Dynamics of the restructuring of above-barrier states and related anomalies in the spectrum radiated by a relativistic electron beam propagating in a crystal

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The behavior of electron wave functions of electrons as their energy increases, so that the interval between neighboring above-barrier bands decreases and the bands touch each other, is analyzed. The changes in the wave functions are determined by the relation between two parameters: the distance $\varkappa d$ from the band edge and the deviation $E - E_c$ from the critical energy. The effects of these changes on the radiation spectrum and possibilities for experimentally observing effects of these changes are discussed.

1. INTRODUCTION

The motion of a fast charged particle along a crystallographic plane in a crystal is governed primarily by the average continuous potential $V(x)$, i.e., by the lattice potential averaged over the coordinates in the (y, z) plane, along which the motion occurs.[1,2] The components of the momentum of a particle along the plane are conserved in such a field. The motion in the transverse direction is governed by the Schrödinger equation

$$\left\{\frac{\hat{p}_x^2}{2E} + V(x)\right\}\psi(x) = \varepsilon\psi(x), \tag{1}$$

where the energy E of the particle plays the role of a mass. The potential $V(x)$ is a periodic function of the coordinate x. The spectrum of allowed values of the transverse energy ε is known to have a band structure in such a field. The structure of the above-barrier states is of particular interest, because as the total energy E of the particle changes, a substantial—even qualitative—restructuring of these states can take place (Fig. 1).

This circumstance was pointed out in Refs. 3 and 4, where it was shown in particular that bands can touch each other as E increases. The effect can be described by saying that at a certain $E = E_c$ the gap between two low-lying bands (specifically, the second and third) of above-carrier states in the spectrum of transverse values of ε disappears. The coefficient of the reflection by an individual unit of this periodic potential vanishes. This effect could be treated[5] as a one-dimensional analog of the Ramsauer effect (Ref. 6, for example). The physical reason for the appearance of a point at which the bands touch was described in Ref. 7, where it was shown that the sign of the parity of the wave functions changes discontinuously at this point. In their study of the effect, however, the author considered only the restructuring of the edges of the touching bands. Analysis shows that for $E \sim E_c$ important changes occur in the interiors of the bands as well as at their edges. This phenomenon is the subject of the present paper. We analyze in detail (Sec. 2) the behavior of wave functions with an arbitrary quasimomentum $\varkappa$ for electron energies both near and away from the band-touching point $E = E_c$. We are particularly interested in the regions adjacent to the edges of the bands, with $0 \leqslant x \ll \pi/d$. We show (Sec. 4) that this restructuring of wave functions leads to anomalies in the photon emission spectrum when an electron undergoes a transition between these bands. We also show that at $E \sim E_c$ there are substantial structural changes in states with quasimomenta $\varkappa$ up to $\varkappa \sim 0.2\pi/d$.

We also examine the possibility (Sec. 3) that other bands can touch as the electron energy increases. We show that for the actual potential of the crystal planes (in contrast with the Kronig-Penney potential) a series of band touch at their edges with $\varkappa = 0$ as E increases in the above-barrier region. For the Kronig-Penney potential the picture is considerably more complicated. All of the specific calculations are carried out for the (110) plane of a silicon crystal at a temperature $T = 293$ K. In the calculations we use a Molière potential[8] averaged over the thermal displacements of the atoms (the Debye temperature is $T_D = 495$ K; Ref. 9). We are using a system of units with $\hbar = c = 1$.

2. DYNAMICS OF THE RESTRUCTURING OF THE WAVE FUNCTIONS

The wave functions $\psi(x)$, which describes the transverse motion of an electron, can always be written in the form

$$\psi(x) = c_s\psi_s(x) + c_a\psi_a(x), \tag{2}$$

where $\psi_s(x)$ and $\psi_a(x)$ are respectively even and odd functions. If we place the origin of coordinates at the center of a unit of the periodic potential, which is symmetric with respect to this center,

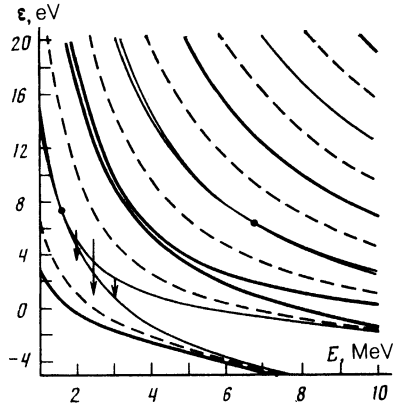

FIG. 1. Band structure of the electron spectrum at low energies. Solid lines—Edges of bands ($\varkappa = 0$ and $\varkappa = d/\pi$); dashed lines—middle of bands ($\varkappa = 0.5d/\pi$); circles—band-touching points; arrows—transitions at quasimomenta $\varkappa = 0.1\,d/\pi$, $\varkappa = 0.5\,d/\pi$, and $\varkappa = 0$.

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$$V(-x)=V(x), \tag{3}$$

the functions $\psi_s(x)$ and $\psi_a(x)$ separately satisfy the differential equation (1) with a given eigenvalue of the energy of the transverse motion, ε. The wave function in the periodic potential must of course satisfy the Bloch theorem,

$$\psi(x+d)=e^{i\varkappa d}\psi(x), \tag{4}$$

where d is the period of the potential (the distance between neighboring crystallographic planes). Applying the Bloch theorem to the outermost points of the unit, $x=+d/2$ and $x=-d/2$ (which are separated by a period), we find

$$\begin{aligned} &c_s\psi_s(d/2)+c_a\psi_a(d/2)=e^{i\varkappa d}(c_s\psi_s(d/2)-c_a\psi_a(d/2)),\\ &c_s\psi_s'(d/2)+c_a\psi_a'(d/2)=e^{i\varkappa d}(-c_s\psi_s'(d/2)+c_a\psi_a'(d/2)). \end{aligned} \tag{5}$$

These relations are essentially boundary conditions which make it possible to reduce the problem to an analysis of the interval $-d/2\leqslant x\leqslant d/2$ alone in constructing the periodic solution of Schrödinger equation (1) in which we are interested.

The requirement that Eqs. (5) be compatible determines the spectrum of allowed eigenvalues of the energy ε, and the equations themselves (which are in this case equivalent) establish the relationship between the coefficient c_s and c_a.

At the edge of the band with $\varkappa=0$, Eqs. (5) for the coefficients c_s and c_a splits up into the independent equations

$$c_a\psi_a(d/2)=0, \quad c_s\psi_s'(d/2)=0 \tag{6}$$

and allows solutions of two types: even solutions, $c_s=1$, $c_a=0$, at energies $\varepsilon=\varepsilon_s$ for which the condition

$$\psi_s'(d/2)|_{\varepsilon=\varepsilon_s}=0. \tag{7}$$

holds; and odd solutions, $c_s=0$, $c_a=i$, at energies $\varepsilon=\varepsilon_a$ for which the condition

$$\psi_a(d/2)|_{\varepsilon=\varepsilon_a}=0 \tag{8}$$

holds.

At a certain value $E=E_c$ of the electron energy we can have a situation in which conditions (7) and (8) are satisfied simultaneously, i.e., at the same value $\varepsilon=\varepsilon_R>0$. The physical meaning of this degeneracy $\varepsilon_s=\varepsilon_a=\varepsilon_R$ is that allowed energy bands touch each other. In this case Eqs. (5) impose no restrictions on the coefficients c_s and c_a.

With $0<\varkappa d\ll\pi$ and $\varepsilon_s\neq\varepsilon_a$ system (5) takes the form (to within terms which are quadratic in the small parameter $\varkappa d/\pi$)

$$\begin{aligned} &c_a\psi_a(d/2)=ic_s\psi_s(d/2)\varkappa d/2,\\ &c_s\psi_s'(d/2)=-ic_a\psi_a'(d/2)\varkappa d/2. \end{aligned} \tag{9}$$

In this case, both of the coefficients c_s and c_a are nonvanishing, and the wave function (2) does not have a definite parity. The admixture of the state of opposite parity is proportional to the small parameter $\varkappa d/\pi$, however, and for $\varepsilon\approx\varepsilon_s$ the wave function is approximately of even parity:

$$c_s\approx 1,\ c_a\approx -i\{\psi_s(d/2)/\psi_a(d/2)\}_{\varepsilon=\varepsilon_s}\varkappa d/2. \tag{10}$$

For $\varepsilon\approx\varepsilon_a$ the wave function is approximately of odd parity:

$$c_a\approx i,\ c_s\approx\{\psi_a'(d/2)/\psi_s'(d/2)\}_{\varepsilon=\varepsilon_a}\varkappa d/2. \tag{11}$$

It can be seen from (10) and (11) that the admixtures of the "foreign" parity are indeed small if the electron energy E is substantially different from the critical value E_c and if the values of $\psi_a(d/2)$ on the even branch $\varepsilon\approx\varepsilon_s$ and of $\psi_s'(d/2)$ on the odd branch $\varepsilon\approx\varepsilon_a$ are nonzero. As the energy of the electron changes and approaches the band-touching point, however, the roots ε_s and ε_a move closer together, so the denominators in (10) and (11) decrease, and the relative importance of the state of foreign parity increases sharply. In this case the admixtures are no longer small, and the situation requires further analysis.

Let us analyze the solutions of Eqs. (6) with $E=E_c$. Writing the functions $\psi_a(d/2)$ and $\psi_s'(d/2)$ at energies ε close to ε_R in the form

$$\begin{aligned} &\psi_a(d/2)|_{\varepsilon=\varepsilon_R+\Delta\varepsilon}\approx d\psi_a/d\varepsilon|_{\varepsilon=\varepsilon_R}\Delta\varepsilon,\\ &\psi_s'(d/2)|_{\varepsilon=\varepsilon_R+\Delta\varepsilon}\approx d\psi_s'/d\varepsilon|_{\varepsilon=\varepsilon_R}\Delta\varepsilon, \end{aligned} \tag{12}$$

we can rewrite Eqs. (6) as

$$\begin{aligned} &c_a d\psi_a/d\varepsilon|_{\varepsilon=\varepsilon_R}\Delta\varepsilon=-ic_s\psi_s|_{\varepsilon=\varepsilon_R}\varkappa d/2,\\ &c_s d\psi_s'/d\varepsilon|_{\varepsilon=\varepsilon_R}\Delta\varepsilon=ic_a\psi_a'|_{\varepsilon=\varepsilon_R}\varkappa d/2. \end{aligned} \tag{13}$$

We thus see that there exist two solutions for these equations, which differ in the sign of the quantity $\Delta\varepsilon$,

$$\Delta\varepsilon=\pm\frac{\varkappa d}{2}\left[\frac{\psi_s\psi_a'}{(d\psi_a/d\varepsilon)(d\psi_s'/d\varepsilon)}\right]^{1/2}_{\varepsilon=\varepsilon_R}, \tag{14}$$

and thus in the sign of the imaginary part,

$$c_a=\mp ic_s\left[\frac{\psi_s(d\psi_s'/d\varepsilon)}{\psi_a'(d\psi_a/d\varepsilon)}\right]^{1/2}_{\varepsilon=\varepsilon_R}. \tag{15}$$

The wave functions in the upper zone, $\psi_\uparrow$, and the lower zone, $\psi_\downarrow$, are therefore complex conjugates (to within terms quadratic in $\varkappa d/\pi$),

$$\psi_\uparrow=\psi_\downarrow^*;$$

i.e., the states which they describe are time-reversed copies of each other. The functions $\psi_\uparrow$ and $\psi_\downarrow$ depend only weakly on the quasimomentum[1] $\varkappa$. It is of course meaningless to speak in terms of the parity of such states, since even in the limit $\varkappa\to 0$ we have

$$|c_s|\sim|c_a|.$$

Let us examine the behavior of the solutions of Eqs. (9) as we move away from the band-touching point. We first write the functions $\varepsilon_s(E)$ and $\varepsilon_a(E)$ in the form

$$\begin{aligned} &\varepsilon_s(E)=\varepsilon_R+\alpha(E-E_c),\ \alpha\equiv d\varepsilon_s/dE|_{E_c},\\ &\varepsilon_a(E)=\varepsilon_R+\beta(E-E_c),\ \beta\equiv d\varepsilon_a/dE|_{E_c}. \end{aligned} \tag{16}$$

Analysis shows that for the Molière potential we have

$$\beta<\alpha<0$$

The quantities ψ_a and ψ_s' in (9) depend on both the transverse energy ε and the total energy E, which is playing the role of a mass parameter, so we can write

$$\psi_a(\varepsilon, E)=\psi_a(\varepsilon_R, E_c)+\frac{\partial\psi_a}{\partial\varepsilon}\Big|_{\varepsilon_R, E_c}\Delta\varepsilon+\frac{\partial\psi_a}{\partial E}\Big|_{\varepsilon_R, E_c}(E-E_c). \tag{17}$$

From the definition of the function $\varepsilon_a(E)$ we find

$$\psi_a(\varepsilon_a(E), E)=0$$

$$\frac{\partial\psi_a}{\partial\varepsilon}\Big|_{\varepsilon_a}\frac{d\varepsilon_a}{dE}+\frac{\partial\psi_a}{\partial E}\Big|_{\varepsilon_a}=0. \tag{18}$$

Expressing $\partial\psi_a/\partial E$ in terms of $\partial\psi_a/\partial\varepsilon$ on the basis of this equation (and expressing $\partial\psi_s'/\partial E$ in terms of $\partial\psi_s'/\partial E/d\varepsilon$ analogously), we find a generalization of Eqs. (13) for $E\neq E_c$:

$$\begin{aligned} c_a\frac{d\psi_a}{d\varepsilon}\Big|_{\varepsilon_R}(\Delta\varepsilon-\beta(E-E_c))&=-ic_s\psi_s|_{\varepsilon_R}\frac{\varkappa d}{2},\\ c_s\frac{d\psi_s'}{d\varepsilon}\Big|_{\varepsilon_R}(\Delta\varepsilon-\alpha(E-E_c))&=ic_a\psi_a'|_{\varepsilon_R}\frac{\varkappa d}{2}. \end{aligned} \tag{19}$$

Hence

$$\Delta\varepsilon=\frac{\alpha+\beta}{2}(E-E_c)\pm\Big[\frac{(\alpha-\beta)^2}{4}(E-E_c)^2+\Big(\frac{\varkappa d}{2}\Big)^2\times\Big\{\frac{\psi_s\psi_a'}{(d\psi_a/d\varepsilon)(d\psi_s'/d\varepsilon)}\Big\}\Big|_{\varepsilon_R}\Big]^{1/2} \tag{20}$$

and

$$c_a=-ic_s\frac{\psi_s}{(d\psi_a/d\varepsilon)}\Big|_{\varepsilon_R}\frac{\varkappa d}{2(\Delta\varepsilon-\beta(E-E_c))}. \tag{21}$$

Near the critical point,

$$\Big|\frac{E-E_c}{E_c}\Big|\ll\frac{\varkappa d}{\pi} \tag{22}$$

relations (20) and (21) reduce to (14) and (15). Far from the point E_c,

$$\Big|\frac{E-E_c}{E_c}\Big|\gg\frac{\varkappa d}{\pi}, \tag{23}$$

in contrast, the situation changes. For example, on the lower branch we have, in the leading approximation,

$$(\Delta\varepsilon)_\downarrow=\begin{cases}\beta(E-E_c), & E>E_c\\ \alpha(E-E_c), & E<E_c\end{cases}. \tag{24}$$

We thus see that at $E<E_c$ the ratio c_a/c_s on the lower branch is proportional to $\varkappa d/(\alpha-\beta)(E-E_c)$ and is therefore small. For $E>E_c$, on the other hand, the leading terms cancel out when (24) is substituted into (21), so in order to determine the ratio c_a/c_s we need to incorporate in $(\Delta\varepsilon)_\downarrow$ the next term of the expansion in $\varkappa d$. As a result, the denominator in (21) turns out to be quadratic, and the ratio c_a/c_s to be inversely proportional to this small parameter. As the electron energy E varies from $E<E_c$ to $E>E_c$, the wave function in the lower band thus undergoes a smooth conversion from a nearly even parity to a nearly odd parity. In the upper band, the wave function undergoes a conversion in the opposite direction. As we see, this process occurs in a certain neighborhood ΔE of the critical point E_c, whose magnitude is determined by the proximity to the edge of the band:

$$\Delta E/E_c\sim\varkappa d/\pi. \tag{25}$$

The ratio of the contributions of the even and odd wave functions, c_s/c_a, is thus determined by the ratio of the small parameters $(E-E_c)/E_c$ and $\varkappa d/\pi$, which characterize the distance from the band-touching point in terms of the electron energy E and the quasimomentum $\varkappa$. At $E=E_c$ this ratio vanishes and thereby becomes independent of the quasimomentum [see (15)]. It follows that the wave functions $\psi_\uparrow$ and $\psi_\downarrow$ change only slightly with distance from the edge of the band at $E=E_c$ (see Fig. 4, in Sec. 4 below).

In the limit $\varkappa\to 0$ the restructuring region becomes smaller, $\Delta E\to 0$, and shrinks to the critical point E_c. The relation becomes c_a and c_s depends in this case on the order in which the limits in terms of $\varkappa$ and ΔE are taken. This order is evidently determined by the relation between the divergence and the energy spread of the electron beam.

3. BAND-TOUCHING POINTS

The anomaly in the wave functions near the point at which the second and third bands touch, which we discussed above, is not unique. A direct numerical calculation shows that a similar situation arises at, for example, an electron energy $E=7$ MeV, where the fourth and fifth bands touch (Fig. 1). On the other hand, the opposite edges of the bands, with quasimomentum $\varkappa=\pi/d$, i.e., the third and the fourth, the fifth and the sixth, etc.—do not touch in motion in a Molière potential.

To analyze the possible existence of band-touching points E_c it is convenient to first consider the limiting case $E\to 0$ (as in Ref. 7). Although values $E<m$ lie in a nonphysical region, the limit $E\to 0$ is formally equivalent to the limit $V(x)\to 0$, since the potential appears in Schrödinger equation (1) only in the combination $2EV(x)$. For the case of free motion in a periodic potential the wave functions are obviously

$$y_s=\cos(kx),\quad y_a=\sin(kx) \tag{26}$$

(here and below, we are for simplicity omitting some normalization coefficients of the wave functions, which are of no importance for the question under discussion here). The permissible values of the wave number k are determined by the Bloch theorem. With $\varkappa=0$ we find the boundaries of the bands from (6):

$$k_n=ng,\quad n=0, 1, 2, \ldots\ (g=2\pi/d). \tag{27}$$

It is obvious that the value $n=0$ corresponds exclusively to the even-parity function $y_s=1$, the ground state. The other values k_n are doubly degenerate; i.e., the boundaries of neighboring bands coincide. We find a corresponding situation at $\varkappa d=\pi$, where the coincident boundaries are found from Eq. (5):

$$\tilde{k}_n=(n-1/2)g,\quad n=1, 2, \ldots. \tag{28}$$

By increasing the energy E slightly, we can now deal with the potential $2EV(x)$ by perturbation theory. In first-order perturbation theory the shift of the energy level is of course determined by the diagonal element of the potential, so the lifting of the degeneracy—the splitting of the energies of the even and odd states—can easily be expressed in terms of the Fourier coefficients of the potential $V(x)$:

$$E_s-E_a=2V_{(2n)}, \quad \varkappa=0,$$
$$E_s-E_a=2V_{(2n-1)}, \quad \varkappa=\pi/d, \tag{29}$$
$$V_{(l)}=1/d\int_{-d/2}^{d/2} V(x)\cos(\lg x)\,dx.$$

For a Molière potential averaged over the thermal vibrations, all of the Fourier coefficients are negative:

l	0	1	2	3	4	5	6	7	8	9
$-V_{(l)}$	7.073	4.652	1.601	0.709	0.337	0.165	0.079	0.038	0.017	0.0076

The splitting thus occurs in such a way that in all cases the lower states are even, and the upper states odd. The boundaries of all of the bands except the lowest differ in parity (Fig. 2).

If, on the other hand, E is quite large, and a given band is pulled below the barrier, its boundaries must be of identical parity. In the above-barrier region there must therefore exist critical points $E=E_c^{(n)}$ at which the levels of an n-pair from (27) trade places.[7]

It is important to note two circumstances here. First, the points E_c could in principle lie in the nonphysical region $E_c<m$. Second the levels $\varepsilon_s^{(n)}(E)$ and $\varepsilon_a^{(n)}(E)$ can evidently cross where the effect of the potential has become important but where these energies are still positive:

$$0\leqslant\varepsilon_{s,a}^{(n)}(E)\leqslant\overline{V} \tag{30}$$

($\overline{V}$ characterizes the depth of the potential well).

Using (27), we find from (30) an estimate of the nth critical energy $E_c^{(n)}$:

$$n^2g^2/4\overline{V}\leqslant E_c^{(n)}\leqslant n^2g^2/2\overline{V}. \tag{31}$$

Substituting half the maximum depth V_0 into this estimate in the role of $\overline{V}$, we find for the first critical point, discussed above,

$$1\text{ MeV}\leqslant E_c^{(1)}\leqslant 2\text{ MeV}. \tag{32}$$

This estimate corresponds to the actual value, $E_c^{(1)}\approx 1.73$ MeV. It can be seen from inequalities (31) that the condition $g^2/2\overline{V}>m$ must hold if this picture is to prevail. In the opposite case, one or several of the critical points will lie in a nonphysical region during motion in the field of planes for which the relation $g^2/2\overline{V}<m$ holds.

Note that the qualitative structure of the spectrum in the above-barrier region (in contrast with that below the barrier) depends strongly on the properties of the potenial, as we will now demonstrate. If we are to have the situation shown in Fig. 2, all of the Fourier coefficients must be negative. It is easy to see that a screened Coulomb potential has these properties (and therefore a superposition of such potentials—the Molière potential—also has these properties). The Kronig-Penney potential, on the other hand, and even a smeared square well—a Fermi potential (in nuclear phyiscs, a Woods-Saxon potential)—have Fourier coefficients of alternating sign. For example, the Kronig-Penney potential which was analyzed in Ref. 4 (in which the ratio of the width of the well to the distance between planes was $2a/d=1/3$) leads to

$$\Delta E^{(n)}|_{E\to 0}=-\frac{V_0}{n\pi}\sin\frac{2\pi n}{3}, \quad \varkappa=0, \quad n\geqslant 1, \tag{33}$$

$$\Delta E^{(n)}|_{E\to 0}=-\frac{V_0}{(n-1/2)\pi}\sin\frac{(2n-1)\pi}{3}, \quad \varkappa=\frac{\pi}{d}. \tag{34}$$

The order of the levels in this potential in the limit $E\to 0$ differs from that which characterizes a realistic potential. As a result, the entire picture is vastly more complicated (Fig. 3).

4. ANOMALIES IN THE RADIATION SPECTRUM NEAR A BAND-TOUCHING POINT

The behavior of the electron wave functions as a function of the electron energy near the point E_c which we described above should be manifested in the spectrum radiated by electrons as they undergo transitions between these touching bands. In the dipole approximation this process is determined by the momentum operator $\hat{p}_x$, so transitions are possible only between states which have the same quasimo-

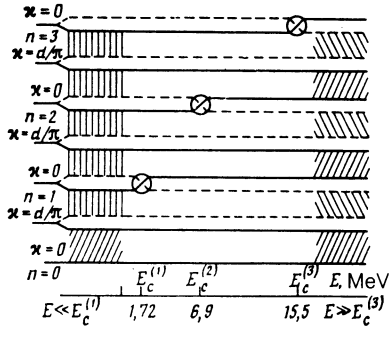

FIG. 2. Changes in the band structure in a real potential. The band edges corresponding to even-parity states are shown by solid lines, and those corresponding to odd-parity states are shown by dashed lines.

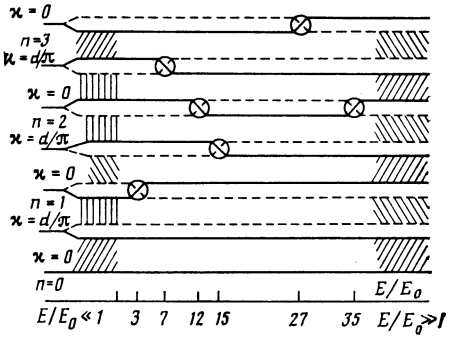

FIG. 3. The same as in Fig. 2, for the Kronig-Penney potential.[3] For the state $\varkappa=d/\pi$, $n=2$, the degeneracy for $E\to 0$ is lifted only in second order in $2EF(x)$.

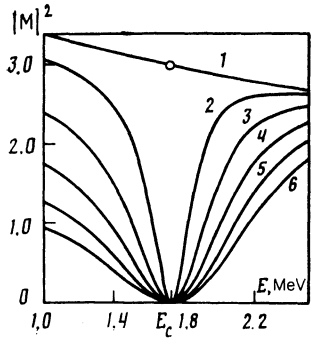

FIG. 4. Square of the matrix element ($|M|^2$) for the $3 \rightarrow 2$ dipole transition versus the energy of the electron. The meaning of the curves is explained in the text.

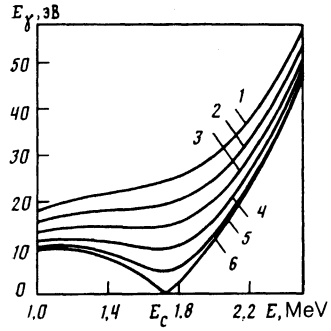

FIG. 6. Energy of the photons emitted in $3 \rightarrow 2$ transitions. The notation is the same as in Fig. 4.

mentum $\varkappa$ but opposite parities. Far from the point $E = E_c$ [see (23)] the states $\psi_\uparrow$ and $\psi_\downarrow$ which we were discussing above have specifically these properties. Near the critical point, however, where condition (22) holds, the wave functions are approximately time-reversed copies of each other, $\psi_\uparrow \approx \hat{T}\psi_\downarrow$, so the matrix element for the process vanishes:

$$M \equiv (\psi_\uparrow | \hat{p}_x | \psi_\downarrow),$$

$$M = M^+ = \hat{T}(\psi_\downarrow | \hat{p}_x | \psi_\uparrow) = (\hat{T}\psi_\downarrow | \hat{T}^{-1} p_x \hat{T} | \hat{T}\psi_\downarrow)$$

$$= -(\psi_\uparrow | \hat{p}_x | \psi_\downarrow) = -M = 0. \qquad (35)$$

Figure 4 shows the square of this matrix element for a transition from the third band to the second for energies E near the point (E_c) at which the second and third bands touch. Curves 1–6 correspond to quasimomenta $\varkappa d/\pi = 0$, 0.01, 0.02, 0.03, 0.04, and 0.05. We see that $|M|^2$ does indeed have a sharp dip near $E \approx E_c$ at all of these quasimomenta $\varkappa$. This dip is a consequence of the behavior of the wave functions which we described above.

Figure 5 represents the emission of photons with an energy E_γ in the forward direction from $l = 1\ \mu$m of the thickness of the crystal during the transition of interest here. This emission can be calculated from the well-known expressions[2]

$$\frac{dN}{d\Omega} = n_i \frac{|M|^2}{m^2} E_\gamma \frac{e^2}{\pi} l, \qquad (36)$$

where $d\Omega$ is an element of solid angle, $n_i(\theta)$ is the population coefficient of the initial state, and $\theta = (g + \varkappa)/p_0$ is the angle of incidence of the electrons. [The curves correspond to various divergences in the beam: curves 1 and 2 to $\Delta(\varkappa d/\pi) = 0.01$, and 3 and 4 to $\Delta(\varkappa d/\pi) = 0.1$. Curves 1 and 3 correspond to a Gaussian distribution, and 2 and 4 to the equivalent square distribution.]

To within a Doppler factor, the energy of the emitted photons, E_γ, is determined by the difference between the transverse energies $\varepsilon_\uparrow$ and $\varepsilon_\downarrow$:

$$E_\gamma \approx 2\left(\frac{E}{m}\right)^2 (\varepsilon_\uparrow - \varepsilon_\downarrow). \qquad (37)$$

Near the critical point, this energy depends strongly on the proximity to the band edge (see Fig. 6, where curves 1–6 correspond to those in Fig. 4).

These results show that as the electron energy is increased from $E = 1$ MeV the peak in the low-energy part of the emission spectrum shifts to the left, shrinks, and essentially disappears by $E = E_c = 1.73$ MeV. As E increases further, the peak reappears, grows rapidly, and shifts to the right. This effect could be observed experimentally; it would be noticeable even at beam divergences $\Delta\theta \lesssim 1$ mrad.

Another interesting aspect is that behavior of the matrix elements M_{31} and M_{21} (corresponding to transitions from the third and second bands to the first; Fig. 7) which is caused by the effect which we pointed out above: that the functions $\psi_\uparrow$ and $\psi_\downarrow$ are independent of the quasimomentum $\varkappa$ at $E = E_c$. The energies E_γ of the photons emitted in the $3 \rightarrow 1$ and $2 \rightarrow 1$ transitions are fairly close together (at $E \sim E_c$), so these transitions would be rather difficult to separate experimentally. However, even in the total yield of

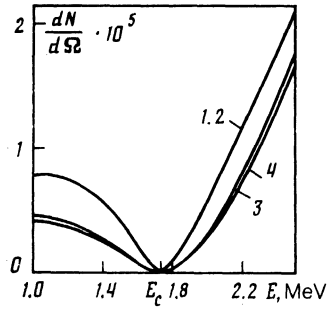

FIG. 5. Emission of photons in $3 \rightarrow 2$ transitions. The meaning of the curves is explained in the text.

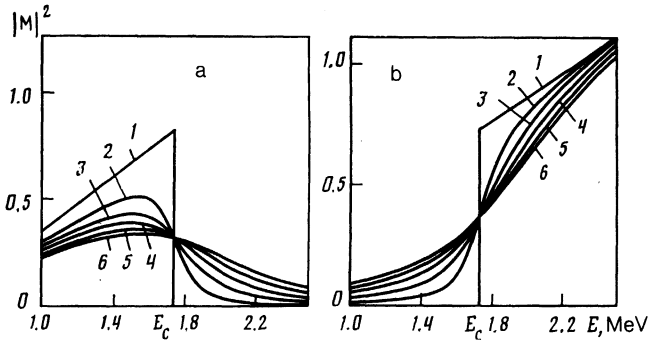

FIG. 7. The same as in Fig. 4, for (a) the $3 \rightarrow 1$ and (b) the $2 \rightarrow 1$ transitions.

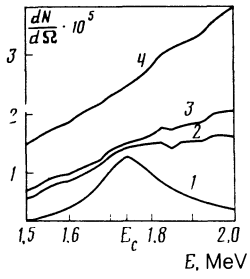

FIG. 8. Total emission of photons in the $3 \rightarrow 1$ and $2 \rightarrow 1$ transitions. The meaning of the curves is explained in the text.

photons one could observe anomalies near $E = E_c$; such observations would require beams with a small divergence (Fig. 8, where curves 1–4 correspond to divergences $\Delta\theta = 0.02$ mrad, 0.1 mrad, 0.2 mrad, and 1 mrad.)

Babakhanyan *et al.*[4] have predicted a value $E_c = 1.47$ MeV (on the basis of a Kronig-Penney potential). Tulupov[7] has mentioned that a parity-change effect should occur at 1.3 MeV $< E_c <$ 1.4 MeV. The value which we found, $E_c = 1.73$ MeV, agrees with a value recently found experimentally,[5] $E_c = 1.8 \pm 0.05$ MeV.

When an electron beam is incident on a crystal at a zero angle, $\theta = 0$, far from the critical point E_c, the parity at the band edges is definite. In this case the levels of negative parity (the third level for $E < E_c$ and the second for $E > E_c$) are not populated, and a dipole transition from levels of positive parity to the ground state (which has a positive parity) is not allowed. Consequently, there should be no radiation accompanying the $2 \rightarrow 1$ or $3 \rightarrow 1$ transition.

As the critical point is approached, both levels can be filled and also transitions from these levels to the ground level become possible by virtue of the restructuring of states which we discussed above. As a result, radiation ($E_\gamma \approx 400$ eV) can be observed at $E \approx E_c$.

We wish to thank N. N. Nasonov for useful discussions.

[1)]Both the even-parity and odd-parity parts of the wave function have zero expansion terms, in contrast with the situation near resonance, where one of them is proportional to $\varkappa$.

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