[2)]The asterisk labels relative quantities.
[3)] For exciton clusters we can expect a dielectric–metal transition of a type of its own with increasing N.
[4)]The results of[11] for CdS are similar, but are not marked on Fig. 4, inasmuch as in this case the lines for different N overlap and the interval of N to which the binding energies measured in[11] pertain remains unclear.

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Theory of tunneling in crystals at arbitrary ratios of the widths of the forbidden and allowed bands

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A quasiclassical theory of tunneling in crystals in an electric field is developed. The theory takes into account the finite widths of the allowed energy bands. The two-band Slater-Koster model is used to calculate the tunneling probability. It is shown that for crystals with narrow allowed bands, the customarily employed Kane model yields an erroneous estimate of the tunneling probability. Criteria are obtained for the applicability of the Kane model, and a correct tunnel probability is calculated for the case when these criteria do not hold. Tunneling accompanied by photon absorption in a crystal is investigated with account taken of the finite widths of the allowed bands. The dependence of the tunneling probability on the angles between the electric-field intensity vector and the symmetry axes of the crystal is investigated; this dependence does not appear in Kane's model. It is demonstrated that this dependence can yield additional information on the crystal symmetry and crystal structure.

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The investigation of tunneling in crystals in an external electric field is of considerable interest for solid-state electronics. Interband tunneling in a constant electric field determines, for example, the current flow in Esaki diodes.[1,2] Theoretical descriptions of the tunneling process in crystal are contained in many papers for the case of constant[3–6] and time-alternating (laser emission)[7,8] electric field. In most cited papers they used Kane's two-band model,[9] which corresponds to the following dispersion law (the dependence of the energy ε on the quasimomentum $\hbar\mathbf{k}$):

$$\varepsilon(\mathbf{k}) = (\Delta^2 + \Delta\hbar^2k^2/\mu)^{1/2}. \quad (1)$$

Here Δ is the half-width of the forbidden band and μ is the reduced effective mass of the electron and hole. The results of expression (1) are greatly limited in scope. In Kane's model (1), the allowed energy bands are assumed to be infinitely broad in comparison with the forbidden band. This assumption can be justified for tunneling processes only for the special class of narrow-band crystals (e.g., of the InSb type).

The decisive circumstance for the quasiclassical tun-

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neling theory that is natural for our problem is that the electron energies in the valence and conduction bands constitute two branches of a single analytic function $\varepsilon(\mathbf{k})$ of the complex quasimomentum $\hbar\mathbf{k}$, which are connected by a branch point k^*.[3,4] In Kane's model (1) we have $k^* = k_0^* = i(\mu\Delta)^{1/2}/\hbar$, i.e., the position of the branch point is determined only by the width of the forbidden band and does not depend on the widths of the valence and conduction bands. It will be shown below that allowance for the finite widths of the allowed bands alters significantly the positions of the branch points ($k^* \neq k_0^*$), and this predetermines an exponential error in the quasiclassical tunnel-probability estimate based on (1). It can be verified that if the width of the forbidden band turns out to be of the same order as the widths of the allowed bands, then allowance for the finite widths of these bands is of fundamental importance, and the use of the dispersion law (1) leads to erroneous results. In addition, the tunneling probability becomes dependent on the angles between the electric-field intensity vector and the crystal symmetry axes, a dependence that does not exist when the spherically symmetrical dispersion law (1) is used. A band model with an allowed band of finite width, based on the tight-binding method, was considered as applied to tunneling problem in[5,6]. The results of[5] pertain only to crystals with a very broad forbidden band and with weak coupling of the narrow allowed bands (i.e., to a situation that is the inverse of the one described by Kane's model (1)). The results of[6], furthermore, pertain to a special configuration of an inhomogeneous field in a tunnel diode (in the form of a rectangular step), and consequently is likewise not general in character.

The question thus arises of constructing a consistent theory of tunneling in a crystal in an electric field for arbitrary ratios of the widths of the forbidden band and the allowed bands. This makes it possible to establish definite criteria for the applicability of the existing results that pertain to the alternate limiting cases discussed above, and to obtain an estimate of the tunneling probability in the intermediate situation.

The basis for the construction of this theory, in our opinion, can be the two-band model of Slater and Koster,[11] which takes into account both the analytic connection between the dispersion laws in the valence and conduction bands, on the one hand (just as in Kane's model (1)), and the finite widths of the allowed energy bands, on the other. For a primitive cubic lattice, confining ourselves in the tight-binding method to the overlap of the wave functions of the nearest atoms in the unit cell of the crystal, and assuming for simplicity that the widths of the valence and conduction bands are equal, we can obtain according to[11] for $\varepsilon(\mathbf{k})$

$$\varepsilon(\mathbf{k}) = (u^2(\mathbf{k}) + v^2(\mathbf{k}))^{1/2}, \tag{2}$$

$$u(\mathbf{k}) = \Delta + A[3 - \cos k_x a - \cos k_y a - \cos k_z a], \tag{3}$$

$$v(\mathbf{k}) = B[\sin^2 k_x a + \sin^2 k_y a + \sin^2 k_z a]^{1/2}. \tag{4}$$

Here a is the lattice constant. The parameters A and B can be determined by a direct quantum-mechanical calculation. It is preferable, however to determine them by identifying (2) with a dispersion law obtained by using more accurate numerical methods of calculating the band structure, or by comparing the experimentally obtained values of $\varepsilon(\mathbf{k})$ in high-symmetry points of the Brillouin zone with the corresponding values that follow from (2). The parameters A and B are connected with the effective mass μ by the relation

$$\mu^{-1} = (A + B^2\Delta^{-1})a^2\hbar^{-2}. \tag{5}$$

We direct the external electric-field intensity vector $\mathbf{F}$ along one of the edges of the unit cube (say along the x axis). Then the vector $\mathbf{k}$ has a component $\mathbf{k}_\perp = (k_y, k_z)$ perpendicular to the direction of $\mathbf{F}$, this component is conserved in the transition, and an important role in what follows is played by the positions of the branch points k_x^* of expression (2) at $\mathbf{k}_\perp = 0$ (see, e.g.,[3,12]). Let us find

$$\begin{aligned} &k^*_{x(1,3)} = \pm i\varkappa_1 \pm \frac{\pi}{2a}[1 - \operatorname{sign}(\alpha-\beta)] + \frac{2\pi}{a}n, \\ &k^*_{x(2,4)} = \pm i\varkappa_2 + \frac{2\pi}{a}n, \quad n = 0, \pm 1, \pm 2, \ldots \\ &\operatorname{sign}(\alpha-\beta) = 1, \quad \alpha > \beta, \quad \operatorname{sign}(\alpha-\beta) = -1, \quad \alpha < \beta, \\ &\alpha = \frac{A}{\Delta}, \quad \beta = \frac{B}{\Delta}, \quad \varkappa_1 = \operatorname{Arch}|z_1|, \quad \varkappa_2 = \operatorname{Arch} z_2, \\ &z_{1,2} = \frac{\alpha(\alpha+1)}{\alpha^2-\beta^2}\left\{1 \pm \frac{\beta[(1+\alpha)^2 - (\alpha^2-\beta^2)]^{1/2}}{\alpha(\alpha+1)}\right\}. \end{aligned} \tag{6}$$

The position of the branch points of $\varepsilon(\mathbf{k})$ in the complex k_x plane at $\mathbf{k}_\perp = 0$ is shown in Figs. 1a and 1b. As follows from (6) and from Fig. 1, at $\alpha < \beta$ the minimal distance between the points $k^*_{x(1)}$ and $k^*_{x(2)}$ ($k^*_{x(3)}$ and $k^*_{x(4)}$) is π/a. Under the condition

$$\left|\frac{1}{e_0 F}\int_0^{\pi/a} \varepsilon(k_x)\,dk_x\right| > 1 \tag{7}$$

the pairs of points $k^*_{x(1,3)}$ and $k^*_{x(2,4)}$ can be considered independently. If at the same time

$$\left|\frac{1}{e_0 F}\int_0^{i\varkappa_{1,2}} \varepsilon(k_x)\,dk_x\right| > 1, \tag{8}$$

then each of the branch points $\varepsilon(\mathbf{k})$ can be considered independently. The two inequalities above signify in essence the possibility of using the quasiclassical approximation to estimate the transition probability. We use the quasiclassical "imaginary time" method,[12] according to which the probability amplitude R of an interband transition, with account taken of one isolated branch point, is given by

$$R = \exp\left\{\frac{2i}{\hbar}\int_0^{t_2^{(0)}} \varepsilon(k_x(t))\,dt\right\}. \tag{9}$$

The dependence of k_x on t is determined by the equation of motion $\hbar\dot{k}_x = e_0 F$, and the time $t_2^{(0)}$ is determined by the condition $k_x(t_2^{(0)}) = i\varkappa_2$. In (9) it is taken into account that at $\alpha < \beta$ the point $i\varkappa_2$ is closer to the real axis than $i\varkappa_1$, and accordingly the $k_x^* = i\varkappa_2$ is exponentially larger than the contribution $k_x^* = i\varkappa_1$. A contribution of the same absolute value is made to the transition probability by the points $t_2^{(n)}$ determined by the condition

$$k_x(t_2^{(n)}) = i\varkappa_2 + \frac{2\pi}{a}n \quad (n = \pm 1, \pm 2, \ldots).$$

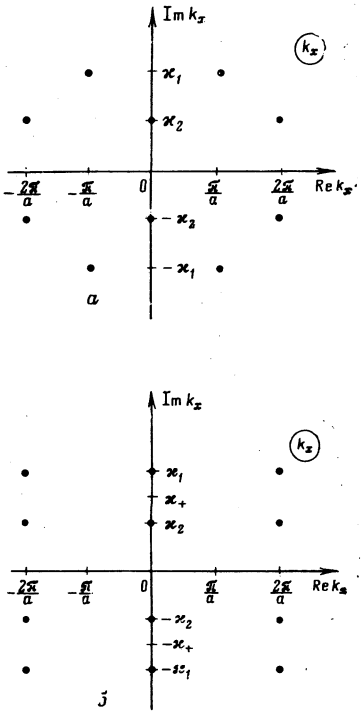

FIG. 1. a) Arrangement of the branch points of the dispersion of $\varepsilon(\mathbf{k})$ in the complex k_x ($k_\perp = 0$) plane at $\alpha < \beta$. b) Arrangement of the branch points of the dispersion of $\varepsilon(\mathbf{k})$ in the complex k_x ($k_\perp = 0$) plane at $\alpha > \beta$.

The contributions of all these points must be summed. The existence of an infinite number of equidistant branch points of $\varepsilon(\mathbf{k})$ is obviously due to the appearance in the allowed band, following application of a homogeneous electric field, of Wannier-Stark levels.[13] Their appearance is a direct consequence of the use of the Slater–Koster model, in which account is taken of the periodic dependence of the energy on the quasimomentum. This circumstance constitutes one more advantage of the discussed model over Kane's model, in which no Wannier–Stark levels appear and they must be introduced as an additional fact that does not follow from the theory (for example, in the calculation of the probability of the interband transition per unit time[3]).

If $\alpha > \beta$, a situation is possible in which

$$\left| \frac{1}{e_0 F} \int_{i\varkappa_2}^{i\varkappa_1} \varepsilon(k_x)\, dk_x \right| < 1, \tag{10}$$

whereas (7) and (8) are satisfied as before. The inequality (10) is the result of the coalescence of the points $i\varkappa_1$ and $i\varkappa_2$ as $\beta \to 0$. (At $\beta \to 0$, $i\varkappa_1 \to i\varkappa_+$, $i\varkappa_2 \to i\varkappa_+$.) Satisfaction of (10) means that the point $k^*_{x(1)} = i\varkappa_1$ cannot be considered independently of the point $k^*_{x(2)} = i\varkappa_2$ (or $k^*_{x(3)} = -i\varkappa_1$ independently of $k^*_{x(4)} = -i\varkappa_2$). Satisfaction of (8) makes it possible to separate the point pair $k^*_{x(1,2)}$ from the pair $k^*_{x(3,4)}$. In this situation formula (9) is wrong and to obtain the tunnel probability we can resort to the equations of motion based on the adiabatic approximation for the transition amplitudes.[3,7,8] The wave function for the electron in the crystal is represented in the presence of an electric field in the form

$$\Psi(\mathbf{r}, t) = \int d\mathbf{k}\, a_c(\mathbf{k}, t)\, \psi_{c\mathbf{k}'}(\mathbf{r}) + \int d\mathbf{k}\, a_v(\mathbf{k}, t)\, \psi_{v\mathbf{k}'}(\mathbf{r}). \tag{11}$$

Here $\psi_{c,v\mathbf{k}}(\mathbf{r})$ are the Bloch functions corresponding to the conduction (C) and valence (V) bands, and $\mathbf{k}' = \mathbf{k} + e_0\mathbf{F}t/\hbar$. The amplitudes $a_C(\mathbf{k}, t)$ and $a_V(\mathbf{k}, t)$ satisfy the system of equations

$$i\hbar \frac{da_c}{dt} - \varepsilon a_c = i a_v \frac{\hbar\varepsilon}{2v} \frac{d}{dt}\left(\frac{u}{\varepsilon}\right), \qquad i\hbar \frac{da_v}{dt} + \varepsilon a_v = -i a_c \frac{\hbar\varepsilon}{2v} \frac{d}{dt}\left(\frac{u}{\varepsilon}\right). \tag{12}$$

Equations (12) should be solved with the initial conditions

$$a_c(-\infty) = 0, \quad |a_v(-\infty)| = 1.$$

The transition probability amplitude R is given by $|R| = |a_C(+\infty)|$. Near an isolated branch point, following Dykhne,[14] we can put in (12) $u = iv$, recognizing that near its zero $\varepsilon(t)$ is a steep function of t, whereas u and v are individually smooth functions of t. The determination of $a_C(+\infty)$ from (12) then reduces to the problem of above-the-barrier reflection, and

$$|a_c(+\infty)| = \left| \exp\left\{ \frac{2i}{\hbar} \int_0^{t_2} \varepsilon(t)\, dt \right\} \right| \qquad (\varepsilon(t_2) = 0),$$

which agrees with the result (9) of the "imaginary time" method. To consider also a situation wherein the inequality (10) is satisfied, we introduce two new functions X_1 and X_2:

$$X_{1,2} = \frac{1}{(2\varepsilon v)^{1/2}} [(\varepsilon \pm u)^{1/2} a_c \mp (\varepsilon \mp u)^{1/2} a_v]. \tag{13}$$

which satisfy the equations

$$\ddot{X}_{1,2} + \frac{1}{\hbar^2} \omega^2_{1,2} X_{1,2} = 0, \tag{14}$$

$$\omega^2_{1,2} = \varepsilon^2(t) \pm i\hbar v \frac{d}{dt}\left(\frac{u}{v}\right) - \hbar^2 \{v, t\}. \tag{15}$$

Here $\{v, t\} = \frac{3}{4}(\dot{v})^2/v^2 - \ddot{v}/2v$ is the so-called Schwartz derivative, and $X_{1,2}$ satisfy the initial conditions ($t \to -\infty$):

$$X_{1,2}(t \to -\infty) = \mp \left(\frac{\varepsilon \mp u}{2\varepsilon v}\right)^{1/2} \exp\left\{ \frac{i}{\hbar} \int_{t'}^{t} \varepsilon(t'')\, dt'' \right\}. \tag{16}$$

Here t' is an arbitrary point on the real time axis. Far from the branch points $\varepsilon(t)$ we can use the quasiclassical approximation for the solution of Eqs. (14) (the Schwartz derivative $\{v, t\}$ can in this case be omitted[15] since it makes no contribution to the principal term of the asymptotic solution of the solution of (14)). The remainder of the calculation program consists of obtaining for (14) an analytic solution which is the same in the entire small region of the complex k_x ($k_x = e_0 F t/\hbar$) that spans the close branch points $k^*_{x(1)}$ and $k^*_{x(2)}$. It is then necessary to join together the obtained solution to the quasiclassical solutions, valid as $t \to \pm\infty$, of the same equations, with account taken of the initial conditions (16).

We consider first the case of sufficiently broad allowed bands, when u and v can be written in the form

($\mathbf{k}_\perp = 0$)

$$u=\Delta+\alpha_0 t^2, \quad v=\beta_0 t, \quad \alpha_0=\frac{A}{2\hbar^2}(e_0Fa)^2, \quad \beta_0=\frac{B}{\hbar}e_0Fa. \tag{17}$$

The transition to the Kane model (1) in Eq. (17) means $Z=0$, i.e., the requirement that the effective mass (see (5)) be formed only by the interband coupling ($B\neq 0$). Formula (17) thus corresponds to a situation more general than (1) (including also the case $A>B$). Near the pair of branch points t_1 and t_2 of the function $\varepsilon(t)=(u^2+v^2)^{1/2}$, which are located in the upper half-plane (case $A>B$), we can put approximately $v=i\beta_0(\Delta/\alpha_0)^{1/2}$ (since as $\beta_0\to 0$ we have $t_1\to t_+$, $t_2\to t_+$, $t_+=i(\Delta/\alpha_0)^{1/2}$ and in this case $v(t)$ is a much smoother function of t than $u(t)$). The equations for $X_{1,2}$ take the form

$$\frac{d^2X_{1,2}}{ds^2}+\left[\left(\delta+\frac{s^2}{b^2}\right)^2-1\pm\frac{2s}{b^2}\right]X_{1,2}=0, \tag{18}$$

$$s=\beta_0(\Delta/\alpha_0)^{1/4}t/\hbar, \quad \delta=(\Delta\alpha_0)^{1/4}/\beta_0, \quad b=\Delta^{3/4}/\alpha_0^{1/4}\delta^{1/4}\hbar. \tag{19}$$

Equations of the type (18) were considered in a number of papers[16,17] in connection with the problem of the quasiclassical spectra of molecules in the approximation where the terms are linear and are not coupled adiabatically. Near the pair of branch points $s_{1,2}=ib(\delta\pm 1)^{1/2}$, Eqs. (18) take the form

$$\frac{d^2X_{1,2}}{ds^2}-\left[\frac{1}{4\nu^2}(s-s_+)^2\pm\frac{1}{2\nu}+1\right]X_{1,2}=0, \tag{20}$$

$$s_+=ib\delta^{1/2}, \quad \nu=\frac{b}{4\delta^{1/2}}. \tag{21}$$

Equations (20) have solutions in the form of the parabolic-cylinder functions $D_{-(\nu+1)}[\pm\nu^{-1/2}(s-s_+)]$ for X_1 and $D_{-\nu}[\pm\nu^{-1/2}(s-s_+)]$ for X_2. It is these solutions that must be joined to the quasiclassical solutions, valid respectively as $t\to\pm\infty$, of the initial equations (14). The details of the calculations in accord with the program described above can be found in[17,18]. Leaving out the details, we find

$$|R|=\frac{(2\pi\nu)^{1/2}}{\Gamma(1+\nu)}\exp(\nu\ln\nu-\nu)\exp\left(-\frac{1}{2}Q\right), \tag{22}$$

$$Q=\frac{4}{e_0F}\operatorname{Im}\int_0^{ix_2}\varepsilon(k_x)\,dk_x.$$

Here $\Gamma(1+\nu)$ is the gamma function. To find the contribution made to the transition probability by a pair of close branch points of $\varepsilon(\mathbf{k})$ in the general case (formula (2)) we can use the associated-equation method.[15,19] The equations associated with (14) can be chosen to be in the form of (20). The parameter ν is then determined from the condition

$$\frac{i}{2\nu}\int_{-2i\nu}^{2i\nu}(\sigma^2+4\nu^2)^{1/2}\,d\sigma=\frac{1}{e_0F}\int_{ix_2}^{ix_1}\varepsilon(k_x)\,dk_x.$$

Formula (22) then remains valid for $|R|$, where we must put

$$\nu=-\frac{1}{\pi e_0F}\int_{ix_2}^{ix_1}\varepsilon(k_x)\,dk_x. \tag{23}$$

At $\nu\gg 1$ Eq. (22) leads to (9). At $\nu\ll 1$ we have

$$|R|=(2\pi\nu)^{1/2}\exp\left\{-\frac{4}{e_0F}\operatorname{Im}\int_0^{ix_2}\varepsilon(k_x)\,dk_x\right\}.$$

The last result can be obtained in the first nonzero order of perturbation theory in terms of the interband coupling (see[5] and formula (22) of Keldysh's paper[3]). To obtain the transition probability per unit time it is necessary to sum the contributions of all the branch points located in the upper complex t half-plane at equal distances from the real axis.

If inequality (8) is satisfied, the transition probability as a function of $\mathbf{k}_\perp^2$ is a sharp maximum at $\mathbf{k}_\perp^2=0$. This is why the foregoing analysis was carried out for $\mathbf{k}_\perp^2=0$. To obtain the probability W of generating an electron in the conduction band per unit time and unit volume of the crystal it is necessary to take into account the dependence of the parameter Q on $\mathbf{k}_\perp^2$. It suffices here to expand Q in a series near $\mathbf{k}_\perp^2=0$:

$$Q=Q_0+\frac{\Delta}{e_0Fa}Q_1q_\perp^2, \quad Q_0=Q(q_\perp^2=0), \quad Q_1=\frac{e_0Fa}{\Delta}\frac{\partial Q}{\partial q_\perp^2}\Big|_{q_\perp=0}, \quad q_\perp^2=\frac{\hbar^2\mathbf{k}_\perp^2}{\Delta\mu},$$

where μ is determined by formula (5). It is then necessary to integrate the transition probability with respect to $\mathbf{k}_\perp$ in the volume of the first Brillouin zone. We neglect the weaker dependence of the transition probability on $\mathbf{k}_\perp^2$ via the parameter ν. We obtain

$$W=\frac{e_0^2F^2\mu a}{2(2\pi)^2\hbar^3Q_1}\frac{2\pi\nu}{[\Gamma(1+\nu)]^2}\exp\{2\nu\ln\nu-2\nu-Q_0\}. \tag{24}$$

(If $\alpha<\beta$ we can use for W also formula (24), in which we must put formally $\nu=\infty$.)

We present the result of the calculation of the principal parameters of (24) in the Slater–Koster model (dispersion law (2)):

$$\nu=\frac{2\Delta}{\pi e_0Fa}(\alpha^2-\beta^2)^{1/2}(z_1-p)^{1/2}(z_2-p)^{1/2}\left[(1-x_0^2)\Pi\left(\frac{x_0^2}{p^2},x_0\right)-E(x_0)\right];$$

$$Q_0=\frac{4\Delta}{e_0Fa}|\alpha^2-\beta^2|^{1/2}(1-p^2)^{-1/2}|z_1-p|^{1/2}|z_2-p|^{1/2}\times \tag{25}$$

$$\times\left[K(\sqrt{1-x_0^2})-E(\sqrt{1-x_0^2})+\frac{p^2(1-x_0^2)}{1-p^2}\Pi\left(\frac{1-x_0^2}{1-p^2},\sqrt{1-x_0^2}\right)\right.$$

$$\left.-\frac{\pi p(1-x_0^2)\theta(x_0^2-p^2)}{2[(1-p^2)(x_0^2-p^2)]^{1/2}}\right], \quad x_0=\frac{1-pz_2}{z_2-p}, \quad p=\frac{\alpha}{\alpha+1} \tag{26}$$

(here $(K(x)$, $E(x)$, and $\Pi(n,x)$ are complete elliptic integrals of the first, second, and third kind, $\theta(x)=1$, $x>0$; $\theta(x)=0$, $x<0$);

$$Q_1=2\Delta\operatorname{Im}\int_1\frac{\alpha_z(\alpha+1)+\beta^2-\alpha^2z}{(\alpha+\beta^2)(1-z^2)^{1/2}\varepsilon(z)}\,dz, \quad z=\cos k_xa, \tag{27}$$

Q_1 is also expressed in terms of the elliptic integrals $K(x)$, $E(x)$ and $\Pi(n,x)$, but since Q_1 is contained only in the pre-exponential factor of (24), the corresponding cumbersome expression is not written out here for the sake of simplicity.

Let $\alpha=0$ (in this case the width of the allowed band in the section $\mathbf{k}_\perp=0$ is $(\Delta^2+B^2)^{1/2}-\Delta$)

$$W\sim\exp\left\{-\frac{4\Delta}{e_0Fa}(1+\beta^2)^{1/2}\left[K\left(\frac{1}{(1+\beta^2)^{1/2}}\right)-E\left(\frac{1}{(1+\beta^2)^{1/2}}\right)\right]\right\}. \quad (28)$$

For a narrow forbidden band and broad allowed bands we have $\beta>1$. Then

$$W\sim\exp\left\{-\xi\left(1-\frac{1}{8\beta^2}+\ldots\right)\right\}, \quad \xi=\frac{\pi\Delta^{3/2}\mu^{1/2}}{e_0\hbar F}. \quad (29)$$

If $\xi/8\beta^2<1$, we obtain for the tunneling probability the well known expression corresponding to the Kane model[1,3]:

$$W\sim e^{-\xi}. \quad (30)$$

For allowed bands of finite width at $\xi/8\beta^2>1$, as follows from (29), Eq. (30) leads to an exponential error, and for a reliable estimate of the transition probability it is necessary to use the general formulas (24)–(28).

In the opposite limiting case of weakly coupled ($\beta\ll\alpha$) narrow allowed bands we get

$$Q_0=\frac{4\Delta}{e_0Fa}\left[(1+\alpha)\operatorname{Arch}\frac{1+\alpha}{\alpha}-((1+\alpha)^2-\alpha^2)^{1/2}\right], \quad (31)$$

$$\nu=\frac{\Delta\beta^2}{e_0Fa}\frac{(1+\alpha)^2-\alpha^2}{\alpha^2(1+\alpha)}. \quad (32)$$

Substitution of (31) and (32) in (24) gives a result close to that obtained in[3,5], in the first nonzero order of perturbation theory in the interband coupling ($\beta\ll\alpha$). Deviations from this limiting result, which set in at $\beta\sim\alpha$, are described by the general formulas (24)–(26).

The dispersion law (2) has no spherical symmetry, and therefore the probability of the interband tunneling in an electric field, with allowance for the finite widths of the allowed bands, exhibits a strong dependence on the angles between the direction of the field-intensity vector and the symmetry axes of the crystal. This dependence disappears, of course, on going to Kane's spherically symmetrical dispersion law (1). Assume for simplicity that the electric field intensity vector lies in the plane of the face of the unit cube and makes an angle φ with one of its edges. We choose the coordinate frame such that the x axis is parallel to the intensity vector. In this frame, the dispersion law (2) is rewritten in the form

$$u(\mathbf{k})=\Delta+A[3-\cos(k_x\cos\varphi-k_y\sin\varphi)a-\cos(k_x\sin\varphi+k_y\cos\varphi)a-\cos k_za],$$
$$v(\mathbf{k})=B[\sin^2(k_x\cos\varphi-k_y\sin\varphi)a+\sin^2(k_x\sin\varphi+k_y\cos\varphi)a+\sin^2 k_za]^{1/2}. \quad (33)$$

We write down two principal terms of the expansion of the quantity Q_0, which determines the tunneling probability, in terms of the parameters $\alpha^{-1}=\Delta/A$ and $\beta^{-1}=\Delta/B$ (the case $\alpha^{-1}<1$, $\beta^{-1}<1$):

$$Q_0=Q_{01}+Q_{02}(\varphi), \quad (34)$$

$$Q_{01}=\frac{2\Delta}{3e_0Fa}\alpha r_0\left[(r_0^2+r_1^2)E\left(\frac{r_1}{r_0}\right)-(r_0^2-r_1^2)K\left(\frac{r_1}{r_0}\right)\right], \quad (35)$$

$$Q_{02}(\varphi)=-\frac{\Delta r_0}{2^3\cdot3^2\cdot5e_0Fa}\left[\eta_1K\left(\frac{r_1}{r_0}\right)+\eta_2E\left(\frac{r_1}{r_0}\right)\right](3+\cos4\varphi), \quad (36)$$

Here

$$\eta_1=2(2r_0^2+r_1^2)\left[\frac{20\beta^2}{\alpha}-2\alpha(r_0^2+r_1^2)+5\right]+9\alpha r_1^2r_0^2,$$

$$\eta_2=4(r_1^2+r_0^2)\left[2\alpha(r_0^2+r_1^2)-\frac{20\beta^2}{\alpha}-5\right]-9\alpha r_1^2r_0^2,$$

$$r_{0,1}=2^{1/2}\frac{(\alpha+\beta^2)^{1/2}}{\alpha}\left\{1\pm\left[1-\frac{\alpha^2}{(\alpha+\beta^2)^2}\right]^{1/2}\right\}^{1/2}.$$

If $Q_{02}(\varphi)>1$, the tunneling probability exhibits a strong (exponential) dependence on the angle φ. We consider directly the deviation from the result obtained with the aid of the dispersion law (1). To this end we put $\alpha=0$ in (34)–(36). We get

$$Q_{01}=\frac{\pi\mu^{1/2}\Delta^{3/2}}{e_0\hbar F},$$
$$Q_{02}(\varphi)=-Q_{01}\left(\frac{\Delta}{B}\right)^2\frac{1}{2^5}(3+\cos4\varphi). \quad (37)$$

Thus, the tunneling probability acquires an additional exponential factor

$$\exp\left\{Q_{01}\left(\frac{\Delta}{B}\right)^2\frac{1}{2^5}(3+\cos4\varphi)\right\},$$

which is maximal at $\varphi=0$ and $\pi/2$ and has a minimum at $\varphi=\pi/4$, i.e., when $\mathbf{F}$ is directed along the diagonal of the face of the unit cube. The ratio of the maximum and minimum tunneling probabilities is

$$\frac{W_{max}}{W_{min}}=\exp\left\{\frac{\pi\mu^{1/2}\Delta^{3/2}}{e_0\hbar F}\left(\frac{\Delta}{B}\right)^2\frac{1}{2^4}\right\}.$$

If we take parameter values that are not extremal $Q_{01}=20$ and $\Delta/B=\frac{1}{2}$, then this ratio is equal to 1.4. This difference between W_{max} and W_{min} can be observed in experiment.

We consider next interband tunneling accompanied by photon absorption (the Keldysh–Franz effect). The principal exponential factor that determines the coefficient $\rho(\Omega)$ of absorption of light of frequency Ω in the crystal, in the presence of an electric field and under the condition $2\Delta-\hbar\Omega>0$, is of the form[20]

$$\exp\left\{-\frac{2}{e_0F}\operatorname{Im}\int_0^{k_0}[2\varepsilon(k_x)-\hbar\Omega]dk_x\right\},$$

where k_0 is determined from the condition $2\varepsilon(k_0)-\hbar\Omega=0$. We use for the crystal dispersion law $\varepsilon(\mathbf{k})$ the expression (2) in which we put for simplicity $B=0$ (in this case the width of the allowed band is $2A$). Then

$$\rho(\Omega)\sim\exp\left\{-\frac{4\Delta}{e_0Fa}\left[(1+\alpha-\nu_0)\operatorname{Arch}\frac{1+\alpha-\nu_0}{\alpha}-[(1+\alpha-\nu_0)^2-\alpha^2]^{1/2}\right]\right\},$$
$$\nu_0=\hbar\Omega/2\Delta. \quad (38)$$

Under the condition

$$\frac{1-\nu_0}{\alpha}=\frac{2\Delta-\hbar\Omega}{2A}\ll1$$

(38) leads to the known result[20,21]

$$\rho(\Omega)\sim\exp\left\{-\frac{4(2\Delta-\hbar\Omega)^{3/2}\mu^{1/2}}{3e_0\hbar F}\right\}, \quad (39)$$

which is obtained in the model of simple parabolic bands. At $(2\Delta-\hbar\Omega)/2A\gtrsim1$ formula (39) is incorrect, and the absorption coefficient $\rho(\Omega)$ is determined by formula (38).

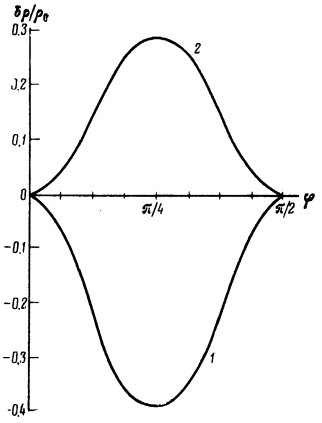

FIG. 2. Angular dependence of the relative change of the light absorption coefficient in an electric field. Curve 1 correspond to a primitive cubic lattice of the crystal, and curve 2 to a face-centered cubic lattice.

Consider the case when the vector **F** is in the plane of a face of the unit cube and makes an angle φ with one of its edges. For a primitive cubic lattice we then obtain $((2\Delta-\hbar\Omega)/2A<1)$

$$\rho(\Omega)\sim\exp\left\{-\frac{4\mu^{1/2}(2\Delta-\hbar\Omega)^{3/2}}{3e_0\hbar F}\cdot\right.$$
$$\left.\times\left[1-\frac{2\Delta-\hbar\Omega}{2^5\cdot 5A}(3+\cos 4\varphi)+\ldots\right]\right\}. \qquad (40)$$

For comparison we present in the same approximation the result for a face-centered cubic lattice ($\varepsilon(\mathbf{k})=\Delta[1+\frac{1}{2}\alpha(3-\cos k_x a\cdot\cos k_y a-\cos k_x a\cos k_z a-\cos k_y a\cdot\cos k_z a)]$):

$$\rho(\Omega)\sim\exp\left\{-\frac{4\mu^{1/2}(2\Delta-\hbar\Omega)^{3/2}}{3e_0\hbar F}\cdot\right.$$
$$\left.\times\left[1-\frac{2\Delta-\hbar\Omega}{2^6\cdot 5A}(9-\cos 4\varphi)+\ldots\right]\right\}. \qquad (41)$$

It is seen from (40) and (41) that the angular dependence of $\rho(\Omega)$ becomes particularly strong in the region of the absorption "tails" that lie in the forbidden band when

$$\eta=\frac{\mu^{1/2}(2\Delta-\hbar\Omega)^{3/2}}{30e_0\hbar FA}>1.$$

Figure 2 shows the angular dependence of the relative change of the absorption coefficient $\delta\rho/\rho_0(\delta\rho=\rho(\Omega,\varphi)-\rho_0(\Omega),\ \rho_0(\Omega)=\rho(\Omega,\varphi=0))$.

The parameter η was chosen equal to unity. It follows from Figs. 2 that the dependence of $\delta\rho/\rho_0$ on φ is quite strong and differs substantially for different types of crystal structure. Thus, an investigation of the absorption of light in the presence of an electric field in crystals with broad allowed bands can yield important information on the crystal symmetry and on the structure of its unit cell. The latter circumstance is quite interesting if account is taken of the high sensitivity of the modulation-spectroscopy methods based on the Keldysh–Franz effect.

It follows from the foregoing that to estimate the tunneling probability in a crystal in the quasiclassical approximation with allowance for the finite widths of the allowed energy bands, it suffices to know the dispersion law $\varepsilon(\mathbf{k})$ in the two-band approximation and the analytic properties of $\varepsilon(\mathbf{k})$ as functions of the complex quasimomentum $\hbar\mathbf{k}$. To clarify the qualitative aspect of the problem and to obtain lucid results, we used here a primitive cubic lattice model, for which we wrote out in turn the simplest dispersion expression that follows from the method of Slater and Koster. However, as shown by Slater and Koster,[14] the method yields analytic expressions for the dispersion laws for lattices with more complicated symmetry and unit-cell structure, with a larger number of phenomenological parameters, and approximating more flexibly the dispersion laws of real crystals. Estimates of the tunneling probability by the quasiclassical method described in the present paper can be obtained without difficulty also in these more complicated cases. Naturally, it is advantageous to do so in comparison of the theory with actual experiment.

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