

field, we regard the abrupt boundary as the limit of a smoothed boundary when the transition region tends to zero. We write down an equation for  $\varphi$  with variable coefficients that hold in the whole of space, and the boundary conditions are obtained by integrating it and then going to the limit of a sharp boundary.

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## Pendellosung radiation of an electron diffracted in a single crystal

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A quantum-mechanical analysis is made of Pendellosung radiation produced by diffraction of an electron in a single crystal, with account taken of the deviation from the Bragg condition in the final state of the electron. The formulas obtained for the angular distribution duplicate the result of I. M. Frank for the radiation of an oscillator moving in a refracting medium and oriented perpendicular to the velocity.

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1. Frank<sup>1</sup> has developed the theory of the emission of a classical oscillator moving in a refracting medium. He has shown that at  $n\beta > 1$  ( $\beta = v/c$ ,  $v$  is the oscillator velocity, and  $n$  is the refractive index) a number of new phenomena appear, namely the anomalous and complex Doppler effects.

It was previously noted<sup>2</sup> that the Pendellosung effect

causes an electron diffracted in a crystal to behave, with respect to emission, like a moving oscillator, i.e., when the electron is diffracted Pendellosung radiation is produced at a frequency and polarization that are determined by the frequency and direction of the oscillations of the diffracted electron. It was shown in Ref. 3 that  $n\beta_{\parallel} > 1$  ( $\beta_{\parallel} = v \cos \theta_B / c$ ,  $\theta_B$  is the Bragg angle), just as in the case considered by Frank,<sup>1</sup> the dependence

of the frequency of the Pendellosung radiation on the direction is determined either by the normal or by the anomalous Doppler effect. It was also indicated that experimental observation of the phenomena of the complex and anomalous Doppler effect in Pendellosung radiation is feasible.

From the point of view of quantum mechanics, Pendellosung radiation is the result of transition of the electron between different branches of the dispersion surfaces (equal-energy surfaces in momentum space) of the electron in the crystal.<sup>3</sup>

However, in the derivation of the formulas for the intensity of the Pendellosung in Ref. 3, no account was taken of the deviation, due to photon emission, from the Bragg condition in the final state of the electron; this led to loss of the longitudinal component of the electron current. As a result, these results are valid only at  $\kappa \cdot \mathbf{g} = 0$ , where  $\kappa$  is the wave vector of the photon and  $\mathbf{g}$  is the reciprocal-lattice vector, i.e., in the case of radiation in a plane parallel to a crystallographic plane.<sup>1)</sup>

In this paper is developed a quantum-mechanical theory of Pendellosung radiation with account taken of the deviation from the Bragg condition in the final state of the electron. It is shown that the equations for the angular distribution of the Pendellosung radiation are substantially different from those in Ref. 3, and duplicate exactly the result obtained by Frank<sup>1</sup> for the emission of a moving oscillator oriented perpendicular to the velocity. Thus, the classical analog of a diffracting electron is a moving oscillator, and this analogy has a distinct physical meaning in the language of dynamic theory of diffraction.

Similar formulas describe also the emission of fast electrons channeled in a crystal.<sup>4-6</sup> The analysis of this radiation is based on the concept of channeling as a finite motion of the particle in the transverse direction, bounded by two planes (for planar channeling) of the crystal (see, e.g., Ref. 7). The radiation accompanying the channeling is in this case the result of transitions between discrete states of the transverse motion of the particle.

2. We consider a system of crystallographic planes in the crystal, characterized by a reciprocal-lattice vector  $\mathbf{g}$  ( $|\mathbf{g}| = 2\pi/d$ , where  $d$  is the distance between the planes).

As follows from the dynamic theory of diffraction in the two-ray approximation, near the Bragg condition an electron of energy  $E$  in a crystal is described by the Bloch functions  $\psi^{(1)}(\mathbf{k}^{(1)}, \mathbf{r})$  and  $\psi^{(2)}(\mathbf{k}^{(2)}, \mathbf{r})$ , corresponding to the two branches of the dispersion surface<sup>8</sup>

$$\psi^{(1)}(\mathbf{k}^{(1)}, \mathbf{r}) = \cos \gamma \exp[i\mathbf{k}^{(1)}\mathbf{r}] + \sin \gamma \exp[i(\mathbf{k}^{(1)} + \mathbf{g})\mathbf{r}], \quad (1)$$

$$\psi^{(2)}(\mathbf{k}^{(2)}, \mathbf{r}) = -\sin \gamma \exp[i\mathbf{k}^{(2)}\mathbf{r}] + \cos \gamma \exp[i(\mathbf{k}^{(2)} + \mathbf{g})\mathbf{r}], \quad (2)$$

where

$$\operatorname{tg} \gamma = -[\Delta + (\Delta^2 + U_g^2)^{1/2}] / U_g, \quad (3)$$

$\Delta = [(\mathbf{k} + \mathbf{g})^2 - k^2] / 2$  is the parameter of the deviation from the Bragg condition,  $V_g = \hbar^2 U_g / 2m$ ,  $-V_g$  is the amplitude of the first harmonic of the periodic potential of the

lattice. The wave vectors  $\mathbf{k}^{(1)}$  and  $\mathbf{k}^{(2)}$  correspond to two branches of the dispersion surface whose equation is of the form

$$(k^2 - K^2) [(k + \mathbf{g})^2 - K^2] = U_g^2, \quad (4)$$

where  $K = [2m(E + V_0) / \hbar]^2 \approx mv / \hbar$ , and  $-V_0$  is the average potential of the lattice. The symmetry of the functions (1) and (2), as follows from (3), is determined by the sign of  $U_g$ . We shall assume that  $U_g > 0$ , and in this case at  $\Delta \approx 0$  we have  $\gamma < 0$ , so that the function  $\psi^{(1)}$  is an antisymmetrical combination of the direct and reflected waves, while the function  $\psi^{(2)}$  is a symmetrical combination. The intensities of the direct and reflected waves in branches (1) and (2) are determined by the quantity

$$\cos^2 \gamma = 1/2 (1 - \Delta / (\Delta^2 + U_g^2)^{1/2}). \quad (5)$$

3. Let electrons with energy  $E_a$  be incident at exactly the angle  $\theta_B$  on the reflecting planes of the crystal in the Laue diffraction scheme (i.e., the crystal boundary is perpendicular to the planes). This excites in the crystal waves belonging to both branches of the dispersion surface, so that the wave function of the electron  $\psi_a$  inside the crystal takes the form<sup>8</sup>

$$\psi_a = 2^{-1/2} [\psi_a^{(1)}(\mathbf{k}_a^{(1)}, \mathbf{r}) + \psi_a^{(2)}(\mathbf{k}_a^{(2)}, \mathbf{r})] \exp[-iE_a t / \hbar]. \quad (6)$$

By virtue of satisfaction of the Bragg condition  $\Delta_a = 0$ , we get from (1)-(3) for the functions  $\psi_a^{(1)}$  and  $\psi_a^{(2)}$

$$\psi_a^{(1)}(\mathbf{k}_a^{(1)}, \mathbf{r}) = 2^{1/2} i \sin \frac{\mathbf{g}\mathbf{r}}{2} \exp \left[ i \left( \mathbf{k}_a^{(1)} + \frac{1}{2} \mathbf{g} \right) \mathbf{r} \right], \quad (7)$$

$$\psi_a^{(2)}(\mathbf{k}_a^{(2)}, \mathbf{r}) = 2^{1/2} \cos \frac{\mathbf{g}\mathbf{r}}{2} \exp \left[ i \left( \mathbf{k}_a^{(2)} + \frac{1}{2} \mathbf{g} \right) \mathbf{r} \right]. \quad (8)$$

The dispersion equation (4) is correspondingly simplified:

$$k_a^{(1,2)^2} = K_a^2 \mp U_g. \quad (9)$$

We consider now transitions of the electron from the state  $\psi_a$  to the state  $\psi_b$  with energy  $E_b$  at which a phonon of energy  $\hbar\omega$  and with wave vector  $\kappa$  is emitted:

$$\kappa = \omega n / c. \quad (10)$$

We assume that the emission of the phonon violates only slightly the Bragg condition, i.e., the parameter  $\Delta_b$  in the final state is small compared with  $U_g$ :

$$|\Delta_b| \ll U_g, \quad (11)$$

where

$$\Delta_b = 1/2 [(k_b + \mathbf{g})^2 - k_b^2] = -\kappa \mathbf{g} \quad (k_b = k_a - \kappa). \quad (12)$$

This leads to a limitation on the considered wavelengths of the photons:

$$\lambda \gg \xi_g \operatorname{tg} \theta_B \cos \chi(\kappa \mathbf{g}), \quad (13)$$

where  $\xi_g = (2\pi K \cos \theta_B) / U_g$  is the extinction length.

Inasmuch as  $\lambda \sim \xi_g$  for Pendellosung radiation, and  $\theta_B \ll 1$  (for example,  $\theta_B \approx 0.03$  for electrons of energy 50 keV), the conditions (11) and (13) are practically always satisfied. In this case, retaining in (5) the terms linear in  $\Delta_b / U_g$  we get for the Bloch functions of the final state of energy  $E_b$

$$\psi_b^{(1)}(\mathbf{k}_b^{(1)}, \mathbf{r}) = 2^{1/2} i \left[ \sin \frac{\mathbf{g}\mathbf{r}}{2} - i \frac{\kappa \mathbf{g}}{2U_g} \cos \frac{\mathbf{g}\mathbf{r}}{2} \right] \exp \left[ i \left( \mathbf{k}_b^{(1)} + \frac{1}{2} \mathbf{g} \right) \mathbf{r} \right], \quad (14)$$

$$\psi_b^{(2)}(\mathbf{k}_b^{(2)}, \mathbf{r}) = 2^{1/2} \left[ \cos \frac{\mathbf{g}\mathbf{r}}{2} - i \frac{\kappa\mathbf{g}}{2U_g} \sin \frac{\mathbf{g}\mathbf{r}}{2} \exp \left[ i \left( \mathbf{k}_b^{(2)} + \frac{1}{2}\mathbf{g} \right) \mathbf{r} \right] \right]. \quad (15)$$

Accordingly, we obtain from (4)

$$k_b^{(1,2)} = K_b^2 + \kappa\mathbf{g} \mp U_g. \quad (16)$$

The matrix element of the transition  $a \rightarrow b$  from the branch  $\alpha$  to  $\beta$  ( $\alpha=1, 2; \beta=1, 2$ ) with emission of a photon with polarization  $\mathbf{u}_\lambda$  is of the form

$$H_\lambda^{a\alpha} = 2^{-1/2} \langle \psi_b^{(\beta)}(\mathbf{k}_b^{(\beta)}, \mathbf{r}) | H_\lambda | \psi_a^{(\alpha)}(\mathbf{k}_a^{(\alpha)}, \mathbf{r}) \rangle, \quad (17)$$

where  $H_\lambda$  is the operator of the interaction of the electron with the photon in the medium<sup>9</sup>:

$$H_\lambda = \frac{e}{m\kappa} \left( \frac{2\pi\hbar}{\omega} \right)^{1/2} e^{-i\mathbf{r}\cdot\mathbf{u}_\lambda} (\mathbf{u}_\lambda \cdot i\hbar \nabla). \quad (18)$$

As shown in Ref. 3, the Pendellosung radiation is due to transitions between different branches, with the ordinary and anomalous Doppler effects produced in the transitions 1-2 and 2-1, respectively. Calculation of the corresponding matrix elements yields

$$H_\lambda^{21,12} = -\frac{e}{m\kappa} \left( \frac{\pi\hbar}{\omega} \right)^{1/2} \hbar \left[ \frac{\mathbf{g}\mathbf{u}_\lambda}{2} \mp \frac{\kappa\mathbf{g}}{2U_g} \left( \mathbf{k}_a^{(1,2)} + \frac{1}{2}\mathbf{g} \right) \mathbf{u}_\lambda \right]. \quad (19)$$

We have taken into account the quasimomentum conservation laws:

$$\begin{aligned} \mathbf{k}_b^{(2)} + \kappa - \mathbf{k}_a^{(1)} &= 0 \text{ for the transition } 1 \rightarrow 2, \\ \mathbf{k}_b^{(1)} + \kappa - \mathbf{k}_a^{(2)} &= 0 \text{ for the transition } 2 \rightarrow 1. \end{aligned}$$

It is seen from (19) that despite the smallness of the quantity  $\kappa \cdot \mathbf{g}/2U_g$ , the contribution of the second term to the matrix element can be comparable with the contribution from the first, since  $g/2|\mathbf{k}_a + \mathbf{g}/2| = \tan\theta_B \ll 1$ .

We note that allowance for the deviation from the Bragg condition in the final state is inessential for the Cerenkov radiation due to the transitions 1-1 and 2-2,<sup>3</sup> since it adds a small increment  $\sim \kappa \cdot \mathbf{g}/4U_g$  to the large quantity  $\sim |\mathbf{k}_a + \mathbf{g}/2|$  in the matrix elements.

Introducing the unit vectors  $\mathbf{e}_\parallel$  and  $\mathbf{e}_\perp$  along the directions  $\mathbf{k}_a^{(1,2)} + \mathbf{g}/2$ , and  $\mathbf{g}$ , as well as  $\mathbf{n}_\kappa$  along the direction  $\kappa$ , and also recognizing that

$$|\mathbf{k}_a^{(1,2)} + \frac{1}{2}\mathbf{g}| = k_{a\parallel}^{(1,2)} \approx m v_\parallel / \hbar, \quad (20)$$

we get

$$H_\lambda^{21,12} = -\frac{e}{m\kappa} \left( \frac{\pi\hbar}{\omega} \right)^{1/2} \frac{\pi\hbar}{d} \left[ (\mathbf{e}_\perp \mathbf{u}_\lambda) \mp (\mathbf{e}_\perp \mathbf{n}_\kappa) (\mathbf{e}_\parallel \mathbf{u}_\lambda) \frac{\hbar\omega}{2V_g} \beta_\parallel n \right]. \quad (21)$$

Denoting by  $\mathbf{u}_1$  the polarization vector lying in the plane of the vectors  $\mathbf{n}_\kappa$  and  $\mathbf{e}_\parallel$  ( $\mathbf{u}_2$  lies in this case in a plane perpendicular to the direction of  $\mathbf{e}_\parallel$ ) we obtain for the matrix elements corresponding to different polarizations, in a spherical coordinate system

$$H_1^{21,12} = -\frac{e}{m\kappa} \left( \frac{\pi\hbar}{\omega} \right)^{1/2} \frac{\pi\hbar}{d} \cos\varphi \left( \cos\theta \mp \frac{\hbar\omega}{2V_g} \beta_\parallel n \sin^2\theta \right), \quad (22)$$

$$H_2^{21,12} = -\frac{e}{m\kappa} \left( \frac{\pi\hbar}{\omega} \right)^{1/2} \frac{\pi\hbar}{d} \sin\varphi. \quad (23)$$

Here  $\theta$  and  $\varphi$  are the angles that characterize the direction of the photon emission, the polar axis is chosen along  $\mathbf{e}_\parallel$ , i.e., along the direction of the average propagation of the electron in the crystal parallel to the crystallographic planes, and  $\varphi$  is the angle in the plane

perpendicular to the vector  $\mathbf{e}_\parallel$  and is reckoned from the direction of  $\mathbf{e}_\perp$ .

4. The number  $N$  of photons emitted per unit time is determined by the formula

$$N = \sum_{\substack{\alpha, \beta, \lambda \\ (\alpha \neq \beta)}} \int \frac{2\pi}{\hbar} |H_\lambda^{a\alpha}|^2 \delta(E_a - E_b - \hbar\omega) \frac{n^3 \omega^2}{c^3} \frac{d\omega d\Omega}{(2\pi)^3}. \quad (24)$$

Using the quasimomentum conservation laws as well as the dispersion equations (9), (10), and (16) for the electron and photon, and neglecting the recoil energy, we obtain for the transition 1-2

$$E_a - E_b - \hbar\omega = 2V_g - \hbar\omega(1 - n\beta_\parallel \cos\theta). \quad (25)$$

Analogously for the transition 2-1 we have

$$E_a - E_b - \hbar\omega = -2V_g - \hbar\omega(1 - n\beta_\parallel \cos\theta). \quad (26)$$

From the energy conservation law it follows directly that the transition 1-2 is allowed in the angle region  $\theta > \theta_0$  [ $\theta_0 = \arccos(1/\beta_\parallel n)$ ] outside the Cerenkov cone, and the dependence of the frequency of the emitted photon on the direction is determined by the normal Doppler effect

$$\omega = \omega_0 / (1 - n\beta_\parallel \cos\theta), \quad (27)$$

where

$$\omega_0 = 2V_g / \hbar = 2\pi v_\parallel / \xi_g. \quad (28)$$

The transition 2-1 is allowed in the region of angles  $\theta < \theta_0$  inside the Cerenkov cone, and the dependence of the frequency on the direction is determined in this case by the anomalous Doppler effect:

$$\omega = \omega_0 / (n\beta_\parallel \cos\theta - 1). \quad (29)$$

Substituting the expressions for the matrix elements (22) and (23) in (24) and integrating with respect to the frequencies with the aid of a  $\delta$  function, we obtain for the number of photons emitted per unit time into a unit solid angle an expression that is valid both at  $\theta < \theta_0$  and  $\theta > \theta_0$ :

$$\frac{dN}{d\Omega} = \frac{\alpha n}{4\pi} \beta_\perp^2 \omega_0 \frac{(1 - \beta_\parallel n \cos\theta)^2 - (1 - \beta_\parallel^2 n^2) \cos^2\varphi \sin^2\theta}{(1 - \beta_\parallel n \cos\theta)^4}, \quad (30)$$

where  $\beta_\perp = v_\perp / c$ ,  $v_\perp = \hbar\mathbf{g}/2m = \pi\hbar/md$  is the electron velocity corresponding to the transverse momentum  $\hbar\mathbf{g}/2$ , and  $\alpha = e^2/\hbar c$ .

We note that in this form Eq. (30) is valid also in the relativistic region, if  $m$  is taken to mean the total mass (and not the rest mass) of the electron, since the relativistic matrix elements for the emission of a photon by a free electron, expressed in terms of the electron velocity, coincide with the nonrelativistic ones if the recoil momentum is neglected, and are proportional to the velocity. On the other hand, the relativistic effects in dynamic theory of diffraction are also taken into account by corrections for the electron mass.<sup>8</sup>

In the derivation of (30) we took into account the fact that when (27) and (29) are satisfied we have

$$|H_\lambda^{21,12}|^2 = \frac{e^2}{n^2} \frac{\pi\hbar}{\omega} v_\perp^2 \cos^2\varphi \frac{(\cos\theta - \beta_\parallel n)^2}{(1 - \beta_\parallel n \cos\theta)^2} \quad (31)$$

and

$$|H_z^{21,12}|^2 = \frac{e^2 \pi \hbar}{n^2 \omega} v_{\perp}^2 \sin^2 \varphi. \quad (32)$$

At constant  $n$ , difficulties are raised by the infinitely large Doppler frequency and radiation intensity at  $\theta \approx \theta_0$ , but these difficulties are eliminated if account is taken of the dispersion of the medium, i.e., the  $n(\omega)$  dependence.

In this case the complex Doppler effect arises.<sup>1,10,11</sup> Equation (30), however, retains the same form.

The obtained expression (30) for the intensity of the Pendellosung radiation agrees with the result of Frank<sup>1</sup> for the intensity of the emission of a classical oscillator oriented perpendicular to its velocity  $v_{\parallel}$  in a refracting medium.

Thus, the classical analog of a diffracting electron is a classical charged particle moving along the crystallographic planes with velocity  $v_{\parallel}$  and oscillating harmonically in the direction of the vector  $g$  at a frequency  $\omega_0$  and amplitude  $x_m$ :

$$x_m = \frac{v_{\perp}}{\omega_0} = \frac{\xi_g}{2\pi} \operatorname{tg} \theta_B. \quad (33)$$

The condition  $|\Delta_b| \ll U_g$  of the smallness of the deviation parameter in the form (13) acquires in this case the simple physical meaning that the amplitude of the oscillations of the diffracting electron be small compared with the wavelength of the emitted light. Thus, (13) is in essence the condition that the radiation be of the dipole type.

We note that (30) leads to a substantial directivity of the radiation even at relatively low electron velocities, for example, at  $n\beta \approx 2/3$  (this corresponds to  $n \approx 1.2$  at an electron energy 100 keV) the ratio of the number of photons emitted forward and backwards into a unit solid angle per unit time is  $\sim 25$ .

Integrating (30) over the angles at  $n\beta_{\parallel} < 1$  in the case of constant  $n$  we obtain for the total number of photons emitted per unit time

$$N = \frac{2}{3} \alpha n \beta_{\perp}^2 \frac{\omega_0}{1 - \beta_{\parallel}^2 n^2}. \quad (34)$$

In the optical region, for example at  $\lambda_0 = 2\pi c/n\omega_0 = \xi_g/n\beta_{\parallel} \approx 3000 \text{ \AA}$  (which corresponds to  $\xi_g \approx 2000 \text{ \AA}$  at  $n\beta_{\parallel} \approx 2/3$ ) at  $n = 1.2$  and  $d = 1 \text{ \AA}$  an estimate in accordance with (34) yields  $N = 5.7 \times 10^9$  photons/sec, so that when an electron current of  $1 \mu\text{A}$  ( $\sim 0.6 \times 10^{13}$  electrons/sec) passes through a crystal of thickness  $D = 5 \xi_g = 10000 \text{ \AA}$  there will be emitted  $\sim 2.1 \times 10^8$  photons/sec in the wavelength band from 1000 to 5000  $\text{\AA}$ . In the soft x-ray region, for example at  $\xi_g = 300 \text{ \AA}$  and at an electron kinetic energy 1 MeV ( $\beta_{\parallel} = 0.94$ ), taking into account the fact that  $n \approx 1$  and  $\lambda_0 = 320 \text{ \AA}$  we get from (34) a value  $N \approx 4.2 \times 10^{10}$  photons/sec in the wavelength band from

20 to 600  $\text{\AA}$ , and by virtue of (30) the number of photons with minimal wavelengths emitted forward is  $\sim 10^3$  times larger than backwards. Accordingly, when the same current passes through a crystal of thickness  $D = 5 \xi_g$ , the number of photons emitted predominantly in the short-wave region is  $\sim 1.3 \times 10^8$ .

We note that since  $\beta_{\perp}^2$  in (34) contains the relativistic factor  $(1 - \beta^2)$ , it follows that at  $n \approx 1$  and at high energies ( $\beta_{\parallel} \approx \beta$ ) the value of  $N$  does not depend on the electron energy, while the energy losses increase like  $(1 - \beta_{\parallel}^2)^{-1}$  because of the shift of the photon frequency into the harder region. In the case of channeling, the number of radiated photons increases with energy like  $(1 - \beta_{\parallel}^2)^{-1/2}$ .<sup>5</sup> The cause of the difference is that, in contrast to channeling in diffraction, when the energy increases the amplitude  $x_m$  [Eq. (33)] of the transverse oscillations of the electron decreases like  $(1 - \beta^2)^{1/2}$ , and what is constant is the transverse momentum  $\hbar g$  transferred to the lattice, while the frequency  $\omega_0$  is likewise independent of the particle energy. On the other hand, the equations given above are valid only up to electron energies at which  $\theta_B \geq \theta_c$ , where  $\theta_c$  is the critical channeling angle. For higher energies, when  $\theta_B < \theta_c$ , the angular width of the diffraction begins to exceed the Bragg angle. Multibeam effects then become substantial.<sup>8</sup>

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<sup>1</sup>In Eqs. (20) and (21) of Ref. 3 there were left out also the factors  $\pm 1/(1 - \beta n \cos \theta)$ , which stem from the arguments of the  $\delta$  functions, and the normalization factor 2; see Eq. (30) of the present paper.

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