Quantum theory of inelastic scattering of negatively-charged particles by oriented crystals

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A general quantum-mechanical approach is adopted to investigate how the interaction of a relativistic electron with the phonon and electron subsystems of a crystal affects the stability of motion in axial and planar channels. It is shown that the generally-adopted interpretation of channeling of electrons in terms of quasiperiodic motion accompanied by relatively slow particle "diffusion" in the space of transverse energy and angular momentum is invalid. For electron energies exceeding a few tens or a few hundred of MeV (for axial and planar cases, respectively), there is no channeling in this interpretation. The relevant quantum-mechanical and classical expressions for quantities characterizing the dechanneling process are obtained for electrons of lower energy and for heavy negatively-charged particles of energy exceeding a few hundred GeV.

It is well-known that the Born approximation is invalid for a fast charged particle moving at a sufficiently small angle θ to a crystal axis or plane. This is because higher-order corrections increase rapidly as $\theta \to 0$ (Ref. 1). The basic idea that simplifies the theoretical analysis of the motion of particles at these small angles is that the true interaction potential between particle and crystal can be replaced by a "continuous potential" of the axes and planes along which the particle motion takes place.[2] From the formal point of view, the "continuous potential" is the zeroth component of the Fourier expansion of the crystal potential in terms of the longitudinal coordinate z measured along the family of axes under consideration, or along the two directions (y,z) in the planar case.[3]

The continuous-potential approximation can be used to demonstrate qualitatively new features of the motion of fast charged particles in an oriented crystal. In particular, the set of eigenfunctions of a particle in a crystal includes states associated with an atomic string or plane. These states have a discrete "transverse"-energy spectrum, i.e., a new integral of motion that arises naturally in the continuous-potential approximation.[4,5]

Allowance for the discrete nature of the atomic planes and strings, and for the presence of phonon and electron excitations in the crystal, leads to the broadening of the energy levels associated with transverse motion and to radiationless transitions between them. Further development of the idea of a continuous potential provides a description of the kinetics of charged particles in oriented crystals in terms of a rigorous perturbation theory that is free from the $\theta \to 0$ divergences.

It has been shown[2,3,6] that the motion of heavy positively-charged particles (protons or ions) under channeling conditions is relatively stable. The problem is then essentially quasiclassical and perturbations are small because the positively-charged particles travel mostly at large distances from the atomic planes and strings, so that their interaction with the electron and phonon subsystems in the crystal is appreciably weaker than in the amorphous medium.

For light relativistic particles (electrons or positrons), the situation is different for two basic reasons. First, for energies between 1 MeV and a few tens of MeV, the number of levels in the channel is large,[7] so that it is essential to use a quantum-mechanical analysis and the attendant concepts of energy levels, level width, and transition probabilities. Second, we expect that the channeled motion of negatively-charged particles, will be less stable than that of positively-charged particles. Actually, in the case of electrons, the continuous-potential minima lie on the atomic strings and planes of the crystal, so that particles in bound state experience maximum perturbation because they move in regions of higher electron and nuclear density. On the other hand, for states whose wave function is localized well away from the nuclei (for example, the high angular-momentum states in axial channeling when the electron winds itself on the axis in the form of a helix with a relatively large radius), even a weak perturbation due to valence electrons in the crystal may produce a very significant change in the nature of the motion because the binding energy is low.

A detailed analysis of these questions began in Refs. 8–10 in which we were concerned only with the interaction of fast particles with the phonon subsystem of the crystal[1)] (scattering by the thermal oscillations of nuclei). In the present paper, we examine processes accompanied by the excitation of the electron shells of crystal atoms. These must be taken into account, since the elastic scattering cross section in the crystal is lower than in the amorphous medium because the collisions between a fast particle and the regularly distributed scattering centers are correlated.[8] We shall concentrate our attention on negatively-charged particles.

A further aim of this paper is to analyze the transport equations describing the passage of electrons through oriented crystals in both the quantum-mechanical and quasiclassical limits. The results obtained in section 2 shows that, contrary to the generally held view, stable quasiperiodic trajectories coupled to a string or plane exist in a broad range of energy. The only meaning that can be given to the well-established phrase "electron channeling" is that the electron

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trajectories become highly curved when the electrons travel at a small angle to a crystal string (plane) and there is an attendant redistribution of the particle flux over the cross section of the channel.

1. INELASTIC SCATTERING OF A CHANNELED PARTICLE BY ELECTRONS IN A CRYSTAL

To calculate the transition probability for a fast particle between transverse-energy levels i and f, due to inelastic interactions with the electron subsystem of the crystal, we shall use essentially the same devices and methods that were used for elastic scattering.[8-10] The difference between the exact Hamiltonian for the interaction between a particle and the crystal and the approximate Hamiltonian that includes only the continuous potential of the atomic strings and planes can be looked upon as a perturbation which, in general, produces a change in the state of both particle and crystal. Since the state of the crystal is not fixed in advance, the final expressions must include summation over the "extra" variables describing phonon and electron excitations in the crystal. Summation over the phonon excitations can be carried out analytically, as in Ref. 8, because their energies are low.

Two features of inelastic processes must be taken into account when the sum over electron excitations is evaluated. First, since the excitation of different atoms in the crystal occurs incoherently, it is sufficient to consider scattering by one atom. Second, for large momentum transfers, the velocity of the recoiling electron is close to that of light, so that retarded effects and the relativistic energy-momentum relation for the electron must be taken into account. However, it is possible to show rigorously[11] that, to within[2] $O(I/m)$ (where I is the ionization potential and m the electron mass), the scattering probability can be calculated for transitions with relatively low transferred energy $\Delta\varepsilon \ll m$, and this can be followed by summation over all the final states.

Taking all the above points into account, we obtain the following expression for the $i \to f$ transition probability due to inelastic particle crystal interaction in the planar case:

$$W_{if}^{inel} = \frac{2e^4 n}{\pi} \int_{-\infty}^{+\infty} \frac{d\lambda\, d\varkappa\, d\mu \exp[-u^2(\varkappa-\mu)^2/2]}{(\lambda^2+\varkappa^2)(\lambda^2+\mu^2)} \times b_{ij}(\varkappa) b_{fi}(-\mu) \times [(B(\varkappa,\lambda)B^*(\mu,\lambda))^{00} - (B(\varkappa,\lambda))^{00}(B^*(\mu,\lambda))^{00}]. \quad (1)$$

As in Ref. 8, n is the density of atoms in the plane, e is the electron charge, and u is the amplitude of thermal vibrations. Indexed expressions such as A^{00}, a_{if} represent the following matrix elements:

$$A^{00} = \int d\mathbf{r}_1 \ldots d\mathbf{r}_z |\varphi_0(\mathbf{r}_1, \ldots, \mathbf{r}_z)|^2 A(\mathbf{r}_1, \ldots, \mathbf{r}_z),$$

$$a_{ij} = \int dx\, \psi_j^*(x) \psi_i(x) a(x),$$

where $\psi_{i(f)}(x)$ is the wave function describing the transverse motion of a channeled electron, $\varphi_0(r_1,\ldots,r_z)$ is the wave function describing the ground state of an atom, $r_1,\ldots,r_z$ are the coordinates of atomic electrons (measured from the nucleus), and Z is the atomic number of the crystal. The functions b and B in (1) are respectively given by

$$b(\varkappa) = \exp(-i\varkappa x), \quad B(\varkappa,\lambda) = \sum_{j=1}^{z} \exp(i\varkappa x_j - i\lambda y_j),$$

where x_j, y_j are the corresponding components of the position vector of the jth electron in the coordinate frame in which the z-axis lies along the longitudinal velocity of the channeled particle and the x-axis is perpendicular to the channeling plane.

The probability of a change in the transverse motion of a particle in the case of axial channeling can be obtained in a similar way,[11] and the result is

$$W_{if}^{inel} = 4e^4 d^{-1} \int d^2s\, d^2k\, s^{-2}k^{-2} \exp[-u^2(\mathbf{s}-\mathbf{k})^2/2] \times c_{if}(\mathbf{s}) c_{fi}(-\mathbf{k}) [(C(\mathbf{s})C^*(\mathbf{k}))^{00} - (C(\mathbf{s}))^{00}(C^*(\mathbf{k}))^{00}], \quad (2)$$

where d is the distance between atoms in a string

$$C(\mathbf{s}) = \sum_{j=1}^{z} \exp(i\mathbf{s}\boldsymbol{\rho}_j), \quad c(\mathbf{s}) = \exp(i\mathbf{s}\boldsymbol{\rho});$$

and $\boldsymbol{\rho}_j$ is the transverse position coordinate of the jth electron.

The "inelastic" width of the ith level, i.e., the total probability per unit time that a particle will leave the level i as a result of inelastic processes, can be obtained from W_{if}^{inel} by summing over all the final states $f \neq i$. Using the completeness property of the set of wave functions for the transverse motion, we obtain the following expression for the planar case:

$$\Gamma_i^{inel} = \frac{2e^4 n}{\pi} \int_{-\infty}^{+\infty} \frac{d\lambda\, d\mu\, d\varkappa \exp[-u^2(\varkappa-\mu)^2/2]}{(\lambda^2+\varkappa^2)(\lambda^2+\mu^2)} \times [b_{ii}(\varkappa-\mu) - b_{ii}(\varkappa) b_{ii}(-\mu)] \times [(B(\varkappa,\lambda)B^*(\mu,\lambda))^{00} - (B(\varkappa,\lambda))^{00}(B^*(\mu,\lambda))^{00}]; \quad (3)$$

whereas in the axial case,

$$\Gamma_i^{inel} = 4e^4 d^{-1} \int d^2s\, d^2k\, s^{-2}k^{-2} \exp[-u^2(\mathbf{s}-\mathbf{k})^2/2] \times [c_{ii}(\mathbf{s}-\mathbf{k}) - c_{ii}(\mathbf{s}) c_{ii}(-\mathbf{k})] \times [(C(\mathbf{s})C^*(\mathbf{k}))^{00} - (C(\mathbf{s}))^{00}(C^*(\mathbf{k}))^{00}]. \quad (4)$$

A relatively simple estimate for the inelastic level width in the case of planar channeling of electrons can be obtained for high-lying levels in the limit of large Z and small thermal-vibration amplitudes. For most atomic electrons (except for the outermost-shell electrons), we then have $\langle x^2\rangle_i \gg \langle x_j^2\rangle \gtrsim u^2$ (where $\langle x^2\rangle_i$ is the mean square coordinate of the channeled electron in the ith state and $\langle x_j^2\rangle$ is the mean square of the x-component of the position vector of the jth electron in the atom), so that the exponential in $(B(\varkappa,\lambda))^{00}$ can be expanded in a series, and only the first few terms of the expansion retained. The final result is

$$(B(\varkappa,\lambda)B^*(\mu,\lambda))^{00} - (B(\varkappa,\lambda))^{00}(B^*(\mu,\lambda))^{00} = {}^1/_3(\mu\varkappa+\lambda^2)\langle d^2\rangle, \quad (5)$$

where

$$\langle d^2\rangle = \int d\mathbf{r}_1 \dots d\mathbf{r}_Z |\varphi_0(\mathbf{r}_1, \dots, \mathbf{r}_Z)|^2 \Big(\sum_{j=1}^{Z} \mathbf{r}_j\Big)^2$$

is the dipole moment of the atom. The field inside the atom is radially symmetric so that, in the derivation of (5), we can assume that

$$\langle x_j^2\rangle = \langle y_j^2\rangle = {}^1/_3\langle \mathbf{r}_j^2\rangle, \quad \langle \mathbf{r}_j\rangle = 0.$$

Neglecting corrections $O(u^2/\langle x_j^2\rangle)$, and using (3), we obtain the following estimate:

$$\Gamma_i^{inel} \approx \frac{8\beta e^4 n\langle d^2\rangle}{\langle x^2\rangle_i^{1/2}} \ln\left(\frac{\langle x^2\rangle_i}{a_{TF}^2}\right), \tag{6}$$

where β is a numerical factor of order unity and a_{TF} is the Thomas-Fermi radius.

The mean square atomic dipole moment that appears in (5) and (6) can be calculated, for example, in the Thomas-Fermi model. However, there are some doubts as to the validity of isolated-atom models because weakly-bound electrons belonging to the outermost shell become collectivized in the crystal and are effectively free. The situation can then be described by the electron-gas model in which a_{TF} is replaced with a new parameter, namely, the plasma oscillation frequency.

Let us now estimate the role of valence electrons in inelastic level broadening. From (3), we have the following order-of-magnitude estimate:

$$\Gamma_i^{val} \approx \frac{8\beta_v n Z_v e^4}{d_p} \langle x^2\rangle_i \ln(k_v^{-2}\langle x^2\rangle_i^{-1}), \tag{7}$$

where d_p is the separation between the planes, Z_v is the number of valence electrons per atom, β_v is a numerical constant of the order of unity, k_v is the characteristic momentum of an electron in the electron plasma, and $k_v \sim d_p^{-1}$.

Comparison of (6) with (7) shows that, for the planar channeling of electrons, the ratio of the level widths due to valence electrons and inner-shell electrons is given by

$$\Gamma_i^{val}/\Gamma_i^{inel} \sim (Z_v/Z)\,(\langle x^2\rangle_i^{1/2}/d_p a_{TF}^2).$$

It follows from the above estimates that, for most levels, the contribution of valence electrons to the inelastic width is small and proportional to the ratio Z_v/Z. The only exception occurs for levels lying near the continuous-spectrum limit, for which $\Gamma_i^{val}/\Gamma_i^{inel}$ may not be small because $\langle x^2\rangle_i/a_{TF}^2$ is large.

A similar estimate can be obtained for axial channeling in the case where the wave function of the channeled electron is localized well away from the channel center. The exponential in $(C(s))^{00}$ can then be expanded into a series, and this eventually yields

$$\Gamma_i^{inel} \approx \frac{16\pi\beta e^4}{d} \langle \rho^{-2}\rangle_i \langle d^2\rangle, \tag{8}$$

The contribution of valence electrons is given by the following order-of-magnitude formula:

$$\Gamma_i^{val} \approx \frac{8\pi^3\beta_v Z_v e^4}{dS_0} \langle \rho^2\rangle_i \ln(k_v^{-2}\langle \rho^2\rangle_i^{-1}), \tag{9}$$

where $\langle \rho^{\pm 2}\rangle_i = \int d^2\rho |\psi_i(\rho)|^2 \rho^{\pm 2}$, S_0 is the area per atomic string in the transverse cross section, and β_v is a constant of the order of unity [like β in (8)]. It follows from (8) and (9) that the contribution of valence electrons to the inelastic width increases as the level approaches the continuous-spectrum limit and, in contrast to the planar case, valence electrons play a dominant part in the inelastic broadening of most of the angular momentum states. This is so because the path of an electron traveling in an axial channel can "bend around" atomic chains, and run mostly along the periphery of the channel, where the probability of scattering by inner-shell electrons is small.

Calculations[12] based on the above formulas show that agreement with experimental data[13] is good.

2. KINETICS OF TRANSMISSION OF RELATIVISTIC ELECTRONS THROUGH AN ORIENTED CRYSTAL

It is well known that the general equation for a weakly-perturbed quantum-mechanical system can be reduced to a set of equations for the diagonal elements of the density matrix:

$$\dot{p}_j = -\Gamma_j p_j + \sum_{k\neq j} W_{jk} p_k, \tag{10}$$

where j, k represent the set of quantum numbers characterizing the eigenfunctions of the unperturbed Hamiltonian, p_j is the population of the jth state, W_{jk} is the transition probability between the states j and k per unit time, and the summation sign represents summation over discrete, and integration over continuous, spectra. In the case of channeling at relatively low electron energies, when the number of levels in the channel is low, the kinetics of the population of transverse-motion levels is also described[14] by a set of equations such as (10). The coefficients Γ_j and W_{jk} were evaluated above.

However, the situation changes as the particle energy E increases. Equations (10) were written on the assumption that the perturbation was small. In particular, the probability that a particle will leave a given level in a time of the order of the reciprocal of the transition frequency between neighboring levels must be small, i.e., $\Gamma_j\omega^{-1} \ll 1$. On the other hand, it has been shown[8] that the level widths Γ_j tend to a constant as E increases, whereas the level separation falls as $E^{-1/2}$. Consequently, after a certain electron energy has been reached,[3)] the condition $\Gamma_j\omega^{-1} \ll 1$ ceases to be valid for most levels in the channel. The discrete energy levels actually disappear and, from this moment onward, the transition kinetics is described by a more complicated set of equations than (10), and the quantity Γ_j can no longer be interpreted as the "level width" because one must then take into account the phase relationships between the wave functions of different levels.

A simplification of the problem can be achieved in this case by allowing for the quasiclassical nature of the transverse motion of electrons at these high energies. Actually, when the number of levels in the channel is large, we can transform from the basis of the eigenfunctions of the unperturbed Hamiltonian to a basis of localized wave packets. The transport equation for the distribution $f(\mathbf{r}_\perp, \mathbf{p}_\perp, t)$ of the

particles over the transverse momenta and position coordinates then has the standard form

$$\frac{\partial f}{\partial t}+\frac{\mathbf{p}_\perp}{E}\frac{\partial f}{\partial \mathbf{r}_\perp}-\nabla U\frac{\partial f}{\partial \mathbf{p}_\perp}=\mathrm{St}(t), \tag{11}$$

where U is the continuous potential of the corresponding family of strings or planes and $St(f)$ is the collision integral which, in this case, can be written down in the small-angle (Fokker-Planck) approximation (we recall that the interaction between a fast particle and a crystal is partially represented by the continuous potential).

If there are no collisions, (11) describes the motion of particles in the field of the atomic planes and strings on trajectories that can be parametrized by certain integrals of motion ν (for planar channeling, the variable ν is the "transverse" energy ε, whereas for axial channeling ν is the "transverse" energy ε and angular momentum l of the particle about the nearest string). The presence of the perturbation gives rise to a change in the trajectory parameters as the particle passes through the crystal. When this change occurs slowly enough, the function $f(\mathbf{r}_\perp, \mathbf{p}_\perp, t)$ can be replaced with the distribution over the variable ν, i.e., $f(\nu,t)$. Equation (11) then takes the diffusion from[15-18]

$$\frac{\partial f}{\partial t}=-\frac{\partial}{\partial \nu}(D_1 f)+\frac{1}{2}\frac{\partial^2}{\partial \nu^2}(D_2 f), \tag{12}$$

where D_1 and D_2 are the diffusion coefficients characterizing the change in the parameters of the particle trajectory per unit time (for the planar case, there are two such coefficients, whereas for the axial case there are five because the variable ν is two-dimensional). Equation (12) can also be obtained directly from the set of quantum-mechanical transport equations (10) by transforming from the discrete variables p_j to the mean distribution function $f(\nu)$ (Ref. 19). The diffusion coefficients then have the following form: for the planar case

$$D_r=\sum_f W_{if}(\varepsilon_i-\varepsilon_f)^r, \quad r=1,2; \tag{13}$$

and for the axial case

$$D_{rs}=\sum_f W_{if}(\varepsilon_i-\varepsilon_f)^r(l_i-l_f)^s. \tag{14}$$

These transformations would appear to remove the above difficulty. Actually, since the quasilocal wave packet is constructed for a large number of closely-spaced levels, the width of an individual level and the separation between neighboring levels cannot play as important a role in the quasiclassical case as they do in the quantum-mechanical case. Nevertheless, it will be shown below that the lack of a small parameter associated with the probability of collisional transitions manifests itself even in the quasiclassical approach, and is not removed by a simple transformation to the diffusion equation (12).

Actually, the diffusion coefficients in (12) are determined by taking an average over certain functions $D_r(x)$, $D_{rs}(\rho)$ (see Appendix) along the unperturbed particle trajectory. The condition for the self-consistency of this procedure is therefore that the change in the parameters of the trajectory, i.e., the transvere energy and the angular momentum, in one rotation around the axis (or the oscillation period in the planar channel) should be small. It is only then that electron transport in the channel can be looked upon as relatively slow diffusion of quasiparticles in the space of the adiabatic invariants (see, for example, Ref. 20). Unless this is so, the "adiabatic" approach is not self-consistent, and the general transport equation (11) cannot be reduced to the simpler form (12).

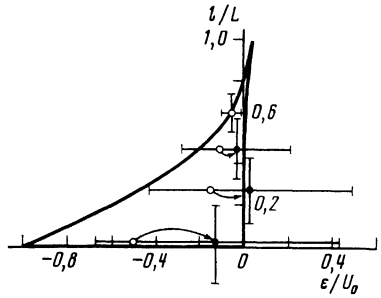

FIG. 1. Region of bound motion in the space of transverse energy and angular momentum for axial channeling of 1-GeV electrons in the ⟨111⟩ direction in silicon single crystals ($U_0 \simeq 100$ eV, $L \approx 50\hbar$). Open circles show the parameters of the trajectories of a number of particles entering the crystal; crosses indicate the "drift" and "spreading" of the initial parameters in one revolution of the particle around the axis.

Let us now examine in greater detail the case of axial orientation of the crystal. In axial electron channeling, the region of bound motion, in which we must consider the diffusion of particles over the transverse energy and angular momentum, is quite complicated (see Fig. 1): for each value of the angular momentum below some maximum, there are two boundary values of the transverse energy corresponding to circular electron trajectories. The characteristic scales of the problem are thus the dimensions of this region, the depth U_0 of the axial channel along the transverse energy axis and the maximum angular momentum L along the angular momentum axis.

Let us now estimate the change in the transverse energy of a particle in one period. This is most simply done for particles with zero angular momentum about the axis. The principal scattering mechanism then involves close encounters with nuclei so that, for approximate estimates, it is sufficient to retain only the first terms in (A.5)–(A.7). Next, we take $\rho(t) \simeq v_0 t$ (where $v_0 = [2(\varepsilon + U_0)/E]^{1/2}$) and, integrating with respect to t between infinite limits, we obtain the following expressions for the mean ($\overline{\delta\varepsilon}$) and mean square ($\overline{\delta\varepsilon^2}$) increase in the transverse energy:

$$\overline{\delta\varepsilon}=\frac{2(Ze^2)^2}{ud}\ln(Eu)\left[\frac{\pi}{E(\varepsilon+U_0)}\right]^{1/2}, \tag{15}$$

$$\overline{\delta\varepsilon^2}=\frac{4(Ze^2)^2}{ud}\ln(Eu)\left[\frac{\pi(\varepsilon+U_0)}{E}\right]^{1/2}. \tag{16}$$

The largest of the numbers $\overline{\delta\varepsilon}$, $(\overline{\delta\varepsilon^2})^{1/2}$ defines the size of the "cell" (in the space of ε) in which any further resolution of the transverse-energy distribution function is not physically meaningful. At high energies, $(\overline{\delta\varepsilon^2})^{1/2}$ decreases more slowly than $\overline{\delta\varepsilon}$: $(\overline{\delta\varepsilon^2})^{1/2} \sim E^{-1/4}$, whereas

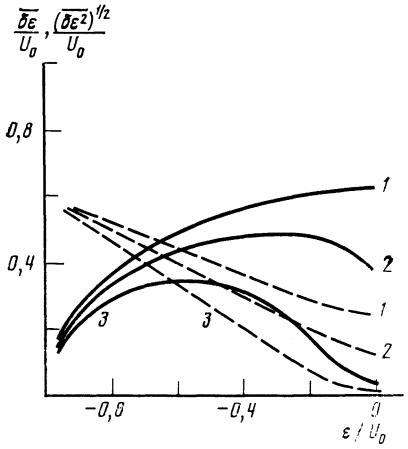

FIG. 2. Dependence of $\overline{\delta\varepsilon}$ (broken curves) and $(\overline{\delta\varepsilon^2})^{1/2}$ (solid curves) on the transverse energy of particles of different angular momentum: 1—zero angular momentum; 2—angular momentum equal to half the maximum possible for given transverse energy; 3—maximum possible angular momentum (silicon, ⟨111⟩ direction, 1-GeV electrons).

$\overline{\delta\varepsilon} \sim E^{-1/2}$. If we demand that $(\overline{\delta\varepsilon^2})^{1/2}$ is less than $0.1U_0$, we obtain the condition

$$E \gtrsim 5 \cdot 10^5 (\varepsilon + U_0) \frac{(Ze^2)^4 \ln^2(Eu)}{U_0^4 u^2 d^2}. \qquad (17)$$

Substituting reasonable values for the parameters in (17), i.e., $\ln(Eu) \sim 10$, $\varepsilon \sim -U_0/2$, we obtain, for example the condition $E \gtrsim 10^{12}$ eV for the ⟨111⟩ axis of silicon single crystals. The diffusion equation (12) thus becomes self-consistent only for gigantic energies of the order of 1000 GeV.

We have examined the most favorable situation, i.e., the case where the particle moves with zero angular momentum about an axis. More detailed analysis shows that the situation remains practically the same for other values of the angular momentum. Figure 2 shows the results of a numerical calculation of $\overline{\delta\varepsilon}$ and $(\overline{\delta\varepsilon^2})^{1/2}$ using (A.5)–(A.13) in a realistic (Hartree-Fock) potential of an atomic string (silicon, ⟨111⟩ direction). It is readily seen that, at energies of 1 GeV, for which the calculation was performed, the relative fluctuation in the transverse energy $(\max\{\overline{\delta\varepsilon}, (\overline{\delta\varepsilon^2})^{1/2}\}/|\varepsilon|)$ and the relative fluctuation $\delta T/T$ in the period of revolution are of order unity. It follows that the diffusion equation in the space of the integrals of motion is physically justified only at energies much greater than 100 GeV. [Figure 1 illustrates the evolution of the "probability cloud" in (ε, l) space at electron energies of 1 GeV: a point succeeds in "spreading" by an amount comparable with U_0 and L in one revolution around the axis.]

The situation is complicated further by the fact that, above about 100 GeV, the motion of electrons is greatly distorted by reaction,[21–23] which is quite strong at these energies of electromagnetic radiation. All this leads us to the conclusion that generally accepted ideas on the channeling of electrons as a form of quasiperiodic motion, accompanied by relatively slow diffusion of particles in the space of transverse energy and angular momentum, are invalid. The diffusion coefficients (13) and (14) can be used only in calculations of the dechanneling of heavy, negatively-charged particles (negative pions, antiprotons, etc.) with energies in excess of 100 GeV.

The above result becomes particularly significant in relation to the problem of the quantitative characterization of electron dechanneling in axial channels, which is currently of interest. The last two or three years have seen the publication of a number of papers on the "adiabatic" approach[17–19] and calculations based upon it.[24–28] Our analysis shows that the results published in these papers have not been adequately justified.[4)] (It is important to remember that the precision of results based on the "adiabatic" approach requires further examination: for integrated parameters such as the total radiated intensity, or number of particles in the channel, the result can be close to the true result, even for $\delta T/T \gtrsim 1$. Thus, for planar electron channeling, the diffusion coefficients are not very dependent on the transverse particle energy, so that averaging along any trajectory, including the unperturbed trajectory, should lead to more or less the same results. On the other hand, in the case of axial electron channeling, the diffusion coefficients are very dependent on the particle trajectory parameters, so that one can hardly expect high precision of the adiabatic approach.)

Thus, the correct description of electron dechanneling kinetics for $\Gamma_j \omega^{-1} \gtrsim 1$ involves the solution of either the quantum-mechanical transport equations in their general form or the four-dimensional Fokker-Planck equation in the space of transverse momenta and coordinates. Either approach presents us with a very complicated mathematical problem.

Numerical simulation of the trajectories of channeled particles, as developed by the present authors in Ref. 29, is a possible way of resolving the problem.

We note in conclusion that the absence of quasiperiodic channeled motion of electrons should have a particularly radical effect on the electromagnetic radiation emitted by them. Because of the absence of periodicity of motion, the spectral and angular properties of the radiation emitted by electrons in "bound" states are close to those of radiation emitted by over-barrier particles. Moreover, as the particles traverse the crystal, over-barrier states are found to be more highly populated than subbarrier states. It would appear that these facts explain the good agreement between measured spectra[30–32] and theoretical calculations[33] based on the assumption that, when the crystal is thick enough, the radiation emitted by high-energy electrons is due to free-free transitions in the continuous potential (this is the so-called emission by quasichanneling, predicted in Ref. 34 and subsequently investigated in several papers;[35–39] see also the reviews in Refs. 40 and 41). This conclusion is also in agreement with Ref. 42, in which a study was reported of the hard part of the spectrum of radiation emitted by electrons traveling at small angles to the crystal axes.

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APPENDIX

The transition probabilities W_{if} reproduced above and in Ref. 8 can be used to find the diffusion coefficients in (12)

in an explicit form. The summation over f in (13) and (14) can be accomplished with the aid of relationships of the form

$$\sum_f (\varepsilon_f-\varepsilon_i)^2|F_{if}|^2=-([\hat{H}_\perp,F^+][\hat{H}_\perp,F])_{ii},$$

where $\hat{H}_\perp$ is the transverse-motion Hamiltonian, F is an arbitrary function, and the subscript if signifies the corresponding matrix elements. As a result, the diffusion coefficient is expressed in terms of a certain function of the transverse coordinate, averaged over the ith state of the particle:

$$D_r=(D_r(x))_{ii}, \quad D_{rs}=(D_{rs}(\rho))_{ii}. \tag{A.1}$$

In the quasiclassical limit, the matrix element is replaced with an integral over the period of the motion:

$$(D(\mathbf{r}))_{ii}\to T^{-1}\int_0^T dt\, D(\mathbf{r}_v(t)),$$

where $\mathbf{r}_v(t)$ is the particle trajectory. The functions $D_r(x)$ and $D_{rs}(\rho)$ in (A.1) under the matrix element symbol are the "local" scattering characteristics that depend on the transverse coordinate of the particle. Each contains an elastic and an inelastic term.

It was shown in Ref. 11 that the contribution of elastic scattering to $D_r(x)$ and $D_{rs}(\rho)$ is[5)]

$$D_1^{el}(x)=\frac{n}{4\pi E}\int dq\left\{\int dX_a P(X_a)\left|\frac{d\Phi_q(|x-X_a|)}{dx}\right|^2-\exp(-q^2u^2)\right.$$
$$\left.\times\left|\int dX_a P(X_a)\frac{d\Phi_q(|x-X_a|)}{dx}\right|^2\right\}, \tag{A.2}$$

$$D_{10}^{el}(\rho)=\frac{1}{2Ed}\left[\int d^2R_a P(\mathbf{R}_a)\left|\frac{\partial}{\partial\rho}\tilde{\Phi}(|\rho-\mathbf{R}_a|)\right|^2-\left|\frac{\partial}{\partial\rho}\int d^2R_a P(\mathbf{R}_a)\tilde{\Phi}(|\rho-\mathbf{R}_a|)\right|^2\right], \tag{A.3}$$

$$D_{02}^{el}(\rho)=\frac{1}{d}\int d^2R_a P(\mathbf{R}_a)\left|\frac{\partial}{\partial\varphi}\tilde{\Phi}(|\rho-\mathbf{R}_a|)\right|^2, \tag{A.4}$$

where $\Phi_q(x)$, $\tilde{\Phi}(\rho)$ are the corresponding Fourier components of the potential $\Phi(r)$ of an individual atom:

$$\Phi_q(x)=\int dz\,dy\, e^{iqy}\Phi((x^2+y^2+z^2)^{1/2}),$$

$$\tilde{\Phi}(\rho)=\int dz\,\Phi((\rho^2+z^2)^{1/2});$$

$P(X_a)$, $P(\mathbf{R}_a)$ is the probability density of thermal displacements of atoms from their equilibrium positions:

$$P(X_a)\approx(2\pi u^2)^{-1/2}\exp(-X_a^2/2u^2),$$
$$P(\mathbf{R}_a)\approx(2\pi u^2)^{-1}\exp(-R_a^2/2u^2);$$

and φ is the azimuthal angle of a particle relative to the string. Integration with respect to q in (A.2) is performed between the limits $-E\lesssim q\lesssim E$ (precise values are unimportant because the divergence is logarithmic).

Substituting $\ln(Eu)\gg 1$, $u^2/A_{\mathrm{TF}}^2\ll 1$, we can rewrite (A.2)–(A.4) in a more convenient form:

$$D_1^{el}(x)\approx\frac{n}{2E}\left\{4\pi(Ze^2)^2\ln(Eu)P(x)+u^2\int_{-\infty}^{+\infty}\frac{dy}{\eta^2}\left[x^2\left(\frac{\partial^2\tilde{\Phi}(\eta)}{\partial\eta^2}\right)^2+\frac{y^2}{\eta^2}\left(\frac{\partial\tilde{\Phi}(\eta)}{\partial\eta}\right)^2\right]_{\eta=(x^2+y^2+2u^2)^{1/2}}\right\}, \tag{A.5}$$

$$D_{10}^{el}(\rho)\approx\frac{1}{2Ed}\left\{8\pi(Ze^2)^2\ln(Eu)P(\rho)+u^2\left[\left(\frac{\partial^2\tilde{\Phi}(\eta)}{\partial\eta^2}\right)^2+\frac{1}{\eta^2}\left(\frac{\partial\tilde{\Phi}(\eta)}{\partial\eta}\right)^2\right]_{\eta=(\rho^2+2u^2)^{1/2}}\right\}, \tag{A.6}$$

$$D_{02}^{el}(\rho)\approx\frac{\rho^2}{d}\left\{4\pi(Ze^2)^2\ln(Eu)P(\rho)+u^2\left[\frac{1}{\eta^2}\left(\frac{\partial\tilde{\Phi}(\eta)}{\partial\eta}\right)^2\right]_{\eta=(\rho^2+2u^2)^{1/2}}\right\}. \tag{A.7}$$

The first term in (A.5)–(A.7) is due to "close encounters" between the channeled particle and the atomic nuclei.[43] The second term describes the small-angle deflection of a particle from an equilibrium trajectory, and constitutes the analog of the diffusion coefficient due to scattering by fluctuations in the electrostatic field of the crystal lattice, obtained in Ref. 2.[6)] The two terms in (A.5)–(A.7) together reproduce approximately the behavior of the corresponding diffusion coefficient in a broad range of variation of the transverse coordinate. At short distances from the string or plane (x, $\rho\lesssim 2u$), the first term is dominant. On the contrary, for x, $\rho\gtrsim 2u$, the first term decreases rapidly and the "fluctuation" term must therefore be taken into account.

For diffusion coefficients due to inelastic scattering, we can use the result of Section 1 to obtain similarly

$$D_1^{inel}(x)\approx(2\pi e^4 n/E)\,q(x)\ln(Ea_{TF}), \tag{A.8}$$

$$D_{10}^{inel}(\rho)\approx(4\pi e^4/Ed)\,q(\rho)\ln(Ea_{TF}), \tag{A.9}$$

$$D_{02}^{inel}(\rho)\approx(4\pi e^4\rho^2/d)\,q(\rho)\ln(Ea_{TF}), \tag{A.10}$$

where $q(x)$, $q(\rho)$ is the density of the electron cloud in a crystal, averaged along the plane (axis). In reality, $D_r^{\mathrm{inel}}(x)$, $D_{rs}^{\mathrm{inel}}(\rho)$ have a more complicated form. In particular, when $x,\rho\sim a_{\mathrm{TF}}$, the functions D_r^{inel} and D_{rs}^{inel} contain terms corresponding to "dipole" scattering, and are proportional to $\langle d^2\rangle$. Nevertheless, (A.8)–(A.10), which take into account only the "close encounters," provide an accurate enough approximation to $D_r^{\mathrm{inel}}(x)$, $D_{rs}^{\mathrm{inel}}(\rho)$, so that the probability of "dipole" scattering decreases rapidly with increasing x or ρ, and the electron density $q(x)$, $q(\rho)$ differs from zero everywhere inside the channel.

The remaining coefficients are related to D_1, D_{10}, and D_{02} as follows:

$$D_2(x)=4(\varepsilon-U(x))D_1(x), \tag{A.11}$$

$$D_{20}(\rho)=4\left(\varepsilon-U(\rho)-\frac{l^2}{2E\rho^2}\right)\times\left(D_{10}(\rho)-\frac{D_{02}(\rho)}{2E\rho^2}\right)+\frac{l^2D_{02}(\rho)}{E^2\rho^4}, \tag{A.12}$$

$$D_{11}(\rho)=(l/E\rho^2)D_{02}(\rho), \quad D_{10}(\rho)=0. \tag{A.13}$$

where $U(x)$, $U(\rho)$ is the continuous potential of the atomic plane and string, respectively.

[1)]In contrast to scattering by the electron subsystem of the crystal, scattering by phonons will also be referred to as "elastic."[8]

[2)]Here and henceforth, $\hbar = c = 1$.

[3)]Estimates show that the corresponding energies amount to a few tens of and a few hundred of MeV for the string and plane, respectively.

[4)]We note that, in Ref. 24 and in the subsequent papers by these workers,[25–27] there is a purely mathematical error, namely, when they pass to over-barrier motion, the authors of Ref. 24 assume that the coefficient of diffusion over angular momentum is zero (see Ref. 24, Appendix), whereas the problem itself indicates that it should tend to infinity.

[5)]We recall that these formulas contain the Coulomb divergence, so that we have written out only those terms for which the degree of divergence at the upper limit is not stronger than logarithmic.

[6)]It follows from (A.5) that both "planar fluctuations"[2] and oscillations of atoms in the plane of channeling at right-angles to the direction of longitudinal motion are important.

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