

Dechanneling of fast particles in crystals as a random process

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The interaction of a fast charged particle with individual atoms in a crystal is used as the starting point in a study of statistical properties of a fluctuation force acting on such a particle as it travels at a small angle with respect to a crystallographic plane. This analysis makes it possible to derive an equation for the distribution function in the two-dimensional phase space of the variables that describe the motion transverse to the plane. The feasibility of simplification in the limiting cases of high and low energies is considered and the results are compared with those given in the literature.

1. INTRODUCTION

We consider the process of motion of a fast particle in the field of slowly fluctuating force centers when the following condition is obeyed:

$$t_a \ll t_u \quad (1.1)$$

(t_u is the characteristic time over which the field created by a given center changes and t_a is the time taken by the fast particle to travel across the region of interaction with the field of the center). This is exactly the situation when relativistic charged particles traverse a crystal: the period of the thermal vibrations of atoms governed by the Debye temperature T_D is

$$t_u \sim 2\pi\hbar/kT_D \sim 10^{-13} \text{ s}, \quad (1.2)$$

whereas the region of the interaction with an atom is of the order of the screening radius $a \approx 0.2 \text{ \AA}$, which such a particle crosses in a time $t_a \sim a/c \sim 10^{-19} \text{ s}$. We shall consider this particular process, but the whole of the analysis and the results obtained are of much more general validity.

When the condition (1.1) is satisfied, we can regard the thermal displacements of atoms as random quantities and not as a random process, and it is usual to assume that such displacements have a Gaussian distribution:

$$W(\mathbf{u}_n) = (2\pi\sigma^2)^{-3/2} \exp(-\mathbf{u}_n^2/2\sigma^2). \quad (1.3)$$

The variance is found from the Debye model which shows that σ is much less than the screening radius. For example, in the case of silicon at normal temperature we have $\sigma \approx 0.08 \text{ \AA}$.

The problem of the passage of fast particles through a crystal is of greatest interest in the case when the direction of such motion makes a small angle ψ relative to some crystallographic axis or plane, i.e., under the channeling conditions investigated extensively in recent years (see, for example, the review in Ref. 1 and various monographs^{2–7}). Fast longitudinal motion of a particle with an energy $E_{||} \approx E$ can then be regarded as free. On the other hand, slow transverse motion is characterized by an energy $E_{\perp} = E\psi^2/2$, which is comparable with the potential V_0 of the field in a crystallographic plane or along an axis (it amounts to several tens of electron volts) and, therefore, such motion is governed by the interaction with this field.

The channeling theory is usually developed so that the motion in the average potential is considered first. Then, an allowance is made (by a variety of methods) for what are

known as the multiple scattering effects due to the difference between the true potential and its average value. This approach is largely related to the concept of the continuous potential introduced by Lindhard,¹ i.e., to the concept of self-averaging of the potential because of the fast longitudinal motion. For example, when the motion takes place at a small angle with respect to the (y, z) plane, the potential $V(x)$ describing the transverse motion is

$$V(x) = (1/S_0) \int dy dz V(x, y, z) \quad (1.4)$$

[S_0 is the area of the (y, z) plane per one atom]. The Lindhard approach is exceptionally fruitful in the description of the dynamics of motion, but the averaging in Eq. (1.4) suppresses information on fluctuations. Therefore, such information has to be obtained anew by one method or another.

We shall approach in a somewhat different way the same problem of the influence of fluctuations of the potential and the motion under the channeling conditions but without adopting the approximations mentioned above. First of all, we separate the irregular part of the interaction of the fast particle with the crystal because of the thermal displacements of its atoms. We determine the statistical properties of the random force by constructing the characteristic functional and we study the motion both far and close to a crystallographic plane. The random force due to the thermal displacements of atoms in a crystal is found to be delta-correlated (Sec. 2) in a wide range of values of the impact parameters.

In Sec. 3 we discuss a different mechanism for the appearance of an irregular force: it is due to the difference between the interaction of the fast particle with individual electrons of an atom and the interaction with the average electron distribution, included in the potential of an atom. This mechanism is important in the case of motion at large distances from crystallographic planes, since the interaction with individual electrons decreases much more slowly with the distance than the interaction with an electrically neutral atom.

Since the random force in stochastic differential equations of motion can be regarded, as shown in Secs. 2 and 3, as Gaussian and delta-correlated, in Sec. 4 we derive an equation for the distribution function in terms of the transverse coordinates and velocities. The feasibility of deriving an equation of the parabolic type, namely the Fokker–Planck equation, is related (see, for example, Ref. 8) precisely to

these properties of the random forces and is in no way related to the weakness of these forces. In general, the phase space of planar channeling is two-dimensional. In the limiting cases of $\omega\tau \gg 1$ and $\omega\tau \ll 1$ (ω is the characteristic frequency of the vibrational motion in a channel and τ is the evolution time of a beam of particles) the situation simplifies greatly and we can derive simpler equations describing the evolution in one-dimensional phase space. In particular, in the hf limit, which is reached at sufficiently high energies, the Fokker–Planck equation reduces the equation of Ref. 3, which describes the evolution of the distribution function in the transverse energies and which is obtained by the authors of Ref. 3 by a completely different approach utilizing the semiclassical limit of a quantum-mechanical equation.

Finally, in Sec. 5 we analyze in detail the scenarios of the development of the processes of dechanneling of electrons and positrons at high energies in the limit $\omega\tau \gg 1$. A comparison with the experimental data shows that the description obtained by the approach adopted here is satisfactory.

2. STOCHASTICITY DUE TO THERMAL DISPLACEMENTS OF ATOMS

For a given motion in the (y, z) plane the potential governing the transverse motion depends on time as a parameter:

$$V(x, t) = \sum_n V_a(x\mathbf{e}_x + vt - \mathbf{r}_n - \mathbf{u}_n), \quad (2.1)$$

where \mathbf{v} is the velocity of a particle in the (y, z) plane; V_a is the potential of one atom; \mathbf{r}_n and \mathbf{u}_n are, respectively, the equilibrium position and the thermal displacement of the n th atom.

We can distinguish the irregular part¹⁾ in Eq. (2.1) which is due to thermal displacements $\{\mathbf{u}_n\}$ of the atoms:

$$\delta V(x, t, \{\mathbf{u}_n\}) = \sum_n \{V_a(\mathbf{r}(t) - \mathbf{r}_n - \mathbf{u}_n) - \langle V_a(\mathbf{r}(t) - \mathbf{r}_n - \mathbf{u}_n) \rangle\}, \quad (2.2)$$

where for brevity we shall use

$$\mathbf{r}(t) = x\mathbf{e}_x + vt. \quad (2.3)$$

The part δV is the generator of the random force $F(t, x)$ and the time dependence of the latter is linked, not to changes in the random quantities $\{\mathbf{u}_n\}$, but to the circumstance that in the course of motion in the (y, z) plane a fast particle interacts at different moments with atoms displaced by different amounts from the equilibrium position. In other words, the random field of each atom is individual and, therefore, it is localized. On the other hand, the regular fields of atoms in a crystal are coherently additive and, therefore, they are periodic and of the long-range type.

The statistical properties of the random force $F(t, x)$ are governed by the following characteristic functional:

$$\Phi[\xi(t)] = \left\langle \exp \left[i \int dt \xi(t) F(t, x) \right] \right\rangle, \quad (2.4)$$

where the averaging is carried out over all the quantities $\{\mathbf{u}_n\}$.

In the above formulation of the problem we are interested in arbitrary functions $\xi(t)$ which change over a time char-

acteristic of the transverse motion $t_x \gtrsim d/c\Psi_c$ (d is the width of the investigated channel, i.e., the distance between the adjacent crystallographic planes, and ψ_c is the Lindhard angle). Such times are long compared with the interaction time t_a :

$$\frac{t_x}{t_a} \sim \frac{d}{a} \frac{1}{\Psi_c} \gg 1; \quad (2.5)$$

consequently, the integral in the argument of the exponential function can be represented in the form

$$J = \sum_n \xi(t_n) \int dt F_n(t, x), \quad (2.6)$$

where t_n is the time at which the fast particle passes the n th atom and $F_n(t, x)$ is the contribution of this atom to the total random force $F(t, x)$.

If we assume that the displacement of the atoms are small²⁾ compared with the screening radius governing the scale of variation of the atomic field, $u \ll a$, we find that

$$F_n(t, x) = -\mathbf{u}_n \frac{\partial}{\partial \mathbf{r}_n} \frac{\partial}{\partial x} V_a(\mathbf{r}(t) - \mathbf{r}_n). \quad (2.7)$$

Using Eqs. (2.6) and (2.7), and averaging over all the quantities \mathbf{u}_n with the aid of Eq. (1.3), we obtain

$$\Phi[\xi(t)] = \exp \left\{ -\frac{\sigma^2}{2} \sum_n \xi^2(t_n) \left[\frac{\partial}{\partial \mathbf{r}_n} \frac{\partial}{\partial x} I(x, \mathbf{r}_n) \right]^2 \right\},$$

(2.8)

where

$$I(x, \mathbf{r}_n) = \int dt V_a([(x - x_n)^2 + b_n^2 + v^2(t - t_n)^2]^{1/2}), \quad (2.9)$$

b_n is the transverse (relative to the velocity \mathbf{v}) component of the radius vector \mathbf{p}_n of the n th atom in the (y, z) plane and $t_n = v\mathbf{p}/v^2$ is the time of closest approach to the n th atom (Fig. 1).

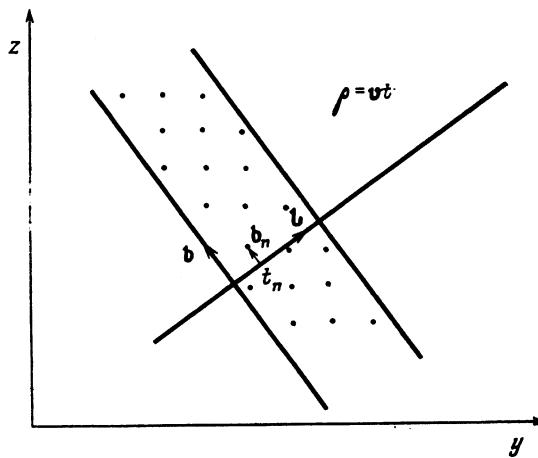


FIG. 1. Schematic representation of a channeling plane.

The functional (2.4) may be given the standard form⁸

$$\Phi[\xi(t)] = \exp \left[-\frac{1}{2} \int dt_1 dt_2 B(t_1, t_2) \xi(t_1) \xi(t_2) \right], \quad (2.10)$$

if we define the correlation function as follows:

$$B(t_1, t_2) = \delta(t_1 - t_2) \sigma^2 \sum_n \delta(t_1 - t_2) G(x - x_n, b_n), \quad (2.11)$$

where

$$G(x - x_n, b_n) = \frac{(x - x_n)^2}{\eta_n^2} I''^2 + \frac{b_n^2}{\eta_n^4} I'^2, \quad (2.12)$$

and $\eta_n = [(x - x_n)^2 + b_n^2]^{1/2}$, the minimum distance from the n th atom to the “observation point” x of interest to us in the argument of the function I and the differentiation in Eq. (2.12) is carried out with respect to this argument.

It therefore follows that atoms distributed at random because of thermal displacements have an effect on a fast particle moving at a small angle to a crystallographic plane, and this effect is equivalent to Gaussian delta-correlated noise.

Bearing in mind that the intervals Δt_n between the interactions with different atoms are considerably shorter than the time t_x of interest to us,

$$\Delta t_n/t_x \sim \Psi \ll 1, \quad (2.13)$$

we average Eq. (2.11) over some intermediate time interval $\Delta t_n \ll T \ll t_x$. We then obtain

$$\langle B(t_1, t_2) \rangle_T = 2\mathcal{D}(x) \delta(t_1 - t_2), \quad (2.14)$$

$$\mathcal{D}(x) = (\sigma^2/2T) \sum_n G(x - x_n, b_n). \quad (2.15)$$

The summation in the above equation is carried out over all the atoms with which the interactions occur during the time interval T of interest to us. In each of the parallel planes (i.e., at fixed values of x_n) these atoms form a strip of width vT and the boundaries of this strip are perpendicular to the velocity vector \mathbf{v} of the fast particle (Fig. 1). Introducing the distribution function of atoms in this strip

$$f(\rho) = \sum_m \delta(\rho - \rho_m), \quad (2.16)$$

we convert Eq. (2.15) to

$$\mathcal{D}(x) = \sum_{(x_n)} (\sigma^2/2T) \int_s d\rho f(\rho) G(x - x_n, b_n) \quad (2.17)$$

(the summation is carried out over planes with different coordinates x_n). In the case of the motion in the field in a plane far from crystallographic axes, which is considered here, the distribution function averaged along a strip of width l (in the direction of motion V) ceases to depend on the impact parameter b :

$$\frac{1}{l} \int_0^l dl' f(\rho) = \frac{1}{S_0}. \quad (2.18)$$

This allows us to obtain the following final expression:

$$\mathcal{D}(x) = \frac{v\sigma^2}{2S_0} \sum_{(x_n)} \int_{-\infty}^{\infty} db G(x - x_n, b). \quad (2.19)$$

It is understood that the contribution from distant atoms to the noise level $\mathcal{D}(x)$ is small: the function $I(\eta)$ and its derivatives decrease rapidly. If the atomic potential is of the screened Coulomb type,

$$\varphi_a(r) = \frac{Z_a e}{r} e^{-r/a}, \quad (2.20)$$

the function $I(\eta)$ represents a modified Bessel function

$$I(\eta) = \frac{2Z_a Z_p e^2}{v} K_0(\eta/a), \quad (2.21)$$

and for large values of the argument $\eta \gg a$, we have

$$I(\eta) \approx (2\pi)^{1/2} \frac{Z_p Z_a e^2}{v} e^{-\eta/a} (\eta/a)^{-1/2}. \quad (2.22)$$

The Molière potential, quite satisfactory for real crystals, represents a sum¹⁰ of three terms of the form (2.22):

$$\begin{aligned} \varphi_a(r) &= \frac{Z_a e}{r} \sum_{j=1}^3 \alpha_j \exp(-\beta_j r/a), \\ \alpha_j &= \{0.1; 0.55; 0.35\}, \quad \beta_j = \{6.0; 1.2; 0.3\}; \\ a &= 0.4685 \cdot Z_a^{-1/2}. \end{aligned} \quad (2.23)$$

The quantity $\mathcal{D}(x)$ governing the noise level corresponds to this potential and can be represented in the form

$$\mathcal{D}(x) = \mathcal{D}_0 g(x), \quad (2.24)$$

where the dimensional factor

$$\mathcal{D}_0 = \frac{4(Z_p Z_a e^2)^2}{v S_0 a} \quad (2.25)$$

determines the scale, and $g(x)$ is a dimensionless structure function

$$g(x) = \frac{\sigma^2}{a} \int_0^\infty \frac{db}{\eta^2} \left[\frac{(x - x_n)^2}{a^2} \Sigma_{(0)}^2 + \frac{2(x - x_n)^2}{\eta a} \Sigma_{(0)} \Sigma_{(1)} + \Sigma_{(1)}^2 \right]. \quad (2.26)$$

Here, $\Sigma_{(0)}$ and $\Sigma_{(1)}$ are combinations of modified Bessel functions

$$\Sigma_{(0)} = \sum_j \alpha_j \beta_j^2 K_0(\beta_j \eta/a), \quad \Sigma_{(1)} = \sum_j \alpha_j \beta_j K_1(\beta_j \eta/a). \quad (2.27)$$

In determining the characteristic potential $\Phi[\xi(t)]$ we used the above approximation given by Eq. (2.7). We now discuss in greater detail a situation when the path of a fast particle passes so close to an atom

$$(x - x_n)^2 + b_n^2 \leq \sigma^2, \quad (2.28)$$

that the approximation (2.7) loses its meaning. Then, the averaging over the thermal displacements of atoms $\{\mathbf{u}_n\}$ should be carried out avoiding linearization in the displacement amplitudes. This is a soluble problem, although the solution is very time-consuming. We therefore consider one

case, most unfavorable from the point of view of the validity of the approximation (2.7), of the central interaction $x = n_n$, $b_n = 0$. Noting that when the condition (2.28) is obeyed, the integral in the argument of the exponential function can be simplified by using the asymptotic form of the function K_0 for small arguments

$$K_0(\eta/a) \approx \ln \frac{2a}{\eta} - 0.577, \quad (2.29)$$

we can readily find the contribution of this interaction to the characteristic functional:

$$\Phi_n[\xi(t)] = \frac{1}{2\pi\sigma^2} \int du_x du_b \times \exp \left[-\frac{u_x^2 + u_b^2}{2\sigma^2} - i\xi(t_n) \frac{2Z_p Z_a e^2}{v} \frac{u_x}{u_x^2 + u_b^2} \right]. \quad (2.30)$$

Adopting polar coordinates in the space of the thermal displacements (u_x, u_b) , we can reduce the above expression to the following integral:

$$\Phi_n[\xi(t_n)] = \int_0^\infty du u \exp(-u^2/2) J_0(\xi/u), \quad (2.31)$$

[$\xi = (2Z_p Z_a e^2/v\sigma)\xi(t_n)$, and J_0 is the Bessel function of order zero], which can be calculated numerically. Figure 2 shows the characteristic function Φ_n (depending on ξ^2) together with the Gaussian functions

$$\Phi_n^G(\xi) = \exp \left(-\frac{1}{2} \kappa^2 \xi^2 \right), \quad \kappa^2 = \{1.0; 1.1; 1.2\}, \quad (2.32)$$

which correspond to passage at distances

$$(x - x_n)^2 + b_n^2 = \sigma^2/\kappa \quad (2.33)$$

in the approximation of Eq. (2.7). It is clear from Fig. 2 that even in the most unfavorable case of the central interaction the function Φ_n is smooth and quite close to the Gaussian function corresponding to the passage through the outer

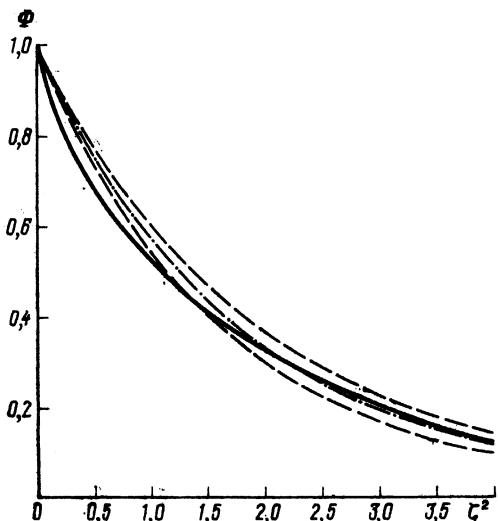


FIG. 2. Characteristic function for zero impact parameter.

edge of the thermal layer of the atom. Therefore, allowing also for the fact that the situation of the type described by Eq. (2.29) has in general only a small statistical weight $\sim \sigma^2/d^2$, we can use Eq. (2.19) where the contribution of the terms with $\eta \ll \sigma/\kappa^{1/2}$ is truncated at their values corresponding to $\eta = \sigma/\kappa^{1/2}$.

The structure function $g(x)$ which is then obtained determines the coordinate dependence of the quantity $\mathcal{D}(x)$ plotted in Fig. 3. This function decreases rapidly for values of the coordinate x (which is the distance to the nearest plane) exceeding the amplitude of the thermal vibrations of an atom. In the asymptotic case $x \gg \sigma$, we readily obtain

$$g(x) \approx \frac{\pi^{\frac{1}{2}} \sigma^2}{4 a^2} \alpha_s^2 \beta_s^{-3} \frac{\exp(-2\beta_s x/a)}{(\beta_s x/a)^{\frac{1}{2}}} \quad (2.34)$$

(the term with $j = 3$ in the Molière potential has the longest range). Therefore, in the case of motion near one of the planes the contribution to the value of $\mathcal{D}(x)$ of the other planes is unimportant. However, where the motion occurs in the center of the channel, we must include the contribution to $\mathcal{D}(x)$ made by two adjacent planes forming a given channel.

We now find the structure function near a crystallographic plane. Since the main contribution comes from the "close" collisions characterized by $\eta \ll a$, for which we have

$$G(0, \eta) = \begin{cases} \sigma^2/\eta^4, & \eta \geq \sigma/\kappa^{1/2}, \\ 1/\kappa^2 \sigma^2, & \eta \leq \sigma/\kappa^{1/2}, \end{cases} \quad (2.35)$$

we obtain

$$g(0) = \frac{4}{3} \kappa^{\frac{1}{2}} \frac{a}{\sigma} \quad (2.36)$$

and

$$\mathcal{D}(0) = \frac{16}{3} \kappa^{\frac{1}{2}} \frac{(Z_p Z_a e^2)^2}{v S_0 \sigma}. \quad (2.37)$$

We must draw attention to the nontrivial dependence on the amplitude of the thermal vibrations, which are the source of noise. This is because at short distances, in contrast to the case of large distances, the fluctuation force is not a linear function of the thermal displacements.

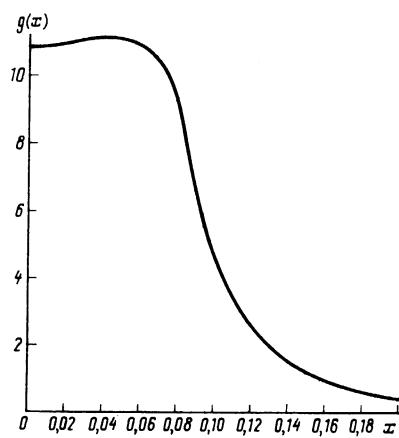


FIG. 3. Structure function $g(x)$ near a crystallographic plane.

3. STOCHASTICITY DUE TO ATOMIC ELECTRONS

In the random process associated with the thermal vibrations of atoms in the crystal which is discussed above, the elementary potential is that of the atom as a whole. Therefore, the noise level is proportional to the square of the charge and, because of the electrical neutrality and the high symmetry of an atom, it decreases quite rapidly (exponentially) with the distance. Another source of stochasticity is fluctuations of the electron distribution in an atom, i.e., the difference between the real interaction with atomic electrons and the average contribution to the atomic total potential:

$$\delta V_n^{(e)}(\mathbf{r}) = Z_p \sum_{i=1}^{z_a} \left(\frac{e^2}{|\mathbf{r}-\mathbf{r}_i|} - \langle\langle \frac{e^2}{|\mathbf{r}-\mathbf{r}_i|} \rangle\rangle \right). \quad (3.1)$$

Here, the double angular brackets denote quantum-mechanical averaging of the square of the electron wave functions in an atom:

$$\langle\langle \dots \rangle\rangle = \int \prod_i d\mathbf{r}_i |\Psi(\mathbf{r}_1, \dots, \mathbf{r}_{z_a})|^2 \dots \quad (3.2)$$

The fluctuation potential $\delta V_n^{(e)}(\mathbf{r})$, created by electrons of the n th atom, depends on the coordinates of these electrons $\{\mathbf{r}_i\}$ as parameters. The statistical properties of the random force generated by this atom

$$F_n^{(e)}(x, t) = -\frac{\partial}{\partial x} \delta V_n^{(e)}[\mathbf{r}(t) - \mathbf{r}_n, \{\mathbf{r}_i\}] \quad (3.3)$$

are governed by the characteristic functional

$$\Phi_n[\xi(t)] = \langle\langle \exp \left[i \int dt F_n^{(e)}(x, t) \xi(t) \right] \rangle\rangle. \quad (3.4)$$

As in the preceding case, the total functional of the interaction with the whole crystal is factored for the individual atoms, which is due to the limited dimensions of the region of interaction with a single atom (it is of the order of the Bohr radius $a_B \approx 0.5 \text{ \AA}$), compared with the distance between different atoms (which is of the order of the lattice constant amounting to several angstroms).

The feasibility of further simplification of the characteristic functional depends on the use of the multiplicative properties of many-electron wave functions. For example, in the Hartree-Fock approximation, when the many-electron wave function is a Slater determinant, the characteristic functional Φ_n describing the interaction with the n th atom represents the following product:

$$\Phi_n[\xi(t_n)] = \prod_{i=1}^{z_a} \int d\mathbf{r}_i |\varphi_i(r_i)|^2 \exp \left[-i\xi(t_n) \int dt F_{ni}(x, t) \right]. \quad (3.5)$$

If, for the sake of simplicity, we use an exponential distribution (quite close to reality)

$$|\varphi_i(r_i)|^2 \rightarrow \frac{\lambda^3}{8\pi} \exp(-\lambda r_i), \quad (3.6)$$

then even if we ignore the “close” interactions and linearize the fluctuation force F_{ni} with respect to the electron coordinates in an atom \mathbf{r}_i , we obtain a very complex expression:

$$\Phi_n[\xi(t_n)] = \prod_{i=1}^{z_a} \left[\frac{\lambda^2}{\lambda^2 + \xi^2(t_n) \cdot 4e^4 Z_p^2 / v^2 \eta_n^4} \right]^2. \quad (3.7)$$

It therefore follows that the process generated by electron fluctuations is not Gaussian and, therefore, it cannot in general be described by a Fokker-Planck equation of parabolic type.

On the other hand, at large distances from a plane, where the process in question is most important because of the slower (obeying a power law and not an exponential function) decrease with the distance, the situation simplifies. In fact, in this case the function Φ_n can be described by an expansion

$$\Phi_n[\xi(t_n)] = 1 - \frac{8Z_a Z_p^2 e^4 \xi^2(t_n)}{\lambda^2 v^2 \eta_n^4}, \quad (3.8)$$

which is close to an expansion of a Gaussian function:

$$\Phi_n^G[\xi(t_n)] = \exp \left[-\frac{8Z_a Z_p^2 e^4 \xi^2(t_n)}{\lambda^2 v^2 \eta_n^4} \right]. \quad (3.9)$$

Consequently, at long distances $x \gg 1/\lambda$ we can regard the interaction with electron fluctuations as a Gaussian process which is delta-correlated in the sense of different atoms, with a correlation function is³⁾

$$\mathcal{D}^{(e)}(x) = \frac{8\pi Z_a Z_p^2 e^4}{v \lambda^2 S_0 x^3}, \quad (3.10)$$

or if we use the mean-square radius $\langle\langle r^2 \rangle\rangle$ in the distribution parameter of Eq. (3.6), we find that

$$\mathcal{D}^{(e)}(x) = \frac{2\pi}{3} \frac{Z_a Z_p^2 e^4}{v S_0} \frac{\langle\langle r^2 \rangle\rangle}{x^3}. \quad (3.11)$$

The electron distribution giving rise to the Molière potential, corresponds to the mean-square radius

$$\langle\langle r^2 \rangle\rangle = 6a^2 \sum_j \alpha_j / \beta_j^2 \approx 25,6a^2. \quad (3.12)$$

It should be noted that Eq. (3.11), which is valid when the displacement x of the fast particle is large, can be derived also without postulating factorization of the atomic electron functions and without knowing the explicit form of the electron distribution.

Far from a plane the interaction with electron fluctuations dominates the formation of noise:

$$\frac{\mathcal{D}^{(e)}(x)}{\mathcal{D}(x)} = \frac{2}{3\pi^{1/2}} \frac{1}{\alpha_s^2} \frac{1}{Z_a} \frac{\langle\langle r^2 \rangle\rangle}{\sigma^2} \left(\frac{a}{x\beta_s} \right)^2 \exp(2\beta_s x/a). \quad (3.13)$$

The role of interaction with electron fluctuations at short distances is similar to that described above for the passage of a fast particle through the thermal layer of an atom. The only difference is that the role of the truncation parameter is now played not by the amplitude σ of the thermal vibrations, but by the mean-square radius of the electron distribution. Therefore, the following ratio applies near a plane:

$$\frac{\mathcal{D}^{(e)}(0)}{\mathcal{D}(0)} \sim \frac{1}{Z_a} \sigma (\langle\langle r^2 \rangle\rangle)^{-1/2}, \quad (3.14)$$

so that the main role is played by the interaction with atoms as a whole. The correlation function $\mathcal{D}^{(e)}$ is linear (and not quadratic like \mathcal{D}) in the charge Z_a because the fluctuation force is incoherent in the case of individual electrons of an atom.

It therefore follows that at not too large distances from a crystallographic plane we can ignore the weak electron noise $\mathcal{D}^{(e)}$ compared with the much stronger, in this region, thermal noise \mathcal{D} . However, at larger distances where electron fluctuations become dominant, this process becomes Gaussian. Consequently, we can regard random forces as Gaussian in a wide range of the values of the variable x , which is of interest in connection with the problem of dechanneling of fast particles moving under planar channeling conditions, the case considered here.

4. FOKKER-PLANCK EQUATION

It follows that when we consider the motion of a fast charged particle in the transverse direction, we have to allow not only for the determinate force F_d due to the regular part of the crystal potential $V(x)$, but also for the random force $F(t, x)$:

$$\ddot{Ex} = F_d(x) + F(t, x), \quad (4.1)$$

where E is the energy of the particle, playing the role of a mass coefficient in the slow transverse motion.⁴⁾ This equation can be written in the standard form for stochastic differential equations:

$$y = \dot{x}, \quad \dot{y} = f_d(x) + f(t, x), \quad (4.2)$$

where y is the velocity of the motion parallel to the x axis (which should not be confused with the coordinate in the plane) and

$$f_d(x) = F_d(x)/E, \quad f(t, x) = F(t, x)/E \quad (4.3)$$

the normalized (to the mass coefficient) determinate and random forces. It follows from the above that the random force can be reasonably regarded as Gaussian and delta-correlated:

$$\langle f(t, x) f(t', x) \rangle = 2D(x) \delta(t - t'), \quad D(x) = \mathcal{D}(x)/E^2. \quad (4.4)$$

The evolution in the phase space (x, y) is then described (see, for example, Refs. 8 and 11) by the distribution function $P_i(x, y)$ satisfying the Einstein-Fokker-Planck equation

$$\partial_t P_i(x, y) = \{-y\partial_x - f_d(x)\partial_y + D(x)\partial_y^2\} P_i(x, y) \quad (4.5)$$

subject to the initial conditions

$$P_0(x, y) = \delta(x - x_0) \delta(y - y_0). \quad (4.6)$$

Having found $f_d(x)$ and $D(x)$ from Eq. (4.5), we can (in principle) find all the information on the investigated transverse motion. It should be pointed out that smallness of $D(x)$ is in no way essential for the validity of the Fokker-Planck equation.

We are interested in that part of the phase space which corresponds to the subbarrier motion, i.e., to channeling proper. Then, as in the investigation of an oscillator with a noisy frequency,⁸ it is convenient to replace the variables $(x,$

$y)$ representing the coordinate and velocity, with the variables (A, φ) , representing (in the absence of noise) two integrals of motion, the amplitude and initial phase of vibrational motion in a channel

$$x = x_i(t; A, \varphi), \quad y = y_i(t; A, \varphi). \quad (4.7)$$

The physical meaning of going over to the phase space of the integrals of determinate motion is this: since the whole evolution in this space is due to the noise, the Fokker-Planck equation simplifies to

$$\partial_t P_i(A, \varphi) / \Delta = D(x_i) \left[\frac{1}{\Delta} \left(\frac{\partial x_i}{\partial \varphi} \partial_A - \frac{\partial x_i}{\partial A} \partial_\varphi \right) \right]^2 P_i(A, \varphi), \quad (4.8)$$

where Δ is the Jacobian of the transformation (4.7) and the “determinate” coordinates x_i and the velocity y_i are given by the following equations of motion:

$$\dot{x}_i(t; A, \varphi) = y_i(t; A, \varphi), \quad \dot{y}_i(t; A, \varphi) = f_d(x_i(t; A, \varphi)). \quad (4.9)$$

It should be noted that the idea of going over to the integrals of motion in the Fokker-Planck equation was put forward already in Ref. 12.

Since in the case of vibrational motion at a frequency ω (which generally depends on the amplitude A) the time t and the initial phase occur in the form of a single combination $\Phi = \omega t + \varphi$ and, therefore,

$$\partial x_i / \partial \varphi = \dot{x}_i / \omega, \quad (4.10)$$

we can readily use Eq. (4.9) to find

$$\Delta = \frac{1}{\omega} \frac{\partial}{\partial A} \left[\frac{y_i^2}{2} + \frac{V(x_i)}{E} \right] = \frac{1}{\omega} \frac{\partial}{\partial A} \frac{E_\perp}{E}. \quad (4.11)$$

Like the energy of transverse motion, the Jacobian Δ is thus independent of the time t and of the initial phase φ , and is only a function of the amplitude: $\Delta = \Delta(A)$.

Equation (4.8) can be rewritten also in the form

$$\partial_t P_i(A, \varphi) = D(x_i) \left[\left(\frac{y_i}{\omega} \partial_A - \frac{\partial x_i}{\partial A} \partial_\varphi \right) \frac{1}{\Delta} \right]^2 P_i(A, \varphi). \quad (4.12)$$

It is convenient to replace the amplitude A directly with E_\perp , the energy of transverse motion, as is usual in studies of channeling. Then the Fokker-Planck equation becomes

$$\partial_t P_i(E_\perp, \varphi) = \mathcal{D}(x_i) \left[y_i \partial_{E_\perp} - \omega \frac{\partial x_i}{\partial E_\perp} \partial_\varphi \right]^2 P_i(E_\perp, \varphi). \quad (4.13)$$

We can see that the dechanneling in the planar case must be considered allowing for the evolution in the two-dimensional phase space of transverse motion: in either the space (x, y) or (A, φ) or (E_\perp, φ) . The situation simplifies greatly and an equation in a one-dimensional phase space can be obtained (it is usual to employ the transverse energy space) if the characteristic evolution time τ and the transverse motion period in the channel differ in scale, i.e., if

$\omega\tau \gg 1$ and $\omega\tau \ll 1$ hold. We consider these limiting cases in greater detail, but at this stage we simply note that they are encountered at, respectively, high and low energies of the particles passing through the crystal. In fact, the frequency of vibrational motion in a channel is inversely proportional to the total energy of the particle, which acts as the mass coefficient. However, the evolution time is roughly proportional to this energy, so that the parameter $\omega\tau$ is the proportional to the square root of the energy:

$$\omega\tau \propto (E/E_c)^{1/2}. \quad (4.14)$$

The quantity E_c which occurs here depends on the actual conditions and amounts to several tens of megaelectron volts.

In the hf limit $\omega\tau \gg 1$ the distribution function behaves like a wave packet whose center of gravity travels "rapidly" along a determinate path in the (x, y) phase space or is standing in the phase plane (A, φ) , while the packet itself then "slowly" spreads. Since the distribution function $P_t(A, \varphi)$, like the distribution function $P_t(E_\perp, \varphi)$, changes little in one vibration period in a channel, it is reasonable to average the Fokker-Planck equation over this period of time. As a result, the distribution function $P_t(E_\perp, \varphi)$ obeys

$$\partial_t P_t(E_\perp, \varphi) = (\mathcal{D}_1 \partial_{E_\perp} + \mathcal{D}_2 \partial_{E_\perp}^2 + \mathcal{D}_3 \partial_\varphi^2 + \mathcal{D}_4 \partial_{E_\perp} \partial_\varphi + \mathcal{D}_5 \partial_\varphi) P_t(E_\perp, \varphi), \quad (4.15)$$

where the coefficients \mathcal{D}_i depend on the transverse energy: $\mathcal{D}_i = \mathcal{D}_i(E_\perp)$. In particular, we have

$$\begin{aligned} \mathcal{D}_1(E_\perp) &= \langle \mathcal{D}(x, (\Phi, E_\perp)) \rangle_\Phi, \\ \mathcal{D}_2(E_\perp) &= \langle \mathcal{D}(x, (\Phi, E_\perp)) y_i^2(\Phi, E_\perp) \rangle_\Phi, \end{aligned} \quad (4.16)$$

and we can easily show that

$$\mathcal{D}_1(E_\perp) = \partial_{E_\perp} \mathcal{D}_2(E_\perp). \quad (4.17)$$

Consequently, we can also obtain an equation for the distribution function of the transverse energies:

$$P_t(E_\perp) = \int d\varphi P_t(E_\perp, \varphi) \quad (4.18)$$

by integrating Eq. (4.17)

$$\partial_t P_t(E_\perp) = \partial_{E_\perp} \mathcal{D}_2(E_\perp) \partial_{E_\perp} P_t(E_\perp). \quad (4.19)$$

This equation is similar to Eq. (6.34) of Ref. 3, where the authors used a completely different approach and, consequently, made different assumptions.

The opposite limiting case of $\omega\tau \ll 1$ corresponds to strong diffusion. The system then acquires an energy or velocity much faster than it travels along the coordinate x . This coordinate can also be regarded as a parameter and in Eq. (4.5) we can ignore what is known as the sideways motion (or drift) term describing the "determinate" evolution compared with that occurring by diffusion

$$\partial_t P_t(x, y) = D(x) \partial_y^2 P_t(x, y). \quad (4.20)$$

The solution of this equation subject to the initial conditions of (4.6) is

$$P_t(x, y) = \frac{\exp[-(y-y_0)^2/4D(x)t]}{[4\pi D(x)t]^{1/2}} \delta(x-x_0). \quad (4.21)$$

In the case of an arbitrary initial distribution $P_0(x)$ in

position for a given initial velocity y_0 , we have

$$P_t(y) = \int dx P_0(x) \frac{\exp[-(y-y_0)^2/4D(x)t]}{[4\pi D(x)t]^{1/2}}. \quad (4.22)$$

The variance of the velocity distribution is, as we can see, a linear function of the diffusion coefficient $D(x)$:

$$\langle (y-y_0)^2 \rangle_y = 2D(x)t \cdot P_0(x), \quad (4.23)$$

so that the rise of the average transverse energy (or, which is equivalent, of the average square of the angle of multiple scattering) is governed by the value of the diffusion coefficient averaged over position:

$$\langle E_\perp \rangle = \langle E_\perp \rangle_0 + \frac{t}{E} \int dx P_0(x) \mathcal{D}(x). \quad (4.24)$$

On the other hand, not all the characteristics are governed by this average: in accordance with Eq. (4.22), the diffusion coefficient is generally included in a very complicated manner.

We conclude this section by pointing out two circumstances: firstly, the lf limit is realized at relatively low energies [it is understood that all these energies are much greater in the crystal potential $V(x)$]. Since in the case of light particles (electrons and positrons) we should use a quantum-mechanical description of these energies, the results obtained in this limit represent the passage of protons and ions with energies up to several MeV. The theory of Ref. 5 is developed specifically for such particles and averaging over the coordinates (integration over the relevant volume) is then one of the starting points.

Secondly, in both limiting cases the transition to a one-dimensional phase space is performed by averaging. However, in the low-energy limit the averaging procedure is carried out over the coordinates, whereas in the high-energy limit it is carried out over time.

5. DECHANNELING AT HIGH ENERGIES

We now investigate dechanneling in the limit $\omega\tau \gg 1$ when the evolution is described by Eq. (4.19) for the distribution function over the transverse energies $P_t(E_\perp)$ and we note that the diffusion coefficient $\mathcal{D}(E_\perp)$ which occurs in this equation is usually calculated using the relationship

$$\mathcal{D}(E_\perp) = \mathcal{D}_2(E_\perp) = \frac{2}{E} \frac{\oint dx \mathcal{D}(x) [E_\perp - V(x)]^{1/2}}{\oint dx / [E_\perp - V(x)]^{1/2}}. \quad (5.1)$$

We consider the initial stage of the dechanneling process on the assumption that at $t = 0$ the particles are at the bottom of the channel (negative for $x = 0$ or positive for $x = d/2$):

$$P_0(E_\perp) = \delta(E_\perp). \quad (5.2)$$

Assuming that in the initial stage the distribution function differs from zero only at energies small compared with the depth of the potential well, to first order in the ratio V_0 , we have

$$\mathcal{D}(E_\perp) = \mu E_\perp, \quad (5.3)$$

and assuming that the potential at the center of the channel is parabolic and inverted parabolic for, respectively, positive and negative particles, we find that

$$\mu_{(+)} = \mathcal{D}(d/2)/E, \quad \mu_{(-)} = \frac{2}{3} \mathcal{D}(0)/E. \quad (5.4)$$

When the diffusion coefficient depends linearly on the energy E_\perp , the distribution function becomes exponential

$$P_t(E_\perp) = \frac{1}{\mu t} \exp(-E_\perp/\mu t) \quad (5.5)$$

with an increasing width μt , and the characteristic spreading time is $\tau = V_0/\mu$. the proportion of the particles transferred to the above-barrier fraction by the time t is then

$$n_>(t) = \int_{V_0}^{\infty} dE_\perp P_t(E_\perp) = e^{-\tau/t}. \quad (5.6)$$

If we determine the moments of the distribution function

$$M_n(t) = \int dE_\perp E_\perp^n P_t(E_\perp) = n! (\mu t)^n, \quad (5.7)$$

we find that the higher moments of this function rise more rapidly than the lower moments and for $n \gg 1$ we have

$$\tau^{(n)} = \tau / (n!)^{1/n}. \quad (5.8)$$

However, then the ratio of the moments

$$\frac{M_{n+k}(t)}{M_n(t) M_k(t)} = \frac{(n+k)!}{n! k!} \quad (5.9)$$

is independent of time.

The more rapid growth of the higher moments implies that with time the role of corrections to the linear approximation of Eq. (5.3) should become stronger. We now consider this problem in greater detail. To next order (relating to the depth of the potential V_0) in the transverse motion energy, we find from Eq. (5.1) that

$$\mathcal{D}(E_\perp) = \mu E_\perp + \gamma E_\perp^2, \quad (5.10)$$

where

$$\gamma_{(+)} = -\frac{1}{2E} \left[\frac{d^2 \mathcal{D}(x)}{dx^2} \Big|_{x=d/2} \right] / \frac{d^2 V(x)}{dx^2} \Big|_{x=d/2}, \quad (5.11)$$

$$\gamma_{(-)} = -\frac{4\mathcal{D}(0)}{45EV_0}$$

[here, as in Eq. (5.4), the diffusion coefficient for $x = d/2$ must include, as pointed out above, the contribution of two adjacent planes, i.e., Eq. (3.10) should be doubled].

It is quite obvious that as the transverse motion energy increases the diffusion coefficient behaves differently for positive and negative particles ($\gamma_{(+)} > 0$, whereas $\gamma_{(-)} < 0$), giving rise to quite different scenarios of the subsequent evolution. An analysis can be made conveniently in terms of the moments of the distribution function, the equations for which can easily be derived from Eq. (4.19):

$$\dot{M}_n(t) = \mu n^2 M_{n-1}(t) + \gamma n(n+1) M_n(t). \quad (5.12)$$

Using in our estimates the “linear” approximation of Eq. (5.7), we find that the ratio of the second to the first term

increases in proportion to time and by $t = \tau^{(n)}$ should reach the following value in the case of positive particles:

$$e[(\mathcal{D}''/\mathcal{D})/V''/V]_{x=d/2}, \quad (5.13)$$

which is much greater than unity. In the case of negative particles, this ratio is not so large: it should reach only $\sim 1/3$.

Therefore, the second term in Eq. (5.12) begins to influence the evolution long before $t = \tau^{(n)}$. We can easily obtain the solution of the system of Eq. (5.12) by employing the recurrence relation

$$M_n(t) = \mu n^2 \int_0^t dt' \exp[\gamma n(n+1)(t-t')] M_{n-1}(t'), \quad M_0(t) = 1. \quad (5.14)$$

For example, we have

$$M_1(t) = \frac{\mu}{2\gamma} (e^{2\gamma t} - 1), \quad (5.15)$$

$$M_2(t) = \frac{\mu^2}{6\gamma^2} (e^{6\gamma t} - 3e^{2\gamma t} + 2). \quad (5.16)$$

Hence, it is clear that the process develops differently for positive and negative particles. In the case of positive particles the algebraic increase of the moments changes gradually to exponential and after a sufficiently long time the increments are quadratic functions of the order of the moment:

$$M_n(t) \propto \exp[\gamma n(n+1)t]. \quad (5.17)$$

Such a fast rise of the moments, when

$$\frac{M_{n+k}(t)}{M_n(t) M_k(t)} \propto e^{2\gamma n k t}, \quad (5.18)$$

means that the structure of the distribution function becomes quite complex. In a qualitative treatment of the process we can use a simplified model. We assume that the process consists of two stages. In the first (linear) stage the particles are accelerated up to a certain small energy E_0 . During the second stage, which begins from this energy, we have

$$P_0^M(E_\perp) = \delta(E_\perp - E_0), \quad (5.19)$$

so that the linear term can be ignored compared with the quadratic one. The distribution function then becomes

$$P_t^M(E_\perp) = \frac{\exp[-\gamma t/4 - (1/4\gamma t) \ln^2(E_\perp/E_0)]}{(4\pi\gamma t E_\perp E_0)^{1/2}}, \quad (5.20)$$

and the proportion of particles in the subbarrier fraction is

$$n_{<}^M(t) = \Phi \left[\frac{(\gamma t)^{1/2}}{2} + \frac{\ln(V_0/E_0)}{2(\gamma t)^{1/2}} \right] - \Phi \left[\frac{(\gamma t)^{1/2}}{2} \right] \quad (5.21)$$

(Φ is the error integral). After a sufficiently long time such that

$$t \gg \frac{1}{4\gamma} \ln^2 \frac{V_0}{E_0},$$

this expression simplifies to

$$n_{<\mu}(t) \approx \frac{e^{-\gamma t/\mu}}{2(\pi\gamma t)^{1/2}} \ln \frac{V_0}{E_0}. \quad (5.22)$$

Hence, we can see that during this stage of the process the dechanneling time is governed by a quantity $\tau_\gamma = 4/\gamma$, which is considerably less than the characteristic linear stage of the evolution $\tau_\mu = V_0/\mu$:

$$\frac{\tau_\gamma}{\tau_\mu} \propto (\beta_s d/a)^2 \frac{\alpha_s}{6} \exp(-\beta_s d/2a). \quad (5.23)$$

In this situation the rise time of the n th moment depends even more strongly on the order of the moment than in the linear approximation:

$$\tau_\gamma^{(n)} = [\gamma n(n+1)]^{-1}. \quad (5.24)$$

In the case of negative particles we have $\gamma_{(-)} < 0$, so that the second term in Eq. (5.12) prevents the growth of the moments. In the asymptotic case the solution would become steady-state.

$$M_n(t) = (-\gamma/\mu)^n / (n+1) = (7.5V_0)^n / (n+1), \quad (5.25)$$

which however corresponds to moments which are too high and, therefore, is unsatisfactory; the motion becomes sub-barrier much earlier.

In the case of negative particles it is reasonable to assume, as shown above, that τ_μ represents the lower limit in estimates of the dechanneling time. In terms of the dechanneling lengths, this corresponds to the expression

$$l_{(-)} \propto 2 \frac{Ev^2 a \sigma}{Z_a Z_p e^2}. \quad (5.26)$$

On the other hand, in the case of positive particles it is more realistic to obtain estimates using τ_γ , which is considerably shorter than the corresponding value τ_μ [see Eq. (5.23)]. Consequently, in the case of positive particles, we find that

$$l_{(+)} \propto 10^{-5} \frac{Ev^2 d^5}{Z_p e^2 a^3}. \quad (5.27)$$

In particular, for electrons and positrons of energy $E = 1.2$ GeV, which move in a silicon crystal along the (1, 1, 0) plane, we obtain

$$l_{(-)} \sim 20 \text{ } \mu\text{m}, \quad l_{(+)} \sim 300 \text{ } \mu\text{m}. \quad (5.28)$$

These estimates are in reasonable agreement with those found experimentally:¹³

$$l_{(-)} = 29 \text{ } \mu\text{m}, \quad l_{(+)} = 190 \text{ } \mu\text{m}. \quad (5.29)$$

Note that, in accordance with the description of the properties of the diffusion coefficient given above (Sec. 3), the dechanneling length for positive particles is independent of the charge Z_a of atoms in a crystal.

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¹⁾ The same approach was used to study the problem of emission of radiation.

²⁾ The passage of a particle through the thermal layer of an atom, when this approximation is hardly applicable, will be discussed in greater detail later.

³⁾ We used here the method of summation over atoms in a crystal described earlier (Sec. 2).

⁴⁾ Here and later we shall assume that $c = 1$.

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