-1)}(\mathbf{r}) + \sum_{k\neq i} H_{ik}^{bg} \varphi_k^{(2\beta)}(\mathbf{r}) \Big],$$
$$\varphi_n^{(2\beta)}(\mathbf{r}) = \hat{G}_n H_{ni}{}^{bg} \varphi_i^{(2\beta)}(\mathbf{r}), \qquad (26)$$
$$\varphi_n^{(2\beta-1)}(\mathbf{r}) = \hat{G}_n H_{ni}{}^d \varphi_i^{(2\beta-2)}(\mathbf{r}).$$

In the formulas (25) and (26) the integer $\beta \geqslant 1$.

We now separate from the total inelastic scattering wave function the part that describes multiple collisions of both $\hat{H}^{bg}$ and $\hat{H}^d$ nature, the result of which would be a finite loss of energy $\varepsilon^d_{\text{in}}$, characteristic for the specified collisions, by the scattered particle. This part of the inelastic scattering wave function is determined by the formula

$$\varphi_{n,d}(\mathbf{r}) = \sum_{\beta=1}^{\infty} \varphi_n^{(2\beta-1)}(\mathbf{r}) = \hat{G}_n H_{ni}{}^d \sum_{\beta=1}^{\infty} \varphi_i^{(2\beta-2)}(\mathbf{r}) = \hat{G}_n H_{ni}{}^d \varphi_i(\mathbf{r}). \qquad (27)$$

In deriving Eq. (27) we employed the identity (25) and the last equation of the system (26). We recall that the wave function $\varphi_i(\mathbf{r})$ in Eq. (27) satisfies Eq. (10).

Comparing Eq. (27) to Eq. (22) we find immediately that in the two-state approximation $\hat{\mathscr{R}}_n \equiv \hat{I}$. From this result we can draw an important conclusion. It is easy to see that the formula (27), derived in the two-state approximation, does not satisfy the quantum-mechanical reciprocity theorem.[1,2] This can be understood intuitively, starting from the fact that the significance (for polarization processes) of the initial (i) and final (n) states of the particle in the formula (27) is different (or, in other words, starting from the asymmetric nature of the wave fields of the initial and final states relative to their damping).

Thus we can draw the following conclusion, important for the discussion of the applicability of the two-state approximation for describing scattering of particles in matter:[2,8] When the two-state approximation is used to study inelastic scattering processes, the reciprocity theorem, which is connected with the symmetry of scattering processes under time reversal, is not satisfied.

6. COMPETITION BETWEEN INELASTIC COLLISIONS WHEN A FAST ELECTRON UNDERGOES DIFFRACTION CHANNELING IN A SINGLE CRYSTAL

The principal mechanisms which transform the energy of a fast charged particle of intermediate energy moving in matter into the energy of the scattering medium are generation of delocalized electronic excitations (bulk plasmons), excitation of electrons in the inner shells of atoms (single-electron excitations), and phonon generation.[8,9] In the physics of the interaction of charged particles with crystals, these inelastic processes were of interest primarily from the standpoint of describing their effect on the channels for elastic diffraction channeling.[10] To this end, the role of inelastic collisions in the polarization of the crystalline system and their contribution to the imaginary part of the crystal potential were investigated.[4,11-14] Later the theory of diffraction channeling was developed in the direction of taking into account systematically the multiple character of the inelastic and inelastic collisions of a particle and describing correctly the interference of elastic and inelastic scattering channels.[3,6,15-23] At the same time, the problem of the interaction of the inelastic scattering channels of different nature during diffraction channeling of charged particles in crystals was still neglected.

It should be noted that when the distinguished inelastic scattering channel is the channel for generation of a bulk plasmon, the effect of background inelastic collisions, i.e., collisions of the particle with phonons and electrons in the inner shells of atoms, should result in a strong orientational dependence of the angle-integrated cross section for plasmon generation on the direction of incidence of the fast charged particle relative to the system of the crystallographic planes that is under consideration. This effect of the competing inelastic collisions, which are of a substantially multiple character, is ultimately due to the marked spatial localization of the corresponding scattering centers. We note that the spatial localization of scattering centers in the case of collisions with phonons and inner-shell electrons is manifested, for example, in the fact that the corresponding anomalous absorption coefficient is of the same order of magnitude as the normal absorption coefficient;[8,9] at the same time, the anomalous absorption coefficient for electron-plasmon interaction is only a few percent of the normal absorption coefficient.[24]

6.1. Inelastic wave field and asymptotic Green's function of a fast electron in backscattering from a single crystal

Consider an elementary act of generation of a bulk plasmon by a fast electron, Laue-diffracted by some system $\{\mathbf{G}\}$ of crystallographic planes in a semi-infinite crystal occupying the space $z>0$. We assume that plasmon generation occurs only after the wave field of the diffracting particle has already formed:

$$l_{pl}\gg\xi_G,$$

where l_{pl} is the mean free path of a fast electron with respect to generation of a bulk plasmon by the electron and ξ_G is the extinction length.[4)] We also assume that after the plasmon has been generated by the diffracting electron, the latter electron is incoherently scattered through a large angle and exits from the same side of the crystal on which it entered the crystal. This space-time picture corresponds completely to the picture considered in Ref. 6, neglecting competition between inelastic collisions, and does not include processes with the reverse sequence of events: first incoherent scattering of a particle by a large angle, followed by generation of a bulk plasmon.[5]

In accordance with the formula (22) of the general theory, the wave field of the fast electron which has emitted a plasmon is determined by the following relation, taking into account the competition between inelastic collisions:

$$\psi_{pl}(\mathbf{r},n)=\int d\mathbf{r}'\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)H_{ni}^{pl}(\mathbf{r}')\tilde{\psi}_D(\mathbf{k},\mathbf{r}'),\qquad(28)$$

where the matrix element H_{ni}^{pl} is calculated in accordance with Eq. (4) using the wave functions Φ_n and Φ_i of the electronic subsystem of the crystal in the excited and ground states from the electron-electron interaction Hamiltonian, responsible for the excitation of delocalized electronic states. The wave function $\tilde{\psi}_D(\mathbf{k},\mathbf{r})$ describes an electron with wave vector $\mathbf{k}$ in the initial state and takes into account the effect of all inelastic scattering channels on the elastic diffraction channeling channel, and $k^2=2m\hbar^{-2}(E-\varepsilon_i)$. In accordance with Eqs. (5) and (17)

$$\Delta\tilde{\psi}_D(\mathbf{k},\mathbf{r})+\frac{2m}{\hbar^2}[E-\varepsilon_i-U_L(\mathbf{r})]\tilde{\psi}_D(\mathbf{k},\mathbf{r})=\frac{2m}{\hbar^2}\int d\mathbf{r}'A_i(\mathbf{r},\mathbf{r}')\tilde{\psi}_D(\mathbf{k},\mathbf{r}'),\qquad(29)$$

where $U_L(\mathbf{r})$ is the crystal potential and $A_i(\mathbf{r},\mathbf{r}')$ is the effective nonlocal potential, arising due to all possible inelastic collisions, for a particle in the input channel. The propagator $\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)$, describing the evolution of the wave field of the electron, which has emitted a plasmon and has undergone incoherent scattering through a large angle, satisfies the equation

$$\Delta\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)+\frac{2m}{\hbar^2}[E-\varepsilon_n]\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)-\frac{2m}{\hbar^2}\int d\mathbf{r}''A_n(\mathbf{r},\mathbf{r}'')\tilde{\mathscr{G}}(\mathbf{r}'',\mathbf{r}',E-\varepsilon_n)=\frac{2m}{\hbar^2}\delta(\mathbf{r}-\mathbf{r}'),\qquad(30)$$

containing the nonlocal potential $A_n(\mathbf{r},\mathbf{r}')$ for a particle in the final state. Equations of the form (29) and (30) can be solved in the optical-potential approximation.

We shall derive the asymptotic form of the propagator $\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)$ in the limit $\mathbf{r}\to\infty$, using the well-known Fourier representation[25,26] in the region $z>0$, $z'<0$:

$$\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)=-\frac{im}{2\pi^2\hbar^2}\int d\mathbf{s}\frac{\exp[i\mathbf{s}(\boldsymbol{\rho}-\boldsymbol{\rho}')-ik_sz+i\varkappa_sz']}{k_s+\varkappa_s}.\qquad(31)$$

In Eq. (31) $\boldsymbol{\rho}$ and z ($\boldsymbol{\rho}'$ and z') are the tangential and normal components of the radius vector $\mathbf{r}$ ($\mathbf{r}'$) with respect to the crystal-vacuum interface $z=0$; the vector $\mathbf{s}=(s_x,s_y)$ is parallel to this surface;

$$k_s=(k_n^2-s^2)^{1/2},\quad \varkappa_s=(k_n^2-s^2-2m\hbar^{-2}U_0^{opt})^{1/2},$$

$$k_n^2=2m\hbar^{-2}(E-\varepsilon_n),$$

and the constant component of the optical potential is

$$U_0^{opt}=\mathrm{Re}\,U_0^{opt}+i\,\mathrm{Im}\,U_0^{opt},\quad \mathrm{Im}\,U_0^{opt}<0.$$

Introducing into Eq. (31) an integration over $\mathbf{P}=(\mathbf{s},s_z)$, where $s_z=-k_s$,

$$\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)=-\frac{im}{2\pi^2\hbar^2}\int d\mathbf{P}\exp[i\mathbf{P}(\mathbf{r}-\mathbf{r}')+iz'(\varkappa_s+s_z)]\times\frac{\delta(s_z+k_z)}{\varkappa_s-s_z},\qquad(32)$$

and using the identity

$$\delta(s_z+k_s)=\frac{k_s}{k_n}\theta(-s_z)\theta(P)\delta(P-k_n),\qquad(33)$$

we obtain the following representation for the propagator:

$$\tilde{\mathscr{G}}(\mathbf{r},\mathbf{r}',E-\varepsilon_n)=-\frac{im}{2\pi^2\hbar^2}\int d\mathbf{P}\delta(P-k_n)\chi(\mathbf{P},z')\times\exp[i\mathbf{P}(\mathbf{r}-\mathbf{r}')],\qquad(34a)$$

$$\chi(\mathbf{P},z')=\exp[iz'(\varkappa_s+s_z)]\frac{\theta(-s_z)k_s}{k_n(\varkappa_s-s_z)}.\qquad(34b)$$

In Eq. (34b) $s=\mathbf{P}\mathbf{e}_\rho$, $s_z=\mathbf{P}\mathbf{e}_z$, and $\mathbf{e}_\rho$ and $\mathbf{e}_z$ are unit vectors which are parallel and perpendicular, respectively, to the crystal-vacuum interface; χ is a function of the angle between $\mathbf{P}$ and $\mathbf{r}-\mathbf{r}'$, varying slowly compared with $\exp[i\mathbf{P}(\mathbf{r}-\mathbf{r}')]$ in the limit $\mathbf{r}\to\infty$. Following Ref. 1, on integrating over $\mathbf{P}$ in Eq. (34a) we obtain

$$\tilde{\mathscr{G}}(\mathbf{r}\to\infty,\mathbf{r}',E-\varepsilon_n)=-\frac{m}{\pi\hbar^2}\frac{\exp[ik_n|\mathbf{r}-\mathbf{r}'|]}{|\mathbf{r}-\mathbf{r}'|}k_n\chi(\mathbf{k}_n,z').\qquad(35)$$

The asymptotic Green's function $\tilde{\mathscr{G}}$ (35) takes into account both the effect of inelastic processes on the propagation of the particle in the medium and the effects due to reflection and refraction at the interface.[5)] Analysis of the formula (35) shows that coherent effects at the interface between two media are significant for angles θ', such that $\cos\theta'\ll(|U_0^{\rm opt}|/E_n)^{1/2}$, between the direction of the outer normal to the interface and the direction of the wave vector of the final state, i.e., for glancing exit angles of the electron from the medium. The contribution of this narrow angular region to the scattering cross section integrated over the exit angle is negligible. Neglecting the indicated coherent defects, we obtain from Eqs. (34b) and (35)

$$\tilde{\mathscr{G}}(r\to\infty,\mathbf{r}',E-\varepsilon_n)=-\frac{m}{2\pi^2\hbar^2}\frac{\exp(ik_nr)}{r}\dot{\psi}_{inc}(\mathbf{k}_n,\mathbf{r}'),\qquad(36a)$$

where

$$\psi_{inc}(\mathbf{k}_n,\mathbf{r})=\exp(i\mathbf{k}_n\mathbf{r})\exp[-\mu_0(\mathbf{k}_n)z/2]\qquad(36b)$$

is the wave function, and

$$\mu_0(\mathbf{k}_n)=-\frac{2m}{\hbar^2(\mathbf{k}_n)_z}\,\mathrm{Im}\,U_0^{opt}$$

is the damping of the wave field of the particle in the final state. In deriving Eqs. (36a) and (36b), we assume that the real part of the optical potential, determined by virtual polarization processes, is much less than the imaginary part of the optical potential, associated with a real polarization process.[4,8,14]

6.2. Cross section for bulk-plasmon generation

Following Refs. 6 and 27, we find from the formulas (28), (36a), and (36b) that the cross section for the generation of a bulk plasmon by a diffracting electron is determined by the formula

$$\sigma_{pl}=-\frac{im}{(2\pi)^3\hbar^2}\iint\frac{\theta(\omega)\,d\omega\,d\mathbf{Q}}{(k^2-2m\omega/\hbar)^{1/2}}\delta(E_\mathbf{k}-E_{\mathbf{k}-\mathbf{Q}}-\hbar\omega)\iint d\mathbf{r}\,d\mathbf{r}'\times\dot{\psi}_{inc}(\mathbf{k}-\mathbf{Q},\mathbf{r})\psi_{inc}(\mathbf{k}-\mathbf{Q},\mathbf{r}')[D_R(\mathbf{r},\mathbf{r}',\omega)-D_A(\mathbf{r},\mathbf{r}',\omega)]\psi_D(\mathbf{k},\mathbf{r})\psi_D^*(\mathbf{k},\mathbf{r}').\qquad(37)$$

The integration in Eq. (37) extends, in particular, over the total energy $\hbar\omega$ lost and the transferred momentum $\hbar\mathbf{Q}$; $D_{R(A)}$ is the retarded (advanced) Green's function of the electric field in the crystal; the wave function $\psi_D(\mathbf{k},\mathbf{r})$ of the diffracting electron in the initial state is determined by Eq. (29); $E_{\mathbf{k}-\mathbf{Q}}=\hbar^2(\mathbf{k}-\mathbf{Q})^2/2m$. In Refs. 8–10 it is shown that in the optical model in the two-wave approximation of dynamic refraction the solution (29) can be represented in the form

$$\psi_D(\mathbf{k},\mathbf{r})=\exp(i\mathbf{k}\mathbf{r})\exp(-{}^1/{}_2\mu_0z)[\psi_0(\mathbf{k},z)+\psi_G(\mathbf{k},z)\exp(-i\mathbf{G}\rho)],\qquad(38a)$$

where

$$\psi_0(\mathbf{k},z)=\cos^2\frac{\beta}{2}\exp(i\varkappa_1z)\exp\left[\frac{\Delta\mu_Gz}{2(1+w^2)^{1/2}}\right]+\sin^2\frac{\beta}{2}\exp(i\varkappa_2z)\exp\left[-\frac{\Delta\mu_Gz}{2(1+w^2)^{1/2}}\right],\qquad(38b)$$

$$\psi_G(\mathbf{k},z)=\sin\frac{\beta}{2}\cos\frac{\beta}{2}\left\{\exp(i\varkappa_2z)\exp\left[-\frac{\Delta\mu_Gz}{2(1+w^2)^{1/2}}\right]-\exp(i\varkappa_1z)\exp\left[\frac{\Delta\mu_Gz}{2(1+w^2)^{1/2}}\right]\right\},\qquad(38c)$$

$$\varkappa_1(w)=[w-(1+w^2)^{1/2}]/2\xi_G,\quad\varkappa_2(w)=[w+(1+w^2)^{1/2}]/2\xi_G.\qquad(38d)$$

Here $\mathbf{G}$ is a reciprocal-lattice vector, parallel to the surface of the crystal; $w=\cot\beta$ is a parameter describing the deviation of the electron wave vector from the exact reflected position; $w=(E_\mathbf{k}-E_{\mathbf{k}-\mathbf{G}})/2|U_G|$. The normal μ_0 and anomalous $\Delta\mu_G$ absorption coefficients and the extinction length ξ_G are related to the optical and crystal Fourier potentials by the relations

$$\mu_0=-2\,\mathrm{Im}\,U_0^{opt}/\hbar v_z,\qquad\Delta\mu_G=-2\,\mathrm{Im}\,U_G^{opt}/\hbar v_z,$$

$$\xi_G=\hbar v/2|U_G|,$$

where v is the velocity of the fast electron.

Assuming that the electronic subsystem of the crystal is homogeneous and isotropic, the expression (37) can be transformed into the form

$$\sigma_{pl}(w)=\frac{S\omega_p}{(2\pi)^3a_Bv_z}\left(k^2-\frac{2m\omega_p}{\hbar}\right)^{-1/2}\iint dz\,dz'\theta(z)\theta(z')\times\int\frac{dq}{q^2}\theta(q_c-q)\exp[-\mu_0(z+z')]\exp\left[i\frac{\omega_p-\mathbf{v}\mathbf{q}}{v_z}(z-z')\right]$$
$$\times\left\{\cos^2\frac{\beta}{2}\exp\left[\frac{\Delta\mu_G(z+z')}{2(1+w^2)^{1/2}}\right]\left[\cos^2\frac{\beta}{2}\exp(i\varkappa_1(z-z'))+\sin^2\frac{\beta}{2}\exp(-i\varkappa_2(z-z'))\right]+\sin^2\frac{\beta}{2}\exp\left[-\frac{\Delta\mu_G(z+z')}{2(1+w^2)^{1/2}}\right]\right.$$
$$\times\left[\sin^2\frac{\beta}{2}\exp(i\varkappa_2(z-z'))+\cos^2\frac{\beta}{2}\exp(-i\varkappa_1(z-z'))\right]+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\exp\left[\frac{\Delta\mu_G(z-z')}{2(1+w^2)^{1/2}}\right]$$
$$\times[\exp(i\varkappa_1z-i\varkappa_2z')-\exp(i\varkappa_1z'-i\varkappa_2z)]+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\exp\left[-\frac{\Delta\mu_G(z-z')}{2(1+w^2)^{1/2}}\right]$$
$$\left.\times[\exp(i\varkappa_2z-i\varkappa_1z')-\exp(i\varkappa_2z'-i\varkappa_1z)]\right\}.\qquad(39)$$

In Eq. (39) S is the surface area of the crystal, $\mathbf{q}$ is the wave vector of the plasmon, q_c is the cutoff wave vector, associated with taking into account the strong Landau damping, ω_p is the plasmon frequency, and $a_B=\hbar^2/me^2$ is the Bohr radius. In deriving Eq. (39) the spatial dispersion of the plasmon was neglected and it was assumed that $\mu_0(\mathbf{k}-\mathbf{Q})\approx\mu_0(\mathbf{k})$.

Each term in braces in the last formula has a distinct physical meaning.[6] The first term describes the contribution made to the integrated scattering cross section by transitions of the fast electron from a wave of type I in the crystal into a plane wave $\mathbf{k}'=\mathbf{k}-\mathbf{Q}$ in the vacuum, which are accompanied by generation of a plasmon and incoherent scattering of the particle by a large angle; the second term describes the contribution of transitions of the electron from a wave of the type II in the crystal into a plane wave $\mathbf{k}'$ in the vacuum; the third and fourth terms are due to interference of the two preceding scattering processes. The last two terms are qualitatively new compared with the analysis given in Ref. 6, where the competition between inelastic collisions in the diffraction channeling of a fast electron in a single crystal was neglected.

Integrals of the general form

$$L(\alpha_1,\omega_1;\alpha_2,\omega_2)=\frac{v}{2\pi^2 v_z}\iint dz\,dz'\theta(z)\theta(z')\times\exp[-(\alpha_1 z+\alpha_2 z')]\times\int\frac{d\mathbf{q}}{q^2}\theta(q_c-q)\exp\left(i\frac{\omega_1-\mathbf{vq}}{v_z}z\right)\exp\left(-i\frac{\omega_2-\mathbf{vq}}{v_z}z'\right),\quad(40)$$

arose in Eq. (39). These integrals are calculated in the Appendix. Keeping in mind the result (A10) of the Appendix and defining the orientational function of the cross section of inelastic diffraction scattering by the relation $F_{pl}(w)=\sigma_{pl}(w)/\sigma_0$, in which

$$\sigma_0=\frac{S\omega_p}{2va_n(k^2-2m\omega_p/\hbar)^{1/2}}L(\mu_0,\omega_p;\mu_0,\omega_p)$$

is the cross section for the generation of a bulk plasmon by an electron in a semi-infinite amorphous medium, which is calculated taking into account the interference of the inelastic scattering channels, the orientational function $F_{pl}(w)$ can be represented as

$$F_{pl}(w)=F_I(w)+F_{II}(w)+F_{int}(w),\quad(41a)$$

where the function

$$F_I(w)=\frac{1}{4}\left[1+\frac{w}{(1+w^2)^{1/2}}\right]\left\{\left[1+\frac{w}{(1+w^2)^{1/2}}\right]\times L(\mu^-,\omega_1^+;\mu^-,\omega_1^+)+\left[1-\frac{w}{(1+w^2)^{1/2}}\right]L(\mu^-,\omega_2^-;\mu^-,\omega_2^-)\right\}L^{-1}(\mu_0,\omega_p;\mu_0,\omega_p)\quad(41b)$$

is due to transitions of the fast electron of the type I→$\mathbf{k}'$, and

$$F_{II}(w)=\frac{1}{4}\left[1-\frac{w}{(1+w^2)^{1/2}}\right]\left\{\left[1-\frac{w}{(1+w^2)^{1/2}}\right]\times L(\mu^+,\omega_2^+;\mu^+,\omega_2^+)+\left[1+\frac{w}{(1+w^2)^{1/2}}\right]L(\mu^+,\omega_1^-;\mu^+,\omega_1^-)\right\}L^{-1}(\mu_0,\omega_p;\mu_0,\omega_p)\quad(41c)$$

is due to transitions of the fast electron of the type II→$\mathbf{k}'$, and

$$F_{int}(w)=\frac{1}{2(1+w^2)}\mathrm{Re}[L(\mu^-,\omega_1^+;\mu^+,\omega_2^+)-L(\mu^+,\omega_1^-;\mu^-,\omega_2^-)]\times L^{-1}(\mu_0,\omega_p;\mu_0,\omega_p)\quad(41d)$$

is determined by the interference of the scattering processes I→$\mathbf{k}'$ and II→$\mathbf{k}'$. The following notation is employed in Eqs. (41b)–(41d):

$$\omega_1^{\pm}=\omega_p\left\{1\pm\frac{|U^G|}{\hbar\omega_p}[w-(1+w^2)^{1/2}]\right\},$$

$$\omega_2^{\pm}=\omega_p\left\{1\pm\frac{|U^G|}{\hbar\omega_p}[w+(1+w^2)^{1/2}]\right\},$$

$$\mu^{\pm}=\mu_0\pm\Delta\mu_G/2(1+w^2)^{1/2}.$$

6.3. Analysis of the orientational function of inelastic diffraction scattering of a fast electron

The result obtained in Sec. 6.2 for the case of a semi-infinite crystal is correct, to a high degree of accuracy, for the case of a thick crystal ($d\gg\mu_0^{-1}$, d is the thickness of the crystal). In contradistinction to our result, the results of Ref. 6 will be quite accurate for a thin crystal ($d\ll\mu_0^{-1}$), in which, however, size effects are not yet manifested. In what follows we shall make a comparative analysis of the processes of emission of a plasmon by a Laue-diffracted fast electron in thin and thick crystals. First, we note that on a fundamental level the cross section for plasmon generation in thick crystals also exhibits orientational resonances, called plasmon-diffraction resonances in Ref. 6. As analysis shows, their approximate position is determined by the logarithmic terms in Eq. (41b) [see also the formula (A10)] in the limit of zero frequency ω in the argument of the function $L(\mu^-,\omega;\mu^-,\omega)$:

$$w_{res}=\pm{}^1/_2(f_G-f_G^{-1}),\quad f_G=|U_G|/\hbar\omega_p.\quad(42)$$

In the case of thin crystals the formula (42) is exact. In thick crystals the height of the plasmon-diffraction resonances is finite (see Fig. 5) and is determined by the energy of the fast electron as well as by the properties of the crystal and its electronic subsystem: plasmon energy, crystal potential (its real and imaginary parts), and the Fermi velocity of the electrons of the medium.

In Ref. 6 it was concluded that in the case of a thin (in the sense indicated above) crystal under conditions of plasmon-diffraction resonance a plasmon with extremely long wavelength (with zero wave vector) can be generated both by an electron in a type-I wave and by an electron in a type-II wave, which differ by the degree to which they are localized in atomic planes.[8,9] The different degree of localization of waves of the types I and II also explained the different degree of manifestation of resonances for $w<0$ and $w>0$. In contradistinction to Ref. 6, it follows from Eq. (41) that a plasmon with extremely long wavelength can be emitted only by an electron in a wave of the type I, while emission of such a plasmon by an electron in a wave of the type II is forbidden ultimately by the law of conservation of energy; this fundamental difference between the waves I and II in the theory of plasmon-diffraction resonance is associated with the fact that the wave vector of the electron in the wave I (to within a reciprocal lattice vector $\mathbf{G}$) is less than the wave vector of an electron in vacuum, while the wave vector of an electron in

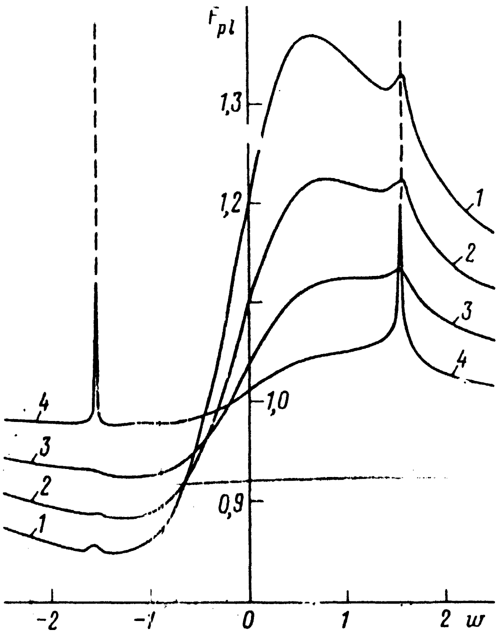

FIG. 5. Orientational functions of inelastic diffraction scattering of a 100 keV electron in the case of thick [curves *1–3*, formula (41) of this paper] and thin [curve *4*, formula (42) of Ref. 6] crystals with different degree γ of spatial localization of the scattering centers; $\gamma = \text{Im}\,U_G^{\text{opt}}/\text{Im}\,U_0^{\text{opt}}$: $\gamma = 0.75$ (*1*), 0.50 (*2*), and 0.25 (*3*); plasmon energy $\hbar\omega_p = 17$ eV, the crystal Fourier potential $|U_G| = 5$ eV, the optical Fourier potential $|\text{Im}\,U_G^{\text{opt}}| = 0.1$ eV, $w_{\text{res}} = 1.553$.

the wave II is greater than the wave vector of an electron in vacuum. Resonance in the region $w < 0$ is suppressed, since the electron located in a wave of type I and responsible for generation of a plasmon with infinite wavelength is, in this case, excited more weakly than an electron located in a wave of type II. Conversely, in the region $w > 0$ the electron is predominantly located in a strongly excited wave of type I and the plasmon-diffraction resonance is more pronounced.

It follows from Eq. (41d) that in the case of thick crystals the interference process from transitions of the type $\text{I} \to \mathbf{k}'$ and $\text{II} \to \mathbf{k}'$, which does not occur in the case of thin crystals, makes a nonzero contribution to the plasmon-generation cross section. As calculations show, however, the contribution of such an interference process is negligible and is at most 0.5% of the total orientational function. We note that the width of the most pronounced plasmon-diffraction resonance in the region $w > 0$ is about $5 \cdot 10^{-4}$ rad, which is of the same order of magnitude as the width of the resonances in the case of thin crystals. Thus detection of resonances in thick crystals could present a significant problem.

Another interesting question is which plasmon-generation mechanism is most sensitive to the presence of the crystal lattice—bremsstrahlung or "Cherenkov." Our calculations show that the contribution of the bremsstrahlung mechanism of bulk-plasmon generation is less than 10% of the total orientational function, so that plasmons generated by the Cherenkov mechanism are more sensitive to the presence of the crystal lattice. As a result of this, the orientational effects in the inelastic diffraction scattering cross section are determined predominantly by the effect of the density.

We now consider the relation between the sign of the density effect and the degree of localization of the scattered electron. In the region $w < 0$ the wave field of the fast electron is localized predominantly in the atomic planes,[8,9] and thus gives rise to strong phonon excitation and excitation of electrons in the inner shells of atoms. Such stimulation of background inelastic processes results in suppression of bulk-plasmon generation in this region of angles of incidence of the fast electron on the surface of the crystal and correspondingly the density effect is negative. For $w > 0$, on the other hand, the electron wave field is localized predominantly between atomic planes. This leads to the fact that the background inelastic processes are significantly weaker and, as a consequence, the cross section for plasmon generation increases (the density effect is positive).

Thus the competition between inelastic collisions in thick crystals results in a pronounced orientational effect in the cross section for the generation of a bulk plasmon by a fast electron when the electron is reflected from the crystal. This orientational effect is due primarily to the effect of the density, i.e., the strong sensitivity of classical Cherenkov plasmons to the direction of incidence of the primary electron relative to the atomic planes. The orientational effect

$$\delta\sigma_{pl} = (\sigma_{pl}^{max} - \sigma_{pl}^{min})/(\sigma_{pl}^{max} + \sigma_{pl}^{min})$$

is about 20%, so that the competition between inelastic scattering channels is easily observable.

7. CONCLUSIONS

In this paper we have formulated a general theory of the interaction of physically different inelastic scattering channels when a fast particle moves in matter. As an illustration of the application of the formalism developed, we examined in detail the consequences of the competition of inelastic collisions during diffraction channeling of a fast electron in a single crystal, when the distinguished inelastic scattering channel is the bulk-plasmon generation channel. This example does not exhaust, of course, all possible manifestations of this effect. We briefly discuss some other consequences of the general formula (22).

Polarization processes, which result in a finite damping of the wave field of the particle under consideration, should decrease the effective cross section for the distinguished inelastic process. This is connected with the fact that the wave functions of the initial and final states in Eq. (22) are different from a plane wave and decay in space, so that (with the corresponding normalization) their magnitude is less than unity. In other words, polarization processes decrease the number of particles in the ground state which are capable of undergoing inelastic scattering of the specified nature and in the process can be recorded as such after exiting from the medium.

In addition, since the decay of the wave field caused by all possible inelastic processes in the matter can have pronounced energy and temperature dependences, the phenomenon of coupling of the inelastic scattering channels can play a determining role in the energy and temperature dependences of the cross section of the particular inelastic scattering process.

I thank B. N. Libenson and V. V. Rumyantsev for pointing out the connection between the processes discussed in this paper, the reciprocity theorem, and the principle of detailed balance.

APPENDIX

Calculating in Eq. (40) the integrals over z and z' we obtain

$$L(\alpha_1, \omega_1; \alpha_2, \omega_2) = \left(\alpha_1 + \alpha_2 + i\frac{\omega_2 - \omega_1}{v_z}\right)^{-1} \times [R(\alpha_1, \omega_1) + R^*(\alpha_2, \omega_2)], \quad (A1)$$

where the complex function $R(\alpha,\omega)$ can be represented in terms of the real functions $I(\alpha,\omega)$ and $P(\alpha,\omega)$:

$$R(\alpha, \omega) = \alpha I(\alpha, \omega) + iP(\alpha, \omega), \quad (A2)$$

$$I(\alpha, \omega) = \frac{v}{2\pi^2 v_z} \int \frac{d\mathbf{q}}{q^2} \theta(q_c - q) \left[\alpha^2 + \left(\frac{\omega - \mathbf{vq}}{v_z}\right)^2\right]^{-1}, \quad (A3)$$

$$P(\alpha, \omega) = \frac{v}{2\pi^2 v_z} \int \frac{d\mathbf{q}}{q^2} \theta(q_c - q) \left(\frac{\omega - \mathbf{vq}}{v_z}\right) \left[\alpha^2 + \left(\frac{\omega - \mathbf{vq}}{v_z}\right)^2\right]^{-1} \quad (A4)$$

The function $I(\alpha,\omega)$ can be easily represented in the form of single integral:

$$I(\alpha, \omega) = \frac{1}{\alpha\pi} \int_0^{q_c} \frac{dq}{q} \left(\operatorname{arctg}\frac{vq - \omega}{\alpha v_z} + \operatorname{arctg}\frac{vq + \omega}{\alpha v_z}\right). \quad (A5)$$

Since in the limit $vq_c/\alpha v_z \sim -(\hbar\omega_p/\mathrm{Im}\, U_0^{\mathrm{opt}})(v/v_F) \gg 1$

$$\frac{\partial I(\alpha, \omega)}{\partial \omega} = \frac{1}{\alpha} \frac{\omega}{\omega^2 + \alpha^2 v_z^2}, \quad (A6)$$

and $I(\alpha, \omega = 0)$ in the same approximation[28] has the form

$$I(\alpha, \omega = 0) = \frac{2}{\alpha\pi} \int_0^{q_c} \frac{dq}{q} \operatorname{arctg}\frac{vq}{\alpha v_z} \approx \frac{1}{\alpha} \ln\frac{vq_c}{\alpha v_z}, \quad (A7)$$

we obtain for Eq. (A3) the approximate result

$$I(\alpha, \omega) = \int_0^{\omega} \frac{\partial I(\alpha, \omega')}{\partial \omega'} d\omega' + I(\alpha, \omega = 0) = \frac{1}{\alpha} \ln\frac{vq_c}{(\omega^2 + \alpha^2 v_z^2)^{1/2}}. \quad (A8)$$

Correspondingly,

$$P(\alpha, \omega) = -\operatorname{arctg}\frac{\omega}{\alpha v_z}, \quad (A9)$$

so that $L(\alpha_1, \omega_1; \alpha_2, \omega_2)$ is determined by the formula

$$L(\alpha_1, \omega_1; \alpha_2, \omega_2) = \left(\alpha_1 + \alpha_2 + i\frac{\omega_2 - \omega_1}{v_z}\right)^{-1} \times \left\{\left[\ln\frac{vq_c}{(\omega_1^2 + \alpha_1^2 v_z^2)^{1/2}} + \ln\frac{vq_c}{(\omega_2^2 + \alpha_2^2 v_z^2)^{1/2}}\right] - i\left(\operatorname{arctg}\frac{\omega_1}{\alpha_1 v_z} - \operatorname{arctg}\frac{\omega_2}{\alpha_2 v_z}\right)\right\}. \quad (A10)$$

1) We shall not consider energy threshold effects.

2) It is assumed that the condition $v \gg v_s$ is satisfied at nonrelativistic energies of the external particle.

3) We note that in the exact expansion (which holds outside the framework of the two-state approximation) topologically more complicated polarization diagrams would be present in Fig. 1a.

4) It is shown in Ref. 6 that this condition is satisfied for electron energy exceeding tens of keV.

5) As $U_0^{\mathrm{opt}} \to 0$ the formula (35) goes over to the well-known Green's function of a particle with energy $E_n = E - \varepsilon_n$ in unbounded space.

6) We employ below the standard terminology of the theory of scattering of particles in crystals (see, for example, Refs. 8 and 9).

1. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Nonrelativistic Theory*, Pergamon, Oxford (1974), Secs. 125 and 142.
2. N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, Clarendon Press, Oxford, 1965.
3. S. L. Dudarev and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **85**, 1748 (1983) [Sov. Phys. JETP **58**, 1018 (1983)].
4. H. Yoshioka, J. Phys. Soc. Jpn. **12**, 618 (1957).
5. V. V. Rumyantsev and B. N. Libenson, Ann. Phys. **111**, 152 (1978).
6. V. V. Rumyantsev and B. N. Libenson, Zh. Eksp. Teor. Fiz. **87**, 1818 (1984) [Sov. Phys. JETP **60**, 1046 (1984)].
7. B. N. Libenson and V. V. Rumyantsev, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 10 (1987) [JETP Lett. **45**, 10 (1987)].
8. Y.-H. Ohtsuki, *Charged Beam Interaction With Solids*, Taylor and Francis, New York, 1983.
9. P. B. Hirsch, A. Howie, R. B. Nicholson, D. W. Pashley, and M. J. Whelan, *Electron Microscopy of Thin Crystals*, Butterworth, London, 1965.
10. H. Hashimoto, A. Howie, and M. J. Whelan, Proc. Roy. Soc. A **269**, 80 (1962).
11. C. R. Hall and P. B. Hirsch, Proc. Roy. Soc. A **286**, 158 (1965).
12. M. J. Whelan, J. Appl. Phys. **36**, 2099, 2103 (1965).
13. S. L. Cundy, A. J. Metherell, and M. J. Whelan, Phil. Mag. **15**, 623 (1967).
14. G. Radi, Acta Crystallogr. A **26**, 41 (1970).
15. A. Howie, Proc. Roy. Soc. A **271**, 268 (1963).
16. S. L. Dudarev and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **88**, 631 (1985) [Sov. Phys. JETP **61**, 370 (1985)].
17. S. L. Dudarev and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **89**, 1685 (1985) [Sov. Phys. JETP **62**, 972 (1985)].
18. S. L. Dudarev, Zh. Eksp. Teor. Fiz. **94**(11), 289 (1988) [Sov. Phys. JETP **67**, 2338 (1988)].
19. E. E. Gorodnichev, S. L. Dudarev, L. B. Rogozkin, and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **96**, 1801 (1989) [Sov. Phys. JETP **69**, 1017 (1989)].
20. V. V. Fedorov, Zh. Eksp. Teor. Fiz. **78**, 46 (1980) [Sov. Phys. JETP **51**, 22 (1980)].
21. V. V. Fedorov, Zh. Eksp. Teor. Fiz. **82**, 473 (1982) [Sov. Phys. JETP **55**, 272 (1982)].
22. V. V. Rumyantsev and B. N. Libenson, Fiz. Tverd. Tela **30**, 1392 (1988) [Sov. Phys. Solid State **30**, 804 (1988)].
23. E. A. Kantsyper and V. V. Rumyantsev, Izv. Akad. Nauk SSSR, Ser. Fiz. **55**, 2362 (1991).
24. W. Munchmeyer, Z. Naturforsch. A **27**, 402 (1972).
25. Yu. N. Barabenenkov, Zh. Eksp. Teor. Fiz. **56**, 1262 (1969) [Sov. Phys. JETP **29**, 679 (1969)].
26. E. E. Gorodnichev, S. L. Dudarev, D. B. Rogozkin, and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **93**, 1642 (1987) [Sov. Phys. JETP **66**, 938 (1987)].
27. B. N. Libenson and V. V. Rumyantsev, Fiz. Tverd. Tela **20**, 65 (1978) [Sov. Phys. Solid State **20**, 34 (1978)].
28. Yu. A. Brychkov, O. I. Marichev, and A. P. Prudnikov, *Handbook of Tables of Indefinite Integrals* [in Russian], Nauka, Moscow, 1986, p. 171.

Translated by M. E. Alferieff