Theory of the channeling effect: II. Influence of inelastic collisions

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The density matrix formalism is employed to derive a kinetic equation in which the coherent nature of diffraction in a regular medium and inelastic processes concurrent with motion of a fast charged particle in a crystal are taken into account simultaneously. The damping length L_2 of off-diagonal density matrix elements responsible for coherence effects, such as the dependence of a nuclear reaction yield on crystal thickness[1], is discussed. It is found that L_2 may be several thousand angstroms. It is shown that for $L > L_2$, damping of off-diagonal elements leads to symmetrization of the particle angular distribution in a planar channel. A theory of multiple scattering of fast charged particles under channeling conditions is developed. The problem reduces to that of two-dimensional diffusion in transverse momentum space with a diffusion coefficient D that changes appreciably on transition from the channel region to the region outside it. It is demonstrated that inside the channel, D is determined mainly by scattering by electrons, and in particular by valence electrons, and that the value of D is small compared to that outside the channel. The solution of the problem for the case of planar channeling yields an explanation for the sharp anisotropy of the angular distribution of particles emerging from a single crystal, and in particular for the elongation of the angular distribution along the family of crystallographic planes considered and, simultaneously, the channel's "screening" effect; it also is possible to bring out some of the features of the angular distribution for incidence angles exceeding the channeling angle ϑ_0, such as the "forced channel crossing" effect at small thicknesses and the "particle capture and delay in channel" effect at large crystal thicknesses.

1. INTRODUCTION

In a preceding paper[1] (henceforth designated I) we developed a quantum theory of channeling, with inelastic processes neglected. We have revealed the purely quantum-theoretical aspects of the phenomenon, which are manifest in the existence of a unique effect of spikes of the yield of the nuclear reaction with increasing thickness ("nuclear echo"), and also in a fine structure of the dependence of the reaction intensity on the angle of entry of the fast particles. Naturally, in the presence of inelastic processes, these effects should become smeared out and ultimately vanish. In the case of "nuclear echo" this is due to the damping of the off-diagonal elements of the density matrix, since it is the deviation of these elements from zero which in fact determines the unique phase gathering following the passage through a definite thickness of the crystal. (We note, to avoid misunderstandings, that the amplitude of the spikes also decreases in the absence of inelastic processes, owing to the inevitable phase difference that sets in with increasing thickness). As shown in I, we are primarily interested in the off-diagonal elements of the density matrix, which correspond to the nearest above-the-barrier states. Consequently, a decisive role in the feasibility of revealing this effect is played by the length L_1 over which the off-diagonal elements of the density matrix are effectively damped outside the channel.

For a particle moving inside the channel, the damping of the off-diagonal density-matrix elements is much slower than for a particle outside the channel. This damping therefore corresponds to a certain effective length L_2 which is larger than L_1. In fact, L_2 is the characteristic dimension over which the memory of the state of the incident particle at the level of the wave function is still preserved. At distances $L \gg L_2$ from the entry surface, this memory is completely erased, and the particle's motion is now described by an equation that contains in fact only diagonal elements of the density matrix.

The transition thickness L_2 is, as will be shown below, relatively large, on the order of several thousand Angstrom units. In such a thickness, however, the angular spreading of the packet is still small in comparison with the channeling angle. At the same time, under conditions in which the off-diagonal elements have already been damped out, the properties of the true angular distribution are close to the properties of the angular distribution averaged over the crystal thickness. In the case of planar channeling, in particular, this causes, as indicated in I, the incident beam to be represented in the angular distribution on a par with the "specularly" reflected beam. With further increase of the thickness, this symmetrical state becomes smeared out as a result of the inelastic processes, within the framework of a multiple-scattering picture that differs from the usual one in an exceedingly strong dependence of the character of the scattering on the direction of motion in the crystal, primarily on going from the region inside the channel to the region outside.

It is interesting that L_2 was in fact measured recently in experiments by Eisen and Robinson[2].

Most experiments on the angular distribution of particles after passing through a single crystal under channeling conditions were in fact performed with crystals of thickness $L \gg L_2$. The experiments revealed quite nontrivial singularities in the character of the angular distribution. Thus, in the case of axial channeling, a star-like structure of the angular distribution is observed, with higher-intensity "prongs" along the crystallographic planes, and the given crystallographic axis lies on the intersection of these prongs[3]. In the case of planar channeling, there is a strongly pronounced stretching of the angular distribution along the planes in question[4,5].

The physical causes of these phenomena have not yet been fully clarified. Yet it is clear from the foregoing that at such thicknesses the entire picture can be described within the framework of the Boltzmann-type equation (for the diagonal elements of the density matrix) with allowance for the strong difference between the types of scattering inside and outside of the channel.

The present paper is devoted to an analysis of inelastic scattering of fast heavy charged particles passing through crystals under channeling conditions. The quantum-kinetic equation obtained for the density matrix is analyzed primarily from the point of view of the damping of the off-diagonal elements, and by the same token, of the determination of the thicknesses L_1 and L_2. The result obtained here raises the hope of experimentally observing coherent spikes of the yield of the nuclear reaction. It is found at $L \gg L_2$ that the kinetic equation can be reduced to a diffusion equation with different values of the diffusion coefficient inside and outside the channel. The angular distribution obtained in this region turns out to be fully equivalent to that observed in the experiment. In particular, it explains the aforementioned singularities in the angular distribution of the particles emerging from the single crystal, and reveals the special role played by multiple scattering in the trapping of particles in the channels, a role observed experimentally in a recently published interesting paper by Markus, Geguzin, and Faĭnshteĭn[6].

2. KINETIC EQUATION FOR THE DENSITY MATRIX

We start with a derivation of the equation for the density matrix of a fast charged particle moving in an arbitrary scattering medium. The Hamiltonian of the entire system as a whole can be represented in the form

$$\hat{H} = \hat{H}_1 + \hat{H}_2,$$

where $\hat{H}_1$ is the Hamiltonian of the particle and includes its interaction with the medium, while $\hat{H}_2$ is the Hamiltonian of the medium (we shall henceforth omit the carets designating the operators).

We introduce the density matrix ρ for the entire system as a whole. The density matrix of the fast particle

$$\rho_1 = \mathbf{Tr}_2 \rho$$

(the trace with subscript 2 denotes summation over the variables of the medium) satisfies the equation ($\hbar = 1$)

$$i\partial\rho_1 / \partial t = [H_0, \rho_1] + \mathbf{Tr}_2 [W, \rho]. \tag{2.1}$$

Here

$$W = H_1 - H_0, \quad H_0 = \mathbf{Tr}_2(\rho_2^{(0)} H_1), \tag{2.2}$$

where $\rho_2^{(0)}$ is the equilibrium density matrix of the medium and is diagonal in the representation of the eigenfunctions of the Hamiltonian H_2.

If the inelastic-scattering operator W is neglected, Eq. (2.1) describes a coherent evolution of the density matrix of the particle in the averaged potential produced by the particles of the medium. The solution of the corresponding problem was given in I. If the inelastic scattering is taken into account, the equation for the density matrix of the entire system can be represented in the following integral form:

$$\rho(t) = \exp\{-i(H_0 + H_2)t\}\rho(0)\exp\{i(H_0 + H_2)t\}$$
$$- i\int_{-t}^{0} \exp\{i(H_0 + H_2)\tau\}[W, \rho(t+\tau)]\exp\{-i(H_0 + H_2)\tau\}d\tau. \tag{2.3}$$

Here

$$\rho(0) = \rho_1(0)\rho_2^{(0)}, \tag{2.4}$$

where $\rho_1(0)$ is the initial density matrix of the particle.

We substitute (2.3) in (2.1) and recognize that the terms containing $\rho(0)$ vanish when (2.2) and (2.4) are taken into account. We confine ourselves in the right-hand side of the resultant equation to an approximation quadratic in the scattering operator W. Then the total density matrix $\rho(t+\tau)$ in the right-hand side can be replaced by $\exp[-iH_0\tau]\rho_1(t)\exp[iH_0\tau]\rho_2^{(0)}$. Bearing in mind that the characteristic times of the incoherent variation of ρ_1 are long in comparison with the duration of the collision, we obtain

$$\partial\rho_1/\partial t + i[H_0, \rho_1] = \mathbf{Tr}_2\int_{-\infty}^{0}[\exp\{i(H_0 + H_2)\tau\}$$
$$\times[W, \exp\{-iH_0\tau\}\rho_1(t)\exp\{iH_0\tau\}\rho_2^{(0)}]\exp\{-i(H_0 + H_2)\tau\}, W]d\tau \tag{2.5}$$

When integrated with respect to time, the contribution of the terms with the principal values of the integrals with respect to energy in the right-hand side of (2.5), a contribution connected with the renormalization of the energy spectrum, turns out to be small in the case of fast particles and can be neglected. Then, after simple transformations, we write the following kinetic equation

$$\partial\rho_{1ss'} / \partial t + i(E_s - E_{s'})\rho_{1ss'} = I_{ss'}, \tag{2.6}$$

$$I_{ss'} = \pi \sum_{\substack{s''s''' \\ \alpha\alpha'}} \rho_{2\alpha}^{(0)} \{W_{ss''}^{\alpha'\alpha} W_{s'''s'}^{\alpha\alpha'} \rho_{1s''s'''}(t)[\delta(E_s + E_{\alpha'} - E_{s''} - E_\alpha)$$
$$+ \delta(E_{s'} + E_{\alpha'} - E_{s'''} - E_\alpha)] - [W_{ss''}^{\alpha\alpha'} W_{s''s'''}^{\alpha'\alpha} \rho_{1s'''s'}(t)$$
$$+ W_{s'''s''}^{\alpha\alpha'} W_{s''s'}^{\alpha'\alpha} \rho_{1ss'''}(t)]\delta(E_{s''} + E_{\alpha'} - E_{s'''} - E_\alpha)\}. \tag{2.7}$$

Here the subscript s labels the particle eigenstates corresponding to the Hamiltonian H_0, while α labels the states of the medium.

We note that the operator W has no matrix elements that are diagonal in the states of the scattering medium. Indeed, a diagonal matrix element over the states of an equilibrium macrosystem is equivalent to thermodynamic averaging of the considered quantity. But in our case $\mathrm{Tr}_2(\rho_2^{(0)}W) = 0$.

When channeling in a crystal is considered, the states of the Hamiltonian H_0 are Bloch functions corresponding to the motion of the particle in an effective periodic potential (see I for details). Accordingly, the subscript s corresponds to a quasimomentum k and a band number n, and in the expanded-band scheme it corresponds to a generalized quasimomentum q. As to the off-diagonal elements of the operator W, in a regular crystal they correspond to inelastic scattering of a fast particle with excitation of the electron and phonon subsystems.

Operating in expanded q-space, we can show that in a regular crystal we always have in (2.7)

$$\mathbf{q}''' - \mathbf{q}'' = \mathbf{q}' - \mathbf{q} + \mathbf{K}, \tag{2.8}$$

where K is the reciprocal-lattice vector. Let us consider the transition to the case of a completely randomized scattering medium. In this case, the eigenfunctions of the Hamiltonian H_0 are plane waves. Under the assumptions that have led to the equation for the density matrix in the form (2.6)–(2.7), allowance for the random distribution of the scattering centers reduces to a corresponding averaging of bilinear combinations of the matrix elements of W. A simple analysis shows that in this case relation (2.8) holds with $\mathbf{K} \equiv 0$.

When considering the problem of scattering of fast particles in a random medium made up of heavy particles, we can neglect the inelastic scattering by the electrons. Neglecting also the recoil energy of the nuclei in the energy δ functions in the right-hand side of (2.6), we arrive at the following equation for a monatomic medium:

$$\partial\rho_{1\mathbf{q}\mathbf{q}'}/\partial t + i(E_\mathbf{q} - E_{\mathbf{q}'})\rho_{1\mathbf{q}\mathbf{q}'} = \frac{N}{8\pi^2}\int d\mathbf{p}'\,|V_{\mathbf{p}'}|^2[\delta(E_\mathbf{q} - E_{\mathbf{q}+\mathbf{p}'}) + \delta(E_{\mathbf{q}'} - E_{\mathbf{q}'+\mathbf{p}'})][\rho_{1\mathbf{q}+\mathbf{p}',\mathbf{q}'+\mathbf{p}'} - \rho_{1\mathbf{q}\mathbf{q}'}]. \tag{2.9}$$

Here N is the density of the atoms of the medium and $V_\mathbf{p}$ is the Fourier component of the potential, averaged over the ground state, of an individual atom.

We note that Eq. (2.9) coincides with an equation first derived by Migdal in[7].

3. DAMPING OF OFF-DIAGONAL ELEMENTS OF THE DENSITY MATRIX

In this section we consider the question of the damping length of the off-diagonal elements outside the channel and inside the channel, primarily in connection with the problem of coherent spikes of the yield of the nuclear reaction with thickness. This effect depends significantly on the off-diagonal elements of the density matrix, which connect the low-lying above-the-barrier states (at an incidence angle smaller than the channeling angle—see I). In this connection, we start with an analysis of the damping of the off-diagonal elements within the framework of Eq. (2.9), where the analysis can be carried through directly to conclusion.

We replace q and q′ in (2.9) by new variables $\mathbf{p} = (\mathbf{q} + \mathbf{q}')/2$ and $\mathbf{g} = \mathbf{q} - \mathbf{q}'$, and put

$$\rho_\mathbf{g}(\mathbf{p}, t) \equiv \rho_{1\mathbf{p}+\mathbf{g}/2,\ \mathbf{p}-\mathbf{g}/2}(t).$$

The main contribution to the right-hand side of (2.9) is made by the region $p' \ll q, q'$. Since we are obviously interested in the case $g \ll \rho$ ($g \sim K$), the energy δ functions cut out under these conditions, as usual, a plane perpendicular to p and containing the vectors p′. We recognize that

$$\frac{M}{(2\pi)^2 p}\int |V_{\mathbf{p}'_\perp}|^2\, d^2\mathbf{p}_\perp' = v\sigma_0,$$

where $v = p/M$ is the particle velocity and σ_0 is the cross section for elastic scattering by a single atom. Then Eq. (2.9) can be transformed into

$$\frac{\partial\rho_\mathbf{g}(\mathbf{p},t)}{\partial t} + \left(Nv\sigma_0 + i\frac{\mathbf{g}\mathbf{p}}{M}\right)\rho_\mathbf{g}(\mathbf{p},t) = \frac{NM}{(2\pi)^2 p}\int d^2\mathbf{p}_\perp'\,|V_{\mathbf{p}_\perp'}|^2\rho_\mathbf{g}(\mathbf{p}+\mathbf{p}_\perp', t). \tag{3.1}$$

Assume that at the initial instant of time we have in a certain fixed coordinate system

$$\rho_\mathbf{g}(\mathbf{p}_\perp, p_z, 0) = \rho_\mathbf{g}^{(0)}(\mathbf{p}_\perp, p_z)$$

and let $p_\perp \ll p_z$. Considering limited time intervals, in which the transverse spreading of the initial distribution is still small, we ignore the variation of p_z (and also of the quantities $|\mathbf{p}|$ and v), assuming this quantity to be constant in the left- and right-hand sides of (3.1). Then the solution of (3.1) can be expressed in the form

$$\rho_\mathbf{g}(\mathbf{p}_\perp, p_z, t) = \exp\left\{-\left(Nv\sigma_0 + i\frac{\mathbf{g}\mathbf{p}}{M}\right)t\right\} \times \int\frac{d^2\mathbf{p}_\perp'}{(2\pi)^2}\int d^2\rho\,\exp\left\{-i\mathbf{p}_\perp'\rho + \frac{M}{g_\perp}\int_x^{x+g_\perp t/M} F(x', y)\,dx'\right\}\rho_\mathbf{g}^{(0)}(\mathbf{p}_\perp - \mathbf{p}_\perp', p_z). \tag{3.2}$$

We have introduced here the function

$$F(\rho) = \frac{NM}{(2\pi)^2 p}\int d^2\mathbf{p}_\perp\,|V_{\mathbf{p}_\perp}|^2 e^{i\mathbf{p}_\perp\rho}, \quad \rho = (x, y), \tag{3.3}$$

The x axis is directed here along the component $g_\perp$ (of the vector g) in the plane perpendicular to the z axis.

To obtain an estimate of the characteristic damping time of the off-diagonal density-matrix elements, we change over from $\rho_\mathbf{g}(\mathbf{p}, t)$ directly to Fourier components of the fast-particle density, bearing in mind the fact that it is precisely this quantity which characterizes, in particular, the coherent effects in the yield of the nuclear reaction. In the plane-wave representation, the expression for the particle density $n(\mathbf{r}, t)$ (see (2.14) in I) is of the form

$$n(\mathbf{r}, t) = \sum_\mathbf{g} e^{i\mathbf{g}\mathbf{r}} n_\mathbf{g}(t), \quad n_\mathbf{g}(t) = \int\frac{d^3\mathbf{p}}{(2\pi)^3}\rho_\mathbf{g}(\mathbf{p}, t). \tag{3.4}$$

Substituting (3.2) in (3.4) and assuming that the initial distribution $\rho_\mathbf{g}^{(0)}(\mathbf{p})$ was characterized by a narrow peak near a certain $\mathbf{p}^0$, we obtain

$$n_\mathbf{g}(t) = n_\mathbf{g}^{(0)}(t)\exp\left\{-Nv\sigma_0 t + \frac{M}{g_\perp}\int_0^{g_\perp t/M} F(\rho)\,d\rho\right\}, \tag{3.5}$$

where $n_\mathbf{g}^{(0)}(t)$ denotes the Fourier component of the particle density in the absence of collisions.

Let the characteristic dimension of the region where the function $f(\rho)$ (3.3) differs noticeably from zero be $1/\kappa_0$. Then, at times exceeding

$$\tilde{t} = M/g_\perp\varkappa_0, \tag{3.6}$$

$n_\mathbf{g}(t)$ takes the asymptotic form

$$n_\mathbf{g}(t) \cong n_\mathbf{g}^{(0)}(t)\exp\left\{-Nv\sigma_0 t + \frac{MI}{g_\perp}\right\}, \quad I = \int_0^\infty F(\rho)\,d\rho. \tag{3.7}$$

Thus, expression (3.6) gives an estimate of the damping time of the off-diagonal density-matrix elements.

A more accurate analysis, carried out for scattering by a screened Coulomb potential, gives for the damping length $\tilde{L} = v\tilde{t}$ at a proton energy E = 5 meV and at $g_\perp$ on the order of the reciprocal-lattice vector a value $\tilde{L} \sim 1000$ Å in the case of silicon and $\tilde{L} \sim 600$ Å in the case of germanium. It is interesting that these values are much larger than $1/N\sigma_0$.

When the fast particle moves inside the channel, the scattering cross section decreases sharply (by one or two orders of magnitude-see Sec. 5 below). This increases by several times the length over which the damping of the off-diagonal elements takes place (the asymptotic damping (3.7) that sets in at large times now becomes much slower than outside the channel). Thus, the characteristic damping length L_2 of the off-diagonal density-matrix elements inside the channel is several thousand Å at a proton energy on the order of several MeV.

It should be noted that it follows from the structure of the general kinetic equation for ρ_1, with (2.8) taken into account, that when the particles are channeled in the crystal, the off-diagonal elements of ρ_1 with indices that differ by an amount equal to the reciprocal lattice vector, are "reinforced" to a certain extent by the diagonal elements. This unique circumstance only increases the length L_2. An analogous situation takes place also in the case of motion outside the channel, if one considers not a random medium but a regular one (density matrix in the Bloch-function representation), and by the same token L_1 is actually larger than $\tilde{L}$.

From the point of view of quantum oscillations of the yield of a nuclear reaction in the case of channeling, we are interested primarily in the damping of the "transverse" off-diagonal density-matrix elements corresponding to the lowest above-the-barrier states that differ by multiples of the reciprocal-lattice vector. At short distances from the entrance surface, the damping of these off-diagonal elements follows a law close to (3.2) and (3.5). However, as seen from the results of I, a sharp decrease of the interaction between the particles and the atoms with the medium, owing to the restructuring of the wave function in the crystal, occurs over distances much shorter than L_1. Therefore the effective damping length responsible for the detuning of the nuclear-echo effect is determined by a value intermediate between L_1 and L_2. Bearing the foregoing estimates in mind, we can state that at proton energies on the order of several MeV one is expected to deal with a length on the order of several thousand Angstrom units. This is longer than the length l_0 over which the first spikes of the yield of the nuclear reaction appeared in the model considered in I (at E = 5 MeV, $l_0 \approx 900$ Å in silicon and $l_0 \approx 700$ Å in germanium). Thus, in all likelihood, given a suitable choice of conditions and good angular collimation of the incident beam of particles, one could realistically observe a size effect in thin films, namely a dependence of the yield of the reaction on the plate thickness.

In concluding this section, we note that the general expression (3.2) is valid also when the limit $g \to 0$ is taken. Then, using a screened Coulomb potential for the interaction, we can usually obtain the expression first derived by Moliere[8] for the angular distribution of the particles with a δ-function angular initial condition.

4. QUASISYMMETRICAL STATES OF A PARTICLE IN A PLANAR CHANNEL

The results of the preceding section lead to the conclusion that damping of the transverse off-diagonal density-matrix elements takes place over distances much shorter than the length L_0 over which the characteristic width of the angular distribution that is described by the evolution of the diagonal elements of the density matrix (see Secs. 5—6 below) becomes of the order of the channeling angle ϑ_0. As a result, there exists in the problem a thickness interval $L_2 < L \ll L_0$ in which the phase "memory" of the initial state has already been erased, but the particle is still "deep" in the channel. This causes loss of the memory of the initial direction of entrance of the particle, and the angular distribution at any thickness becomes quasisymmetrical, i.e., the distribution with respect to the transverse momentum represents to an equal degree both a group of states with momenta close to the initial momentum q_x^0 and a group of states with momenta close to $-q_x^0$ (the x axis is perpenddicular to the system of planes making up the planar channel). The reason is that plane waves with oppositely directed momenta are represented with approximately equal weights in the Fourier expansion of the modulating Bloch function of any sub-barrier state in a one-dimensional potential with weak penetrability between the wells.

The general expression for the angular distribution of the particles after traversing a thickness $L(t = L/v_z)$ is (see I)

$$\rho_1(\varkappa, t) = \sum_{\mathbf{q},\mathbf{q}'} C_{\mathbf{q}}^*(\varkappa) C_{\mathbf{q}'}(\varkappa) \rho_{1\mathbf{q}\mathbf{q}'}(t), \tag{4.1}$$

$$C_{\mathbf{q}}(\varkappa) = \int e^{i\varkappa\mathbf{r}} \psi_{\mathbf{q}}^*(\mathbf{r})\, d\mathbf{r} = \delta_{\varkappa_z,q_z}\delta_{\varkappa_y,q_y} \int e^{i\varkappa_x x}\psi_{q_x}^*(x)\, dx$$
$$= \delta_{\varkappa_z,q_z}\delta_{\varkappa_y,q_y} \sum_{K_x} \delta_{\varkappa_x,q_x+K_x} C_{q_x}(\varkappa_x), \tag{4.2}$$

where $\psi_{q_x}(x)$ is the Bloch function defined in expanded q_x space. It follows from (4.2) that the right-hand side of (4.1) contains only off-diagonal density-matrix elements with indices that differ by reciprocal-lattice vectors perpendicular to the considered system of crystallographic planes.

At $L > L_2$ we can leave the off-diagonal elements out of (4.1), and

$$\rho_1(\varkappa, t) \cong \sum_{\mathbf{q}} |C_{\mathbf{q}}(\varkappa)|^2 \rho_{1\mathbf{q}\mathbf{q}}(t). \tag{4.3}$$

At $L \ll L_2$, neglecting the inelastic processes, we obtain for $\rho_{1qq'}(t)$, assuming that a plane wave with momentum q^0 is incident on the entrance surface:

$$\rho_{1\mathbf{q}\mathbf{q}'}(t) \approx C_{\mathbf{q}}(\mathbf{q}^0) C_{\mathbf{q}'}^*(\mathbf{q}^0) \exp\{-i(\varepsilon_{q_x} - \varepsilon_{q'_x})t\}. \tag{4.4}$$

Here ϵ_{q_x} is the energy corresponding to the Bloch state with quasi-momentum q_x.

Figure 1 shows the evolution of the angular distribution as a function of the thickness during the first stage, when the inelastic processes can be neglected; this evolution was obtained using a potential of the Kronig-Penney type as an example. The figure shows quite clearly how nearly specular successive reflections take place from each of the planes.

It is interesting that the angular distribution of Fig. 1 reveals quite clearly "tails" in the angular distribution, equivalent to scattering through a large angle, on the order of the channeling angle ϑ_0. This is caused by the existence of above-the-barrier states which are inevitably represented in the initial distribution of the particles even at entrance angles that are small in comparison with ϑ_0. Thus, the admixture of particles in such states is in no way connected with inelastic scattering. We note that in the simplified classical picture the presence of these states apparently corresponds to the random part of the beam produced on entering the crystal (in Lindhard's terminology[9]).

At $L_2 < L \ll L_0$, using (4.3) and (4.4), we obtain a distribution that does not vary with the thickness. The form of this distribution is shown in Fig. 2. We see that a quasisymmetrical distribution is indeed produced. Such a distribution was apparently observed in the experiments of Eisen and Robinson[2], who noted the onset of symmetrization in the angular distribution, starting at a certain thickness. It is interesting that in silicon this thickness turned out to be of the order of (5—7) $\times 10^3$ Å at a proton energy 0.4 MeV. This cale correlates with the estimate obtained in the preceding section. On the other hand, in the experiments of Lutz et

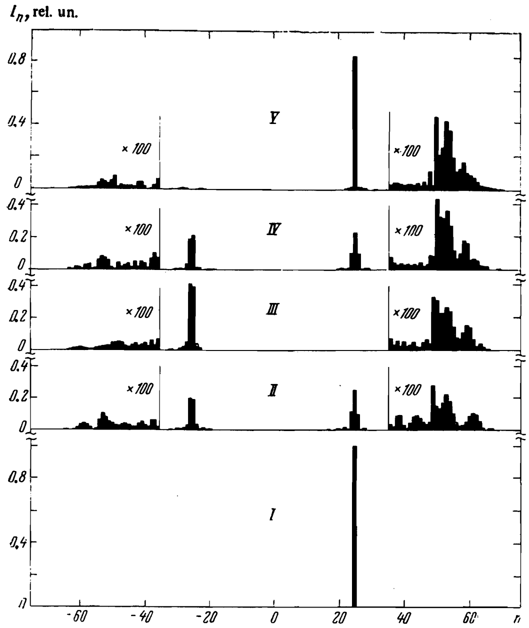

FIG. 1. Evolution of the angular distribution of protons as a function of the crystal thickness L in the case of planar channeling, neglecting inelastic processes and using an effective model potential of the Kronig-Penney type as an example: I - L = 0, II - L = 136, III - L = 232, IV - L = 408, V - L = 544 (L is in units of q_z^0/MV_0). The parameters of the potential are: period d = 2Å, height of barrier $V_0 = 4.5 \times 10^4/Md^2$ width of barrier b = 0.08Å. $I_n = I(q_{xn})$ are the intensities of the discrete beams with momenta $q_{xn} = (n + 1/4)$ (K_x^0 is the elementary reciprocal lattice vector), which are the only beams produced in the crystal when a plane wave with $q_x^0 = (101/4)K_x^0$ is incident on it (the components q_{yn} and q_{zn} of the momenta of the diffracted beams coincide with the corresponding values q_y^0 and q_z^0 of the incident beams).

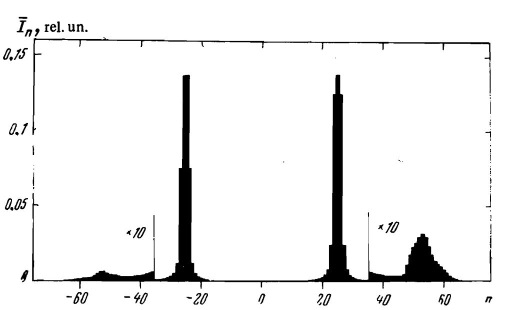

FIG. 2. Angular distribution of the particles, which remains unchanged with changing thickness, calculated for $L \gg L_2$ under the assumption that the inelastic scattering leads only to damping of the off-diagonal density-matrix elements. $\bar{I}_n$ are the intensities of the same diffracted beams as in Fig. 1, averaged over a small interval of n:

$$\bar{I}_n = \frac{1}{3}\sum_{k=-1}^{1} I_{n+k}$$

al.[10] a clear-cut picture of specular reflections of the beams was observed up to thicknesses on the order of 3×10^3 Å at $\{001\}$-plane channeling of α particles with energy 2 MeV in single-crystal gold. Thus, at least up to such thicknesses, inelastic processes played no significant role and the coherent picture was preserved.

5. DIFFUSION APPROXIMATION IN CHANNELLING

In accordance with the results of the preceding sections, we can state that at a crystal thickness $L \gg L_2$ we should in fact consider the kinetic equation only for the diagonal density-matrix elements. Using in this case the general expression (2.6)—(2.7), we obtain directly

$$\frac{\partial \rho_{1qq}}{\partial t} = \int \frac{dq'}{(2\pi)^2} \sum_{\alpha,\alpha'} |W_{qq'}^{\alpha\alpha'}|^2 \delta(E_{q'} + E_{\alpha'} - E_q - E_\alpha) \times [\overset{(0)}{\rho}_{2\alpha'} \rho_{1q'q'}(t) - \overset{(0)}{\rho}_{2\alpha} \rho_{1qq}(t)]. \qquad (5.1)$$

A solution of this equation, substituted in relation (4.3), should yield a complete description of the angular distribution of the particles after passage through a thick crystal. We note that an equation of the type (5.1) could be obtained from the initial equation by averaging in this equation the left- and right-hand sides over times that are long in comparison with the period $\hbar/(\epsilon_{q_x} + K_x - \epsilon_{q_x})$ of the oscillations of the off-diagonal elements (in classical language, this time was of the order of the period of the oscillations of the particle in the channel). However, it is only when $L > L_2$ that we can be certain that it suffices to consider only the diagonal part of the density matrix in the problem.

Since we are, of course, interested in the evolution of the distribution of the particles with respect to the transverse momentum, it is advisable to integrate the left- and right-hand sides of (5.1) with respect to dq_z. We limit the crystal thickness to a value at which the total particle-energy loss is relatively small. Then, considering scattering through limited angles, we obtain for the function

$$\tilde{\rho}(q_\perp, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \rho_{1qq}(t)\, dq_z \qquad (5.2)$$

the equation

$$\frac{\partial \tilde{\rho}(q_\perp, t)}{\partial t} = \int d^2 q_\perp' w(q_\perp, q_\perp') [\tilde{\rho}(q_\perp', t) - \tilde{\rho}(q_\perp, t)]. \qquad (5.3)$$

Here $w(q_\perp, q_\perp')$ denotes a quantity that plays the role of the transition probability, per unit time, between the states $q_\perp$ and $q_\perp'$:

$$w(q_\perp, q_\perp') = \frac{M}{(2\pi)^2 q^0} \sum_{\alpha,\alpha'} |W_{kk'}^{\alpha\alpha'}|^2 \overset{(0)}{\rho}_{2\alpha}, \qquad (5.4)$$

where $k = (q_\perp, q_z^0)$, $k' = (q_\perp', q_z^0)$ and q^0 is the momentum of the particles incident on the crystal.

We confine ourselves for simplicity to the case of planar channeling. We direct the x and y axes perpendicular and parallel to the considered family of crystallographic planes, respectively. Then q_y degenerates into the ordinary momentum, and q_x remains a quasimomentum in the expanded one-dimensional q_x space.

In the expanded zone scheme, the transition probability is subject to discontinuities at the end points of the Brillouin zone as a function of the variables q_x and q_x', or, equivalently, as a function of the discrete variable number of the zone. Bearing in mind that $K_x^0 \ll q_x^*$ ($q_x^* = [2M(V_{\text{eff}}^{\max} - V_{\text{eff}}^{\min})]^{1/2}$ is the momentum corresponding to the channeling angle ϑ_0), we are interested in the distribution of $\tilde{\rho}(q_\perp, t)$ over intervals that are large in comparison with the elementary reciprocal-lattice vector K_x^0. By virtue of this we use the smoothed-out value of the transition probability $w(q_\perp, q_\perp')$, which, of course, does not change the result at all.

As shown in the preceding section, motion in the channel, starting with a definite thickness, gives rise to a practically symmetrical angular distribution. Then, naturally, $\tilde{\rho}_{q_x q_x} \cong \tilde{\rho}_{-q_x', -q_x}$ (actually, this relation, being the relation between the diagonal elements proper, is established from the very outset for the subbarier states if $K_x^0 \ll |q_x| < q_x^*$). It is therefore advantageous to make use of the explicit form of this symmetrization, which takes place for subbarrier states as a result of the coherent action of the medium, and to introduce a symmetrized density matrix

$$\rho_+(q_x, q_y, t) = {}^1/_2[\tilde\rho(q_x, q_y, t) + \tilde\rho(-q_x, q_y, t)].$$

For this matrix we have from (5.3) the equation

$$\frac{\partial\rho_+(\mathbf{q}_\perp, t)}{\partial t} = 2\int_0^\infty dq_x' \int_{-\infty}^\infty dq_y' \, w_+(q_x, q_x', |q_y' - q_y|)[\rho_+(\mathbf{q}_\perp', t) - \rho_+(\mathbf{q}_\perp, t)]; \tag{5.5}$$

$w_+(q_x, q_x', |q_y' - q_y|)$ is the even part of the probability (5.4) with respect to the variable q_x' (in this case w_+ is automatically even also in the variable q_x). This circumstance has enabled us to confine ourselves in (5.5) to the half-space $q_x \geq 0$ in the solution of the problem.

In the general case, the expression for the probability w_+ can be represented in the form

$$w_+ = \tilde w(q_x + \Delta_x/2, |\Delta_x|, |\Delta_y|), \quad \Delta_\beta = q_\beta' - q_\beta, \quad \beta = x, y.$$

Bearing in mind the small-angle character of the scattering, we change over from the integral equation (5.5) to a differential equation of the Fokker-Planck type, using the well-known procedure (see, for example,[11]):

$$\frac{\partial\rho_+}{\partial t} = \frac{\partial}{\partial q_x} D_x^+(q_x)\frac{\partial\rho_+}{\partial q_x} + D_y^+(q_x)\frac{\partial^2\rho_+}{\partial q_y^2}, \tag{5.6}$$

$$D_\beta^+(q_x) = \int_{-\infty}^\infty d\Delta_y \int_{-q_x}^\infty d\Delta_x \tilde w(q_x, |\Delta_x|, |\Delta_y|)\Delta_\beta^2. \tag{5.7}$$

We have left the linear "hydrodynamic" term out of the right-hand side of (5.6), since this term simply vanishes at finite q_x, when the lower limit of integration can be replaced by $-\infty$, and this term does not play any role at small q_x near zero, by virtue of $\partial\rho_+/\partial q_x|_{q_x=0} = 0$.

Let us examine the values of the diffusion coefficients $D_\beta^+(q_x)$ inside the channel. To this end, we analyze first the contribution made to the diffusion coefficients by scattering from the vibrating nuclei without excitation of the electronic subsystem. The corresponding scattering probability, in accord with (5.4), can be written in the form

$$w_n(\mathbf{q}_\perp, \mathbf{q}_\perp') = \frac{M}{(2\pi)^2 q^0}\left\langle\left|\sum_j (V_j - \langle V_j\rangle)_{\mathbf{kk}'}\right|^2\right\rangle. \tag{5.8}$$

Here $V_{j\mathbf{kk}'}$ is the matrix element of the interaction with the j-th atom, averaged over the ground state of the electronic subsystem. The symbol $\langle\ldots\rangle$ denotes averaging over the phonon subsystem.

We consider a crystal consisting of atoms of one sort, and approximate the particle interaction with an individual atom, averaged over the ground state of the electronic subsystem, by a screened Coulomb potential. Then we obtain directly

$$V_{j\mathbf{kk}'} = \frac{2\pi Ze^2}{(\varkappa_0^2 + \Delta_y^2)^{1/2}}(\exp\{i\Delta_y R_{jy} - |x - R_{jx}|[\varkappa_0^2 + \Delta_y^2]^{1/2}\})_{q_x q_x'}. \tag{5.9}$$

Here $\mathbf{R}_j$ is the radius vector of the j-th nucleus, x is the particle coordinate, and κ_0 is the reciprocal of the screening radius.

Making use of the fact that D_x^+ varies little with q_x within the channel, we obtain approximately

$$D_x^+(q_x) \cong \int_{-\infty}^\infty d\Delta_y \int_0^\infty dq_x' \, w_+(q_x, q_x', |\Delta_y|)(q_x' - q_x)^2.$$

In accordance with the mean-value theorem and with the properties of the function w_+, we can write

$$D_x^+(q_x) = \frac{1}{2}\int_{-\infty}^\infty d\Delta_y \overline{\Delta_x^2}(q_x, \Delta_y)\int_{-\infty}^\infty d\Delta_x w(q_x, q_x + \Delta_x, |\Delta_y|).$$

We substitute (5.8) and (5.9) in this expression and use the completeness theorem when integrating with respect to $d\Delta_x$. In the approximation in which the oscillations of the individual atoms are independent, we arrive at the simple relation

$$D_x^{+n}(q_x) = \frac{\pi(Ze^2)^2 MN}{q^0}\int_{-\infty}^\infty \frac{\overline{\Delta_x^2}(q_x, \Delta_y)Q_n(q_x, \Delta_y)}{\varkappa_0^2 + \Delta_y^2} d\Delta_y,$$

$$Q_n(q_x, \Delta_y) = \int_{-\infty}^\infty [\langle\exp\{-2|x - R_{jx}|(\varkappa_0^2 + \Delta_y^2)^{1/2}\}\rangle \tag{5.10}$$

$$- \exp\{-\overline{u^2}\Delta_y^2\}\langle\exp\{-|x - R_{jx}|(\varkappa_0^2 + \Delta_y^2)^{1/2}\}\rangle^2]|\psi_{q_x}(x)|^2 dx,$$

where N is the density of the crystal atoms and $\overline{u^2}$ is the mean-squared thermal displacement of the atom along one of the coordinate axes.

Bearing in mind the exponential decrease of the wave function $\psi_{q_x}(x)$ in the region that is classically inaccessible to the particle inside the potential barrier (see I), we can readily conclude from (5.10) that

$$D_x^{+n}(q_x) \sim D_\infty \exp\{-2\varkappa_0|x_0(q_x) - R_{jx}^0|\},$$

where R_{jx}^0 is the equilibrium position of the nucleus, $x_0(q_x)$ is the classical turning point, nearest to this position, for a particle in the state q_x, and D_∞ is the value of the diffusion coefficient outside the channel and far from its boundaries.

This shows directly, if we use any reasonable estimate for κ_0, that for the overwhelming majority of the subbarrier states (with the possible exception of states directly adjacent to the top of the barrier), the diffusion coefficient $D_x^{+n}(q_x)$ is a very small quantity.

We note that at $|\Delta y| \lesssim \kappa_0$ we have as a rule $\overline{u^2}\Delta_y^2 < 1$. This leads to

$$Q_n(q_x, \Delta_y) \cong \overline{u^2}(\varkappa_0^2 + 2\Delta_y^2)\int_{-\infty}^\infty \exp\{-2|x - R_{jx}^0|(\varkappa_0^2 + \Delta_y^2)^{1/2}\}|\psi_{q_x}(x)|^2 dx \tag{5.11}$$

and as a result we obtain an additional source of smallness, which is physically connected with the fact that the regular lattice proper does not lead to incoherent scattering[1)].

We turn now to electron scattering. To determine $(D_x^{+e})_v$ due to scattering by valence electrons, we can use the same expressions (5.10), provided we leave out the second term in the square brackets, replace the coordinate of the nucleus by the coordinate of the electron, and take the symbol $\langle\ldots\rangle$ to mean averaging over the state of the electron subsystem (κ_0 should be replaced here by κ_e, and the factor Z^2 by Z_v). Assuming as an estimate that the spatial distribution of the valence electrons is homogeneous, we obtain simply

$$(D_x^{+e})_v = \frac{\pi Z_v e^4 MN}{q^0}\int_{-\infty}^\infty \frac{(\overline{\Delta_x^2}(\Delta_y))_v d\Delta_y}{(\varkappa_e^2 + \Delta_y^2)^{3/2}}.$$

Here Z_v is the number of valence electrons per atom and κ_e is the corresponding screening momentum.

An estimate of the contribution of the scattering by the internal electrons cannot, of course, be obtained as simply. It is clear only that in most cases the contribution of this scattering mechanism is, as a rule, small, by virtue of the already noted character of the behavior of the wave function of the particle in the region under the barrier.

Comparing the results, we can conclude that

$$\frac{D_x^{+n}(q_x)}{D_x^{+e}(q_x)} < \frac{Z^2}{Z_v} \exp\{-2|x_0(q_x) - R_{jx}^0|\varkappa_0\}.$$

We see from this expression that the ratio of the scatterings by electrons and by nuclei is radically altered in the channel, and a situation wherein electron scattering predominates is quite realistic[2]. In any case, however, the value of D_x^+ itself inside the channel turns out to be small in comparison with the value D_∞ outside the channel. If scattering by electrons predominates inside the channel, then D_x^+ decreases by a factor $\sim(Z_v/Z^2$ to $1/Z)$. Naturally, this should alter radically the character of the multiple scattering of the particles in channeling.

We have analyzed so far only the coefficient $D_x^+(q_x)$. It is seen from (5.7) that for $D_y^+(q_x)$ we should have the same expressions as for $D_x^+(q_x)$, with the substitution $\Delta_x^2(q_x, \Delta_y) \to \Delta_y^2$. It is clear from the structure of the formulas that in this case we have

$$D_y^+(q_x) \approx D_x^+(q_x).$$

In all the formulas considered above for D^+ we have ignored the standard difficulty of diffusion theory of multiple scattering by screened Coulomb centers connected with the logarithmic divergence of D_β^+ at large momentum transfers. To overcome this difficulty, it is necessary to take into account the finite width of the distribution over the transverse momentum when calculating the integrals with respect to $d^2\Delta_\perp$ in the expressions for the diffusion coefficients (for details see[12]).

Equation (5.6) with allowance for the explicit values of the diffusion coefficients (5.7) in the channel and outside the channel describes the picture of the transverse diffusion of particles incident on the crystal at an angle smaller than the channeling angle. This automatically establishes the symmetrization of the particle states, which was effectively taken into account from the very beginning (see Eq. (5.5)).

On the other hand, if the particle beam is incident at an angle $\vartheta > \vartheta_0$, then the picture must be refined somewhat. The point is that diffusion outside the channel proceeds in the usual manner, and so long as the particles are not drawn into the channel, no special symmetrization takes place in the distribution. For the total function $\tilde{\rho}$ outside the channel, we then have a diffusion equation of the type (5.6), with the substitution $D_\beta^+ \to D_\beta$, where D_β is defined by

$$D_\beta(q_x) = \frac{1}{2}\int_{-\infty}^{\infty} d\Delta_y \int_{-\infty}^{\infty} d\Delta_x w\left(q_x + \frac{\Delta_x}{2}, q_x - \frac{\Delta_x}{2}\ |\Delta_y|\right)\Delta_\beta^2$$

with the usual probability characteristic of scattering outside the channel (we shall henceforth ignore the role of the narrow transition layer near the channel boundary, and consider a problem that is strictly local and therefore distinctly subdivided into regions inside and outside the channel; accordingly, D_β^+ outside the channel coincides with D_β).

As soon as the particles enter the channel, however, the coherent action of the medium leads to symmetrization of the distribution inside the channel, and this occurs within times that are short in comparison with all other characteristic times in the problem. Therefore, if in addition to ρ_+ we introduce the function ρ_-:

$$\rho_-(q_x, q_y, t) = {}^1\!/_2[\tilde{\rho}(q_x, q_y, t) - \tilde{\rho}(-q_x, q_y, t)], \qquad (5.12)$$

then the latter will always be equal to zero inside the channel and in the general case different from zero outside the channel.

The rapid symmetrization of the distribution brings about a special connection between the points q_x^* and $-q_x^*$ at the channel boundaries (q_x^* is the momentum corresponding to the channeling angle), as manifest by a non-diffusion exchange of part of the flux at these points. Indeed, owing to the coherent action of the medium, part of the flux G from the point q_x^* is transferred to the point $-q_x^*$ "hydrodynamically." The conditions at the channel boundaries are then

$$-D_1\frac{\partial\tilde{\rho}}{\partial q_x}\bigg|_{q_x=\pm q_x^*\pm 0} = -D_0\frac{\partial\tilde{\rho}}{\partial q_x}\bigg|_{q_x=\pm q_x^*\mp 0} + G, \qquad (5.13)$$

where D_0 and D_1 are the values of the diffusion coefficients inside and outside the channel near its boundaries. Recognizing that

$$\rho_-(q_x, q_y, t) = 0 \text{ for } |q_x| \leq q_x^*, \qquad (5.14)$$

we can easily obtain from (5.13)

$$D_0\frac{\partial\rho_+}{\partial q_x}\bigg|_{q_x=q_x^*-0} = D_1\frac{\partial\rho_+}{\partial q_x}\bigg|_{q_x=q_x^*+0}, \quad G = -D_1\frac{\partial\rho_-}{\partial q_x}\bigg|_{q_x=q_x^*+0} \qquad (5.15)$$

Equations of the type (5.6), written out for the regions inside and outside the channel, together with the conditions (5.14) and (5.15) and the continuity condition for $\tilde{\rho}$, solve completely the problem of multiple scattering in channeling.

6. ANALYSIS OF THE PICTURE OF MULTIPLE SCATTERING UNDER CONDITIONS OF PLANAR CHANNELING

To reveal the qualitative picture of the character of multiple scattering of fast particles in planar channeling, we consider in the present section the solution of the diffusion problem assuming the diffusion coefficients to be constant inside and outside the channel:

$$D_x^+(q_x) = D_y^+(q_x) = \begin{cases} D_0 & \text{for } |q_x| < q_x^* \\ D_1 > D_0 & \text{for } |q_x| \geq q_x^* \end{cases} \qquad (6.1)$$

Let the initial distribution of the beam be δ-like, i.e.,

$$\rho_+(q_x, q_y, 0) = {}^1\!/_2[\delta(q_x - q_x^0) + \delta(q_x + q_x^0)]\delta(q_y). \qquad (6.2)$$

The problem of finding ρ_+ then reduces in fact to a solution of Eq. (5.6) with allowance for (6.1), for the boundary condition (5.5), and for the initial condition (6.2). It is convenient here to use the Laplace transform with respect to time and the Fourier transform with respect to the "coordinate" q_y, and to seek the solution as a function of q_x in explicit form. Taking into account the initial and boundary conditions and taking the inverse transforms, we arrive after straightforward but cumbersome manipulations at the following expression for ρ_+:

$$\rho_+(q_x, q_y, t) = f_1(q_x, q_y, t) + f_2(q_x, q_y, t),$$

$$f_1(q_x, q_y, t) = \frac{1}{\pi^2}\int_0^\infty dp\, e^{-p^2 t}\cos(p\eta^{1/2} q_y)$$

$$\times \int_0^\infty \frac{\exp\{-\zeta^2 t\} R(q_x^0, \zeta, p) R(q_x, \zeta, p)\, d\zeta}{\lambda^2(\zeta, p)\sin^2\lambda(\zeta, p) + \eta^{-1}\zeta^2\cos^2\lambda(\zeta, p)},$$

$$f_2(q_x, q_y, t) = \frac{1}{\pi}\int_0^\infty e^{-p^2\eta t}\cos(p\eta^{1/2} q_y)$$

$$\times \sum_{\zeta_n(p)} \frac{\exp\{-\zeta_n^2(p)t\} S(q_x^0, \zeta_n, p) S(q_x, \zeta_n, p)}{\eta^{-1/2} + p^2\{[p^2 - \zeta_n^2(p)][(1-\eta)p^2 - \zeta_n^2(p)]^{1/2}\}^{-1}} \quad (6.3)$$

Here

$$R(q_x, \zeta, p) = \zeta \cos[\zeta\eta^{1/2}(|q_x| - 1)]\cos\lambda(\zeta, p)$$
$$-\eta^{1/2}\sin[\zeta\eta^{1/2}(|q_x| - 1)]\sin\lambda(\zeta, p) \text{ for } |q_x| \geq 1,$$
$$R(q_x, \zeta, p) = \zeta\cos[q_x\lambda(\zeta, p)] \text{ for } |q_x| < 1;$$
$$\lambda(\zeta, p) = [\zeta^2 + (1-\eta)p^2]^{1/2}; \quad (6.4)$$
$$S(q_x, \zeta_n, p) = \exp\{-\eta^{1/2}[(1-\eta)p^2 - \zeta_n^2(p)]^{1/2}(|q_x| - 1)\}\cos\zeta_n(p)$$
$$\text{for } |q_x| \geq 1,$$
$$S(q_x, \zeta_n, p) = \cos[q_x\zeta_n(p)] \text{ for } |q_x| < 1,$$

and the summation over ζ_n is the sum of the residues at the poles of the Laplace transform, with ζ_n determined as the roots of the equation

$$\eta^{1/2}\zeta_n \operatorname{tg}\zeta_n = [(1-\eta)p^2 - \zeta_n^2]^{1/2}, \quad (6.5)$$

located in the interval $0 \leq \zeta_n \leq p(1-\eta)^{1/2}$.

In expressions (6.3)—(6.5) and in the following ones, q_x, q_y, t, and ρ_+ are taken to mean the dimensionless quantities

$$q_x / q_x^*, \; q_y / q_y^*, \; tD_0 / (q_x^*)^2, \; (q_x^*)^2\rho_+, \quad (6.6)$$

and we designate the ratio of the diffusion coefficients by

$$\eta = D_0 / D_1$$

(as $\eta \to 1$, the function f_2 vanishes, while f_1 goes over into the well-known solution for homogeneous space).

In the analysis of the multiple-scattering picture, there are two physically different cases, when the directions of incidence of the initial beam are such that $|q_x^0| < 1$ and $|q_x^0| > 1$. It is convenient to consider these cases separately.

Case A: $|q_x^0| < 1$

Analyzing the behavior of $\tilde{\rho}$, which at $|q_x^0| < 1$ coincides identically with ρ_+, in the case of short times, corresponding to the condition

$$t^{1/2} / [1 - |q_x^0|] \ll 1,$$

we can easily obtain

$$\tilde{\rho}(q_x, q_y, t) \cong \frac{1}{8\pi t}\left[\exp\left\{-\frac{(q_x - q_x^0)^2}{4t}\right\} + \exp\left\{-\frac{(q_x + q_x^0)^2}{4t}\right\}\right]\exp\left\{-\frac{q_y^2}{4t}\right\} \text{ for } |q_x| < 1. \quad (6.7)$$

It is seen from this expression that at sufficiently short times the presence of channel boundaries has not yet come into play, and the diffusion is determined completely by the coefficient D_0 (see the notation in (6.6)).

To describe the evolution of the particle distribution in the channel, we put for simplicity $q_x^0 = 0$ and investigate the region of small q_x and q_y at arbitrary times. In this case

$$\tilde{\rho}(q_x, q_y, t) = \tilde{\rho}(0, 0, t) + A(t)q_x^2 + B(t)q_y^2. \quad (6.8)$$

At short times, the constant-level lines of the function $\tilde{\rho}$, as seen from (6.7), are circles. At long times, the contribution of f_2 to $A(t)$ and $B(t)$ can be neglected. Determining the asymptotic form of f_1 and taking the second derivatives with respect to q_x and q_y at zero, we obtain

$$A(t) \cong -\eta(2-\eta) / 32\pi t^2, \quad B(t) \cong -\eta^2 / 32\pi t^2.$$

Hence

$$\lim_{t\to\infty} [A(t)/B(t)] = 2D_1/D_0 - 1. \quad (6.9)$$

Thus, in the considered case the level lines of the function $\tilde{\rho}$ in the region of small q_x and q_y become deformed in the course of time from circles to ellipses, becoming more and more elongated along the y axis, with a maximum ratio (6.9) of the squares of the semi-axes (at $D_1 > D_0$; if $D_1 = D_0$, then the circular symmetry is preserved).

This result is quite remarkable for the entire picture of diffusion in channeling. Indeed, let us bear in mind that in a real case $D_1 \gg D_0$. Then at times $t \sim 1$ the fast diffusion in the region outside the channel comes abruptly into play, and causes the distribution at $t \gtrsim 1$ to be sharply delineated within the width of the channel. Since diffusion with the characteristic coefficient D_0 takes place at the same time along the channel, the distribution of $\tilde{\rho}$ exhibits a clearly pronounced tendency to become elongated along the y axis. A situation close in fact to diffusion under conditions of total absorption on the channel boundaries produces in the direction of x gradients (dictated by D_1) that are large in comparison with the gradients along the y direction (which are dictated by D_0). It is precisely this circumstance which is reflected in the result (6.9). Thus, under conditions of planar channeling there should occur a strongly pronounced anisotropy of the particle distribution, and the scale of the anisotropy should correlate uniquely in the experiment with the ratio D_1/D_0.

The strong difference between the diffusion coefficients inside the channel and outside the channel lead to an interesting effect of "screening" of the channel. Its gist lies in the fact that the particles emerging from the channel and returning to its boundary at noticeable "distances" q_y as a result of fast diffusion experience, as it were, reflections from the channel boundaries, namely, the particles diffuse principally along the channel (in momentum space), and not into its interior. As a result, over a large interval of q_y, the density of the scattered particles outside the channel is much larger than the density inside the channel (a "white channel" against a "grey background"). We emphasize once more that this effect is a consequence only of the ratio $D_1/D_0 \gg 1$, which is characteristic of the channeling effect. This phenomenon was treated earlier as a manifestation of the "blocking" effect (see, for example,[3]).

We note that simultaneously there takes place a unique "shunting" effect, wherein particles that have experienced diffusion outside then channel can again be trapped in the channel at distances much larger than the distances characteristic of diffusion in the channel along the y axis. This should alter noticeably the character of the distribution of the particles in the channel itself, especially at intermediate distances ($q_y^2/4t > 1$).

The described picture is very clearly pronounced in Figs. 3 and 4, where the constant-density lines $\tilde{\rho}$ are plotted in accordance with (6.3) for different values of t. First to be noted is a very sharp distribution anisotropy that increases continuously with time. The stretching of the distribution of $\tilde{\rho}$ along the y axis near its maximum value has already become noticeable at $t = 1$, and is the stronger the larger t and the larger the ratio D_1/D_0.

The figures corresponding to the times $t = 0.5$ and $t = 1$ show quite distinctly the manifestation of the

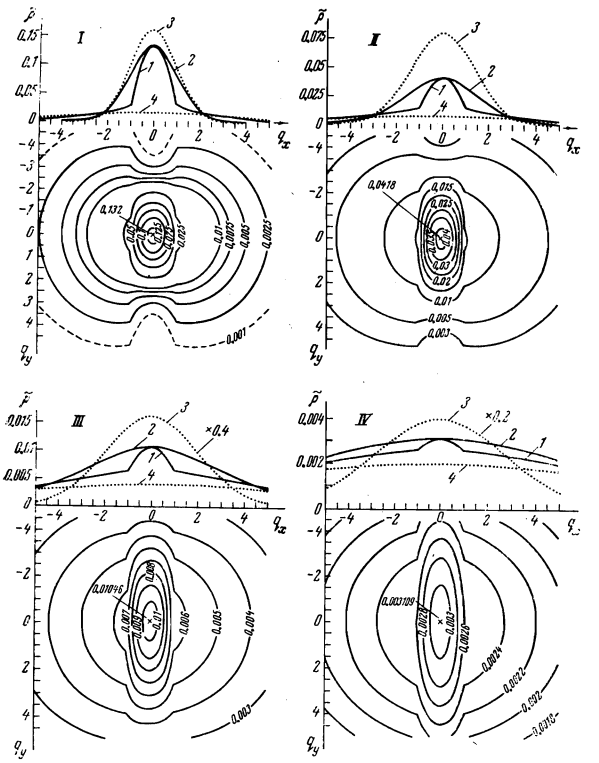

FIG. 3. Constant-level lines and profiles of the function $\tilde{\rho}$, calculated in accordance with (6.3) for the case $\eta = 0.1$. Initial value $q_x^0 = 0$. The distributions presented correspond to the following instants of time t: I - 0.5, II - 1, III - 2, IV - 4. Curves 1 and 2 give the sections of $\tilde{\rho}$ by the planes $q_y = 0$ and $q_x = 0$, respectively, while curves 3 and 4 give the distributions that describe the diffusion in homogeneous space with coefficients D_0 and D_1, respectively.

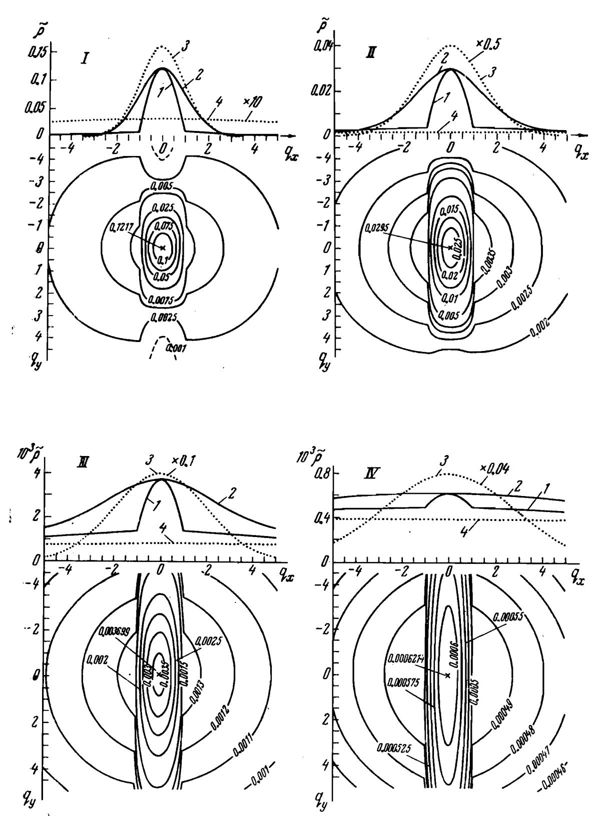

FIG. 4. The same distributions as in Fig. 3, constructed for the case $\eta = 0.02$.

channel "screening" effect. Indeed, at noticeable q_y, the density $\tilde{\rho}$ inside the channel turns out to be appreciably smaller than outside the channel. At the same time, a "shunting" effect comes into play, wherein the particle flux density vector is directed away from the walls towards the center of the channel. With increasing time, the region where the "screening" and "shunting" effects come into play moves away from the origin and corresponds to values of q_y not found in the figures at times $t > 1$ (see also[12]).

Finally, we note that the relative value of the maximum in the region of the channel decreases with increasing time and in the limit as $t \to \infty$ the distribution tends to become uniform, as it should.

Case B: $|q_x^0| > 1$

To determine $\tilde{\rho}$ in this case it is necessary to add to the function ρ_+, which is determined by the same general expressions (6.3), the function ρ_- (5.12). The latter is determined in the form of a continuous function that is equal to zero in the channel and satisfies equation (5.6) outside the channel (with allowance for (6.1)) with the initial condition

$$\rho_-(q_x, q_y, 0) = {}^1/_2[\delta(q_x - q_x^0) - \delta(q_x + q_x^0)]\delta(q_y).$$

It is easy to see that ρ_- is simply

$$\rho_-(q_x, q_y, t) = \operatorname{sign}(q_x q_x^0)\frac{\eta}{8\pi t}\left[\exp\left\{-\frac{\eta(|q_x| - |q_x^0|)^2}{4t}\right\}\right. \tag{6.10}$$

$$\left. - \exp\left\{-\frac{\eta(|q_x| + |q_x^0| - 2)^2}{4t}\right\}\right]\exp\left\{-\frac{\eta q_y^2}{4t}\right\} \text{ for } |q_x| \geq 1;$$

$$\rho_-(q_x, q_y, t) = 0 \text{ for } |q_x| < 1.$$

For short times

$$t^{1/2}\eta^{-1/2} / (|q_x^0| - 1) \ll 1,$$

we obtain directly, by determining $\tilde{\rho}$ with allowance for (6.10),

$$\tilde{\rho}(q_x, q_y, t) = \rho_+(q_x, q_y, t) + \rho_-(q_x, q_y, t)$$

$$\cong \frac{\eta}{4\pi t}\exp\left\{-\frac{\eta[q_y^2 + (q_x - q_x^0)^2]}{4t}\right\} \text{ for } |q_x| > 1.$$

It was perfectly natural that at such times the picture of the distribution is equivalent to the situation of homogeneous space with diffusion coefficient D_1.

The exponential decrease towards the channel boundary, from the outside, is accompanied at short times by an even sharper exponential decrease inside the channel ($D_0 \ll D_1$). At the same time, the coherent action of the medium leads to symmetrization of the distribution with respect to q_x inside the channel within very short times (as already noted above, these times are small in comparison with all the other characteristic times in the problem). This results in a unique "forced channel crossing," manifest in the fact that the particle density near the opposite boundary of the channel is immediately appreciably larger than that at the center of the channel. The total number of particles remaining in the "forced" channel, however, turns out to be small.

The particles that forced have executed the channel crossing leave the channel rapidly, whereas the particles that fall in the channel stick in it, increasing at first the total number of particles in the channel. After times that are already characteristic of diffusion with a coefficient D_0, the minimum on the channel axis gives way to a distribution peak, and the subsequent evolution of the distribution of the particles trapped in the channel recalls the picture described in case A.

The validity of the foregoing statements can be checked by considering the behavior of the density distribution at small q_x and q_y in the channel, for which the general representation (6.8) is valid. In the case of long times, $t \gg 1$, we have

$$A(t) = -\frac{\eta}{16\pi t^2}\left[\left(1-\frac{\eta}{2}\right)-\frac{\eta(q_x^0)^2}{4t}\right]\exp\left\{-\frac{\eta(q_x^0)^2}{4t}\right\},$$

$$B(t) = -\frac{\eta^2}{32\pi t^2}\exp\left\{-\frac{\eta(q_x^0)^2}{4t}\right\}.$$

It follows therefore that the minimum of $\tilde{\rho}$ as a function of q_x turns into a maximum at $q_x = 0$ (which is, generally speaking, a saddle point) in the case of long times, and roughly speaking, that the accumulation of particles in the channel gives way to diffusion from the channel. The maximum of the distribution shifts to this point from the region outside the channel. The $\tilde{\rho}$ level lines near the origin then take the form of ellipses that become elongated along the y axis with increasing t. Their semiaxis ratio, just in the case A, tends to $(2D_1/D_0 - 1)^{1/2}$ as $t \to \infty$.

All the obtained results can be very clearly traced by analyzing the curves obtained in accordance with (6.3) and (6.10) and shown in Fig. 5. The curves for the short times demonstrate quite lucidly the effect of "forcing" of the channel. A sharp density spike is seen on the left edge of the channel ($q_x = -1$, as well as a distribution corresponding in the interior of the channel

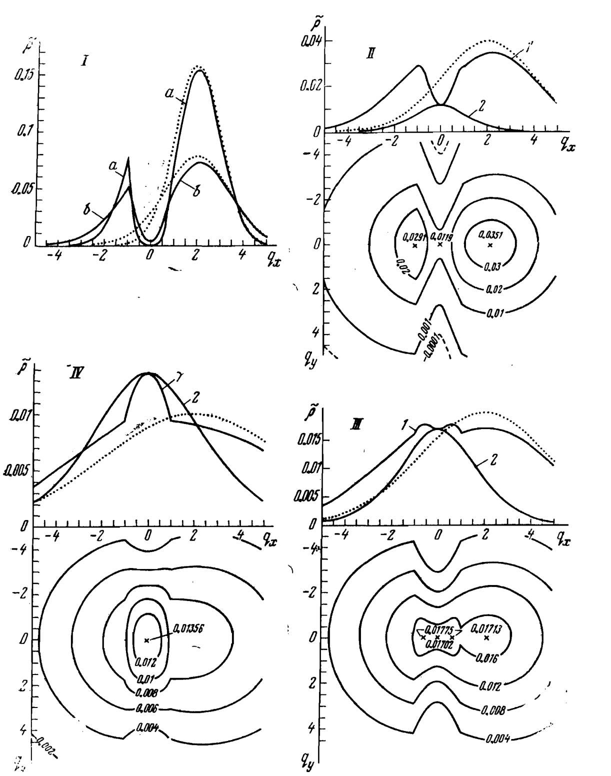

FIG. 5. Constant-level and profile lines of the function $\tilde{\rho}$, constructed in accordance with (6.3) and (6.10) for the case $\eta = 0.1$. The initial value is $q_x^0 = 2$. The distributions presented here correspond to the following instants of time t: I, curve a – t = 0.05, I, curve b – t = 0.1; II, t = 0.2, III, t = 0.4, IV t = 0.8. Curves 1 and 2 give the intersections of $\tilde{\rho}$ with the planes $q_y = 0$ and $q_x = 0$, respectively. The points show the distributions describing the diffusion in uniform space with a diffusion coefficient D_1. In case I, the curves show only the distribution of $\tilde{\rho}$ in the plane $q_y = 0$.

to a saddle point at $q_x = q_y = 0$. In the case of longer times, a delay of the particles in the channel is observed, accompanied by a strong anisotropy of the distribution within the channel and by the appearance of a "screening" effect, two phenomena typical of the picture of diffusion of particles from the channel (see also[12]).

7. COMPARISON WITH EXPERIMENTAL RESULTS

The theory developed in the preceding sections for multiple scattering of fast particles under conditions of channeling explains all the main experimental results obtained in this region. On the other hand, it is interesting to verify that all the theoretically deduced features of the physical picture become observable in one form or another in experiment.

We note first of all that the momentum distribution of the particles is connected with the diagonal density matrix ρ_{1qq} by the relation (4.3). Being interested only in the distribution with respect to the transverse momentum, or in the angular distribution, we can change over in this expression from $\rho_{1qq}(t)$ to the function $\tilde{\rho}(q_\perp, t)$ (5.2), which we have obtained precisely in the preceeding section. The function $|C_q(\kappa)|^2$ at $|\kappa_x| < q_x^*$ is close to a superposition of δ functions at the points $q_x = \pm\kappa_x$, and is close to a δ function at point $q_x = \kappa_x$ when $|\kappa_x| > q_x^*$. Consequently the angular distribution $\rho_1(\kappa_\perp, t)$ is close to the function $\tilde{\rho}(\kappa_\perp, t)$. As a consequence, all the experimental data can be compared with the results obtained for the distribution function $\tilde{\rho}(q_\perp, t)$.

The first experiments in which the angular distributions of fast heavy charged particles were measured in planar channeling were those of Gibson et al.[4]. They were the first to observe a sharp anisotropy of the angular distribution with stretching along the channel. The experimental distribution of the particles is qualitatively very close to the picture shown in Figs. 3–4.

Dearnaley et al.[5] have revealed very clearly the character of the anisotropy by measuring the distribution of the particles in two planes, one of which is parallel to the plane of the channel and the other perpendicular to it. It is interesting that the shapes of the obtained curves are very close to those of the distributions in the planes $q_y = 0$ and $q_x = 0$, as shown in Figs. 3–4. Dearnaley et al. were apparently the first to observe the effect of the sharp increase of the intensity on the opposite edge of the channel while the density remained low inside the channel if the proton-beam incidence angle was larger than the channeling angle ϑ_0. This nontrivial result, which was not explained adequately either in that reference or in any subsequent one, is none other than the "forced crossing" of the channel, which was described in detail in the preceding section (see Fig. 5).

The effect of trapping and retention of the particles in the channel at initial-beam incidence angles larger than ϑ_0 was first revealed in distinct form by Markus, Geguzin, and Faĭnshteĭn[6]. They have pointed out that when the proton energy is increased at a fixed crystal thickness and a fixed geometry, the capture effect can give way to a picture characterized by a value of the particle density in the channel that is smaller than the diffusion background outside the channel. It is easily seen that the explanation of this phenomenon lies in the decrease of the diffusion coefficient with energy, and consequently, at a fixed thickness, in a change of the characteristic time t. When such a decrease takes place, the particle distribution changes from that represented by curves IV and III in Fig. 5 to that represented by curves II and I in the same figure.

In[5], as well as in many other papers, "screening" of the channel was clearly observed, namely, the particle density inside the channel, at a large distance from the initial direction of incidence, turned out to be small in comparison with the diffusion background outside the channel.

Finally, we note that Golovchenko[13] recently performed a detailed investigation wherein the angular distribution of the particles was varied under conditions of planar channeling and with systematic variation of the angle of incidence from values $\vartheta < \vartheta_0$ to $\vartheta > \vartheta_0$. He used 1.8-MeV protons and thin gold crystals. The experimental results are in good qualitative agreement with the distributions given in Figs. 3–5[3)].

It should be stated that all the physical arguments advanced in the analysis of particle diffusion in an individual planar channel remain fully in force also for a system of planar channels in the case of axial channeling. The formation of a star-like angular distribution with prongs of increased intensity along the planar channels, and the drop of the intensity at large distances in the channels below the intensity of the surrounding background, can be obtained directly from a diffusion equation similar to that used above for an individual planar channel.

[1)]The expression for the total cross section $\sigma_n(q_x)$, per atom, for scattering by oscillating nuclei without excitation of the electronic subsystem is obtained from (5.10) by making the substitution $\overline{\Delta_x^2}(q_x, \Delta_y) \to 2$ and dividing the result by Nv_0. Taking (5.11) and the rapid convergence of the integral with respect to $d\Delta_y$ into account, we readily obtain the estimate

$$\sigma_n(q_x) \sim u^2\varkappa_0^2 \exp\{-2\varkappa_0|x_0(q_x) - R_{jx}^0|\}\sigma_0,$$

where σ_0 is the cross section for elastic scattering by an individual atom in free space.

[2)]For the ratio of the total cross sections of the nuclear and electronic scattering in the channel we have an even stronger bound

$$\sigma_n(q_x) / \sigma_e(q_x) < (Z^2 / Z_v)\overline{u^2}\varkappa_e^2 \exp\{-2|x_0(q_x) - R_{jx}^0|\varkappa_0\}.$$

[3)]One of the authors (Yu. Kagan) is grateful to Prof. Gibson for the opportunity of becoming acquainted with Golovchenko's dissertation prior to publication.

[1]Yu. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. 58, 226 (1970) [Sov. Phys.-JETP 31, 124 (1970)].
[2]F. H. Eisen and M. T. Robinson, Phys. Rev., B4, 1457 (1971).
[3]M. W. Thompson, Contemp. Phys., 9, 375 (1968).
[4]W. M. Gibson, C. Erginsoy, H. E. Wegner, and B. R. Appleton, Phys. Rev. Lett., 15, 357 (1965).
[5]G. Dearnaley, I. V. Mitchell, R. S. Nelson, B. W. Farmery, and M. W. Thompson, Phil. Mag., 18, 985 (1968).
[6]A. M. Markus, Ya. E. Geguzin, and A. L. Faĭnshteĭn, Zh. Eksp. Teor. Fiz. 61, 332 (1971) [Sov. Phys.-JETP 34, 175 (1972)].
[7]A. B. Migdal, Dokl. Akad. Nauk SSSR 105, 77 (1955).
[8]G. Moliere, Zs. Naturforsch., 3A, 78 (1948).
[9]J. Lindhard, Mat.-Fys. Medd. Dan Vid. Selsk., 34, 14 (1965).
[10]H. O. Lutz, R. Ambros, C. Mayer-Böricke, K. Reichelt, and M. Rogge, Zs. Naturforsch., 26A, 1105 (1971).
[11]L. Landau, Phys. Zs. Sowjetunion, 10, 154 (1936).
[12]Yu. Kagan and Yu. V. Kononets, Theory of Channeling Effect. II. Influence of Inelastic Collisions, 1972. Preprint IAE-2249, Moscow, 1972.
[13]J. A. Golovchenko, Ph. D. Thesis, Rensselaer Polytechnic Institute, Troy, New York, 1972.(unpublished).

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