

Quantum theory of the inelastic scattering of channeled particles

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A kinetic equation is derived for the density matrix in the problem of fast-ion scattering by a single crystal, including the effect of plane channeling. The nonoscillatory part of the spatial density of the channeled particles is separated out in the quasiclassical approximation. Based on the formulas obtained for the kinetic coefficients in the Fokker-Planck equations, an analysis is made of the roles of various inelastic scattering mechanisms. The results of classical and quantum theory are compared.

1. INTRODUCTION

The use of quantum-mechanical methods to analyze the interactions of fast charged particles with crystals is justified for several reasons. For example, the band structure of the spectrum of particles with energies above the barrier level is responsible for the appearance of interference phenomena in the angular distribution of the charged particles. The related oscillatory structure of the distribution near the critical angle for heavy ions (protons) has been observed experimentally^[1]. The motion of light particles in a channel is also essentially quantum in nature, since there exist only a few levels in the potential well formed by the channel walls^[2].

Although the effects due to coherent diffraction of the incident beam have undergone ample theoretical investigation, the question of their existence in a number of experiments still remains open^[3]. This is largely due to the difficulties of a theoretical analysis of such processes as elastic (coherent) scattering in an ideal lattice and inelastic scattering by the thermal oscillations of the lattice and the electrons. These difficulties arise from the fact that the channeling effect can display separate features in a quantum or a classical picture. For this reason the scattering problem, in particular, requires the use of multiple-wave approximations within the framework of the dynamic theory of diffraction^[4-6].

In the following we shall solve the problem of the scattering of a plane wave by a single crystal, including the effect of plane channeling. A similar problem was discussed by Kagan and Kononets^[5,6], who obtained expressions for the angular and spatial distributions of the scattered particles and analyzed them numerically in the Kronig-Penney potential approximation. It is useful, however, to consider the possibility of obtaining rigorous analytical results in cases when a quasiclassical treatment or simple model potentials are applicable.

2. STATEMENT OF THE PROBLEM

Let us assume a high-energy particle beam to be incident upon the surface of a single crystal. In the small-angle approximation the scattering problem can be regarded as transient, since the thickness L of the crystal in the incident direction of the beam is uniquely related to the time of evolution of the particle wave function $\Psi(\mathbf{r}, t)$ in the field of the crystal: $t = L/v$ (where v is the particle velocity). Since we shall neglect the braking effect (the corresponding criterion will be stated below), we can assume that the coordinates

of the lattice atoms are fixed and do not vary during the scattering time.

When the direction of beam incidence is far from any densely-packed direction in the lattice, Ψ varies with time almost as in an amorphous medium. Assuming an amorphous target, Migdal^[7] obtained an equation for the particle density matrix $\rho = \Psi^*(\mathbf{r}', t)\Psi(\mathbf{r}, t)$, which contains all the information about the angular and spatial distributions. When the beam approaches a low-index direction, the structure of the target begins to affect the scattering process; the mean free path increases, the energy loss is reduced, and so on^[8].

To take into account the plane channeling effect it is sufficient to assume that the atoms lie randomly in the YZ atomic planes with uniform density Nd (d is the distance between planes, N is the number of atoms per cm^3) and oscillate, with mean square amplitude \bar{u}^2 , in the X direction normal to the given family of planes. This picture corresponds to the case of beam incidence far from any dense-packed directions in the plane, and allows us to neglect the ordered arrangement of atoms in each plane and to simplify the statement of the scattering problem^[9].

It is convenient to write the particle density matrix in the representation of the eigenfunctions of the averaged (over the atomic positions) Hamiltonian with a one-dimensional periodic potential $Y(x) = \langle V \rangle$, where V is the potential of the particle interaction with the lattice atoms, and

$$\begin{aligned} \langle V \rangle &= \sum_j \langle V^0(\mathbf{r}-\mathbf{R}_j) \rangle = Nd \int dy dz ds W(s) \\ &\times \sum_k V^0(x+s+kd, y, z) = \sum_k Y^0(x+kd), \quad (2.1) \\ W(s) &= (2\pi\bar{u}^2)^{-1/2} \exp(-s^2/2\bar{u}^2). \end{aligned}$$

Here $V^0(\mathbf{r})$ is the binary potential of the interaction, the index j enumerates the positions \mathbf{R}_j of the lattice atoms, and $Y^0(x)$ are the averaged potentials of the atomic planes. The eigenfunctions for a potential in the form (2.1) can be written as

$$\psi_s = \exp(ip_y y + ip_z z) \varphi_{np_x}(x), \quad s = p_y, p_z, p_x, n, \quad (2.2)$$

where φ_{np_x} are the one-dimensional Bloch functions corresponding to a state with quasimomentum p_x in the n -band (in the reduced band scheme $\hbar = c = 1$, and the normalized volumes are omitted).

In the case of the scattering of heavy positive ions, the band structure of the spectrum can be neglected for the great majority of states with energies $\epsilon_{np_x} \sim Y_{\text{max}} \sim 10-10^2 \text{ eV}$ (Y_{max} is the barrier height), to which the

channeling effect is related. At the same time, in conditions of weak channeling the allowed energy bandwidth $\Delta\epsilon_a$ is on the order of the level splitting in a single potential well; this is due to the possibility of a tunneling transition into a neighboring potential well. The estimate^[10]

$$\Delta\epsilon_a \sim \frac{\omega}{\pi} \exp(-a[2m(Y_{\max}-\epsilon)]^{1/2}),$$

where ω is the frequency of the classical oscillations of a particle with energy ϵ in the channel and a is the screening parameter, indicates that, starting at several eV below the barrier energy, $\Delta\epsilon_p$ becomes much smaller than the forbidden gap width $\Delta\epsilon_f \sim \omega \sim 10^{-1}$ eV. Thus the transverse motion of the channeled particle (along the X axis) can be described within the framework of a multiple-wave model in the potential formed by the two neighboring atomic planes:

$$Y_c = Y^0(x+d/2) + Y^0(x-d/2).$$

We first consider nuclear collisions. The difference between the potential of particle interactions with the lattice and the continuous potential leads to transitions between the states (2.2). The Liouville equation for the particle density matrix in representation (2.2) can be obtained by generalizing the result that Migdal^[7] obtained for an amorphous medium to the case of an arbitrary distribution of the coordinates of the lattice atoms (see the Appendix):

$$\frac{\partial \rho_{n'n}}{\partial t} + i(E_n - E_n) \rho_{n'n} = \pi \left\{ \sum_{s'''} \langle \Delta V_{n'n} \Delta V_{s'''} \rangle \rho_{s'''} [\delta(E_{s'''} - E_n) + \delta(E_n - E_{s'''})] - [\langle \Delta V_{s'''} \Delta V_{n'n} \rangle \rho_{n'n} + \langle \Delta V_{n'n} \Delta V_{s'''} \rangle \rho_{s'''}] \delta(E_n - E_{s'''}) \right\}, \quad (2.3)$$

where $\Delta V_{S_1 S_2}$ is the matrix element of the operator $\Delta V = V - \langle V \rangle$ over the states (2.2), and

$$E_s = \epsilon_{n p_x} + p_y^2/2m + p_z^2/2m.$$

Equation (2.3) differs from the result obtained by Kagan and Kononets^[6] in that Eq. (2.3) includes an additional term in the δ -functions on the right-hand side, equal to the difference in the lattice energies before and after the collision. In our approximation, where the positions of the target atoms are "frozen," the total energy of the particle is conserved; a more rigorous approach (see^[6]) would take into account energy exchange between the particle and the lattice phonons. In the final analysis this difference amounts to the appearance of a correction of order p_{\perp}/p in the collision term of Eq. (2.3), where p_{\perp} is the average transverse transmitted momentum of the particle and p is the total momentum. To verify this we need only perform the sum over the longitudinal transmitted momentum $q_z = p_{z1} - p_{z2}$ in the right side of Eq. (2.3). For sufficiently thin single crystals, such that $p_z/p \ll 1$, the braking can be neglected and all calculations can be carried out in the approximation of frozen target atoms.

We are similarly uninterested in the relaxation of the distributions in the surface layer of the target, but shall consider only the diagonal elements of the density matrix. There are two reasons for this. First, the non-diagonal elements of the density matrix undergo damping in connection with the scattering of the waves (2.2). The corresponding scattering length L_1 depends, generally speaking, on the transverse energy. For states with $\epsilon_{n p_x} \sim Y_{\max}$ the principal scattering mechanism is nuclear, and $L_1 \sim L_{\text{nuc}} \sim \alpha/N\sigma^{[6]}$ (σ is the total cross section of a single center, and $\alpha > 1$). For deep

levels only scattering by the valence electrons is significant, so that $L_1 \sim Z^2 L_{\text{nuc}}$ (Z is the charge of the target atoms).

Second, even in the absence of damping, i.e., when the right side of Eq. (2.3) is zero, the contribution to the angular and spatial distributions from the terms that contain nondiagonal elements of the density matrix $L > L_1$ is found to be small in many cases. We may illustrate this by considering the yield of a nuclear reaction I:

$$I = \langle n(x, t) \rangle_{\tau} = \int n(x, t) W(x+d/2) dx, \quad (2.4)$$

where the spatial density of the particles for an arbitrary direction of beam incidence p_x has the form

$$n_{p_x}(x, t) = \sum_{n, n'} \rho_{n, n'}(0) \varphi_n(x) \varphi_{n'}(x) \exp[-i(\epsilon_n - \epsilon_{n'})t]. \quad (2.5)$$

(Here and below $s = n, p_x$.)

Because of the quasiclassical form of the wave functions φ_s , the value of I is specified primarily by the contribution from states for which the overlap between φ_s and the nuclear density W is significant. For such states lying in the interval $\Delta\epsilon \lesssim Y_{\max}$, the oscillation frequencies $\omega \sim \epsilon_{n+1, p_x} - \epsilon_{n, p_x}$, due to the strong anharmonicity of the potential near the atomic planes, depend on the energy of transverse motion ϵ_{n, p_x} . For this reason, starting at a time

$$t > \tau \sim \left(\frac{d\omega}{d\epsilon} \Delta\epsilon \right)^{-1},$$

the phases in the arguments of the exponentials in Eq. (2.5) will be distributed approximately uniformly. Accordingly, the result of taking the sum in Eq. (2.5) for $t > \tau$ will be to leave only terms that contain diagonal elements of the density matrix. In other words, the oscillations of the nuclear reaction yield with time will damp out in times $t \gtrsim \tau$. Taking into account that the change in the particle oscillation frequencies for $\Delta\epsilon \sim Y_{\max}$ is not very large in most cases (a factor of 2-3), it is clear that $\tau \sim 1/\omega$.

A classical analog of this phenomenon is the familiar tendency to the establishment of statistical equilibrium¹⁾ in the phase space of the transverse motion of a particle^[8]. For heavy particles in channels formed by the planes of lowest index, $\tau v \sim L_{\text{nuc}}$.

The considerations mentioned above refer only to the comparatively high levels. Near the bottom of the potential well the anharmonicity becomes insignificant, and relaxation of the oscillations in the angular distribution will occur only as the result of inelastic scattering by the valence electrons.

3. SPATIAL DISTRIBUTION OF PARTICLES IN THE CHANNEL

In the absence of inelastic collisions, the spatial distribution of particles in the channel will be specified by the initial population of the levels $\rho_s(0)$. For $t > L_1/v$ we have

$$n(x) = \sum_s \rho_s(0) |\varphi_s|^2, \quad (3.1)$$

where

$$\rho_s(0) = |c_s|^2, \quad c_s = \int e^{i p_x x} \varphi_s(x) dx. \quad (3.2)$$

Let us calculate $n(x)$ in the quasiclassical approximation. We shall make use of the quasiclassical condition $p\theta_{CR}d \gg 1$, where θ_{CR} is the critical channeling angle. In the allowed region of the potential Y_C , the wave function takes the form^[10]

$$\varphi_s = \frac{a_s}{p^{1/2}} \sin \left(\int_x^{x_n} p(x') dx' + \frac{\pi}{4} \right), \quad |a_s|^2 = \left(\int_0^{x_n} \frac{dx}{p} \right)^{-1}. \quad (3.3)$$

Here $p = [2m(\epsilon - Y_C(x))]^{1/2}$, and x_n is the turning point. Using the stationary-phase method to calculate the integral in Eq. (3.2), with (3.3) taken into account, we find for the coefficients

$$c_s = \left[\frac{2\pi}{mY_C'(x_0)} \right]^{1/2} a_s \cos \left(p x_0 + \int_{x_0}^{x_n} p dx' \right) \quad (3.4)$$

when $\epsilon_0 < \epsilon_S < \epsilon_0 + Y_{\max}$ ($\epsilon_0 = p_x^2/2m$); the coefficients are zero for any other values of ϵ_S . In Eq. (3.4) x_0 is specified by the condition $Y_C(x_0) + \epsilon_0 = \epsilon_S$.

By using Eqs. (3.3) and (3.4), we separate from (3.1) the nonoscillatory part of the density:

$$n_{\text{reg}}(x) = \frac{\pi}{2m} \sum_s \frac{|a_s|^2}{|Y_C'(x_0)| p(x)}. \quad (3.5)$$

Summing in the Poisson fashion, and taking into account the quantization condition for nonintegral n ^[10]

$$|a_s|^2 = \frac{2m}{\pi} \frac{d\epsilon}{dn}, \quad (3.6)$$

we may replace the sum in Eq. (3.5) by an integral over the energy:

$$n_{\text{reg}}(x) = \int d\epsilon (|Y_C'(x_0)| p(x))^{-1}. \quad (3.7)$$

The integration in Eq. (3.7) is carried out over states with $\epsilon \lesssim Y_{\max}$. The expression (3.7) that we have obtained for the density agrees exactly with the classical result^[8].

Generally speaking, it is not legitimate to widen the interval of integration in the region near the barrier because of the band structure of the spectrum, which is due to the periodicity of the potential. Note that the structure of the level populations including tunneling effects does not differ significantly from Eq. (3.3) (see^[11]), i.e., the states ϵ_{np_x} that are filled are those for which $\epsilon_0 \lesssim \epsilon_{np_x} \lesssim \epsilon_0 + Y_{\max}$.

4. MULTIPLE SCATTERING

Using Eqs. (2.2) and (2.3) from the first section, we consider the kinetic equation for the diagonal elements of the density matrix of particles in the channel:

$$\frac{\partial \rho_s}{\partial t} = 2\pi \sum_{s'} \langle |\Delta V_{qq'}^{ss'}|^2 \rangle (\rho_{s', p+q} - \rho_{s, p}) \delta(E_{s', p+q} - E_{s, p}), \quad p = p_y, p_z. \quad (4.1)$$

Here $\Delta V = \sum_j V^0(\mathbf{r} - \mathbf{R}_j) - Y_C$, where the sum is taken over the atoms of the neighboring planes that form the channel. We shall be interested in the transverse motion of the particles in the channel, since in Eq. (4.1) we have to perform a sum over q_Z . If in addition we make use of the equation

$$\langle \Delta V_{qq'}(x_1) \Delta V_{qq'}(x_2) \rangle = 2Nd \langle U_{qq}(x_1) U_{qq}(x_2) \rangle_T, \quad (4.2)$$

$$U_{qq'}^0(x) = V_{qq'}^0(x),$$

we obtain finally

$$\frac{\partial}{\partial t} \rho_{s, p_y} = \frac{2mNd}{p} \sum_{s', q_y} \langle |\Delta V_{qq'}^{ss'}|^2 \rangle (\rho_{s', p_y+q_y} - \rho_{s, p_y}). \quad (4.3)$$

In accordance with the arguments presented in Sec. 2, we shall neglect the dependence of the density matrix on the quasimomentum in Eq. (4.3). Since for heavy ions in a low-index plane channel the number of levels is large ($\sim 10^2$) and the characteristic transmitted momentum $q_{\perp} \ll p$, we shall use the diffusion approximation. To this end we rewrite Eq. (4.3) in integral form:

$$\frac{\partial}{\partial t} \rho_{\epsilon, p_y} = \sum_{q_y} \int d\epsilon' [G(\epsilon, \epsilon') \rho_{\epsilon', p_y+q_y} - G(\epsilon', \epsilon) \rho_{\epsilon, p_y}], \quad (4.4)$$

$$G(\epsilon, \epsilon') = \frac{2mNd}{p} g(\epsilon) |U_{q_y}^{\epsilon\epsilon'}|^2.$$

($g(\epsilon)$ is the density of states), and in the expansion of the collision integral we keep only terms of first and second order in the variables $\eta = \epsilon_{n'} - \epsilon_n$, and of second order in q_y , just as in the case of the Fokker-Planck equation. Finally, we have

$$\frac{\partial}{\partial t} \rho_{\epsilon, p_y} = \frac{\partial}{\partial \epsilon} w_{\epsilon} \rho_{\epsilon, p_y} + \frac{\partial}{\partial \epsilon} D_{\epsilon} \frac{\partial}{\partial \epsilon} \rho_{\epsilon, p_y} + D_{\perp} \frac{\partial^2}{\partial p_y^2} \rho_{\epsilon, p_y}, \quad (4.5)$$

$$w_{\epsilon} = \int G \left(\epsilon + \frac{\eta}{2}, \epsilon - \frac{\eta}{2} \right) \eta d\eta \approx A_n^{(1)} - \frac{1}{2} \frac{\partial}{\partial \epsilon} A_n^{(2)},$$

$$D_{\epsilon} = \int G \left(\epsilon + \frac{\eta}{2}, \epsilon - \frac{\eta}{2} \right) \eta^2 d\eta \approx A_n^{(2)},$$

$$D_{\perp} = \frac{\alpha}{2} \sum_{n', q_y} \langle |U_{q_y}^{nn'}|^2 \rangle_T q_y^2,$$

where $\alpha = 2Nd m/p$, and the coefficients $A^{(i)}$ are given by

$$A_n^{(i)} = \alpha \sum_{n', q_y} \langle |U_{q_y}^{nn'}|^2 \rangle_T (\epsilon_{n'} - \epsilon_n)^i. \quad (4.6)$$

We now use Parseval's theorem to perform the sum over q_y , obtaining

$$A_n^{(i)} = \alpha \int dy \sum_{n'} \langle \{ [U^{nn'}(y)] \}^i \rangle_T (\epsilon_{n'} - \epsilon_n)^i, \quad (4.7)$$

$$D_{\perp} = \frac{\alpha}{2} \int dy \sum_{n'} \left\langle \left| \frac{\partial U^{nn'}}{\partial y} \right|^2 \right\rangle_T.$$

We can calculate the sum over n' in Eq. (4.7) by making use of a summation theorem, which is proved precisely as in the problem of calculating the average energy loss of colliding particles^[10]. Denoting by \hat{U} the time-derivative operator of the quantity \hat{U} , we have

$$\sum_{n'} |U^{nn'}|^2 (\epsilon_{n'} - \epsilon_n) = \frac{i}{2} (\hat{U} \hat{U} - \hat{U} \hat{U})_{nn}, \quad (4.8)$$

$$\sum_{n'} |U^{nn'}|^2 (\epsilon_{n'} - \epsilon_n)^2 = -\frac{1}{2} (\hat{U} \hat{U} + \hat{U} \hat{U})_{nn}.$$

Substituting in Eq. (4.8) the expression for the operator^[10]

$$\hat{U} = \frac{1}{2m} \left(\hat{p} \frac{\partial}{\partial x} \hat{U} + \frac{\partial}{\partial x} \hat{U} \hat{p} \right) \quad (4.9)$$

and the operator \hat{U} that is obtained from Eq. (4.9) by replacing \hat{U} with \hat{U} , we obtain finally

$$A_n^{(1)} = \frac{Nd}{p} \int dy \left\langle \left[\left(\frac{\partial U}{\partial x} \right)^2 \right]^{nn} \right\rangle_T, \quad (4.10)$$

$$A_n^{(2)} = \frac{2Nd}{p} \int dy \left\langle \left[\left(\frac{\partial U}{\partial x} \right) \left(\frac{\partial Y}{\partial x} \right) U + \frac{1}{4m} \left\{ \left(\frac{\partial^4 U}{\partial x^4} \right) + 4 \left(\frac{\partial^3 U}{\partial x^3} \right) \frac{\partial}{\partial x} + 4 \left(\frac{\partial^2 U}{\partial x^2} \right) \frac{\partial^2}{\partial x^2} \right\} \right]^{nn} \right\rangle_T.$$

The contraction of the corresponding sum for D_{\perp} gives simply

$$D_{\perp} = \frac{\alpha}{2} \int dy \left\langle \left[\left(\frac{\partial U}{\partial y} \right)^2 \right]^{nn} \right\rangle_T. \quad (4.11)$$

If the density of states varies inconsiderably in the range of difference values $\epsilon_{n'} - \epsilon_n$ where $U_{nn'}$ is significantly different from zero—and this is precisely the situation that occurs for heavy ions in low-index channels—then the following formula^[12] relating the kinetic coefficients in Eq. (4.5) is correct:

$$W = \frac{1}{2T_\epsilon} \frac{\partial}{\partial \epsilon} T_\epsilon D_\epsilon. \quad (4.12)$$

Here T is the period of the oscillations in the channel. In this case Eq. (4.5) coincides with the classical result^{[13] 2)}:

$$\frac{\partial}{\partial t} \rho_{\epsilon, p_y} = \frac{1}{2} \frac{\partial}{\partial \epsilon} T_\epsilon D_\epsilon \frac{\partial \rho_{\epsilon, p_y}}{\partial \epsilon} + D_\perp \frac{\partial^2}{\partial p_y^2} \rho_{\epsilon, p_y}. \quad (4.13)$$

In the quasiclassical approximation, the procedure for calculating the matrix element in Eqs. (4.10) and (4.11) is formally identical to taking the average of the given operator over the period of the oscillation in the channel. Recalling that the scattering angle in a binary collision is^[8]

$$\theta_y = -U'_y/2E, \quad (4.14)$$

we can immediately obtain for the diffusion coefficient D_\perp its classical limit^[9]:

$$D_\perp = NdEm \int dy \frac{2}{T_\epsilon} \int_0^{T_\epsilon} dt \theta_y^2 [x(t), y]. \quad (4.15)$$

It is easy to verify that the same arguments can be used for the average increase in the energy of transverse motion along X , which is given approximately by Eq. (4.6).

In the latter regard a few points should be noted. The first two terms on the right side of Eq. (4.5) describe, on the one hand, the fluctuation acceleration, or in this case the increase in the average transverse energy of a particle in the channel, and on the other hand, the increase of the energy dispersion with time. In fact, let us assume that at the initial instant of time only one level ϵ_n is populated, so that $\rho_\epsilon(0) = \delta(\epsilon - \epsilon_n)$. Then, as Eq. (4.5) shows, the average increase in the energy is

$$\frac{d\epsilon}{dt} = -A^{(1)} + \frac{\partial A^{(2)}}{\partial \epsilon} \sim A^{(1)}. \quad (4.16)$$

Thus as time passes the delta peak in the energy distribution will widen and shift in the direction of higher transverse energies. When the transverse energy of the particle becomes higher than the potential barrier, the subsequent behavior of ρ will be essentially the same as in the case of an amorphous medium.

5. THE HARMONIC APPROXIMATION

The kinetic coefficients of Eq. (4.8) can be calculated exactly in the case of a harmonic potential well: $Y_C = m\omega^2 x^2/2$. Strictly speaking, such an approximation is correct only for low-lying states.

In the following calculations we shall use the standard Lindhard potential^[8], which for large $r = (x^2 + y^2)^{1/2}$ can be written in the simplified form

$$U(r) = \gamma/r^2, \quad \gamma = 3Ze^2 a^2. \quad (5.1)$$

Here

$$\omega^2 = \frac{2}{m} \int \frac{\partial^2}{\partial x^2} U\left(\frac{d}{2}, y\right) dy = \frac{2^2 \pi \gamma N}{md^2}. \quad (5.2)$$

We expand the integrand in Eq. (4.10) as a series in powers of x near $x = 0$, up to terms of order $O(x^3)$.

The corresponding small parameter of the expansion is clearly ϵ_n/ϵ_{cr} , where $\epsilon_{cr} = m\omega^2 d^2/8$ is the analog of the critical energy of the channeled particles, $\epsilon_{cr} \sim Y_{max}$. Expression (4.6) for the kinetic coefficients can easily be put in the form of a sum of two terms by expanding the quantities that appear within the averaging sign $\langle \dots \rangle_T$ in a series in powers of u^2 . By using the wave functions $\varphi_n(x)$ in the harmonic potential^[10] for the term that does not depend on the thermal vibrations, we obtain

$$A_n^{(1)} = \frac{1}{2} \frac{\partial A^{(2)}}{\partial \epsilon_n}, \quad A_n^{(2)} = \frac{5m^2 \omega^4 \epsilon_n}{2^7 \pi p N} + \frac{7.5m\omega^2}{2^6 \pi p N d^2} \left(\epsilon_n^2 + \frac{3}{4} \omega^2 \right), \quad (5.3)$$

$$\epsilon_n = \omega(n + 1/2).$$

Ignoring the diffusion in p_y , Eq. (4.3) can be written in the form

$$\frac{\partial \rho_\epsilon}{\partial t} = \frac{1}{2} \frac{\partial}{\partial \epsilon} A^{(2)} \frac{\partial \rho_\epsilon}{\partial \epsilon}. \quad (5.4)$$

It follows from Eqs. (5.3) and (4.12) that the transverse energy of a particle increases at the average rate

$$\frac{d\epsilon}{dt} = A^{(1)} = \frac{5m^2 \omega^4}{2^7 \pi p N} \left(1 + 7.5 \frac{\epsilon_n}{\epsilon_{cr}} \right). \quad (5.5)$$

Specific estimates of the expression (5.5) show that it is comparable in order of magnitude to its classical value^[9], but that the dependence on the transverse energy is weaker; the latter is a consequence of the harmonic approximation.

The contribution from thermal oscillations, accurate to terms of order $\sim u^2$, is calculated in an entirely similar manner. Thus

$$A_r^{(1)} = \frac{Nd \bar{u}^2 \epsilon_n}{mp} \left[\int dy \left\{ \left(\frac{\partial U(d/2, y)}{\partial x} \right)^2 + U \frac{\partial^2 U(d/2, y)}{\partial x^2} \right\} \right]. \quad (5.6)$$

A comparison of Eqs. (5.5) and (5.6) gives

$$A_r^{(1)} = \frac{7.5m^2 \omega^4 \bar{u}^2}{32\pi p N d^2} \epsilon_n = \frac{60\bar{u}^2 A^{(1)}}{d^2}. \quad (5.7)$$

It should not be forgotten that the calculation presented above of the kinetic coefficients near the bottom of the well, where the harmonic approximation is applicable, is of purely methodological value, since the principal mechanism of inelastic scattering is electronic.

6. SCATTERING BY VALENCE ELECTRONS

Thus far we have analyzed only nuclear collisions. The contribution to the diffusion that arises from scattering by electrons can be estimated independently by assuming that the electrons are distributed uniformly over the entire width of the channel with density $Z_V N$, where Z_V is the number of valence electrons.

In accordance with Eq. (4.10), we obtain

$$A_{el}^{(1)} = \frac{m_e Z_V N}{p} \int dx dy \left(\frac{\partial U}{\partial x} \right)^2. \quad (6.1)$$

Noting the relationship between the derivative $\partial U/\partial x$ and the scattering angle (cf. Eq. (4.10)), we may use an approximate value for the derivative^[9]. For a screened Coulomb potential

$$\frac{\partial U}{\partial x} \approx \frac{4e^2 \kappa}{b^2 [1 + (\kappa r)^2]}, \quad b \approx 1.6. \quad (6.2)$$

Here κ is the inverse Debye radius. Substituting (6.2) in Eq. (6.1), we obtain

$$A_{el}^{(1)} = \frac{\pi e^4 Z_V N}{p b^2} \ln [1 + (\kappa r_{min})^{-2}]. \quad (6.3)$$

The cutoff radius r_{min} in Eq. (6.3) eliminates the

logarithmic divergence in $A^{(1)}$ caused by short-range collisions. In simple cases, for instance in calculating $D_{\perp}(\rho_V)$, it is comparatively simple to determine r_{\min} (see^[6]). In our case, computational difficulties make it impossible to determine $A^{(2)}$ from Eq. (4.8) as simply as we determined $A^{(1)}$. In addition, the use of the self-consistent procedure for determining r_{\min} that was discussed in detail in^[6] is made even more difficult by the fact that the dependence of $A^{(2)}$ on r_{\min} is not logarithmic, but a power law: $A^{(2)} \sim 1/r_{\min}^6$.

Because the dependence of $A^{(1)}$ on r_{\min} is rather weak, however, we can still use Eq. (6.3) to obtain an order-of-magnitude estimate of the average energy increase due to scattering by electrons (which eventually leads to dechanneling). By comparing the results obtained for electronic and nuclear collisions, we come to the conclusion, already familiar from classical analyses, that the contribution from electronic scattering is predominant at small values of the transverse energy of the particle in the channel.

APPENDIX

From the Schrodinger equation in the presentation (2.2),

$$i \frac{\partial \Psi_s}{\partial t} = E_s \Psi_s + \sum_{s'} \Delta V_{ss'} \Psi_{s'}, \quad (A.1)$$

$$\Delta V = V - \langle V \rangle$$

we obtain an equation for the particle density matrix $\rho_{S_1 S_2} = \Psi_{S_1}^* \Psi_{S_2}$:

$$\frac{\partial \rho_{s_1 s_2}}{\partial t} + i(E_{s_1} - E_{s_2}) \rho_{s_1 s_2} = -i \sum_{s'} (\Delta V_{s_1 s'} \rho_{s' s_2} - \rho_{s_1 s'} \Delta V_{s' s_2}). \quad (A.2)$$

We take the average of Eq. (A.2) over the positions of the lattice nuclei, and formulate equations for the quantities $F_1 = \langle \Delta V_{S_1 S'} \rho_{S' S_2} \rangle$ and $F_2 = \langle \rho_{S_1 S'} \Delta V_{S' S_2} \rangle$ that appear in the right side of the averaged equation (A.2). At this point the chain of equations is decoupled by the use of the formula

$$\langle \Delta V_1 \Delta V_2 \rho \rangle = \langle \Delta V_1 \Delta V_2 \rangle \langle \rho \rangle,$$

which is correct in the Born approximation^[7]. From Eq. (A.1) we have

$$\begin{aligned} \frac{\partial F_1}{\partial t} + i(E_{s_1} - E_{s_2}) F_1 &= -i \Sigma_1 \\ &= -i \sum_{s''} (\langle \Delta V_{s_1 s''} \Delta V_{s'' s'} \rangle \rho_{s' s_2} - \langle \Delta V_{s_1 s''} \Delta V_{s'' s_2} \rangle \rho_{s' s'}), \\ \frac{\partial F_2}{\partial t} + i(E_{s_1} - E_{s_2}) F_2 &= -i \Sigma_2 \\ &= -i \sum_{s''} (\langle \Delta V_{s_1 s''} \Delta V_{s'' s_2} \rangle \rho_{s' s'} - \langle \Delta V_{s_1 s''} \Delta V_{s'' s'} \rangle \rho_{s_1 s''). \end{aligned} \quad (A.3)$$

The solution of Eq. (A.3) with zero-point initial conditions can be written in the form

$$F_k = -i \int_{-\infty}^t \exp[i(E_{s_1} - E_{s_2})(\tau - t)] \Sigma_k, \quad k=1,2. \quad (A.4)$$

In the present problem the sudden-collision approximation is correct, since the time between collisions $\tau_1 \sim d/v$ is much longer than the collision duration time $\tau_2 \sim a/v$ (where a is the screening parameter). In this approximation the substitution of Eq. (A.4) into (A.2) leads to the desired equation (2.3).

¹Strictly speaking, we are dealing here with the establishment of a quasi-equilibrium distribution, characterized by time reversibility and the assemblage of phases over some long period of time (the Poincaré cycle).

²It is easy to verify that this equation can be obtained directly from Eq. (4.3) for $n \gg 1$ by taking a series expansion of the collision term in powers of the difference $n' - n$. The simplification arises from the fact that here we can set $\epsilon_{n'} - \epsilon_n = 2\pi T^{-1}(n' - n)$.

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20