Properties of electromagnetic radiation emitted by an electron diffracted in a single crystal

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The radiation emitted when an electron is diffracted in a crystal that constitutes a homogeneous medium with a refractive index n for the photons is considered. It is shown that due to the "pendulum" effect (Pendellosung), radiation is produced whose frequency and polarization are determined by the frequency and direction, respectively, of the electron's oscillations in the crystal as it is diffracted (pendulum radiation). For $n\beta > 1$ the directional dependence of the pendulum radiation frequency is determined by either the normal or an anomalous Doppler effect. Two Vavilov-Cerenkov radiation cones arise from two electron waves in the crystal belonging to different branches of the dispersion surface. Formulas are obtained for the intensities of the two kinds of radiation.

INTRODUCTION

It follows from the dynamic theory of diffraction (see ^[1], for example) that the motion of a diffracted electron in a crystal can be described qualitatively as follows. The motion of an electron whose path through a crystal is, on the average, parallel to crystallographic planes (the z axis in Fig. 1) with velocity $v\cos\theta_{\rm B}$ will, as the result of beats between waves having different wave vectors that belong to different branches of the dispersion surface [see Eqs. (1) and (2)], vary in direction with a spatial period ξ_g , i.e., the electron will oscillate in the direction of the reciprocal-lattice vector with the frequency ω_0 = $2\pi \operatorname{vcos} \theta_{\rm B}/\xi_{\rm g}$. This is the "pendulum" effect (Pendellösung). The possibility that the electron will at the same time emit or absorb a photon was considered in ^[2] in connection with a mechanism for modulating an electron beam at optical frequencies.

In the present paper it is shown that the described behavior of a diffracted electron leads to interesting features of its radiation at velocities exceeding the phase velocity of light in the crystal, i.e., for nv $\cos \theta_{\rm B}/c > 1$. First, in the angular region inside a Vavilov-Cerenkov radiation cone an anomalous Doppler effect will occur for radiation associated with the pendulum effect; this will be called pendulum radiation. An anomalous Doppler effect for radiation emitted by an oscillator moving at "supraluminal" velocity was predicted by Frank in 1942.^[3] However, no experimental situation has hitherto been found where the effect could be observed. The possibility actually exists in the case of electron diffraction. Secondly, the two electron waves belonging to different branches of the dispersion surface give rise to two Vavilov-Cerenkov cones (because of the different wave vectors). In the region of overlap interference will take place between the electromagnetic waves, which are emitted with identical frequency but at different angles. Consequently, the Cerenkov radiation will be intensity-modulated in this region. The beat period will be determined by the extinction length ξ_g . It is thus found that beats of Cerenkov radiation form an "image," magnified in the ratio λ/λ_e , of electron-wave beats in the crystal (λ is the photon wavelength and λ_{e} is the de Broglie wavelength of the electron).

POSSIBLE QUANTUM TRANSITIONS OF AN ELECTRON DURING ITS DIFFRACTION

Let us consider a system of crystallographic planes characterized by the reciprocal-lattice vector \mathbf{g} (with $|\mathbf{g}| = 1/d$, where d is the interplanar spacing). Let electrons of energy E impinge upon these planes at exactly the Bragg angle θ_{B} , as shown in Fig. 1. Then the propagation of an electron in the crystal is described by a superposition of Bloch wave functions ^[1]:

$$\psi = \frac{1}{\sqrt{2}} \left[b^{(1)} \left(\mathbf{k}^{(1)}, \mathbf{r} \right) + b^{(2)} \left(\mathbf{k}^{(2)}, \mathbf{r} \right) \right] \exp \left(-\frac{i}{\hbar} Et \right), \tag{1}$$

where

$$b^{(1)}(\mathbf{k}^{(1)}, \mathbf{r}) = i \overline{\gamma} 2 \sin \pi g \mathbf{r} \cdot \exp \left[2\pi i (\mathbf{k}^{(1)} + 1/2g) \mathbf{r} \right],$$
(2)

$$p^{(2)}(\mathbf{k}^{(2)}, \mathbf{r}) = \sqrt{2} \cos \pi \mathbf{g} \mathbf{r} \cdot \exp \left[2\pi i (\mathbf{k}^{(2)} + \frac{1}{2}g) \mathbf{r}\right];$$

 $2\pi\hbar k^{(1,2)}$ is the quasimomentum of the electron in the crystal. The indices 1 and 2 pertain to the corresponding branches of the electron's dispersion surface, whose equation satisfying the Bragg condition $|\mathbf{k} + \mathbf{g}| = |\mathbf{k}|$ is ^[1] (see Fig. 2)

$$k^{(1,2)} - K = \mp \frac{U_{\mathfrak{s}}}{2K} = \mp \frac{\cos \theta_{\mathfrak{s}}}{\xi_{\mathfrak{s}}}.$$
 (3)

Here

$$K = (2mE/h^2 + U_0)^{\nu_h} = [2m(E + V_0)/h^2]^{\nu_h} \approx mv/h = 1/\lambda_e, \quad (3a)$$

since we usually have $V_0 \ll E$: V_0 is the average potential in the crystal, $V_g = h^2 U_g/2m$ is the amplitude of the first harmonic of the periodic lattice potential, and $\xi_g = K \cos \theta_B/U_g$ is the extinction length. The negative and positive signs in the right-hand part of (3) pertain to the first and second branches of the dispersion surface, respectively.

The form (1) of the electron's wave function can be understood from the following physical considerations. When a plane wave is incident upon the crystal at the Bragg angle, then because of reflections from the crystallographic planes in the x direction two standing

FIG. 1. Incidence of electrons with momentum hK at Bragg angle $\theta_{\rm B}$ to reflecting planes lying parallel to the (yz) plane. The vectors K, $k^{(\alpha)}$, and $k^{(\alpha)} + g$ lie in the (xz) plane. The maximum intensity of pendulum radiation appears in a plane parallel to the crystallographic planes and is polarized along g, unlike the Cerenkov radiation in the same plane with polarization parallel to the (yz) plane.



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FIG. 2. Form of the dispersion surface in the two-beam approximation. Dashed lines—wave vector K of the incident electron, solid arrows—wave vectors $k^{(\alpha)}$ and $k^{(\alpha)} + g$ of the diffracted electron, curves—two branches of the surface of constant energy E.

waves are formed with $\pi/2$ phase difference [the factors $\sin \pi gr$ and $\cos \pi gr$ in (2)] and propagate in the z direction with the wave vectors $k^{(1)} \cos \theta_B$ and $k^{(2)} \cos \theta_B$ [the exponential factors in (2)]. The difference between $k^{(1)}$ and $k^{(2)}$ results from the fact that the first wave has maxima in the x direction on the crystallographic planes, while the maxima of the second wave are between them.

Denoting the initial state of the electron by a subscript a and the final state, which results from the emission of a photon with energy $\hbar\omega$, by the subscript b, for the matrix element of the $a \rightarrow b$ transition we obtain¹⁾

$$H_{a \to b} = \langle \psi_b | H | \psi_a \rangle$$

= $\frac{1}{2} \left[H_{a \to b}^{1 \to 1} + H_{a \to b}^{1 \to 2} + H_{a \to b}^{2 \to 2} + H_{a \to b}^{2 \to 2} \right], \qquad (4)$

$$H_{a \to b}^{a \to b} = \langle b_b^{(\beta)} (\mathbf{k}_b^{(\beta)}, \mathbf{r}) | H | b_i^{(\alpha)} (\mathbf{k}_a^{(\alpha)}, \mathbf{r}) \rangle$$

$$(\alpha, \beta = 1, 2). \tag{5}$$

where

$$H = \frac{e}{mn} \sqrt{\frac{2\pi\hbar}{\omega}} \exp\left(-2\pi i \varkappa \mathbf{r}\right) \left(\mathbf{u} \cdot i\hbar \nabla\right)$$
(6)

is the interaction operator of the electron and photon in the medium. We assume that the crystal constitutes a homogeneous medium of refractive index n for photons, and that

$$\varkappa = vn/c \quad (\omega = 2\pi v). \tag{7}$$

Thus the $a \rightarrow b$ transition has been divided into four transitions (Fig. 3). As we shall show subsequently, the transitions $1 \rightarrow 1$ and $2 \rightarrow 2$ between identical branches of the dispersion surfaces correspond to Vavilov-Cerenkov radiation, while the transitions $1 \rightarrow 2$ and $2 \rightarrow 1$ between different branches yield pendulum radiation. The ordinary Doppler effect occurs in the $1 \rightarrow 2$ transition, and the anomalous effect occurs in the $2 \rightarrow 1$ transition.

The calculation of the matrix elements (5) yields the result

$$H_{a\to b}^{1\to1} \approx H_{a\to b}^{2\to2} = -\frac{e}{mn} \sqrt{\frac{2\pi\hbar}{\omega}} \cdot 2\pi\hbar \left(\mathbf{k}_{a}^{(1,2)} + \frac{1}{2} \mathbf{g} \right) \mathbf{u}$$

$$\approx -\frac{e}{n} \sqrt{\frac{2\pi\hbar}{\omega}} v \cos \theta_{B} \sin \theta,$$
(8)

where θ is the angle between the z axis and the direction of photon emission. In deriving (8) we neglected the difference between $\mathbf{k}^{(1)}$ and $\mathbf{k}^{(2)}$, assuming

$$\left|\mathbf{k}_{a}^{(1,2)}+\frac{1}{2}\mathbf{g}\right|=k_{az}^{(1,2)}\approx\frac{mv\cos\theta_{B}}{2\pi\hbar},$$
(8a)



and we also assumed that quasimomentum is conserved:

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$$\mathbf{k}_{b}^{(1)} + \mathbf{x} - \mathbf{k}_{a}^{(1)} = 0$$
 for the $\mathbf{1} \rightarrow \mathbf{1}$ transition (9)

$$\mathbf{k}_{b}^{(2)} + \mathbf{x} - \mathbf{k}_{a}^{(2)} = 0$$
 for the 2 \rightarrow 2 transition (10)

Similarly,

$$H_{a+b} = H_{a+b}$$

$$= -\frac{e}{mn} \sqrt{\frac{2\pi\hbar}{\omega}} \cdot 2\pi\hbar \left(\frac{\mathbf{g}}{2}\mathbf{u}\right) \qquad (11)$$

$$= -\frac{e}{mn} \sqrt{\frac{2\pi\hbar}{\omega}} \frac{\pi\hbar}{d} \cos \ll (\mathbf{u}, \mathbf{g}).$$

Here for the $1 \rightarrow 2$ and $2 \rightarrow 1$ transitions the respective laws of quasimomentum conservation are

$$\mathbf{k}_{b}^{(2)} + \varkappa - \mathbf{k}_{a}^{(1)} = 0,$$
 (12)

$$\mathbf{k}_{b}^{(1)} + \varkappa - \mathbf{k}_{a}^{(2)} = 0.$$
 (13)

PENDULUM RADIATION. THE ANOMALOUS DOPPLER EFFECT

Let us consider the $1 \rightarrow 2$ and $2 \rightarrow 1$ transitions. In this case the conservation of quasimomentum (12) and (13), and of energy given by

$$E_b + \hbar\omega - E_a = 0 \tag{14}$$

together with the dispersion equations (3) and (7), determine the frequency of the emitted photon uniquely as a function of its propagation direction. Neglecting recoil momenta, for the $1 \rightarrow 2$ transition we obtain

$$\omega = \omega_{0} / \left(1 - \frac{nv\cos\theta_{B}}{c}\cos\theta \right), \qquad (15)$$

$$\omega_{0} = \frac{2\pi v \cos \theta_{B}}{\xi_{g}} \equiv \frac{2V_{g}}{\hbar}.$$
 (16)

We thus see that the frequency ω is determined by the pendulum effect and that its dependence on the direction of emission is determined by the Doppler effect.

Similarly, for the $2 \rightarrow 1$ transition we can obtain the result

$$\omega = \dot{\omega}_0 / \left(\frac{nv\cos\theta_B}{c}\cos\theta - 1 \right). \tag{17}$$

Here the frequency is reduced as the angle θ diminishes, i.e., an anomalous Doppler effect occurs. This transition is allowed only for $nv \cos \theta_B/c > 1$ at angles

$$\theta < \arccos\left(c/nv\cos\theta_B\right) \tag{18}$$

inside the Vavilov-Cerenkov radiation cone (the $1 \rightarrow 2$ transition is allowed for angles outside the Cerenkov cone). Equation (17) coincides with Frank's formula ^[3] for the anomalous Doppler shift of the frequency in the case of an oscillator moving faster than light in a medium. We can combine (15) and (17) in the form

$$\frac{nv\cos\theta_{B}}{c}\cos\theta = \frac{\omega\pm\omega_{0}}{\omega}.$$
 (19)

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This coincides with the form of the law of energy and momentum conservation when a photon is emitted by a system that has discrete energy levels and is moving with the velocity $v \cos \theta_B$.^[4] The positive and negative signs correspond to the anomalous and normal Doppler effects, respectively. We note that in a medium where $n(\lambda)$ is not a linear function a complex Doppler effect can occur such as was considered by Frank in ^[3]. Thus with respect to the emission of radiation the diffracted electron behaves as a moving quasiparticle with a discrete energy level or as an oscillator moving in the z direction and oscillating in the x direction.

We shall now calculate the intensity of the pendulum radiation. For the transition probability per unit time we have

$$N = \frac{1}{4} \int_{\mathfrak{s}>\mathfrak{s}_{0}} \frac{2\pi}{\hbar} |H_{a\to b}^{(1\to1)}|^{2} \delta\left(\frac{\hbar\omega_{\mathfrak{s}}}{1-\beta n\cos\theta} - \hbar\omega\right) \frac{n^{3}\omega^{2}}{c^{3}} \frac{d\omega \, d\sigma}{(2\pi)^{3}} + \frac{1}{4} \int_{\mathfrak{s}<\mathfrak{s}_{0}} \frac{2\pi}{\hbar} |H_{a\to b}^{(2+1)}|^{2} \delta\left(\frac{\hbar\omega_{\mathfrak{s}}}{\beta n\cos\theta - 1} - \hbar\omega\right) \frac{n^{3}\omega^{2}}{c^{3}} \frac{d\omega \, d\sigma}{(2\pi)^{3}}.$$
(20)

Here $\beta = v \cos \theta_B/c$, $\theta_0 = \arccos(1/\beta n)$, and $do = d\varphi d \cos \theta$ is the element of solid angle. Inserting into (20) the expression (11) for the matrix elements and integrating over the frequencies, for the number of photons emitted per unit time into unit solid angle we obtain

$$\frac{dN}{do} = \frac{\pi n}{8} \frac{\hbar}{mc^2} \frac{e^2}{mc} \frac{\omega}{d^2} \sin^2 \sphericalangle(\mathbf{x}, \mathbf{g}).$$
(21)

Here the frequency ω is determined from either (15) or (17), depending on the range of angles θ .

At energies from 50 keV to 5 MeV and depending on the crystal and system of crystallographic planes, the extinction lengths ξ_g lie within wide limits from 200 to 10 000 Å,^[11] i.e., the pendulum radiation frequency can be anywhere from the infrared to the soft x-ray portion of the spectrum. In the optical region, e.g., for λ_0 = $2\pi c/n\omega_0 = \xi_g c/nv \cos \theta_B \approx 2000$ Å, where n = 2 (which corresponds to $\xi_g \approx 2000$ Å for nv \approx c), when an electron current of J = 1 μ A (~10¹² electrons/sec) passes through a crystal of thickness D = 10 000 Å the emission will be ~10⁸ photons-sec-sr.

VAVILOV-CERENKOV EMISSION

Let us consider the $1 \rightarrow 1$ and $2 \rightarrow 2$ transitions. Here energy and quasimomentum conservation lead to the emission condition

$$\cos \theta^{(1,2)} = \frac{c}{n(v^{\pm 1}/_2 \Delta v) \cos \theta_B},$$
 (22)

where $\Delta v = 2\pi\hbar \cos\theta_B/m\xi_g$ is the velocity difference corresponding to the difference between the electron wave vectors belonging to the different branches of the dispersion surface: $k^{(1)} - k^{(2)} = \cos\theta_B/\xi_g$.

Equation (22) coincides with the conditions for the emission of Cerenkov radiation by particles moving in a medium at velocities $(v \neq \Delta v/2)\cos \theta_B$. Thus for $n(v + \Delta v/c)\cos \theta_B/c > 1$ two cones of Cerenkov radiation will be emitted by the diffracted electron, i.e., each frequency will be emitted in two directions. Consequently, in the region of overlap, spatial beats will arise between waves of identical frequency but different propagation directions. Indeed, the amplitude of a transition accompanied by photon emission will be

$$a(t) = -\frac{i}{\hbar} \left\{ \frac{1}{2} \int_{0}^{t} H_{a \to b}^{(i \to i)} \exp\left[-i(\omega_{ab}^{(i)} - \omega)t\right] dt \right\}$$

 $+\frac{1}{2}\int_{0}^{t}H_{a+b}^{(2+2)}\exp\left[-i(\omega_{ab}^{(2)}-\omega)t\right]dt\bigg\},$ (23)

where

$$\omega_{ab}^{(1,2)} = \frac{E_a(k_a^{(1,2)}) - E_b(k_b^{(1,2)})}{\hbar} = \frac{\omega n}{c} (v \mp \Delta v/2) \cos \theta_B \cos \theta.$$
(24)

Integrating (23) and assuming $\Delta v \ll v$ and $H_{a \rightarrow b}^{1 \rightarrow 1} \approx H_{a \rightarrow b}^{2 \rightarrow 2}$, we obtain for $2\pi\omega \ll t \ll 2\pi\Omega$:

$$a(t) = -\frac{1}{\hbar} H_{a \to b}^{i \to i} \cos \Omega t \cdot \left[\exp\left\{ -i\left(\frac{\omega n v \cos \theta_B}{c} \cos \theta - \omega\right) t \right\} - 1 \right] \\ \times \left[\frac{\omega n v \cos \theta_B}{c} \cos \theta - \omega \right]^{-i}, \qquad (25)$$

where

$$=\frac{\omega\Delta v}{2v}=\omega\frac{\lambda_e\cos\theta_B}{2\xi_s}\ll\omega.$$
 (26)

The periodic dependence on time in (25) resulted from interference between the $1 \rightarrow 1$ and $2 \rightarrow 2$ amplitudes.

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For the number of photons emitted by an electron per unit frequency interval and unit time into unit solid angle, we easily $obtain^{2}$

$$\frac{dN}{do\,d\omega} = \frac{2\pi}{\hbar} |H_{a+b}^{i+1}|^2 \cos^2 \Omega t \delta \left(\hbar \omega \left(\beta n \cos \theta - 1\right)\right) \frac{n^3 \omega^2}{c^3 (2\pi)^3}.$$
 (27)

It follows from (27) that the Cerenkov radiation has the direction $\theta = \arccos(1/\beta n)$ corresponding to the electron's average velocity of propagation in the crystal. When the value of $H_{a \rightarrow b}^{1 \rightarrow 1}$ is substituted in (27), followed by angular integration with the aid of the δ function, for the number of photons in unit frequency interval per unit time we obtain

$$\frac{dN}{d\omega} = \frac{e^2}{\hbar c} \frac{v \cos \theta_B}{c} \cos^2 \Omega t \left(1 - \frac{1}{\beta^2 n^2}\right)$$
(28)

or for the energy lost by an electron in unit frequency interval per unit path distance:

$$\frac{dW}{dl\,d\omega} = \frac{e^2}{c^2}\cos^2\frac{2\pi l}{\Lambda}\left(1-\frac{1}{\beta^2 n^2}\right)\omega,\tag{29}$$

where

$$\Lambda = 2\lambda \xi_g / \lambda_e \cos \theta_B \cos \theta \tag{30}$$

is the spatial period of beats between two electromagnetic waves, of frequency ω , emitted at different angles.

With the exception of the oscillating factor, (29) coincides with the Tamm-Frank equation in ^[5]. On the basis of Eq. (30) with $\lambda \approx 2000$ Å for n = 2, $\lambda_e = 0.02$ Å (E = 300 keV, $\beta \approx 0.8$, cos $\theta \approx 0.6$), and $\xi_g \approx 600$ Å, we obtain the beat period $\Lambda \approx 1$ mm.

We note that the pendulum radiation intensity is maximal in a plane parallel to the (yz) plane (Fig. 1); in this case its polarization is perpendicular to that of the Cerenkov radiation. Thus, despite the fact that the pendulum radiation intensity is only $\sim 10^{-4}$ of the Cerenkov radiation intensity, the two kinds of radiation can be separated in accordance with both their directional and polarization differences. Consequently, the anomalous and complex Doppler effects can be observed experimentally.

CONCLUSION

Our principal results can be formulated as follows.

1. As the result of the pendulum effect an electron undergoing diffraction in a single crystal emits pendulum

radiation whose frequency is determined by the frequency of the electron's "oscillations." The directional dependence of the frequency is determined by either a normal or an anomalous Doppler effect. In a real dispersive medium [i.e., for $n = n(\omega)$] a complex Doppler effect is also possible.^[3] For a crystal of 10 000 Å thickness and electron current ~1 μ A the pendulum radiation intensity in the optical region is ~10⁸ photons/sec-sr.

2. Because two electron waves with different wave vectors are present in the crystal during the diffraction process, for $n\beta > 1$ two cones of Vavilov-Cerenkov radiation are produced. The electromagnetic waves, having an identical frequency but different propagation directions in the region of overlap, interfere; consequently, the Cerenkov radiation is intensity-modulated in this region. For each frequency the spatial period of the beats is determined by the extinction length and the ratio between the photon and electron wavelengths.

3. A real possibility exists that anomalous and complex Doppler effects can be observed experimentally under the given conditions.

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²⁾In the case of $t \ge 2\pi/\Omega$ the single δ function in (27) will be replaced by the sum of two δ functions corresponding to the two Cerenkov cones.

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¹⁾If $\lambda \ge \xi_g \tan \theta_B$ the emission of a photon does not violate the Bragg condition; therefore the wave function of the electron in the final state will also have the form (1).