# Spectrum of electrons in a heterostructure quantum well and tunneling between size-quantization subbands in a longitudinal electric field

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The size-quantization spectrum of free electrons in a heterostructure quantum is influenced by the longitudinal wave vector k. Depending on the well parameters, there can be three types of behavior when k is varied: a reduction in the number of subbands on increase in k including disappearance in the range  $k \ge k_1$ ; an increase in the number of subbands with k; absence of subbands at low values of k and their appearance for  $k \ge k_1$ . In a certain range of values the lowest size-quantization level can be a boundary state. Discrete subbands n = 1, 2, 3, ... split off from the continuum of states with a continuous spectrum at branching points  $k^2 = k_1^2, k_2^2, k_3^2, \dots$ , the vicinities of which make a considerable contribution to the tunneling. The dispersion law for electrons in the subbands can readily be written down in the vicinity of the branching points. The motion of electrons in a quantum well cannot be divided into longitudinal and transverse, which leads to the tunneling of electrons in a longitudinal electric field E from one subband to another or from a subband to states with a continuous spectrum. In a given field E the longitudinal tunneling probability depends nonmonotonically on the energy gap between the subbands and is high for transitions to shallow subbands, including the subbands which branch off on increase in k from the states with a continuous spectrum. In the latter case the contribution of the vicinities of the branching points is important; they also make the largest contribution to the tunneling from a discrete subband directly to states with a continuous spectrum. In this case the expressions for the tunneling probability in weak fields do not contain a characteristic exponential smallness.

#### **1. INTRODUCTION**

We shall consider an electron in a quantum well formed by two plane heterojunctions (abrupt or nonabrupt), where this electron is in free motion or is moving longitudinally, i.e., in an electric field parallel to the heterojunction planes, The heterojunctions establish a one-dimensional dependence of the potential energy of the electrons (bottom of the conduction band) U(z) (Fig. 1a) and associated one-dimensional dependences of the band parameters. If the dispersion law is parabolic inside and outside the well, this parameter is the effective mass m(z), which inside the well can be less ("light well," represented by curve 1 in Fig. 1b) or greater than ("heavy well," represented by curve 2 in Fig. 1b) than outside it. If we allow for the nonparabolicity in the two-band approximation, this parameter is the interband gap  $\varepsilon_{g}(z)$  when the Kane velocity s is constant.

Free motion of an electron confined to a quantum well is described by wave functions of the type

$$\psi_{n,\mathbf{k}}(z,\mathbf{r}) = F_n(z,k) e^{i\mathbf{k}\mathbf{r}},\tag{1}$$

where  $\mathbf{r} = (x,y)$  is a vector in the heterojunction plane;  $\mathbf{k} = (k_x, k_y)$  is a two-dimensional wave vector; *n* is the number of a bound state (subband) corresponding to an energy  $\varepsilon_n(k), n = 1, 2, ..., N(k)$ . If the band parameters are independent of *z*, then in the parabolic case the function  $F_n(z,k)$  is independent of *k* and the energy  $\varepsilon_n(k)$  splits into two parts:

$$\varepsilon_n(k) = \varepsilon_n^0 + \varepsilon(k), \qquad (2)$$

where  $\varepsilon_n^0$  is independent of k, whereas  $\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$ (m = const) is independent of n. In the case of the dependences of the type shown in Fig. 1b the separation described by Eq. (2) is impossible and not only is the energy of each discrete state dependent on k, but this is also true of the total number of these states N(k). In a longitudinal electric field  $\mathbf{E} = -\frac{\partial V}{\partial \mathbf{r}}$ , where  $V = V(\mathbf{r})$ , if the effective mass is independent of z, the wave function is

$$\psi_n(z,\mathbf{r}) = F_n(z) \Phi(\mathbf{r}), \qquad (3)$$

where

$$\varepsilon_n = \varepsilon_n^0 + \varepsilon' \tag{4}$$

 $\Phi(\mathbf{r})$  and  $\varepsilon'$  are described by the solution of a two-dimensional problem with the potential  $V(\mathbf{r})$  and are independent of *n*, whereas  $F_n(z)$  and  $\varepsilon_n^0$  remain the same as in the case  $V(\mathbf{r}) = 0$ , i.e., the transverse and longitudinal motion is separated completely. However, such a separation does not occur in the case of a heterowell (when *m* and other band parameters depend on *z*) or in the general case of a nonparabolic well. Then, the problem in a field with the potential  $V(\mathbf{r})$  becomes essentially three-dimensional [or essentially two-dimensional, if the potential *V* varies one-dimensionally or, for example, if it is of the form V(x)]; the initial classification of the states of free motion loses its



FIG. 1. Coordinate dependences of the potential energy of an electron (a) and its effective mass (b) in a quantum heterowell.

meaning. Transitions between different subbands and emission of electrons from discrete subbands to states with a continuous spectrum then become possible.

Earlier treatments have dealt with transitions between subbands<sup>1,2</sup> as well as with thermal emission of electrons from a quantum well<sup>3,4</sup> due to electron scattering by phonons, crystal lattice defects, or inhomogeneities of the well itself. Field emission of electrons to the conduction or valence band from a quantum well under the influence of a transverse field  $E_z(z)$  has also been discussed.<sup>5,6</sup> A special feature of the situation considered here is the absence of scattering mechanisms or of a transverse field outside the well. Transitions between subbands in a longitudinal field resemble the Zener tunneling between bands in a solid, whereas transfer to a continuous spectrum is an analog of the tunnel ionization process.<sup>7</sup>

We shall classify the spectra of free motion of electrons in quantum wells in Secs. 2 and 3. We shall obtain expressions describing the positions of real and imaginary points where the discrete subbands split off from a continuum of states, and we shall write down the dispersion law of electrons in subbands near the branching points. Both are important in the tunneling program. We shall use the one-band parabolic approximation to solve the problem of the Houston probability of a tunneling transition between subbands in a homogeneous electric field (Sec. 4). The probability of a transition from a deep level to a shallower one varies nonmonotonically on increase in the energy gap between the levels. Since it is exponentially small in weak fields, the probability first decreases as the level moves away, but as the shallower level decreases in depth, the probability passes through a minimum and then rises, losing its exponential smallness when the level leaves the well.

The main contribution to the total probability of the tunneling of electrons from a given subband to all the others comes from transitions to the shallowest of these subbands near its branching point; the probability of a transition to a shallow level near its branching point is also free of the exponential smallness in weak fields. An estimate of the tunneling probability from discrete subbands to states with a continuous spectrum shows that in this case too the contribution of the vicinities of the branching points predominates. A discussion of the results is given in Sec. 5.

### 2. BRANCHING POINTS OF DISCRETE SUBBANDS AND DISPERSION LAWS IN THE VICINITIES OF THESE POINTS. ONE-BAND MODEL

We shall first consider the case of the parabolic dispersion law inside and outside the well. A stationary state of an electron is described by the equation

$$-\frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} + \frac{1}{m(z)} \frac{\partial^2}{\partial r^2} \right] \psi + (U(z) + V(r) - \varepsilon) \psi = 0.$$
(5)

In the case of free motion of an electron the wave function is described by Eq. (1) and  $F_n(z,k)$  obeys

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[m^{-1}(z)\frac{dF_n}{dz}\right] + \left[U(z) + \frac{\hbar^2k^2}{2m(z)} - \varepsilon_n\right]F_n = 0.$$
(6)

In the case of U(z) and m(z) shown in Fig. 1 the bound states appear if

$$\int_{-\infty}^{\infty} U(z) dz + \frac{\hbar^2 k^2}{2} \int_{-\infty}^{\infty} (m^{-1}(z) - m_{\infty}^{-1}) dz < 0, \qquad (7)$$

where  $m_{\infty} = m(z \rightarrow \infty)$ .

In the case of a light heterowell [U(z) < 0 and  $m(z) < m_{\infty}$ —see Figs. 1a, 1b, and Eq. (1)] the bound states exist if

$$k^{2} < k_{1}^{2} = 2m_{\infty} \int_{-\infty}^{\infty} U(z) dz / \hbar^{2} \int_{-\infty}^{\infty} \left(1 - \frac{m_{\infty}}{m(z)}\right) dz.$$
(8)

If U(z) is selected in such a way that at k = 0, there are  $N_0 = N(0)$  bound states, it is found that the number of the threshold values  $k_n^2$  (where  $n = 1, ..., N_0$ ) is  $N_0$  and the inequality  $k_n^2 < k_{n-1}^2$  is obeyed (Fig. 2a). These threshold values are the branching points of discrete levels from the continuous spectrum. In this case an increase in  $k^2$  reduces the number of levels at the branching points by unity.

In a heavy heterowell—if U(z) < 0 and  $m(z) > m_{\infty}$  the bound states can exist for any value of  $k^2$  [see Eq. (7)]. However, whereas when  $k^2 = 0$  there are  $N_0$  levels, an increase in  $k^2$  increases the depth of the effective potential well

$$U_{eff}(z) = U(z) + \hbar^2 k^2 (m^{-1}(z) - m_{\infty}^{-1})/2$$

and the number of bound states increases.<sup>7</sup> Their increase by unity occurs at branching points  $k_n^2$ ,  $n = N_0 + 1$ ,  $N_0 + 2$ ,... (Fig. 2b).

If U(z) > 0 and  $m(z) < m_{\infty}$  (light quantum "hump") it follows from Eq. (7) that there may be no discrete states. However, if  $m(z) < m_{\infty}$ , a heavy quantum hump U(z) > 0 is transformed into an effective quantum well beginning from  $k^2 > k_1^2$ , and this quantum well contains bound states. A further increase in  $k^2$  causes these states to increase by one at the points  $k_n^2 > k_{n-1}^2$  (Fig. 2c). If U(z) = 0, i.e., if initially there is no well and no hump, then  $k_1^2 = 0$ .

In the case of a heavy well in Fig. 2b we show not only the real branching points  $k_3^2$ ,  $k_4^2$ , etc., but also the imaginary branching points  $k_1^2$ ,  $k_2^2 < 0$  which play a role in the longitudinal tunneling probabilities (Sec. 4).

In the case of a rectangular well  $(U = -U_0, m = m_0, |z| < a, U = 0, m = m_{\infty}, |z| > a)$  we can readily obtain not only  $k_1^2$ , but  $k_n^2$ , where  $n \ge 2$ :

$$k_n^2 = (m_0^{-1} - m_\infty^{-1})^{-1} \left[ \frac{2U_9}{\hbar^2} - \frac{\pi^2 (n-1)^2}{4m_0 a^2} \right].$$
(9)

The initial number of levels  $N_0$  for  $U_0 > 0$  is the integral part of the quantity  $(8a^2U_0m_0/\pi^2\hbar^2)^{1/2}$ . Near the branching point the dispersion law for the *n*th level is similar to Eq. (2):

$$\varepsilon_n(k) = \varepsilon_n^0(k) + \varepsilon(k), \qquad (10)$$

where  $\varepsilon(k) = \hbar^2 k^2 / 2m_{\infty}$  and

$$\varepsilon_n^{0}(k) = -\frac{\hbar^2 a^2}{8} \frac{(k^2 - k_n^2)^2}{m_{\infty}} \left(1 - \frac{m_{\infty}}{m_0}\right)^2, \quad n \ge 2.$$
(10a)

If n = 1, then a should be replaced with 2a in Eq. (10a); in



FIG. 2. Dependences of  $\varepsilon_n$  on  $k^2$  for S = 0: a) U(z) < 0,  $m(z) < m_{\infty}$ ; b) U(z) < 0,  $m(z) > m_{\infty}$ ; c) U(z) > 0,  $m(z) > m_{\infty}$ .

this case we can also readily generalize the treatment to the case of arbitrary values of U(z) and m(z):

$$\varepsilon_{1}^{0}(k) = -\frac{\hbar^{2}}{8m_{\infty}}(k^{2}-k_{1}^{2})^{2} \left[\int_{-\infty}^{\infty} \left(\frac{m_{\infty}}{m(z)}-1\right) dz\right]^{2}.$$
 (11)

Equations (10a) and (11) are valid for such values of  $k^2$  for which there is an *n*th discrete level (Fig. 2).

## 3. MANY-BAND MODEL

1. The effects considered here and later occur on the energy scale  $\varepsilon(k) \sim |U_0|$  and/or on the scale of the wave vectors  $\sim a^{-1}$  if the changes in the effective mass are not small, i.e., if they are of the order of the mass itself. In the case of narrow-gap semiconductors this requirement is equivalent to the condition of smallness of the change in the gap itself  $\varepsilon_{\varphi}(z)$ . The change in the gap is accompanied by a change in the potential energy of an electron U(z) and by a change in the energy at the top of the valence band  $U(z) - \varepsilon_{\varphi}(z)$ . The many-band approximation, which has to be used in this case, is normally based on one of several calculation schemes.9 By way of illustration, we shall give the results of the use of the Kane scheme with a  $8 \times 8$  matrix Hamiltonian in the isotropic approximation. In the calculations we shall ignore the influence of the distant energy bands (for which the mass of heavy holes is infinitely large) and assume that the Kane velocity s is constant, as in Ref. 10, i.e., we shall assume that it is independent of  $z \left[ \hbar^2 S^2 = \frac{2}{3} P^2 \right]$ , where P is a parameter used in Ref. 9]. Heterojunctions not only alter the energy at the bottom of the conduction band U(z), but also give rise to specific and symbatic changes in the width of the band gap  $\varepsilon_{e}(z)$  and in the separation  $\Delta(z)$ from the spin-split band at the point  $\mathbf{k} = 0$ .

**2.** In the case of a rectangular heterowell  $[U(z) = 0, \varepsilon_g(z) = \varepsilon_{\infty}, \Delta(z) = \Delta_{\infty} \text{ if } |z| > a; U(z) = -U_0, \varepsilon_g(z) = \varepsilon_0, \Delta(z) = \Delta_0 \text{ if } |z| < a]$  the problem reduces to the dispersion equation

$$\left(\frac{\gamma}{m_{\infty}}-\frac{\alpha}{m_{0}}\operatorname{tg}\alpha a\right)\left(\frac{\gamma}{m_{\infty}}+\frac{\alpha}{m_{0}}\operatorname{ctg}\alpha a\right)-S^{2}k^{2}=0,\qquad(12)$$

where

$$\gamma^2 = k^2 - 2m_{\infty} \varepsilon/\hbar^2, \qquad (12a)$$

$$\alpha^2 = 2m_0(\varepsilon + U_0)/\hbar^2 - k^2,$$
  
$$m_0^{-1} = 2s^2[(U_0 + \varepsilon_0 + \varepsilon)^{-1} + \frac{1}{2}(U_0 + \varepsilon_0 + \Delta_0 + \varepsilon)^{-1}],$$

$$m_{\infty}^{-1} = 2s^{2} [(\varepsilon_{\infty} + \varepsilon)^{-1} + \frac{1}{2} (\varepsilon_{\infty} + \Delta_{\infty} + \varepsilon)^{-1}],$$

$$S = s^{2} [(\varepsilon_{\infty} + \varepsilon)^{-1} - (\varepsilon_{\infty} + \Delta_{\infty} + \varepsilon)^{-1} - (U_{0} + \varepsilon_{0} + \varepsilon)^{-1} + (U_{0} + \varepsilon_{0} + \Delta_{0} + \varepsilon)^{-1}].$$
(12b)

If we ignore the spin-orbit splitting of the valence band at k = 0, we find that S = 0 and the condition for branching of discrete electron subbands becomes

$$\varepsilon_n = [(n-1)^2 U_a^2 - U_0(\varepsilon_0 + U_0)]/(\varepsilon_0 + 2U_0 - \varepsilon_\infty), \quad n = 1, 2, \dots,$$
(13)

where  $U_a^2 = \frac{3}{8} (s\pi\hbar/a)^2$ . For the corresponding values  $k_n^2 = k^2(\varepsilon_n)$ , we obtain

$$k_n^2 = \frac{2}{3\varepsilon_n} (\varepsilon_\infty + \varepsilon_n) / s^2 \hbar^2.$$
(14)

It is clear from Eq. (13) that there are two fundamentally different types of behavior: one similar to the behavior in a heavy well characterized by  $\varepsilon_0 < \varepsilon_0 + 2U_0$  and the other similar to the behavior in a light well characterized by  $\varepsilon_0 > \varepsilon_0 + 2U_0$  (Fig. 3). In the former case when  $U_0 > 0$  there is always at least one discrete level ( $K_1^2 < 0$ ); the smallest number of the subbands  $N_0$  is equal to the integral part of  $[U_0(\varepsilon_0 + U_0)/U_a^2]^{1/2}$ , where an increase in  $k^2$  increases the number of subbands: N(k) increases by unity at the branching points found using Eqs. (13) and (14). Obviously, this includes a homostructure (i.e., electrostatic) well, where  $\varepsilon_0 = \varepsilon_{\infty}$  if  $U_0 > 0$ , i.e., the gradual (on increase in  $k^2$ ) increase in the mass of electrons increases the number of levels in a nonparabolic homostructure well. This behavior is equivalent to that shown in Fig. 2b.

In the second case  $(\varepsilon_{\infty} > \varepsilon_0 + 2U_0, U_0 > 0)$  the situation is drastically different: the number of levels equal to  $N_0$  at  $k^2 = 0$  decreases on increase in  $k^2$ , so that the last level disappears when  $\varepsilon = \varepsilon_1 = U_0(\varepsilon_0 + U_0)/(\varepsilon_{\infty} - \varepsilon_0 - 2U_0)$ ; the situation is equivalent to that shown in Fig. 2a. As  $\varepsilon_{\infty}$  approaches  $\varepsilon_0 + 2U_0$ , all the branching points move to infinite values of  $\varepsilon$  and  $k^2$ , so that the initial number of levels  $N_0$  is conserved for all values of  $k^2$ .

In the case of a hump  $(U_0 < 0)$  if  $\varepsilon_0 + 2U_0 > \varepsilon_{\infty}$  and  $\varepsilon_0 + U_0 > 0$ , the situation is similar to that shown in Fig. 2c, i.e., at low values of  $k^2$  there are no discrete levels, but as  $k^2$  increases, then beginning from  $k^2 = k_1^2$  an effective well appears at the position of a hump and quantization also begins from this value. On further increase in  $K^2$  the number of

levels increases. If  $\varepsilon_0 + 2U_0 < \varepsilon_{\infty}$  and  $U_0 < 0$ , no discrete levels appear in the electron band. The dispersion law  $\varepsilon_n(k)$ in a branching point now changes from the law given by Eq. (10) to

$$\mathbf{e}_{n}(k)\left[\mathbf{\varepsilon}_{n}(k) + \mathbf{\varepsilon}_{\infty}\right] = \frac{3}{2}\hbar^{2}s^{2}\left[k^{2} - \gamma_{n}^{2}(k)\right], \qquad (10')$$

where

$$\gamma_n(k) = \frac{a(k^2 - k_n^2)}{2} \frac{(\varepsilon_n + \varepsilon_\infty) (\varepsilon_0 + 2U_0 - \varepsilon_\infty)}{(\varepsilon_n + \varepsilon_0 + U_0) (2\varepsilon_n + \varepsilon_\infty)}, \qquad (10'a)$$

if  $n \ge 2$ ; in the case when n = 1, we have to replace a with 2a.

3. In heterostructures based on compounds of the  $Cd_x Hg_{1-x}$  Te type variation X(z) is usually accompanied by a strong variation of the position of the bottom of the conduction band U(z) and relatively weak variation of the position of the top of the valence band<sup>10-12</sup> (case 1' in Fig. 3):

$$U(z) - \varepsilon_{g}(z) \approx \text{const.}$$
 (15)

In a wide range of values of X(z) the spin-split-off band is separated by a large gap:  $\Delta(z) \ge \varepsilon_g(z)$ , |U(z)|. This allows us to assume in all cases the values

$$S(z) \approx 0, \quad m^{-1}(z) = \frac{2s^2}{(e_s(z) + e - U(z))} \approx \text{const}$$

and reduce the situation under discussion to the one just considered if  $U_a^2 = (s\pi\hbar/2a)^2$  and  $\varepsilon_0 + U_0 = \varepsilon_{\infty}$ . Hence, it follows that

 $\varepsilon_0 + 2U_0 = \varepsilon_\infty + U_0$ 

i.e., the quantum well  $(U_0 > 0)$  becomes enriched with discrete levels as  $k^2$  increases and in the case of a hump  $(U_0 < 0)$  there are no discrete states for any value of  $k^2$ . The dispersion law for a quantum well near the branching points is identical with Eqs. (10') and (10'a) provided we replace  $(3/2)s^2$  with  $s^2$ . Similar behavior of the quantum wells in the situation described here was mentioned in Ref. 8.

4. A special feature of the general case which allows for a finite spin-orbit splitting and deviation of S from 0, is the influence of boundary states at an abrupt heterojunction on the position of the branching point of the n = 1 subband and on the dispersion law near this point (no such states, if S = 0). For the sake of simplicity, we shall consider this feature only in the special situation characterized by

$$|\varepsilon - U(z)| \ll \varepsilon_{g}(z) \ll \Delta(z), \qquad (16)$$

when we can always use the parabolic approximation of the z-dependent effective mass:  $m^{-1}(z) = 2s^2 \varepsilon_g(z)$ . In the case



FIG. 3. Variants of heterowells corresponding to different types of behavior of the branching laws: 1), 1'), 1")  $\varepsilon_{\infty} < \varepsilon_0 + 2U_0$ ; 2)  $\varepsilon_{\infty} > \varepsilon_0 + 2U_0$ .

of a rectangular well, we find that  $m_{\infty}$  and  $m_0$  are constants independent of  $\varepsilon$ , and that  $S = \frac{1}{2}(m_{\infty}^{-1} - m_0^{-1})$ .

We shall find the conditions for branching of discrete levels from a continuum. The branching point is defined by substituting  $\gamma_n = 0$  in Eq. (12), i.e., by assuming that  $k_n^2 = 2m_\infty \varepsilon_n/\hbar^2$ . We then readily obtain the equation  $\alpha_n \tan(\alpha_n a) = \infty$  or  $\alpha_n \cot(\alpha_n a) = \infty$ , for the branching point, and this equation yields values of  $k_n^2$  described by Eq. (9) with n = 2, 3, ..., but not for n = 1. These values do not contain S. If n = 1, it follows from Eq. (12) that  $\alpha_1^2 = -m_0^2 S^2 k_1'^2$  or

$$k_{1}^{\prime 2} = \frac{2m_{0}m_{\infty}U_{0}}{\hbar^{2}(m_{\infty}-m_{0})} \frac{4m_{\infty}}{3m_{\infty}+m_{0}},$$
(17)

which differs by a factor  $4m_{\infty}/(3m_{\infty} + m_0)$  from the expression for  $k_1^2$  that follows from Eq. (9) if we substitute n = 1; the notation  $k_1'^2$  is used to stress this difference.

We shall consider qualitatively the dependences  $\varepsilon_n (k^2)$ . If  $k^2 = 0$ , we find that the values  $\varepsilon_n (0)$  obtained from Eq. (12), are the same as those obtained for S = 0, i.e., if  $S \neq 0$ , the dependences  $\varepsilon_n (k^2)$  begin at the same point as in the case when S = 0, and for  $n \neq 1$  they go over to the continuous spectrum at the same branching points. Therefore, the qualitative nature of all the curves in Fig. 2 is preserved when  $n \neq 1$ ; the quantitative difference between them is determined by the value of S. We shall now consider the curves corresponding to n = 1, for which there are qualitative differences. In a light well  $(m_{\infty} > m_0, U_0 > 0)$  the branching point of Eq. (17) lies to the right of the point  $k_1^2$  in Fig. 2a, i.e., the dependence  $\varepsilon_1 (k^2)$  intersects the curve  $\varepsilon_0 = \hbar^2 k^2 / 2m_0 - U_0$  describing the change in the bottom of the well and the point of intersection is given by

$$k_{0}^{2} = \frac{1-\lambda}{\lambda(1-3\lambda/4)^{2}a^{2}} \left[ \lambda \left(1-\frac{3}{4}\lambda\right)a^{2}k_{1}^{2} - \frac{1}{2} + \frac{1}{2} \left(1+\lambda^{2}a^{2}k_{1}^{2}\frac{1-3\lambda/4}{1-\lambda}\right)^{\frac{1}{2}} \right],$$
(18)

where  $(\lambda = 1 - m_0/m_{\infty}; k_0^2 < k_1^2 < k_1'^2$ . In the interval  $0 < k^2 < k_0^2$  the level  $\varepsilon_1(k^2)$  is the "usual" state with a convex dependence of the electron density on z in the region |z| < a. At the point  $k^2 = k_0^2$  this dependence becomes a constant and for  $k_0^2 < k^2 < k_1'^2$  it is concave, i.e., at the point  $k^2 = k_0^2$  the usual state changes to a boundary state and after surviving as the boundary state for  $k_0^2 < k^2 < k_1'^2$ , it merges at a point  $K^2 = K_1'^2$  with the continuous spectrum. We can show that if  $\Delta \gg \varepsilon_g$ , a boundary state appears in the conduction band if  $\varepsilon_0 + 2U_0 - \varepsilon_{\infty} < 0$ , whereas for the opposite inequality when the discontinuity of the conduction band predominates, a similar boundary state appears in the valence band.

Boundary states at heterojunctions and in heterowells were described by Suris,<sup>13</sup> who derived them for a hole energy band. We can show that a set of boundary states is more extensive and that states of this type can coexist in the valence and conduction bands.

In the limit  $a \to \infty a$  boundary state in a heterowell changes to a surface state when there is only one heterojunction and the dispersion law is

$$\varepsilon = (\hbar^2/2m_0) \{ {}^3/_4 (2-\lambda) k^2 - k_1{}^2 + [(1-\lambda) k^2 (k_1{}^2 - {}^3/_4 k^2)]^{t_0} \}.$$
(19)

Such a state exists in an interval which begins at  $k_0^2|_{a\to\infty} = k_1^2(1-\lambda)/(1-\frac{3}{4}\lambda)$  and terminates at  $k_1'^2$ . At the former point a boundary state splits off from the band  $\varepsilon_0(k^2) = \hbar^2 k^2/2m_0 - U_0$ , whereas in the latter case it merges with the band  $\varepsilon_{\infty}(k^2) = \hbar^2 k^2/2m_{\infty}$  and contact takes place at both points. If  $a < \infty$ , then contact takes place at  $k_1'^2$  (and at all the other branching points), whereas an intersection occurs at the point  $k_0^2$ .

The dispersion laws  $\varepsilon_n (k^2)$  near the branching points are somewhat different from the corresponding laws (10) and (10a) obtained for S = 0. On the right-hand side of Eq. (10a) we have to introduce now a correction factor

$$[1+(\lambda k_n a/\pi (n-1))^2]^2$$
,

whereas for n = 1 we have to use

$$\varepsilon_{i}^{0}(k) = -\frac{1}{2m_{\infty}} \left[ \frac{(1 - i/_{4}\lambda)\hbar(k^{2} - k_{i}'^{2})}{(1 - \lambda)k_{i}' \operatorname{cth}(\lambda k_{i}' a)} \right]^{2}.$$
 (20)

In the case of a heavy well  $(U_0 > 0, \lambda < 0)$  there are no boundary electron states. The expressions for all the real branching points remain the same as before and the dispersion laws to the right of these points are of the same kind as for a light well to the left of the branching points. As in the S = 0 case, the discrete states without real branching points have imaginary points (Fig. 2b) and one of them is described by Eq. (17).

If  $U_0 < 0$  and  $\lambda < 0$ , the state with n = 1 splits off from the continuous spectrum at the point  $k^2 = k_1'^2$  located to the left of the point  $k_2 = k_1^2$  (which is no longer a branching point if  $S \neq 0$ ). Therefore, once again we obtain a boundary state which exists in the interval  $k_1'^2 < k^2 < k_0^2$  and transforms into the usual state at  $k_0^2 < k^2 < \infty$ , where  $k_1'^2 < k_1^2 < k_0^2$ . Figure 4 illustrates two of the three cases shown in Fig. 2 and it allows for the boundary states which appear when  $S \neq 0$ .

### 4. TUNNELING BETWEEN SUBBANDS AND IONIZATION FROM A WELL IN A HOMOGENEOUS LONGITUDINAL ELECTRIC FIELD WHEN THE DISPERSION LAW IS PARABOLIC

1. We shall now consider the motion of an electron in a quantum well in a homogeneous electric field directed along the x axis. As shown in Sec. 1 such motion does not conserve the number of the quantum subband in a heterowell and electrons then tunnel from one subband to another and to



FIG. 4. Dependences of  $\varepsilon_n$  on  $k^2$  for  $S \neq 0$ : a)  $U_0 > 0$ ,  $\lambda > 0$ ; b)  $U_0 < 0$ ,  $\lambda < 0$ .

states with a continuous spectrum. In the case of sufficiently weak fields we can use a method similar to that applied to the Zener tunneling between bands in a solid.<sup>14,15</sup> We shall begin with the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi,$$
 (21)

where  $\hat{H}$  is the same Hamiltonian as in Eq. (5), but with  $V(\mathbf{r}) = -eEx$ . The solution (21) is found in the form of an expansion

$$\psi = \sum_{n, k_x^{\circ}, k_y} c_n(k_x^{\circ}, k_y, t) \psi_n(k_x^{\circ}, k_y, z, t)$$
(22)

in terms of the Houston functions

$$\psi_{n}(k_{x}^{0}, k_{y}, z, t) = F_{n}\left(z, k_{x}^{0} + \frac{eEt}{\hbar}, k_{y}\right)$$

$$\times \exp \int t \left[k_{x}^{0}x + k_{y}y + \frac{eEtx}{\hbar} - \frac{1}{\hbar}\int_{0}^{t} \varepsilon_{n}\left(k_{x}^{0} + \frac{eEt'}{\hbar}, k_{y}\right)dt'\right]\right\}, \quad (23)$$

where  $F_n(z,k_x,k_y)$  is the solution of the equation for free motion in a well described by Eq. (6). The number *n* applies not only to the discrete, but also to the continuous part of the spectrum of quantization along *z*. After substitution of Eq. (22) into Eq. (21), multiplication of Eq. (21) by  $\psi_m^*(k_x'^0,k_y',z,t)$  and integration over the whole volume, we obtain an equation which describes  $c_n(k_y^0,k_y,t)$ :

$$\sum_{n} \left\{ \delta_{mn} \frac{\partial}{\partial t} c_{n}(k_{x}^{0}, k_{y}, t) + \frac{eE}{\hbar} \Gamma_{mn} c_{n}(k_{x}^{0}, k_{y}, t) \right\}$$
$$\times \exp\left[-\frac{i}{\hbar} \int_{0}^{t} (\epsilon_{n} - \epsilon_{m}) dt'\right] = 0, \qquad (24)$$

where the normalization of the functions  $F_n(z,k)$  is allowed for:

$$\int_{-\infty}^{\infty} F_{m}(z,k) F_{n}(z,k) dz = \delta_{mn},$$

the primes of  $k'_x^0$  and  $k'_y$  are omitted,  $\mathbf{k} = (k^0_x + eEt/\hbar, k_y), k_x = k^0_x + eEt/\hbar$ ,

$$\Gamma_{mn} = \int_{-\infty}^{\infty} F_{m} \cdot (z, k) \frac{\partial}{\partial k_{x}} F_{n}(z, k) dz$$
$$= \frac{\hbar^{2} k_{x}}{\varepsilon_{n}(k) - \varepsilon_{m}(k)} \int_{-\infty}^{\infty} \frac{dz}{m(z)} F_{m} \cdot F_{n},$$
$$\Gamma_{nn} = 0.$$
(25)

We shall solve Eq. (24) subject to the initial conditions  $c_n(0) = 1, c_{n'}(0) = 0, n' \neq n$ , i.e., we shall assume that initially an electron is in the *n*th subband with given values of  $k_x^0$  and  $k_y$ . Perturbation theory applied below involves re-

placement of  $c_n(k_x^0, k_y, t)$  in the second term inside the braces of Eq. (24) with  $c_n(k_x^0, k_y, 0)$ . Then, if  $m \neq n$ , we have

$$\sum_{k_{x}^{(n)}}^{\mathbf{k}_{x}} (k_{x}^{0}, k_{y}, t)$$

$$= -\int_{\mathbf{k}_{x}^{0}}^{\mathbf{k}_{x}} dk_{x}' \Gamma_{mn}(k_{x}') \exp\left\{\frac{i}{eE}\int_{\mathbf{k}_{x}^{0}}^{\mathbf{k}_{x}'} dk_{x}''[\varepsilon_{m}(k'') - \varepsilon_{n}(k'')]\right\}.$$

$$(26)$$

We shall consider only the symmetric rectangular wells. For such symmetric wells the value of  $\Gamma_{mn}$  differs from 0 if *m* and *n* have the same parity (or—allowing for the continuous spectrum—the states have the same sign of symmetry). Therefore, only the subbands of the same parity as *n* become filled. In the case of a rectangular well and discrete values of *m* and *n* of the same parity, we find that

$$\Gamma_{mn} = \frac{\hbar^2}{m_{\bullet}} \lambda k_{\pi} \frac{2(\gamma_m \gamma_n)^{\nu_a} A_m A_n}{(\gamma_m + \gamma_n) (\varepsilon_m - \varepsilon_n)}, \qquad (27)$$

where

$$A_{m} = \left\{ 1 + a\gamma_{m} \left[ 1 + \left( \frac{m_{0}\gamma_{m}}{m_{\infty}\alpha_{m}} \right)^{2} \right] + \frac{m_{0}}{m_{\infty}} \left( \frac{\gamma_{m}}{\alpha_{m}} \right)^{2} \right\}^{-1/\epsilon}.$$
 (27a)

We recall that not only  $\varepsilon_m$  and  $\varepsilon_n$ , but also  $\gamma_m$ ,  $\gamma_n$ ,  $A_m$ , and  $A_n$  depend on  $k_x$  and  $k_y$ , i.e., the quantities  $\gamma_m$  and  $\alpha_m$  are described respectively by Eqs. (12a) and (12b). In the case of transitions from a discrete level *n* to states in the continuous spectrum we have to replace  $\Gamma_{mn}$  in Eq. (26) by

$$\Gamma_{n}(q) = \frac{\hbar^{4} \lambda k_{z} \gamma_{n}{}^{t_{0}} A_{n}}{\pi^{t_{0}} m_{\bullet} [\varepsilon(q) - \varepsilon_{n}]^{2}} \left[ \frac{\gamma_{n}}{m_{\bullet}} - \frac{\alpha(q) \tau(q)}{m_{\bullet}} \right] \times \left[ 1 + \left( \frac{m_{\infty}}{m_{\bullet}} \frac{\alpha(q) \tau(q)}{q} \right)^{2} \right]^{-t_{0}}$$
(28)

where  $\tau(q) = \tan[\alpha(q)a]$  for the states with an even function  $F_n$ ,  $\tau(q) = -\cot[\alpha(q)a]$  for the states with an odd function  $F_n$ ,

$$\varepsilon(q) = \hbar^2 (q^2 + k^2) / 2m_{\infty},$$
  
 $\alpha^2(q) = (2m_0/\hbar^2) [\varepsilon(q) + U_0] - k^2.$ 

Perturbation theory allows us to find the probabilities of an electron transition in a time interval t from the *n*th to the *m*th level, which is  $w_m^{(n)} = |c_m^{(n)}(k_x^0, k_y, t)|^2$ , as well as the total probability of transfer of an electron from the *n*th level to states in the continuous spectrum, which is

$$w^{(n)} = \int_{0}^{\infty} dq |c^{(n)}(q; k_{x}^{0}, k_{y}, t)|^{2}.$$
<sup>(29)</sup>

It is assumed that the calculations of the probabilities are valid as long as  $w^{(n)} + \Sigma_m w_m$  remains small.

We begin by considering the case when the discrete subbands *n* and *m* exist for all values of  $k_x$  which is not true of light wells, but which may be true of heavy wells in the case of levels with small values of *n* and *m*. In these calculations it is assumed that  $k_x^0 \rightarrow -\infty$ ,  $k_x \rightarrow \infty$ , i.e., the probability is found for a transition from one level to another level when an

electron is reflected by an infinitely high barrier having a constant slope. We shall then consider a transition from a discrete subband of level *n*, which exists for all values of  $k_x$ , to a subband m, which branches off at the points  $\pm p_m$ , where  $p_m^2 = k_m^2 - k_v^2$ , from a band of continuum state. In one of the limits of Eq. (26) we have a finite result:  $k_x^0 = p_m$ or  $k_x = -p_m$ . In the parabolic approximation adopted here the case of a heavy band is not typical. However, we recall that, firstly, in the qualitative sense it is the heavy bands that model typical structures with compounds of the  $Cd_xHg_{1-x}Te$  type; moreover, all the nonparabolic homowells are similar and discussion of these wells is topical because of the development of the  $\delta$ -doping technology. In all these situations the nonparabolicity makes electrons inside the well much heavier than outside it. Secondly, if the field E is sufficiently weak, it is found that the effective contribution to the tunnel integral comes from relatively narrow intervals of  $k_r$  in the vicinity of the branching points  $\pm p_m$ . Naturally, the results in this interval no longer depend on what happens outside the interval and apply equally to heavy and light wells.

The predominance of the contribution in the vicinities of the branching points observed in weak fields applies also to the case of transitions from a discrete subband in states with a continuous spectrum, but in this case the results are only qualitative.

**2.** Bearing these points in mind, we shall consider the case when  $\lambda < 0$ ,  $U_0 > 0$ , S = 0 (Fig. 2b) and assume that the existence of  $N_0$  bound states at  $k_x = 0$ , which corresponds to the same number of the imaginary branching points:  $k_1^2$ ,  $k_2^2$ ,..., $k_{N_0}^2$ . If we assume that  $N_0 > 3$ , we find that transitions are possible between levels of the same parity, which we shall consider here. The problem reduces to calculation of the integral

$$c_{m}^{(m)} = -c_{n}^{(m)} = -c_{n}^{(m)}$$
$$= \int_{-\infty}^{\infty} dk_{x} \Gamma_{mn}(k) \exp\left\{\frac{i}{eE} \int_{0}^{k_{x}} dk_{x}' \left[\epsilon_{m}(k') - \epsilon_{n}(k')\right]\right\}. \quad (30)$$

We shall consider the specific case when the *m*th level lies above the *n*th level and, on going over to a complex plane  $k_x$ , we shall transfer parallel to itself an integration contour with its real axis directed upward (Fig. 5) over a distance  $ig_m(k_y)$ , where  $g_m^2 = -k_m^2 + k_y^2$ ;  $k_m^2 < 0$  is the abscissa of the imaginary branching point in Fig. 2b.

The quantity  $\Gamma_{mn}(k)$  does not have singularities between the initial and transferred integration contours; only the new contour  $\Gamma_{mn}$  passes through zero at the point



FIG. 5. Integration contour in Eq. (30).

 $ig_m$ . Near this point we have the following value on the contour:

$$\Gamma_{mn} \approx \frac{2\hbar^2 A_n(m)}{\varepsilon_n(m) - \varepsilon_m(m)} \left[ i \frac{am_{\infty}}{\gamma_n(m)} \frac{\lambda^3 g_m^3}{m_0^3} q_\pi \right]^{\eta}, \qquad (31)$$

where  $\gamma_n(m)$ ,  $A_m(m)$ ,  $\varepsilon_n(m)$  and  $\varepsilon_m(m)$  represents the values of the corresponding quantities when  $k^2 = k_m^2$ ;  $q_x$  in Eq. (31) is understood to be the real part of  $k_x$ . The argument of the exponential function in Eq. (30) near  $k_x = ig_m$  can be written in the form

$$\frac{i}{eE}\int_{0}^{k_{x}}dk_{x}'[\varepsilon_{m}(k')-\varepsilon_{n}(k')]\approx -\frac{1}{eE}\int_{0}^{\varepsilon_{m}}d\xi[\varepsilon_{m}(i\xi)-\varepsilon_{n}(i\xi)] +\frac{iq_{x}}{eE}[\varepsilon_{m}(m)-\varepsilon_{n}(m)]-\Omega q_{x}^{2}, \qquad (32)$$

where  $\varepsilon_{m,n}(i\xi)$  corresponds to the values  $k^2 = -\xi^2$  (Fig. 2b);  $\Omega$  is a small positive quantity and its actual nature is unimportant.

Subject to these simplifications, we find that the required probability becomes

$$w_m^{(n)} = |c_m^{(n)}|^2 \approx |Q_{mn}|^2 E^3 \exp\left(-E_{mn}/E\right), \tag{33}$$

where

$$E_{mn} = \frac{2}{e} \int_{0}^{\ell_m} d\xi [\varepsilon_m(i\xi) - \varepsilon_n(i\xi)], \qquad (33a)$$

$$Q_{mn} = 2 \left[ \frac{i \pi a m_{\infty}}{\gamma_n(m)} \right]^{\frac{1}{2}} \hbar^2 A_n(m) \left( \frac{e \lambda g_m}{m_0} \right)^{\frac{1}{2}} \left[ \varepsilon_m(m) - \varepsilon_n(m) \right]^{-\frac{s}{2}}.$$
(33b)

We can easily show that the use of the approximate expressions (31) and (32) in Eq. (30) is justified if  $E_{mn} \ge E$ . Although Eq. (33) contains the parameters  $E_{mn}$  and  $Q_{mn}$ , which are obtained only numerically, we can clearly see the structure of the field dependence and can estimate the order of magnitude of the probabilities.

In particular, it is clear from Eq. (33a) that  $E_{mn} \sim (2g_m/e) \ \overline{(\varepsilon_m - \varepsilon_n)}$ , where the bar denotes averaging in the integral, so that the tunnel probability to the shallow *m*th level increases as the depth of the level decreases. As the *m*th level moves from the *n*th (lower) level, the tunneling probability begins to fall due to an increase in  $\overline{\varepsilon_m - \varepsilon_n}$ , and then it rises because of a reduction in  $g_m$ . If the *m*th level becomes shallow, we can refine the calculation of  $c_m^{(n)}$ . Then, Eq. (30) reduces to

$$c_{m}^{(n)} = \frac{4i\hbar^{2}A_{n}(0)}{\varepsilon_{n}(0)} \left[ \frac{m_{\infty}a\lambda^{3}}{2\gamma_{n}(0)m_{0}^{3}} \right]^{\eta_{n}}$$

$$\times \int_{0}^{\infty} k_{x} dk_{x} (k_{x}^{2} + g_{m}^{2})^{\eta_{x}} \sin\left(\frac{\varepsilon_{n}(0)k_{x}}{eE}\right) \Lambda(k_{x}), \qquad (34)$$

where the argument 0 instead of *m* represents the fact that the level is shallow and  $\Lambda(k_x)$  is a "truncating" function which is close to unity in the relevant values of  $k_x$  and which transforms the integrand to 0 in the limit  $k_x \to \infty$ . We can easily show that apart from the dependence on the actual form of  $\Lambda(k_x)$  [for example, if  $\exp(-\delta k_x)$ ,  $\exp(-\delta^2 k_x^2)$ ,  $(1 + \delta^2 k_x^2)^{-n}$ ,  $n \ge 2$ ,  $\delta \to 0$ ; if  $\delta \approx a$ , the last expression applies], the integral in Eq. (34) is

$$-\frac{g_m^2 eE}{\varepsilon_n(0)} K_2\left(\frac{g_m \varepsilon_n(0)}{eE}\right),$$

where  $K_2(x)$  is the Macdonald function. If the argument of this function  $g_m \varepsilon_n(0)/eE \ge 1$  is large, the use of an asymptotic expression for this function gives Eq. (33) with  $E_{mn} = 2g_m \varepsilon_n(0)/e$ . If the argument of the Macdonald function is small, we obtain the limiting expression for  $w_m^{(n)}$ :

$$w_{m}^{(n)}(0) = \frac{32a\hbar^{4}A_{n}^{2}(0)|\lambda|^{3}m_{\infty}}{\gamma_{n}(0)m_{0}^{3}} \frac{e^{6}E^{6}}{\varepsilon_{n}^{8}(0)}.$$
(35)

Equation (35) is valid on the assumption that its right-hand side is small compared with unity, i.e., it is essential that

$$g_{m}\varepsilon_{n}(0) \ll eE \ll k^{(n)} \frac{(\varepsilon_{n}(0))^{4_{j}} m_{\infty}^{\eta_{k}} m_{0}^{\eta_{k}}}{\hbar^{\eta_{k}} a^{\eta_{k}} | m_{\infty} - m_{0} |^{\eta_{k}}}, \qquad (36)$$

where  $k^{(n)} = [a\gamma_n(0)/32A_n^2(0)]^{1/6} \sim 1$ . If a given level is sufficiently shallow, the range of fields defined by Eq. (36) is always attainable. We shall estimate the upper field limiting this range, such that the tunneling in this field is no longer a small correction. If we assume approximate values  $\varepsilon_n(0) = 0.1 \text{ eV}, a = 10^{-6} \text{ cm}, \text{ and } m_{\infty} = 0.1m$  (here, *m* is the mass of a free electron), we obtain  $E \sim 10^5 \text{ V/cm}$ .

3. In calculations dealing with a tunnel transition from a level *n*, which exists for all values of  $k_x$ , to a level *m*, which branches off at the points  $k_x = \pm p_m$  and exists if  $|k_x| \ge p_m$ , the integral in Eq. (26) can be calculated in the limit  $K_x^0 = p_m$ ,  $k_x = \infty$ , whereas the expressions for  $\varepsilon_m(k)$  and  $\Gamma_{mn}(k)$  can be obtained approximately using the dispersion law (10) near a branching point (which now, in contrast to the preceding case, is real). The relevant coefficient  $c_{m(+)}^{(n)}$  is then described by [compare with Eq. (34)]:

$$c_{m(+)}^{(n)} = \frac{i\hbar^{2}A_{n}(m)}{\left[\varepsilon_{n}(m) - \varepsilon_{m}(m)\right]} \left[\frac{2am_{\infty}\lambda^{3}}{m_{0}^{3}\gamma_{n}(m)}\right]^{l_{1}}$$

$$\times \int_{p_{m}}^{\infty} k_{x} dk_{x} (k_{x}^{2} - p_{m}^{2})^{l_{1}} \exp\left[i\frac{\varepsilon_{m}(m) - \varepsilon_{n}(m)}{eE}(k_{x} - p_{m})\right]\Lambda(k_{x}),$$
(37)

where the argument of *m* still denotes calculation of these quantities at the points  $k_x = \pm p_m$ , so that the function  $\Lambda(k_x)$  has the same meaning as in Eq. (34). Calculation of the integral on the right-hand side of Eq. (37) gives the following expression:

$$c_{m(+)}^{(n)} = \frac{i\pi\hbar^2 A_n(m) p_m^2 eE}{[\varepsilon_n(m) - \varepsilon_m(m)]^2} \left[ \frac{am_\infty \lambda^3}{2m_0^3 \gamma_n(m)} \right]^{\eta_1} \times H_2^{(1)} \left( \frac{\varepsilon_m(m) - \varepsilon_n(m)}{eE} p_m \right),$$
(38)

where  $H_2^{(1)}(x)$  is a Hankel function of the first kind.

We can similarly calculate the coefficient  $c_{m(-)}^{(n)}$  corresponding to tunnelling in the interval  $k_x^0 = -\infty$ ,  $k_x = -p_m$ ; it differs from  $c_{m(+)}^{(n)}$  by a factor governed by the behavior of an electron between the points  $-p_m$  and  $p_m$ . In the adopted approach this factor represents the phase

 $[\exp(i\varphi_m^{(n)})]$ , so that the total probability of a transition from the nth level to the level m branching at the points  $\pm p_m$  is described by

$$w_m^{(n)} = 2|c_{m(+)}^{(n)}|^2 (1 + \cos \varphi_m^{(n)}).$$
(39)

If  $p_m \rightarrow 0$  then also  $\varphi_m^{(n)} \rightarrow 0$ , so that  $w_m^{(n)} = 4|c_{m(+)}^{(n)}|^2$ ; Eq. (39) then transforms in a continuous manner to Eq. (35). If random dephasing occurs between the points  $-p_m$  and  $p_m$ , we find that  $\overline{\cos \varphi = 0}$  and the probability  $w_m^{(n)}$  reduces to  $2|c_{m(+)}^{(n)}|^2$ , i.e., tunnel transitions to the left-and right-hand branch are independent.

Generalizing the results obtained in the subsections 2 and 3 above, we reach the conclusion that an electron in the nth subband subject to a field E is characterized by an exponentially small probability (33) of tunneling to the mth subband of the same parity. As the energy separation between the subbands increases, this probability begins to fall rapidly, as pointed out above. However, as the higher mth level becomes shallower, this probability passes through a minimum and begins to rise exponentially; further reduction in the depth of the level results in saturation (in a given field E) of the probability described by Eq. (35). This relatively high value of the probability is retained for small arguments of the Hankel function in Eq. (38) even when branching of the *m*th level occurs. When the branching point is sufficiently far from  $k_x = 0$ , we obtain

$$|c_{m(+)}^{(n)}|^2 \approx \frac{1}{4} |Q_{mn'}|^2 E^3, \tag{40}$$

where  $|Q'_{mn}|$  is deduced from Eq. (33b) describing  $|Q_{mn}|$  if we replace  $g_m$  with  $p_m$ . The exponentially small factor in Eq. (33) is replaced in Eq. (39) by a factor  $2(1 + \cos\varphi_m^{(n)})$ which oscillates with the field. These oscillations are damped out if dephasing occurs between the points  $-p_m$ and  $p \ m \cdot$  Therefore, the vicinities of the branching points make the greatest contribution to the tunneling from a discrete level to another discrete level.

4. We shall now consider determination of  $|c^{(n)}(q)|^2$ , which is the density of the probability of tunneling from the nth level to states in the continuous spectrum. The results obtained below are purely qualitative, because the states in the continuous spectrum are essentially nonstationary in the presence of a field E.

The integral of Eq. (26) contains a quantity  $\Gamma_n(q)$  described by Eq. (28) and in the present case this integral has an infinite number of pairs of zeros in the denominator which are separated by distances  $\sim a^{-1}$  on the plane of a complex wave number  $k_x$ . If

$$q \ll a^{-i}, \tag{41}$$

then each pair of zeros is located near a branching point, which is real or imaginary, and for the odd value of n (corresponding to an even function  $F_n$ ) these zeros are located near odd branching points, whereas for even n they are located near even branching points. The zeros near imaginary branching points  $\pm ig_m$ are located at  $(k_x^{\pm})^2 = -g_m^2 \pm 2q/a(1-m_{\infty}/m_0)$ , where  $m \neq 1$  (if m = 1, we have to replace a with 2a), i.e., the imaginary points are located at

$$k_{\mathbf{z}}^{\pm} \approx \pm i g_{m} \pm \frac{q}{a g_{m} (1 - m_{\infty}/m_{0})} \,. \tag{42}$$

Near the real branching points  $\pm p_m$ , we similarly have

$$k_{\mathbf{x}}^{\pm} \approx \pm p_m \pm \frac{iq}{ap_m(1-m_{\infty}/m_0)}.$$
(42')

The positions of zeros of the denominator  $\Gamma_n(q)$  in the case of  $N(k_y)$  discrete subbands is plotted in Fig. 6 for  $k_x = 0$ . The number  $N_n$  in this figure is identical with  $N(k_v)$  if the parity of  $N(k_v)$  is the same as the parity of the number n of the level from which electrons are tunneling, but if n and  $N(k_v)$  have different parities, then  $N_n = N(k_v) - 1$ .

We shall assume that at  $k_x = 0$  the highest level  $m = n_n$ is shallow. Then, a considerable contribution to the integral of Eq. (30) comes from relatively small sections of the real axis  $k_x$  near the point  $k_x = 0$  and near all the real branching points. The contribution near the branching point  $p_m$ , where  $m = N_n + 2, N_n + 4,...,$  is given approximately by the integral

$$c^{(n)}(q) \mid_{m}^{\pm} \approx B_{m} e^{\pm i \varphi_{m}} \int_{-\infty}^{\infty} dg \cos b_{m} g (g^{2} + r_{m}^{2})^{-\gamma_{n}}$$
$$= \pm 2B_{m} e^{\pm i \varphi_{m}} K_{0}(b_{m} r_{m}), \qquad (43)$$

(43)

where

$$B_{m}(q) = -\frac{4}{\pi^{\frac{1}{1}}} \gamma_{n}^{\frac{3}{1}}(m) \frac{A_{n}(m)q}{a[q^{2} + \gamma_{n}^{2}(m)]^{2}},$$
  

$$r_{m}(q) = \frac{m_{0}q}{ap_{m}|m_{0} - m_{\infty}|}, \quad b_{m}(q) = \frac{\hbar^{2}(q^{2} + \gamma_{n}^{2}(m))^{2}}{2m_{\infty}eE},$$
  

$$\varphi_{m}(q) = \frac{1}{eE} \int_{0}^{p_{m}} dk_{x}' \Big[ \frac{\hbar^{2}(q^{2} + k'^{2})}{2m_{\infty}} - \varepsilon_{n}(k') \Big].$$

In the calculations based on Eq. (43) it is assumed that  $p_m \gg r_m$ ,  $b_m^{-1}$ , in the opposite case we could not use the infinite limits in the integration procedure. One of these assumptions reduces to the condition  $q \ll a^{-1}\lambda(p_m a)^2$ , which in fact refines the condition of Eq. (41), whereas the other limits from above the electric field:

$$eE \ll \frac{\hbar^2 \gamma_n^2(m) p_m}{2m_\infty}.$$
(44)

If  $b_m r_m \ge 1$ , we can see from Eq. (43) that  $c^{(n)}(q) \mid_m^{\pm}$  is exponentially small; in the opposite limit, we obtain



FIG. 6. Distribution of zeros in the denominator of the function  $\Gamma_n(q)$ [Eq. (28)] in the plane of the complex wave number  $k_x$  in the case when there are  $N(k_y)$  discrete subbands. Here,  $N_n = N(k_y)$  or  $N(k_y) - 1$ , where  $m \ge 1$ .

$$c^{(n)}(q)|_{m} = \approx \mp 2B_{m}e^{\pm i\varphi_{m}}\ln(b_{m}r_{m}/2).$$
 (45)

Consequently, in calculation of the total probability of the transfer to states in the continuous spectrum, based on Eq. (29), the main contribution comes—in accordance with Eqs. (43) and (45)—from the values  $b_m r_m \leq 1$ , i.e., it is necessary to satisfy quite well the condition of Eq. (44).

We shall consider the contribution of the vicinity of the point  $k_x = 0$  in the simpler case when  $n < N_n$ . We then have

$$c^{(n)}(q)|_{0} \approx 2B_{Nn}(q) i\Xi(b_{0}g_{Nn}; b_{0}r_{0}), \qquad (46)$$

where

$$b_{0} = b_{Nn}(q), \quad r_{0}^{4} = 4q^{2}/a^{2}(1 - m_{\infty}/m_{0})^{2},$$
  
$$\Xi(\xi, \eta) = \int_{-\infty}^{\infty} k \, dk \sin k [(k^{2} + \xi^{2})^{2} + \eta^{4}]^{-4}. \quad (46')$$

If we consider  $\Xi(\xi,\eta)$  not only for real, but also for imaginary values of the argument  $\xi$ , we can study both a shallow level  $N_n$  and a level split off from the states with the continuous spectrum in the vicinity of the point  $k_x = 0$ , i.e., we can consider the case when  $|k_x a| \leq 1$ . In the latter case, we obtain  $g_{N_n} = ip_{N_n}$ . The approximate result of Eq. (46) is valid if  $p_{N_{n+2}} \ge b_0^{-1}, r_0, |g_{N_n}|$ , and the predominance of  $p_{N_n+2}$  over  $|g_{N_n}|$  is implied already by the condition that the level  $N_n$  is shallow, whereas the other two conditions are equivalent to Eqs. (41) and (44).

5. The final result of these calculations is the total probability of the transfer of an electron from the *n*th level to states in a continuous spectrum, represented by Eq. (29). As demonstrated above, if electric fields are sufficiently low (which corresponds to  $(eaE \ll U_0)$  and *q* is sufficiently small [this condition corresponds to Eq. (41)], the main contribution to  $c^{(n)}(q)$  comes from the vicinity of the points  $k_x = 0$ as well as the points  $k_x = p_m$ ,  $m = \pm (N_n + 2), \pm (N_n + 4),...,$  so that

$$c^{(n)}(q) \approx c^{(n)}(q) |_{0} + \sum_{m=N_{n}+2}^{\infty} ' (c^{(n)}(q) |_{m} + c^{(n)}(q) |_{m}).$$
(47)

Here, a prime denotes a change in m by 2 when the sum in the above expression is calculated. Substitution of Eq. (43) into Eq. (47) gives

$$c^{(n)}(q) \approx c^{(n)}(q) |_{0} + 4i \sum_{m=N_{n}+2}^{\infty} B_{m} K_{0}(b_{m} r_{m}) \sin \varphi_{m}.$$
(48)

The quantity  $c^{(n)}(q)$  becomes exponentially small well before the condition (41) is violated, so that the expression (48) is sufficient in calculation of the integral in Eq. (29). Substitution of Eq. (47) gives

$$w^{(n)} = w^{(n)}(0) + 2\sum_{m=N_n+2}^{\infty} w^{(n)}(m) + \widetilde{w}^{(n)}, \qquad (49)$$

where

$$w^{(n)}(0) = \int_{0}^{\infty} dq |c^{(n)}(q)|_{0}|^{2}, \quad w^{(n)}(m) = \int_{0}^{\infty} dq |c^{(n)}(q)|_{m}|^{2},$$

and  $\tilde{w}^{(n)}$  is the sum of all the interference terms. The contribution of  $\tilde{w}^{(n)}$  in Eq. (49) applies only if the initially adopted hypothesis of collisionless transport of electrons between the branching points applies at distances of the order of  $a^{-1}|1 - m_{\infty}/m_0|^{-1/2}$  along the  $k_x$  axis, i.e., subject to the condition

$$U_{0} \gg eEa > \hbar/\tau |1 - m_{\infty}/m_{0}|^{\frac{1}{2}}, \qquad (50)$$

where  $\tau$  is the mean free time. If  $|1 - m_{\infty}/m_0| \sim 1$ , this condition is satisfied if  $U_0 \tau \gg \hbar$  or  $U_0 \tau > 10^{-15}$  eV·s. If  $\tau \sim 10^{-13}$  s and  $a \sim 5 \times 10^{-7}$  cm, it follows from Eq. (50) that the field *E* has to exceed 10<sup>4</sup> V/cm. It is meaningless to calculate the total integral from Eq. (29) in weaker fields, because the reflection of an electron by a homogeneous field barrier results in repeated dephasing. However, the partial probabilities  $w^{(n)}(0)$  and  $w^{(n)}(m)$  retain their meaning; they apply to short electron transit times when the momentum  $\hbar k_x$  of an electron changes in the vicinity of the branching points (which may be real or imaginary). Then, if the condition  $U_{0\tau} \gg \hbar$  still applies, the probabilities  $w^{(n)}(0)$  and  $w^{(n)}(m)$  are established in a time much shorter than  $\tau$ .

In calculation of just the partial probabilities  $w^{(n)}(m)$  we are in fact dropping the concept of collisionless transport over the full path  $-\infty < k_x < \infty$  and, consequently, there is no need to limit the treatment to the case when  $m_{\infty} < m_0$ , as assumed at the beginning of the present section. The results obtained below for the partial probabilities are valid in the vicinity of any branching point irrespective of the sign of  $\lambda$ . This applies also to the probability  $w_m^{(n)} = 2|c_{m(+)}^{(n)}|^2$  obtained from Eq. (39) for a transition to a discrete level near its branching point.

Using Eq. (43), we obtain

$$w^{(n)}(m) = (E/E_m^{(n)})^3, \tag{51}$$

where

$$E_m^{(n)} = \frac{[\gamma_n(m)]^{11/3}m_0\hbar^2}{e|\lambda|p_m m_{\infty}^2 (16\pi a)^{\frac{1}{3}} [A_n(m)]^{\frac{1}{3}}} \cdot$$

In calculation of  $w^{(n)}(m)$  we find that the main contribution to the integral with respect to q comes from the range

$$q \leq \frac{2eEam_{\infty}^{2}|\lambda|p_{m}}{\hbar^{2}[\gamma_{n}(m)]^{2}m_{\varrho}} \ll ap_{m}^{2}\left|1-\frac{m_{\infty}}{m_{\varrho}}\right|,$$

which ensures that the inequalities given above, particularly Eq. (41), are satisfied. The field  $E_m^{(n)}$  in Eq. (51) is of the order of  $\zeta(U_0/ea)$ , where  $\zeta \sim 1$  applies to a relatively shallow level *n* and  $\zeta \ll 1$  describes a deep level *n*. Hence, it follows that the probability  $w^{(n)}(m)$  is low in the investigated range of fields, but it is not exponentially small in any field. A comparison of the probability  $w^{(n)}(m)$  of a transition from a level *n* to a state with the continuous spectrum near the *m*th branching point with the probability of a transition to the *m*th level itself  $w_m^{(n)} = 2|c_{m(+)}^{(n)}|^2$ , where  $|c_{m(+)}^{(n)}|^2$  is calculated from Eq. (40), demonstrates that these probabilities agree apart from a factor of 2.

#### **5. DISCUSSION OF RESULTS**

A purely dynamic analysis of the transport of electrons in a homogeneous longitudinal field  $E_x = E$  shows that an electron which initially moves in one of the size-quantization subbands has a finite probability of transfer to other subbands, and also to states with a continuous spectrum. This intersubband tunneling in weak fields E is characterized by an exponential smallness over all parts of a path  $k_x(t)$  in the plane of a two-dimensional wave vector  $(k_x, k_y)$ , with the exception of the vicinity of the points where this path intersects regions in the vicinity of the branching points  $k_x^2 + k_y^2 = k_m^2$ . If  $eEa \ll U_0$ , these regions are much smaller than the distances between neighboring branching regions. Near branching points the probability of a transition to the subband split off most and the total probability of a transition to states in a continuous spectrum both increase with the field as  $E^3$ , i.e., a typical tunnel exponential function no longer occurs in the expression for the probability.

The dynamic approach adopted above is valid only in the range of fairly high fields described by Eq. (50) subject to the condition  $U_0 \tau \gg \hbar$ . In weaker fields an electron travels without collisions only within intervals  $\Delta k_x$ , which are small compared with the separation between the branching regions, but is sufficiently large compared with the intervals that make the dominant contribution to the  $k_y$ -dependent partial tunneling probabilities  $w^{(n)}(0)$  and  $w^{(n)}(m)$  in the vicinity of the branching regions.

Since the motion of an electron in the latter case is of stochastic nature, it is described by a semiclassical kinetic equation

$$\frac{\partial f_n(\mathbf{k})}{\partial t} - \frac{eE}{\hbar} \frac{\partial f_n(\mathbf{k})}{\partial k_x}$$
$$= \operatorname{St} f - f_n(\mathbf{k}) \sum_m w_m^{(n)}(k_y) \frac{e|E|}{\hbar} \delta(k - k_m), \quad (52)$$

where  $f_n(\mathbf{k})$  is the distribution function in the *n*th subband;  $k = |\mathbf{k}|$ ; St *f* is the collision integral describing the scattering between states with different values of **k** both within the subband *n* and between the subbands, i.e., dependent also on  $f_{n'}(\mathbf{k}'), n' \neq n$ . The new term in the kinetic equation is last on the right-hand side where  $W_m^{(n)}(k_y) = w^{(n)}(m) + w_m^{(n)}$  and it describes the loss from the *n*th subband to states with a continuous spectrum and to the subbands which branch off. Equation (52) does not contain terms describing the tunnel return from states with a continuous spectrum and from discrete bands, i.e., in a homogeneous situation this equation can describe only nonequilibrium decay of the electron density in a well under the influence of heating and of the tunneling in a longitudinal field *E*. In an inhomogeneous case this equation, supplemented by the diffusion term  $\mathbf{v}_n(\mathbf{k})\partial f_n/\partial \mathbf{r}$ , can describe the reduction in the electron density in the well and can be used to deal with similar problems.

The authors are grateful to M. I. Dykman for valuable discussions.

- <sup>1</sup>P. J. Price, Ann. Phys. (N.Y.) **133**, 217 (1981).
- <sup>2</sup>A. Riddoch and B. K. Ridley, Physica B (Utrecht) 134, 342 (1985).
- <sup>3</sup>Z. S. Gribnikov, Fiz. Tekh. Poluprovodn. 6, 1380 (1972) [Sov. Phys. Semicond. 6, 1204 (1973)].
- <sup>4</sup>K. Hess, H. Morkoç, H. Shichijo, and B. G. Streetman, Appl. Phys. Lett. **35**, 469 (1979).
- <sup>5</sup>A. Kastalsky, O. Marroux, and R. Bhat, J. Appl. Phys. 62, 305 (1987).
- <sup>6</sup>A. Ziegler and U. Rössler, Solid State Commun. 65, 805 (1988).
- <sup>7</sup>Z. S. Gribnikov and O. É. Raĭchev, Abstracts of Papers presented at Second All-Union Conf. on Physics of Semiconductors, Kishinev, 1988 [in Russian], Vol. 1, p. 14.
- <sup>8</sup>R. E. Doezema and H. D. Drew, Phys. Rev. Lett. 57, 762 (1986).
- <sup>o</sup>V. F. Gantmakher and I. B. Levinson, *Scattering of Carriers in Metals and Semiconductors* [in Russian], Nauka, Moscow (1984).
  - <sup>10</sup>G. Bastard, Phys. Rev. B 25, 7584 (1982).
  - <sup>11</sup>Y.-Ch. Chang, J. N. Schulman, G. Bastard *et al.*, Phys. Rev. B **31**, 2557 (1985).
  - <sup>12</sup>Y. R. Lin-Liu and L. J. Sham, Phys. Rev. B 32, 5561 (1985).
  - <sup>13</sup>R. A. Suris, Fiz. Tekh. Poluprovodn. 20, 2008 (1986) [Sov. Phys. Semicond. 20, 1258 (1986)].
  - <sup>14</sup>L. V. Keldysh, Zh. Eksp. Teor. Fiz. **33**, 994 (1957) [Sov. Phys. JETP 6, 763 (1958)].
  - <sup>15</sup>J. Callaway, Energy Band Theory, Academic Press, New York (1964).

Translated by A. Tybulewicz