Quantum theory of channeled electron and positron scattering in a crystal

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A quantum theory of elastic scattering of planarly and axially channeled electrons and positrons in a thin crystal is developed. The role of coherent (without phonon excitation) and incoherent scattering by the atoms of the plane (chain) is investigated. It is shown that the incoherent scattering, which leads to dechanneling, does not amount to scattering by an isolated atom. Allowance for the ordered disposition of the atoms in the crystal plane (chain) leads to the suppression of the probability for transition between the states of the transverse motion of a particle in the channel, including the reduction of the total width of the levels of the transverse motion. It is also shown that, when the particle moves along the plane in directions strongly differing from the directions of the principal axes, the scattering is incoherent and is determined by the thermal vibrations of the nuclei. As the direction of the particle momentum approaches the directions of the principal axes, the role of the process in which the particle is coherently scattered by the nuclei of the crystal lattice without recoil increases, and can become decisive. At the same time there occurs a relative increase in the probability for large-angle scattering. The coherent scattering becomes resonance scattering upon the fulfillment of certain conditions.

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As is well known, the computer simulation of the passage of particles through crystals has led to the prediction of the effect whereby fast ions moving along the principal crystallographic axes of a single crystal have anomalously long mean free paths.[1,2] The phenomenon of channeling was discovered experimentally,[3,4] and subsequently explained theoretically.[5]

To investigate the problem of proton dechanneling, Lindhard[5] used the approximation in which the energy of the transverse motion of the channeled particle is assumed to increase monotonically. More rigorous and detailed investigations of this problem by classical[6-9] and quantum[10,11] methods have shown that the law of variation of the energy associated with the transverse motion of a channeled particle has a diffusional character. It should be emphasized that the diffusional law of variation of the transverse energy is due to the presence of a large number of energy levels for the transverse motion of the ion in the crystal channel. The diffusion rate for protons is determined largely by the inelastic scattering by the electrons.[6,7] In the case of channeling of negative particles, the dominant mechanism determining the diffusion rate is the elastic scattering by the atoms of the crystal. The existing diffusion coefficients resulting from the scattering on the thermal vibrations of the atoms are derived essentially under the assumption that this scattering occurs on isolated atoms.[12] The purpose of the present paper is, in particular, to correctly take into account the effect of the periodicity of the disposition of the atoms in (on) the channeling plane (axis) on the role of the thermal vibrations in the scattering.

Furthermore, in the case of light charged particles (electrons and positrons) the classical diffusion approximation breaks down at low energies, when the number of levels in the channel is small. The question of the stability of these levels and, in a more general sense, the theory of the elementary acts of quantum scattering in the presence of channeling are the subject of this paper.

§1. FORMULATION OF THE PROBLEM

All the processes of electron (positron) scattering in a crystal can be divided into elastic processes, i.e., those that do not change the state of the crystal, and inelastic processes, which are accompanied by the transfer of energy from the fast particle to the crystal. Let us first consider the elastic processes of electron scattering in the case of channeling in a plane. This case will be considered in detail, since it seems to us to be the most interesting case: in the case of planar channeling of electrons it is precisely the elastic scattering that plays the major role in the broadening of the levels of the transverse motion (see §7). The characteristics of the elastic scattering of positrons as compared with the elastic scattering of electrons and the case of axial channeling of electrons will be discussed below (§§ 4 and 5).

Let an electron enter a crystal at an angle smaller than the Lindhard angle with respect to a crystallographic plane. We shall assume that the thickness of the crystal is greater than the distances over which complete reconstruction of the wave function of the free electron motion into quasistationary states of the channeled particle occurs.[10,11] The Hamiltonian for the interaction of the electron with the crystal is given by the sum of the Hamiltonians for the interaction with each of the charged particles forming the crystal (with allowance, generally speaking, for the retardation). For the elastic processes, the interaction Hamiltonian reduces to a sum of the energies associated with the interaction with the individual atoms of the crystal[1)]:

$$\hat{v}(\mathbf{r})=\sum_{a} V(|\mathbf{r}-\mathbf{r}_a|). \tag{1.1}$$

For an electron energy $E \gtrsim 1$ MeV, $\hat{v}(\mathbf{r}) \ll E$ in the im-

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portant interaction region; therefore, the relativistic Dirac equation for an electron in the external potential $\hat{v}(\mathbf{r})$ can be reduced up to terms $O(\hat{v}^2(\mathbf{r})/E^2)$ (see, for example, Refs. 13 and 14) to an equation of the form

$$[-\Delta+m^2-2E\hat{v}(\mathbf{r})]\varphi(\mathbf{r})=E^2\varphi(\mathbf{r}). \tag{1.2}$$

As the zeroth approximation to the interaction Hamiltonian (1.1), let us take the continuous potential of the plane (near which the channeled electron moves), averaged over the transverse thermal vibrations of the nuclei:

$$U(x)=n\int dydz\langle V\rangle_{th}, \tag{1.3}$$

where n is the density of the atoms in the plane under consideration; the y and z coordinates are measured along the plane, while the x coordinate is measured in the transverse direction; the angle brackets with the subscript *th* here and in the subsequent formulas pertaining to plane channeling denote averaging over the thermal vibrations along the x axis. The vibrations of the various atoms are assumed to be independent of each other. Each of the coordinates is assumed to be distributed according to the law

$$P(x_a)=(2\pi u^2)^{-1/2}\exp[-(x_a-x_a^0)^2/2u^2], \tag{1.4}$$

where x_a is the coordinate of the nucleus of the atom, u is the amplitude of the thermal vibrations, and x_a^0 is the equilibrium position. Then

$$\langle f\rangle_{th}=\int_{-\infty}^{+\infty}dx_aP(x_a)f(x_a). \tag{1.5}$$

In the zeroth approximation, Eq. (1.2) has the form

$$[-\Delta+m^2-2EU(x)]\varphi=E^2\varphi. \tag{1.6}$$

The wave functions of the zeroth approximation that satisfy Eq. (1.6) can be represented in the form of a product of the wave function of the free motion in the (y,z) plane and the wave function of the transverse motion $\psi_n(x)$ satisfying the Schrödinger equation with a relativistic mass:

$$\left[-\frac{1}{2E}\frac{d^2}{dx^2}+U(x)\right]\psi_n(x)=\varepsilon_n\psi_n(x). \tag{1.7}$$

Let us introduce the two-dimensional coordinate $\rho=(y,z)$ and the two-dimensional momentum $\mathbf{p}=(p_y,p_z)$, and write $\varphi(\mathbf{r})$ in the form

$$\varphi(\mathbf{r})=\exp(i\mathbf{p}\rho)\psi_n(x)/2\pi. \tag{1.8}$$

The normalization condition has the form

$$\int\varphi^*(\mathbf{r})\varphi(\mathbf{r})d\mathbf{r}=\begin{cases}\delta(\mathbf{p}-\mathbf{p}')\delta_{nn'}, & \varepsilon_n<0\\ \delta(\mathbf{p}-\mathbf{p}')\delta(\varepsilon_n-\varepsilon_{n'}), & \varepsilon_n\geqslant 0\end{cases},$$

where $\delta(\mathbf{p}-\mathbf{p}')$ is the Dirac delta function and $\delta_{nn'}$ is the Kronecker symbol.

For a channeled electron the relations $\mathbf{p}^2\gtrsim m^2\gg\varepsilon_n^2$ are satisfied; therefore, the total electron energy E can be represented in the form of a sum, $E=E_\parallel+\varepsilon_n$, of the energies of the longitudinal ($E_\parallel=(\mathbf{p}^2+m^2)^{1/2}$) and transverse ($\varepsilon_n$) motions.

A graphic model for the zeroth approximation of the channeling is the peculiar one-dimensional single-electron "atom" uniformly and rectilinearly moving in a definite direction. In such an approach the difference between the true interaction potential (1.1) and the continuous potential (1.3) should be treated as a perturbation leading to the shift and broadening of the energy levels of this "atom." In the first approximation the level width with respect to elastic scattering is determined by the probability for transition of the electron from the initial state i into any other state f in unit time:

$$W_i=\Gamma_i=(2\pi)^{-1}\int|M_{if}|^2p_2dp_2d\theta d\tau_f\delta(E_{1\parallel}+\varepsilon_i-E_{2\parallel}-\varepsilon_f), \tag{1.9}$$

$$M_{if}=\langle\exp(i\mathbf{p}_2\rho)\psi_f^*(x)\left|\sum_a V(|\mathbf{r}-\mathbf{r}_a|)\right|\exp(-i\mathbf{p}_1\rho)\psi_i(x)\rangle. \tag{1.10}$$

Here θ is the scattering angle in the channeling plane; $d\tau_f$ is a range of final transverse-motion states, the integral over which includes a sum over all the levels (except the initial level) of the discrete spectrum and integration over the energy of the continuous spectrum.

The square of the matrix element (1.10) should further be averaged over the thermal vibrations of the crystal atoms (see, for example, Refs. 15–17). Such averaging of the square of the matrix element is entirely equivalent to the consideration of the inelastic processes of phonon production (annihilation). Indeed, in allowing for the excitation of the phonon state of the crystal, we should introduce into the formula (1.10) for the transition matrix element additional variables describing the phonon state of the crystal lattice. Since the final state of the crystal is not fixed in channeling experiments, we must sum the expression (1.9) over all the final states of the lattice. The phonon energy of the crystal excitation is of the order of a fraction of an electron volt, and therefore it can be neglected in comparison with the characteristic change in the transverse energy of the channeled electron. This means that the integral over the variables of the channeled-electron state does not depend on the crystal-excitation energy. In that case we can use the completeness of the system of phonon-state functions for the crystal, finding as a result that the procedure for taking the phonon excitation of the crystal into account is equivalent to the averaging of the square of the matrix element M_{if} over the initial state of the crystal, i.e., the averaging over the thermal vibrations of the atoms.[15] In this case each displacement coordinate of a nucleus is distributed according to the law (1.4), and the averaging is performed with the aid of the formula (1.5).

Thus, the assertion that in the present paper we investigate only the elastic processes of channeled-electron scattering should be understood in the sense that we do not consider the processes of excitation of the electronic states of the crystal (the excitation and ionization of the bound states of the inner and outer shells of the atoms and the valence band, the heating up of the conduction-band electrons, etc.).

§2. COHERENT AND INCOHERENT SCATTERING UNDER CONDITIONS OF PLANAR CHANNELING

Let us average the square of the matrix element over the thermal vibrations of the atoms. We shall, for simplicity, assume that the dechanneling of the electron is brought about by its interaction with the atoms of one plane. In actual fact this approximation is a fairly good one, since the mean distance from the electron to the plane near which the electron oscillates is smaller than the distance to the other planes. The generalization to the case in which the other planes are taken into account is trivial.

Using the fact that the longitudinal and transverse thermal vibrations of the atoms of the crystallographic plane are independent of each other, we obtain, omitting the tedious intermediate calculations (see the Appendix), the following result:

$$|M_{if}|^2 \to \overline{|M_{if}|^2} = |M_{if}|^2_{coh} + |M_{if}|^2_{inc}, \tag{2.1}$$

where

$$|M_{if}|^2_{inc} = n\{\langle|(V_q)_{if}|^2\rangle_{th} - \exp(-q^2u^2)|(\langle V_q\rangle_{th})_{if}|^2\} \tag{2.2}$$

is the incoherent part, due to the thermal vibrations of the crystal-lattice atoms, of the square of the scattering amplitude, while

$$|M_{if}|^2_{coh} = |(\langle V_q\rangle_{th})_{if}|^2 \exp(-q^2u^2)n(2\pi)^2\Delta^{-1}\sum_{g}\delta(\mathbf{q}-\mathbf{g}) \tag{2.3}$$

is the coherent (without phonon excitation) part, due to the periodicity of the potential (1.1), of the square of the scattering amplitude. Here $\mathbf{g}$ denotes the various reciprocal-lattice vectors in the plane; n, the density of atoms in the plane; Δ, the area of the unit cell, equal to the product of two translation vectors; u, the amplitude of the thermal vibrations of the atoms of the plane;

$$V_q(x-x_a) = \int d\rho \exp(iq\rho)V(|\mathbf{r}-\mathbf{r}_a|),$$

the two-dimensional Fourier transform of the potential of a single atom of the crystal; and $\mathbf{q} = \mathbf{p}_2 - \mathbf{p}_1$, the momentum transfer in the longitudinal direction; the brackets with the sign if denote the corresponding matrix element:

$$(A)_{if} = \int dx\psi_i(x)\psi_f^*(x)A(x).$$

As is well known, the differential cross section for elastic scattering of a relativistic particle on a potential with finite range a has a forward peak at angles $\theta \lesssim (p_1a)^{-1} \ll 1$. Using the law of conservation of total energy, the fact that the scattering angle in the plane is small, and the condition $E_\parallel \gg m$, we can derive for the momentum transfer q in the longitudinal direction the expression

$$q^2 \approx (\Delta\varepsilon_\perp)^2 + p_1p_2\theta^2, \tag{2.4}$$

where $\Delta\varepsilon_\perp$ is the change in the transverse energy and $p_1 \approx p_2$.

The contribution of the coherent part (2.3) to the probability for dechanneling will be investigated in detail in §3. Here we shall limit ourselves to the incoherent part (2.2) of the square of the scattering amplitude, since, as will be shown below, in the case in which the electron moves in directions strongly differing from the directions of the principal axes the transverse-energy-level width (as well as the probability for transition between two discrete levels of the transverse motion) is determined precisely by the incoherent term in (2.1).

Performing the dp_2 integration in the expression (1.9), and neglecting the quantity $(\Delta\varepsilon_\perp)^2u^2 \ll 1$, we can write the expression for the level width Γ_i in the form

$$\Gamma_i = np_2\pi^{-1}\int_0^\infty d\theta \int_{f\neq i} d\tau_f\{\langle|(V_q)_{if}|^2\rangle_{th} - \exp(-q^2u^2)|(\langle V_q\rangle_{th})_{if}|^2\}. \tag{2.5}$$

The first term of the difference in the curly brackets describes the scattering on the "amplitude-smeared" transverse oscillations of the density of atoms randomly disposed in the channeling plane. The electron-scattering probability can then be expressed in terms of the cross section for scattering on an isolated atom. The classical analog of this term was considered by Ohtsuki[12] in his investigation of dechanneling caused by the thermal vibrations of the nuclei of the crystal. The approximation in which the atoms are assumed to be randomly disposed in the channeling plane is in fact valid if the amplitude of the thermal vibrations of the nuclei is significantly greater than the mean distance from the electron to the plane $\langle x^2\rangle^{1/2}$ or the atom-screening distance a. In the self-consistent description of channeling, when the level widths are smaller than the level spacing (see above), the thermal-vibration amplitude u is, on the contrary, smaller than (or of the order of) the quantities a and $\langle x^2\rangle^{1/2}$ even in the heaviest elements. In this case the presence of the second term in the integrand in (2.5) is important. For $u^2/\langle x^2\rangle \sim 1$ or $u^2/a^2 \sim 1$, this term is comparable to the first term, and for $u^2/\langle x^2\rangle \ll 1$ and $u^2/a^2 \ll 1$ it causes a significant reduction in the scattering probability.

The expression (2.5) can be simplified further because of the weak dependence of $V_q(x-x_a)$ on the energy ε_f of the final state of the transverse motion. The dominant contribution to the dechanneling probability is made by the final states of the continuous spectrum that lie close to the edge of the spectrum ($\Delta\varepsilon = \varepsilon_i - \varepsilon_f \sim u_0 = 10-100$ eV). The Fourier transform $V_q(x)$ of a potential $V(r)$ with screening radius a significantly depends on q^2 only in the region $q^2 \gtrsim a^{-2}$, which corresponds to the quantity $q \gtrsim 10$ keV. Such a momentum transfer can be given only by the second term in (2.4), i.e., by the term $p_1p_2\theta^2$. Thus, we can, with a good degree of accuracy, assume that $V_q(x-x')$ does not depend on the energy of the final state of the transverse motion, set $q^2 = p_1^2\theta^2$ in (2.5), and use the completeness property of the system of wave functions $|f\rangle$ of the transverse motion:

$$\int_{f\neq i} d\tau_f|f\rangle\langle f| = \delta(x-x') - |i\rangle\langle i|.$$

It can be shown that the accuracy of such a procedure $\sim O((p_1a)^{-1/2})$. We then obtain for the width of the i-th level the expression

$$\Gamma_i = n\pi^{-1}\int_0^\infty dq\{(\langle V_q^2\rangle_{th})_{ii} - \langle|(V_q)_{ii}|^2\rangle_{th} - \exp(-q^2u^2)[((\langle V_q\rangle_{th})^2)_{ii} - |(\langle V_q\rangle_{th})_{ii}|^2]\}. \tag{2.6}$$

Notice that in deriving (2.6) we used neither the explicit form of the wave functions of the continuous spectrum, nor the explicit form of the averaged continuous potential of the planes. The conditions under which we can use the completeness property of the system of wave functions of the transverse motion will also be fulfilled when we take the periodicity of the continuous potential of the crystal planes into account.

The transition from ordered disposition of the atoms in the plane to disordered disposition formally corresponds to the passage to the limit $u\to\infty$. As has already been noted, the first two terms in (2.6) represent the probability for scattering on a single atom displaced through a distance x_a relative to the plane, with subsequent averaging over x_a with the probability density $P(x_a)$. For $a/u\ll 1$ and $\langle x^2\rangle^{1/2}/u\ll 1$ the third and fourth terms are small compared to the first two, and (2.6) assumes the form normal for scattering on randomly disposed atoms:

$$\Gamma_i=n\int dx_a\gamma_i(x_a)P(x_a)\left[1+O\left(\frac{\langle x^4\rangle-\langle x^2\rangle^2}{u^2a^2(1+u^2/a^2)^2}\right)\right], \tag{2.7}$$

where

$$\gamma_i(x_a)=\pi^{-1}\int\limits_0^\infty dq\{(V_q^2)_{ii}-|(V_q)_{ii}|^2\}. \tag{2.8}$$

Actually, the considered limiting case is illustrative as a passage to the limit of amorphous targets, and does not occur in crystals at normal temperatures. Much more real is the limit of small thermal vibrations, i.e., the limit in which $u/a\ll 1$, $u/\langle x^2\rangle^{1/2}\ll 1$, when the last two terms in (2.6) are comparable to the first two. As a result, we obtain (for $u/a\ll 1$, $u/\langle x^2\rangle^{1/2}\ll 1$)

$$\Gamma_i=n\pi^{-1}\int\limits_0^{u^{-1}} dq\left\{q^2u^2[(V_q^2|_{x_a=0})_{ii}-|(V_q|_{x_a=0})_{ii}|^2]\right.$$
$$\left.+u^2\left(\left(\frac{dV_q}{dx}\bigg|_{x_a=0}\right)^2\right)_{ii}+O(u^3)\right\}. \tag{2.9}$$

As $u\to 0$, the contribution of the incoherent part to the level width decreases according to a square law. But at substantial u values the level width for any crystal is determined precisely by the incoherent part of the scattering even in the $u\ll\min\{\langle x^2\rangle^{1/2}, a\}$ case, in which it is quite strongly suppressed (the only exception is the case considered in §3). The incoherent-scattering-suppression effect manifests itself most distinctly in crystals with a small atomic number Z, since the effective screening distance a decreases with increasing Z.

It should be noted that such suppression of the incoherent scattering is due to the periodicity of the crystal lattice, and not to the specific nature of the channeling. As calculations in the Born approximation show, a similar suppression of the scattering through angles $\theta\lesssim(pu)^{-1}$ occurs also in the case of the motion of a fast electron in a single crystal along directions strongly differing from the channeling directions. But it is precisely in the channeling regime that small-angle scattering is most important, a fact which explains the very strong dependence of the level width on the thermal-vibration amplitude.

If we formally neglected the transverse thermal vibrations of the atoms in the plane, then the last term in the curly brackets in the integrand in (2.9) would be absent. If we took into account the transverse, but neglected the longitudinal, thermal vibrations of the atoms, then the first term would be absent. It is not difficult to see that the two terms have the same order of smallness. Therefore, in the case in which electron scattering in a planar channel is considered the transverse and longitudinal thermal vibrations of the atoms of the crystallographic planes of the crystal are, in contrast to the case of axial channeling, equally important (see §5).

It should be noted that the level widths Γ_i do not directly determine the dechanneling probability, since the dominant contribution to the width at high energies is made by the transitions between the states of the discrete spectrum, transitions which do not lead directly to the departure of the particle from the channel. The probability for dechanneling can be close to Γ_i only when there are a small number (one or two) of bound-state levels for the transverse motion, and the thickness T of the crystal is sufficiently small, i.e., $T<1/\Gamma_i$.

At high energies (i.e., in the case of a large number of levels) and in a sufficiently thick crystal, the dechanneling process is described by kinetic equations.[6,7,11] The coefficients in these kinetic equations will be expressible, in particular, in terms of the "dynamical" probabilities W_{nm} for transitions between the levels of the transverse motion. Using the results of this section, we easily obtain the following relation for the W_{nm}:

$$W_{nm}=n\pi^{-1}\int\limits_0^\infty dq[\langle|(V_q)_{nm}|^2\rangle_{th}-\exp(-q^2u^2)|(\langle V_q\rangle_{th})_{nm}|^2], \tag{2.10}$$

which reduces, when $u^2/\langle x^2\rangle\ll 1$, a condition which is well satisfied for the majority of the transverse-motion states, to the expression

$$W_{nm}|_{u^2/\langle x^2\rangle\ll 1}=n\pi^{-1}\int\limits_0^{u^{-1}} dq\left[q^2u^2|(V_q|_{x_a=0})_{nm}|^2+u^2\left|\left(\frac{dV_q}{dx}\bigg|_{x_a=0}\right)_{nm}\right|^2\right]. \tag{2.11}$$

In the case of a large number of levels the quasiclassical matrix elements $\langle n|V_q|m\rangle$ in the expressions (2.10) and (2.11) decrease rapidly as the difference $n-m$ between the quantum numbers increases (the scattering becomes small-angle scattering). In the classical limit, the probabilities W_{nm} are replaced by the differential probabilities $dW/d\varphi$, where φ is the scattering angle in the plane perpendicular to the channeling plane, while the quasiclassical matrix elements $\langle n|V_q(x)|m\rangle$ with nearly equal quantum numbers (i.e., for which $n-m\ll n,m$) are replaced, in accordance with the general principles of quantum mechanics, by the Fourier transforms of the quantity $V_q[x(t)]$, which depends on the time in accordance with the solution, $x=x(t)$, to the classical equation of motion. We can also find in these terms $\langle\varphi^2\rangle$, the mean-square scattering angle in the plane perpendicular to the channeling plane, in terms of which the diffusion coefficients in the kinetic equations are expressed.[6,7]

Using the formulas obtained, we can also find easily the probability per unit time for scattering of a channeled electron through a particular angle in the channeling plane. In doing this, we can distinguish two physically interesting cases:

a) the probability for scattering without a change in the state of the transverse motion;

b) the scattering probability averaged over the beam.

For the case b) we obtain

$$(dw/dq)_{\text{б}}=n\pi^{-1}\int\limits_{-\infty}^{+\infty}dxQ(x)\left(\langle V_q{}^2\rangle_{th}-\exp(-q^2u^2)\,|\langle V_q\rangle_{th}|^2\right),$$

where $Q(x)=\sum_i C_i|\psi_i(x)|^2$ is the transverse-coordinate distribution function of the particles; C_i is the probability for occupation of the i-th transverse-motion level; and $q=p\Theta$, Θ being the scattering angle in the channeling plane.

For the case a) the scattering probability has the form

$$(dw/dq)_a=n\pi^{-1}\{\langle|(V_q)_{ii}|^2\rangle_{th}-\exp(-q^2u^2)\,|(\langle V_q\rangle_{th})_{ii}|^2\}.$$

For $qu\gg1$ the cross section $(dw/dq)_a$ can be approximately written in the form

$$(dw/dq)_a\approx n\pi^{-1}K(q)\int\limits_{-\infty}^{+\infty}|\psi_i(x_a)|^4P(x_a)\,dx_a,$$

where $K(q)$ is the square of the three-dimensional Fourier transform of the potential of an isolated atom.

When the number of levels is small, but the crystal is sufficiently thick ($T>1/\Gamma_i$), we must use the density-matrix formalism to derive the quantum kinetic equations.[10,11] The coefficients in these equations will be expressed in terms of both the probabilities W_{nm} for transitions between the discrete levels and the probabilities for transitions directly into the continuous spectrum (i.e., the Γ_i).

§3. THE ROLE OF THE COHERENT TERM IN THE ELASTIC SCATTERING OF ELECTRONS

Let us investigate the contribution of the coherent part (2.3) to the scattering probability. The characteristic values of the reciprocal-lattice-vector transfers g in (2.3) satisfy the condition

$$U_0\ll|\mathbf{g}|\ll|\mathbf{p}_1|, \tag{3.1}$$

where U_0 is the depth of the well of the planar channel.

Let us consider the case of the simplest lattice:

$$\mathbf{g}_{mn}=\{2\pi m/d,\ 2\pi n/d\},$$

where $m,n=1,2,\ldots$ and d is the distance between the atoms. To each value of m and n corresponds some axis with a direction vector perpendicular to the given $\mathbf{g}_{nm}$. The final electron momentum in the plane is connected with the initial momentum by the relation $\mathbf{p}_2=\mathbf{p}_1+\mathbf{g}_{nm}$; therefore, in the initial (final) state the electron moves in a direction making a small angle $\theta_+(\theta_-)$ with the corresponding axis:

$$\theta_\pm\approx|\mathbf{g}_{nm}|/2|\mathbf{p}_1|\pm\Delta\varepsilon_\perp/|\mathbf{g}_{nm}|. \tag{3.2}$$

All the formulas of the present paper have meaning only when the initial and final states of the longitudinal motion can be represented with a sufficient degree of accuracy by plane waves, which is possible only when

$$|\theta_\pm|\geqslant(3\div4)\,\theta_L{}^{nm}, \tag{3.3}$$

where θ_L^{nm} is the critical Lindhard angle for the given axis.[5] In the opposite case the effect of the strong potential of the axis completely distorts the picture of the planar channeling.

In the region of low energies ($E\approx1-10$ MeV), the critical angles of the axial channeling are quite large; therefore, when the particle moves in the region allowed by the condition (3.3), the coherent scattering is accompanied either by a transverse-energy change significantly greater in magnitude than the depth of the well of the planar channel, or by momentum transfers by a reciprocal lattice with high Miller indices ($(n^2+m^2)^{1/2}\gtrsim10$). In the first case ($|\Delta\varepsilon_\perp|\gg U_0$) the final state of the transverse motion lies far from the edge of the continuous spectrum. Transitions into such states are of low probability because of the smallness of the matrix element $\langle f|V_g|i\rangle$. Physically, this is due to the fact that the longitudinal motion of a channeled electron is a high-energy motion ($E_\parallel\gtrsim m$), while the energy of the transverse motion is small ($\varepsilon_\perp\sim U_0=10-100$ eV), and therefore even a small change in the longitudinal momentum leads—because of the conservation of the sum of the energies of the longitudinal and transverse motions—to a relatively large change in the transverse energy. In the second case the change in the transverse energy can be small, but this process corresponds to large-angle scattering ($\theta\gg(p_1a)^{-1}$) in the channeling plane, and is substantially suppressed by the smallness of the Fourier components $V_g(x)$ of the potential. Thus, when the electron moves along directions strongly differing from the directions of the principal axes, the coherent part in (2.1) is strongly suppressed in comparison with the incoherent part.

But because of the fact that, as the energy $E_\parallel$ increases, the critical Lindhard angles decrease (like $E_\parallel{}^{-1/2}$), there are among the directions allowed by the condition (3.3) those for which the above-adduced arguments are invalid. Classical estimates show that, when the electron motion occurs in a narrow range of angles near the capture boundary for any of the principal axial channels, the situation is possible in which the coherent part (2.3) is comparable to the incoherent part (2.2). The contribution of the coherent part to the level width Γ_i becomes dominant upon the fulfillment of the condition

$$(2\pi/ud)^2(E_\parallel/2U_0)^{-3/2}\exp(-g^2u^2)\,(\Delta\varepsilon_\perp(g))^{-4}\gg1, \tag{3.4}$$

where

$$\Delta\varepsilon_\perp(g)=(\mathbf{p}_1{}^2+m^2)^{1/2}-((\mathbf{p}_1+\mathbf{g})^2+m^2)^{1/2};$$

g and $\Delta\varepsilon_\perp(g)$ should satisfy the condition (3.3).

The condition (3.4) was derived under the assumption that the final state of the transverse motion belongs to the continuous spectrum. The case in which $\Delta\varepsilon_\perp(g)$ is exactly equal to the distance between two discrete levels of the transverse motion requires special treatment; the scattering in this case is resonance scattering. Formally, the coherent part (2.3) is infinite in this case ($|M_{if}|^2_{\text{coh}}\sim\delta(0)$). Actually, the appearance of the infinite factor is due to the fact that we neglected the finiteness of the crystal and the finiteness of the lifetime of the discrete quantum states. In reality, the magnitude of the effect will be determined by the number of centers acting coherently over the smaller of the distances T and $1/\Gamma$, where T is the crystal thickness measured in the direction of flight of the electron and $\Gamma = \Gamma_i + \Gamma_f$ is the total width of the initial and final states. The large factor that arises at resonance compensates for the smallness, discussed above, of the matrix element $\langle i | V_g | f \rangle$. In this case the contribution of the coherent term to the probability W_{if} for transition between the levels i and f becomes decisive upon the fulfillment of the condition

$$(2\pi/d)^2 u L_{min} \exp(-g^2u^2) \gg 1, \quad L_{min} = \min\{1/\Gamma, T\}. \tag{3.5}$$

The condition (3.5) can easily be satisfied. This is due to the simple fact that, when the condition (3.3) is satisfied, only levels of the transverse motion that are sufficiently far apart can be in resonance, whereas the probability for incoherent scattering is highest for the closest levels, and decreases rapidly as the difference between the quantum numbers increases.

The total level width Γ_i can be determined by the $i \to f$ resonance transition probability upon the fulfillment of a condition similar to (3.4) [much more rigid that (3.5)]:

$$\left(\frac{2\pi}{ud}\right)^2 \left(\frac{2U_0}{E_\parallel}\right)^2 (\Delta\varepsilon_\perp(g))^{-4} \frac{\exp(-g^2u^2) L_{min}}{(\langle x_f^2 \rangle)^{1/2}} \bigg|_{\Delta\varepsilon_\perp = \varepsilon_i - \varepsilon_f} \gg 1, \tag{3.6}$$

where $\langle x_f^2 \rangle$ is the mean square of the coordinate x in the state f.

As the total energy of the particle increases, the number of energy levels of the transverse motion increases, and their disposition approaches the equidistant one. Therefore, the resonance condition can be fulfilled not only for a certain pair of levels, but at once for many pairs of levels along the entire depth of the well for the transverse motion. This circumstance can lead to a resonant increase in the probability for the dechanneling of the entire stream of channeled particles (see also Ref. 24).

Thus, as the angle between the direction of the longitudinal momentum of the channeled electron and the direction of any of the principal axes of the crystal decreases, the role of the process of coherent elastic scattering by the nuclei of the crystal lattice without phonon excitation (i.e., without recoil, since the lattice, as a whole, absorbs the momentum) increases, and can become decisive. In this case the role of the large-angle scattering in the plane perpendicular to the channeling plane increases, and that of the low-angle scattering decreases. Let us note that the increase in the role of the large-angle scattering in the absence of planar channeling but under conditions when the angles between the particle momentum and the crystal chains are small is shown in Refs. 18 and 19.

§4. CHARACTERISTICS OF THE PLANAR CHANNELING OF POSITRONS

For positrons, the Hamiltonian for the elastic interaction with the crystal has, as before, the form (1.1), but the potential $V(|\mathbf{r} - \mathbf{r}_a|)$ of the isolated atom is now a repulsive one, and therefore the Hamiltonian in the zeroth approximation should be chosen in the form of a sum of the continuous potentials of the two neighboring planes between which the channeled positron moves:

$$U_+(x) = U(x) + U(-x), \tag{4.1}$$

where $U(x)$ is given by the formulas (1.3)–(1.5) with $x_a^0 = d_p/2$, d_p being the interplanar distance.

In all the formulas of the present section the coordinate x is measured from the midpoint between the planes; the coordinates of the closest planes are then equal to $\pm d_p/2$. The formula (4.1) determines the shape of the well of the planar channel in the region $-d_p/2 \leqslant x \leqslant d_p/2$. The wave functions in the zeroth approximation have the form (1.8), where $\psi_n(x)$ is determined by Eq. (1.7) with the potential $U_+(x)$ instead of $U(x)$.

All the arguments adduced in §3 in respect to the smallness of the coherent part when the particle moves along directions strongly differing from the directions of the principal axes remain valid. Consequently, in this case the width Γ_i of the i-th level of the transverse positron motion with respect to elastic scattering and the probability W_{if} for transition between the states of the transverse motion will be given by an incoherent term similar to (2.2):

$$\Gamma_i = 2n\pi^{-1} \int_0^\infty dq \{ (\langle V_q^2 \rangle_{th})_{ii} - \langle |(V_q)_{ii}|^2 \rangle_{th}$$
$$- \exp(-q^2u^2) [(\langle V_q \rangle_{th}^2)_{ii} - |(\langle V_q \rangle_{th})_{ii}|^2] \}, \tag{4.2}$$

$$W_{if} = 2n\pi^{-1} \int_0^\infty dq [\langle |(V_q^2)_{if}|^2 \rangle_{th} - e^{-q^2u^2} |(\langle V_q \rangle_{th})_{if}|^2]. \tag{4.3}$$

The appearance of the factor 2 is due to the fact the atoms of the two nearest planes, and not just the atoms of one plane, as was the case for electrons, effectively participate in the scattering.

The use of expansions, similar to the limiting cases (2.7)–(2.9), in terms of a small and a large thermal-vibration amplitude allows us to draw the following conclusions about the qualitative characteristics of elastic positron scattering. As for electrons, the incoherent scattering is suppressed as a result of the periodic disposition of the atoms in the plane; at the same time the magnitude of the effect decreases as the atomic number Z of the crystal increases. Furthermore, for positrons the probability for elastic scattering is further suppressed by the weakness of the field in the region where the particle is located (especially for the lower levels) in comparison with the case of electrons, since the scatterers are located in a region classically inaccessible to the positrons.

As the level approaches the edge of the well, the probability for elastic positron scattering increases significantly; therefore, in contrast to the case of electrons, an accumulation of particles at the upper levels should not occur (see §6 below). Let us note in this connection that the width of the levels of the transverse positron motion is determined by the elastic scattering only for sufficiently high levels. For the majority of the levels the dominant broadening mechanism is the inelastic scattering accompanied by electron-shell excitation.[6,7]

As in the case of electrons, as the direction of the longitudinal momentum of the positron approaches the directions of the principal axes of the crystal, the contribution of the coherent elastic scattering increases in comparison with the incoherent scattering. We shall, however, not carry out a detailed investigation of the role of the coherent term here, since its magnitude should be compared not with the incoherent part of the elastic scattering, but with the inelastic scattering, which, for positrons, is more important.

§5. AXIAL CHANNELING OF ELECTRONS

We shall, in considering axial channeling, limit ourselves to the simplest case of "well-channeled" electrons, in which we assume the atomic axes to be sufficiently far apart and the electron states "deep" enough for the continuous potential that describes the electron motion in the zeroth approximation to be considered to be azimuthally symmetric (the single-chain approximation). In the axial case the transverse particle motion is two-dimensional; therefore, it is most convenient to carry out the computations in the cylindrical system of coordinates (ρ, z), where the z axis coincides with the chosen axis and the coordinate vector $\boldsymbol{\rho} = (\rho, \varphi)$ lies in the perpendicular plane. The continuous potential of the axis is given by formulas similar to (1.3)–(1.5):

$$U(\rho)=d^{-1}\int_{-\infty}^{+\infty} dz\langle V\rangle_{th}, \tag{5.1}$$

where d is the distance between the atoms in the chain. The coordinate $\boldsymbol{\rho}_a$ giving the displacement of the atom from the equilibrium position is assumed to be distributed according to the law

$$P(\boldsymbol{\rho}_a)=\frac{1}{2\pi u^2}\exp\left\{-\frac{\rho_a^2}{2u^2}\right\}. \tag{5.2}$$

The perturbation operator has, as before, the form of the difference between the potentials (1.1) and (5.1), the sum in (1.1) extending over all the atoms of the axis in question. The averaging over the thermal vibrations is performed similarly to the planar case. It is easy to see that in the axial case, in contrast to the planar case, the contribution of the coherent part to the level width, as well as to the probability for transition between the discrete levels, can be neglected. Indeed, the maximum depth U_0 of the channeling well for all the elements does not exceed 1 keV, whereas the characteristic frequencies of the perturbation due to the periodic disposition of the atoms on the axis are such that the smallest of the discretely transferable transverse energies $\Delta\varepsilon_\perp \sim 2\pi/d \gtrsim 10$ keV. The transitions into states with such a large transverse energy are of low probability (classically, they correspond to scattering through angles significantly greater than the Lindhard angle); therefore, the probability for transition between the various states of the transverse motion is determined in the case of axial channeling by the incoherent part of the square of the scattering amplitude.

Further, the dominant contribution to the level width is made by the transitions that are accompanied by a small change, $\Delta\varepsilon_\perp \lesssim U_0$, in the transverse energy, transitions for which, with allowance made for the energy conservation law, $(p_f - p_i)^2 u^2 \ll 1$ [here $p_i(p_f)$ is the longitudinal momentum of the electron in the initial (final) state]. This indicates that the longitudinal vibrations of the atoms of the chain can be neglected, in contrast to the planar case, in which the longitudinal and transverse vibrations were found to be essentially of equal intensities. Using the completeness property of the system of wave functions of the transverse motion, as well as the fact that the quantity $(\Delta\varepsilon_\perp)^2 a^2$ is small in the effective domain of integration over the transverse energies (a is the dimension of the atom), we obtain for the i-th level width with respect to elastic scattering the expression

$$\Gamma_i=d^{-1}\{(\langle\tilde{V}^2\rangle_{th})_{ii}-\langle|\tilde{V}_{ii}|^2\rangle_{th}-d^2(U^2)_{ii}+d^2|U_{ii}|^2\}, \tag{5.3}$$

where

$$\tilde{V}(\boldsymbol{\rho}-\boldsymbol{\rho}_a)=\int_{-\infty}^{+\infty} dz V(z, \boldsymbol{\rho}-\boldsymbol{\rho}_a).$$

In the formulas (5.1)–(5.3) the symbols $(\ldots)_{ii}$ and $\langle\ldots\rangle_{th}$ have the following meaning:

$$\langle A\rangle_{th}\equiv\int d^2\rho_a P(\boldsymbol{\rho}_a)A(\boldsymbol{\rho}_a),$$

$$(A)_{ii}\equiv\int d^2\rho|\psi_i(\boldsymbol{\rho})|^2 A(\boldsymbol{\rho}),$$

where $\psi_i(\rho)$ is the wave function of the transverse motion. The formula (5.3) can clearly be generalized to the case of many chains. To do this, we must include in (5.3) terms corresponding to the scattering by the atoms of the neighboring chains and replace $\psi_i(\rho)$, which corresponds to the azimuthally symmetric potential (5.1), by the solution to the Schrödinger equation with a realistic potential taking account of the requisite number of atomic axes.

Passage to the limiting cases of large and small thermal-vibration amplitudes in (5.3) yields a result similar to (2.7)–(2.9). Specifically, in the limit of large u (5.3) reduces to a sum of cross sections for scattering on the individual atoms, while in the limit of small u it indicates the suppression of the incoherent-scattering probability.

§6. SPECIFIC CALCULATION OF THE LEVEL WIDTHS

For numerical estimates, one of the most convenient approximations to the continuous potential (1.3) is[14]

$$U(x)=-U_0\,\mathrm{ch}^{-2}(x/b), \tag{6.1}$$

where U_0 and b are parameters depending on the shape of the crystal and the channeling plane.

The energy levels for Eq. (1.6) with the potential (6.1) are completely determined by the parameter

$$\nu={}^1/_2((1+8EU_0b^2)^{1/2}-1), \tag{6.2}$$

the discrete spectrum being given by

$$\varepsilon_n=-U_0(\nu-n)^2/\nu(\nu+1), \tag{6.3}$$

$$\psi_n(x)=\left[\frac{(\nu-n)\Gamma(2\nu+1-n)}{n!b}\right]^{1/2}P_\nu^{n-\nu}\left(\mathrm{th}\frac{x}{b}\right),$$

where E is the energy of the channeled electron; n is the level number, $0 \leqslant n < \nu$; ε_n and $\psi_n(x)$ are the corresponding energy and wave function, $P_\nu^{\mu}(y)$ and $\Gamma(x)$ being the Legendre and the gamma function respectively.

As the model potential of the atom, we can take the screened Coulomb interaction

$$V(|\mathbf{r}|)=e^{-\gamma r}Ze^2/r, \tag{6.4}$$

where Ze is the nuclear charge and γ is the reciprocal screening distance. The potential (6.4) is one of the three terms of the Molière potential, which is extremely close to the real potential; therefore, all the results obtained with the potential (6.4) can be trivially carried over to the case of the Molière potential.

The wave function of a bound state in a potential of the type (6.1) near $x = 0$ has the oscillatory form:

$$\psi_n(x)=A_n(x)\cos[{}^1/{}_2\pi n+x\omega_n(x)],$$

where the "amplitude" $A_n(x)$ and the "frequency" $\omega_n(x)$ change little over distances of the order of the distance between the nodes of the wave function (perhaps the only exception is the level with $n = 0$, at which the wave function does not have zeros at all). Thus, when the condition $\omega_n(0) \lesssim \gamma \ll u^{-1}$ is satisfied, we can use the approximate expression for the wave functions of the discrete spectrum of the transverse motion:

$$\psi_m(x)\approx A_m\cos({}^1/{}_2\pi m+\omega_m x);$$

then the integration in, for example, the formula (2.9) can be performed explicitly:

$$\begin{aligned}\Gamma_m|_{\omega_m\leqslant\gamma\ll u^{-1}}={}&n\pi^{-1}u^2(Z\alpha)^2|A_m|^2\biggl\{(1+(-1)^m)\operatorname{Arsh}\frac{1}{u\gamma}-\frac{1}{2}\\&-\frac{\pi|A_m|^2}{4}\left(\frac{1}{\gamma}+\frac{1}{(\gamma^2+4\omega_m^2)^{1/2}}\right)-\frac{(-1)^m\pi|A_m|^2}{4\omega_m^2}[(\gamma^2+4\omega_m^2)^{1/2}-\gamma]\\&-\frac{(-1)^m(\gamma^2+2\omega_m^2)}{4\omega_m(\gamma^2+\omega_m^2)^{1/2}}\ln\frac{(\gamma^2+\omega_m^2)^{1/2}+\omega_m}{(\gamma^2+\omega_m^2)^{1/2}-\omega_m}\biggr\}+O(u^3),\end{aligned} \tag{6.5}$$

where $\alpha = 1/137$ is the fine-structure constant. From the explicit form of $\psi_m(x)$, (6.3), we find

$$|A_m|^2=\frac{(\nu-m)\Gamma((m+1)/2)\Gamma((2\nu-m+1)/2)}{\pi b\Gamma((m+2)/2)\Gamma((2\nu-m+2)/2)},$$

$$\omega_m=\frac{2\Gamma((m+2)/2)\Gamma((2\nu-m+2)/2)}{b\Gamma((m+1)/2)\Gamma((2\nu-m+1)/2)}.$$

The formula (6.5), although it is based on the model potentials (6.1), (6.4), demonstrates a general property of the scattering probabilities Γ_i, which depends only on the parity of the functions $U(x)$, $V(|\mathbf{r}|)$, and $P(x_a)$: the even-parity states are scattered somewhat more strongly and live for a shorter time than the odd-parity states, and the greater the atomic number Z of the crystal is, the stronger is this effect. In the limit of high longitudinal-motion energies, when the number of levels in the well is large, the indicated dependence of the scattering probability on the parity of the level disappears. The formula (6.5) then goes over into the expression

$$\begin{aligned}\Gamma_m|_{\gamma\ll u^{-1}\ll\omega_m}\approx{}&n(2\pi)^{-1}u^2(Z\alpha)^2|A_m|^2\biggl\{[1+(-1)^m\exp(-2\omega_m^2u^2)]\\&\times\left(2\operatorname{Arsh}\frac{1}{u\gamma}-1\right)+|A_m|^2\left(\frac{u}{3}-\frac{\pi}{2\gamma}\right)\biggr\}\end{aligned} \tag{6.6}$$

(the term with $(-1)^m$ is retained in order to observe the order of magnitude of the effect of the level parity).

Let us note here the following important circumstance: at high energies the level width is determined by transitions to several nearest levels; therefore, Γ_m in fact determines the diffusion coefficient in the kinetic equation describing the dechanneling process. The expression for Γ_m contains the factor $|A_m|^2$, which decreases as the level approaches the edge of the well; therefore, the rate of electron diffusion over the levels of the transverse motion also decreases as the well edge is approached (see also Ref. 20). In such a situation the particles can collect at the top levels, as a result of which the dechanneling rate for the entire electron stream will be determined not by the rate of diffusion over the depth of the well, but by the probability for departure of a particle from the top levels into the continuous spectrum (it should be remembered that the presence of inelastic processes, as well as of a coherent part in the elastic scattering can further complicate the diffusion picture).

The formula (6.6) allows us to draw another very interesting conclusion: in the limit $E_\parallel\to\infty$, $\varepsilon_\perp = \text{const}$, the level width $\Gamma_{\varepsilon_\perp}\sim E^0$. In fact, such a limit corresponds to $\nu\to\infty$, $m/\nu\to\text{const}$. Only the factor $|A_m|^2$ in (6.6) then depends essentially on ν. But it follows from the explicit form of $|A_m|^2$ that $|A_m|^2\sim\nu^0$ for $\nu\to\infty$. It is easy to realize that this result is not a consequence of the model potentials (6.1)–(6.4). Indeed, for $E_\parallel\to\infty$, when the quasiclassical approach is valid, the matrix elements in the formula (2.6) can be replaced by time integrals of the quantity $V_q(x(t))$, where $x(t)$ is the solution to the classical equation of motion:

$$\langle i|V_q(x)|i\rangle\to\frac{1}{T}\int_0^T dt\,V_q(x(t)).$$

The dependence on $E_\parallel$ is determined by the equation

$$E_\parallel(d^2x/dt^2)=-\nabla U(x)$$

with the initial condition

$$x(0)=x_0,\quad dx/dt|_{t=0}=v_0(E_\parallel).$$

The dependence $v_0(E_\parallel)$ is determined from the condition

$$\varepsilon_\perp=U(x_0)+E_\parallel v_0^2/2=\text{const},$$

whence $v_0\sim E_\parallel^{-1/2}$. By going over to the new variable $\tau = tE^{-1/2}$, we can easily verify that the magnitude of the matrix element does not depend on $E_\parallel$.

Thus, the width of the levels remains constant, while their spacing decreases like $E_\parallel^{-1/2}$ as $E_\parallel\to\infty$. Consequently, starting from some electron energy, the level spacing is smaller than the level width. This result implies that we are outside the limits of applicability of the weak-binding approximation, as a result of which the quantity Γ_i can no longer be interpreted as the level width. To find the true level width in this case, we must solve the system of quantum kinetic equations with the coefficients W_{nm} obtained in the present paper.

§7. OTHER LEVEL-BROADENING MECHANISMS

All the formulas of the present paper were derived with allowance for only the processes of elastic channeled-electron scattering by the atoms of the crystal. In actual fact three other mechanisms contribute to the broadening of the levels of the transverse motion: the inelastic scattering (i.e., the processes accompanied by electron-shell excitation), the radiative transitions between the levels of the transverse motion, and the band broadening. All these mechanisms act additively, and can be considered independently.

The inelastic-scattering processes may play a decisive role in the scattering of sufficiently high levels of the transverse motion, when the electron on the average moves far away from the plane (at a distance greater than the screening radius for the atoms of the crystal lattice), as a result of which the elastic scattering turns out to be suppressed.

The radiative transitions are investigated in detail in Refs. 21 and 22, where it is shown that they begin to play an important role at energies $E \gtrsim 10$ GeV. In the energy region 1–100 MeV they make a negligible contribution to the level width as compared to the scattering by the electrons and nuclei of the crystal.

The band broadening of the levels, which is due to the periodicity of the continuous potential of the planes, does not, in contrast to the scattering, lead directly to a decrease in the lifetime of the electron at the level in question. But in fact in experiments in which level lifetimes are measured (say, by measuring the line width of the spontaneous γ emission) the splitting of a level into a band will give rise to a large number of transitions with nearly the same frequency, which will be received by the measuring apparatus as one broad line. The magnitude of the band splitting is, as is well known, determined by the probability for tunneling through the potential barrier separating neighboring wells of the crystal planes. In the vicinity of $x = d_p/2$, where d_p is the interplanar distance, the potential barrier is well-described by the parabola

$$v(x)=(-U_0)(\beta+(1-\beta)(2x-d_p)^2/d_p^2), \tag{7.1}$$

where β is a constant of the order of 0.03–0.05. Quasi-classical estimates with the potential (7.1) show that, in the case of planar channeling of electrons, the band-broadening effect can be neglected in the case of levels lying below the limit

$$|\varepsilon_n| \approx U_0(\beta+0{,}5/\nu), \tag{7.2}$$

where the coefficient of tunneling through the barrier and the band width do not, as a percentage of the level spacing, exceed 5% (see also Ref. 23); ε_n and ν are given by the formulas (6.2) and (6.3) respectively.

In the case of planar channeling of positrons, the potential barrier between the channels is well-described by the formula (6.1). Here we obtain for the limit below which the band broadening can be neglected the estimate

$$\delta\varepsilon_\perp \approx 1{,}5U_0/\nu, \tag{7.3}$$

where $\delta\varepsilon_\perp$ is the distance to the edge of the potential well of the channeling.

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APPENDIX

Let us represent the square of the matrix element (1.10) in the form

$$\begin{aligned}|M_{if}|^2 &= \Big|\int d^2\rho\, dx \exp(i\mathbf{q}\rho)\psi_f^*(x)\psi_i(x)\sum_a V[((x-x_a)^2+(\rho-\rho_a)^2)^{1/2}]\Big|^2\\ &= \Big|\sum_a \exp(i\mathbf{q}\rho_a)\int \psi_f^*(x)\psi_i(x)V_q(x-x_a)\,dx\Big|^2\\ &= \sum_a \Big|\int \psi_f^*(x)\psi_i(x)V_q(x-x_a)\,dx\Big|^2 + \sum_{a,b;\,a\neq b}\exp[i\mathbf{q}(\rho_a-\rho_b)]\\ &\times\Big[\int\psi_f^*(x)\psi_i(x)V_q(x-x_a)\,dx\Big]\Big[\int\psi_f^*(y)\psi_i(y)V_q(y-x_b)\,dy\Big]^*,\end{aligned}$$

where $V_q(x-x_a)$ is the Fourier transform of the potential of a single atom. Averaging over the coordinate x_a with the aid of (1.3)–(1.5) with $x_a^0 = 0$, we obtain

$$\begin{aligned}|M_{if}|^2 &= N\Big\langle\Big|\int\psi_f^*(x)\psi_i(x)V_q\,dx\Big|^2\Big\rangle_{th}\\ &+ \sum_{a,b;\,a\neq b}\exp[i\mathbf{q}(\rho_a-\rho_b)]\Big|\int\psi_f^*(x)\psi_i(x)\langle V_q\rangle_{th}\,dx\Big|^2,\end{aligned}$$

where N is the number of atoms in the plane under consideration. The averaging over ρ_a is performed analytically, after which we have

$$\begin{aligned}|M_{if}|^2 &= N\Big\langle\Big|\int\psi_f^*(x)\psi_i(x)V_q\,dx\Big|^2\Big\rangle_{th} \qquad \text{(A1)}\\ &+ \exp(-q^2u^2)\Big[\Big|\sum_a\exp(i\mathbf{q}\rho_a^0)\Big|^2 - N\Big]\Big|\int\psi_f^*(x)\psi_i(x)\langle V_q\rangle_{th}\,dx\Big|^2.\end{aligned}$$

Here the ρ_a^0 are the coordinates of the crystal-lattice sites in the plane. Let us represent ρ_a^0 in the form $\rho_a^0 = \{d_x n, d_y m\}$, where d_x and d_y are the lattice constants along the x and y axes, and go over in (A1) from summation over a to summation over m and n. A sum of the type

$$\sum_n \exp(iq_x d_x n)$$

is a sum of the terms of a geometric progression; therefore,

$$\Big|\sum_{n=0}^{N_x}\exp(iq_x d_x n)\Big|^2 = \frac{\sin^2(q_x d_x N_x/2)}{\sin^2(q_x d_x/2)}.$$

In the limit $N \gg 1$ we obtain

$$\lim_{N_x\to\infty}\Big|\sum_{n=0}^{N_x}\exp(iq_x d_x n)\Big|^2 = \frac{2\pi N_x}{dx}\sum_{i=-\infty}^{+\infty}\delta\Big(q_x - \frac{2\pi}{d_x}i\Big). \tag{A2}$$

As can be seen, (A1) with allowance for (A2) splits up into a sum of two terms, which are denoted in §2 by $|M_{if}|^2_{\text{inc}}$ and $|M_{if}|^2_{\text{coh}}$.

1) $\hbar = c = 1$.

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