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ZENER TUNNELING IN SEMICONDUCTORS

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Abstract—The Zener current in a constant field is calculated both with and without the WANNIER–ADAMS reduction of the interband-coupling terms. The Zener current is only slightly different in the two cases, a fact which has already been noted by WANNIER. The apparent reduction of interband coupling is interpreted as a polarization correction. A detailed calculation of the Zener current is made for a simple two-band model which is applicable to InSb. The evaluation of the tunneling integral follows closely a calculation due to KELDYSH.

1. INTRODUCTION

THE possibility that electrons might tunnel through the forbidden band of an insulator in a strong electric field was first suggested by ZENER[1]. Measurements of the current–voltage characteristic of a reverse-biased diode have been interpreted in terms of Zener tunneling.[2] However, other investigations[3] of the so-called "soft-breakdown" characteristic have shown considerable variation from sample to sample in a manner which is hard to reconcile with a Zener tunneling between the valence and conduction bands. More recently, forward current–voltage characteristics in heavily doped junctions have been clearly shown by ESAKI[4] to result from Zener tunneling.

The tunneling problem has been treated theoretically by HOUSTON[5] and MCAFEE *et al.*[6]. WANNIER[7] and ADAMS[8] have shown that the leading terms in the Hamiltonian causing interband transitions can be removed by a perturbation transformation which transforms the original Bloch functions in the field-free crystal to Bloch functions in the presence of the field. At first sight, this transformation appears to affect significantly the calculation of the Zener current. FRANZ[9] and later WANNIER[10] have concluded, however, that this is not the case. Section 2 of the present paper shows in detail that the formula for Zener tunneling is not significantly affected by the WANNIER–ADAMS transformation. The change that does result is partly due to a direct modification of the energy bands by the presence of the electric field and partly due to the introduction of terms which permit transitions with the use of higher or lower bands as virtual intermediate states. The WANNIER–ADAMS transformation is interpreted as taking account of valence-electron polarization, which has very little effect on the Zenner current for small fields.

The most recent calculation of Zener tunneling has been made by KELDYSH[11]. Although KELDYSH was apparently unaware of the WANNIER–ADAMS transformation, his approach is entirely justified, as we show in Section 2. In Section 2 we introduce energy eigenfunctions which provide a simpler and more rigorous treatment than the method used by KELDYSH. However, we arrive at the same integral for the tunneling probability. In Section 3 we follow KELDYSH's method of evaluating the tunneling integral for the case of two simple interacting bands, an approximation which holds well for InSb. Our results agree with KELDYSH's except for a rather large numerical factor. The present calculation is also useful in that it specifies the circumstances for which the band-structure assumptions made by KELDYSH are valid. In Section 4 the results are discussed and numerical examples are given.

2. ZENER CURRENT AND POLARIZATION EFFECTS

The time-independent Schroedinger equation in the presence of a uniform electric field in the

x-direction may be written:

$$\left[E_n(k)-iF\frac{\partial}{\partial k_x}-E\right]a_n(k)-\sum_{n'}FX_{nn'}a_{n'}(k)=0 \tag{1}$$

where F is the force on the electron, $E_n(k)$ is the energy of an electron in the periodic lattice and E is the total energy. We are using ADAM's[12] "crystal momentum" representation where the basis functions are Bloch functions $\psi_n(k,r)$. The position operator x has been decomposed into an intraband operator $i\partial/\partial k_x$ and an "interband" operator $X_{nn'}(k)$. The operator X may also have an intraband component X_{nn} which may be conveniently absorbed in the energy by writing:

$$E_n^{(1)}(k)=E_n(k)-FX_{nn}(k) \tag{2}$$

where the superscript 1 denotes that the energy contains the electric field to first order. The off-diagonal matrix elements $X_{nn'}$ are given by the equation:

$$X_{nn'}=i\int u_{nk}^*\frac{\partial}{\partial k}u_{n'k}\,dr \tag{3}$$

where u_{nk} is the periodic part of ψ_{nk} normalized in the unit cell. The integration in equation (3) extends over the unit cell.

If the interband terms in equation (1) are ignored, the eigenfunctions may be written down immediately:

$$E_n^{(1)}(k)=\kappa^{-\frac{1}{2}}\exp\left\{\frac{i}{F}\int_0^{k_x}[E-E_n^{(1)}(k')]\,dk'_x\right\}\times$$

$$\times\delta(k_y-k_{y0})\delta(k_z-k_{z0}) \tag{4}$$

The "δ functions" are normalized in the first Brillouin zone. The normalization constant κ is the length of the line (k_x, k_{y0}, k_{z0}) subtended by the first Brillouin zone. This treatment is only rigorously correct when the subtended line is a principal vector of the reciprocal lattice. In the general case, the electron traverses a non-periodic path through k-space and the integration should cover the entire path. A different set of values k_{y0}, k_{z0} would obtain on each line segment of the total path, so the analysis would be appreciably more complicated. When the subtended segment is a principal vector, it is easy to install proper boundary conditions which determine the eigenvalues, E. The proper boundary condition is that the phase factor of equation (4) should be the same for the end points k_1, k_2 of the line of integration, since these points are identical. This leads to the condition:

$$\int_{k_1}^{k_2}[E-E_n^{(1)}(k')]\,dk_x'=2\pi nF \tag{5}$$

$$\Delta E=2\pi F/\kappa \tag{6}$$

where ΔE is the spacing between successive eigenvalues.

In an appendix we discuss the spatial dependence of the eigenfunctions of equation (4) and show that they have the expected character of dying away exponentially in the forbidden region between bands in the manner of a WKB function.

Using the eigenfunctions of equation (4), the interband terms in equation (1) then give the following matrix elements, $M_{nn'}^{(1)}$ connecting states of equal energy in different bands:

$$M_{nn'}^{(1)}=-(F/\kappa)\int X_{nn'}(k)\times$$

$$\times\exp\left\{\frac{i}{F}\int_0^{k_x}[E_n^{(1)}(k')-E_{n'}^{(1)}(k')]\,dk_x'\right\}dk_x \tag{7}$$

The probability per unit time, w, of making a transition from band n to band n' is given by the usual formula:

$$w=\frac{2\pi}{\hbar}|M_{nn'}^{(1)}|^2\rho(E) \tag{8}$$

where $\rho(E)$, the density of states, is obtained immediately from equation (6), since $\rho=(1/\Delta E)$.

$$\rho(E)=(\kappa/2\pi F) \tag{9}$$

The k_{y0} and k_{z0} components of k are constants of the motion which do not change on making a transition from one band to another.

The use of equation (8) is not completely standard, since the density of states does not tend to infinity with infinite volume in the usual manner. For a small field the density of states, as given by equation (9), will be very large but finite. The use of equation (8) is correct only for times $t\ll\tau=\hbar/\Delta E=\hbar\kappa/F$. τ is the time required to traverse the band once when κ is a principal k-vector. For times longer than τ the energy spacing between levels can be resolved and the use of equation (8) is invalid.

In most cases phonons will scatter the electron in a time considerably shorter than τ, so that the energy spacing ΔE would be unresolvable. The use of equation (8) is then permissible. A completely rigorous treatment

of the Zener tunneling problem would require the introduction of phonons from the start.

Another approximation implicitly involved in the use of equation (8) is the assumption that $M^2\rho(E)$ varies slowly from one discrete level to the next, so that the sum over states may be replaced by an integral. If we evaluate $M_{nn'}$ for states differing in energy by an amount $\mathscr{E}$ we obtain:

$$\frac{dM^2\rho(E)}{d\mathscr{E}}\cdot\frac{\Delta E}{M^2\rho(E)}=4\sqrt{(2)}\pi\,\frac{m_r^{\frac{1}{2}}E_G^{\frac{1}{2}}}{\hbar\kappa}$$

where ΔE is given by equation (6). We find that this quantity is generally smaller than 1 for most cases of interest, but not sufficiently smaller that the approximation is highly accurate. (We used parabolic bands to evaluate the above expression.)

We now propose to demonstrate that the expression giving the interband transition probability, w, remains essentially the same even though the interband term in equation (1) is formally transformed to be of higher order in F, in the manner of WANNIER[13] and ADAMS[14].

We make a perturbation transformation on equation (1), eliminating interband terms to first order in F:

$$d_n(k)=e^{iT}a_n(k) \tag{10}$$

$$T=iFX_{nn'}/(E_n^{(1)}-E_{n'}^{(1)}) \tag{11}$$

Equation (1) then becomes, to second order in F:

$$\left[E_n^{(2)}(k)-iF\frac{\partial}{\partial k_x}-E\right]d_n(k)+\sum_{n'\neq n}F^2Q_{nn'}d_{n'}(k)=0 \tag{12}$$

$$E_n^{(2)}(k)=E_n^{(1)}(k)+F^2\sum_{n'\neq n}|X_{nn'}|^2/(E_n^{(1)}-E_{n'}^{(1)}) \tag{13}$$

$$Q_{nn'}=\left[\tfrac{1}{2}\sum_{n''\neq n,n'}X_{nn''}X_{n''n'}\left(\frac{1}{E_n^{(1)}-E_{n''}^{(1)}}+\frac{1}{E_{n'}^{(1)}-E_{n''}^{(1)}}\right)\right]+i\frac{\partial}{\partial k_x}\left(\frac{X_{nn'}}{E_{n'}^{(1)}-E_n^{(1)}}\right) \tag{14}$$

We have used equation (2). Equation (13) gives the correction to the energy bands due to the polarization of the Bloch functions by the applied field.

Equation (12) has the same formal structure as equation (1); hence the previously given calculation of the wave functions and transition probabilities will proceed entirely similarly. The new wave functions are the same as the q_n's given by equation (4), except that $E_n^{(2)}$ replaces $E_n^{(1)}$. The new interband transition matrix elements, $M_{nn'}^{(2)}$, corresponding to the $M_{nn'}^{(1)}$ of equation (7), become:

$$M_{nn'}^{(2)}=(F^2/\kappa)\int Q_{nn'}(k)\times$$

$$\times\exp\left\{\frac{i}{F}\int_0^{k_x}[E_n^{(2)}(k')-E_{n'}^{(2)}(k')]\,dk_x'\right\}dk_x \tag{15}$$

In demonstrating the approximate equivalence of equation (15) to (7), we ignore the bracketed term in equation (14). This term involves at least three distinct bands n, n', n'' and hence is a true higher-order term not included in the earlier treatment. Substituting the unbracketed term for $Q_{nn'}$ yields:

$$M_{nn'}^{(2)}=\frac{iF^2}{\kappa}\int\frac{\partial}{\partial k_x}\left(\frac{X_{nn'}}{E_{n'}^{(1)}-E_n^{(1)}}\right)\times$$

$$\times\exp\left\{\frac{i}{F}\int_0^{k_x}[E_n^{(2)}(k')-E_{n'}^{(2)}(k')]\,dk_x'\right\}dk_x \tag{16}$$

Integrating the right-hand side by parts* gives:

$$M_{nn'}^{(2)}=-\frac{F}{\kappa}\int\left(\frac{E_n^{(2)}-E_{n'}^{(2)}}{E_n^{(1)}-E_{n'}^{(1)}}\right)X_{nn'}\times$$

$$\times\exp\left\{\frac{i}{F}\int_0^{k_x}[E_n^{(2)}-E_{n'}^{(2)}]\,dk_x'\right\}dk_x \tag{17}$$

* G. H. WANNIER has obtained a similar result (private communication).

The contribution from the end points is zero by virtue of the boundary condition of equation (5) together with the periodicity of E_n and $X_{nn'}$ in k-space. (We have proved this rigorously only for the case when the line of integration is a principal lattice vector, but it is undoubtedly true in general.) Equation (17) then differs from equation (7) only to the extent that the second-order energy gaps $E_n^{(2)}-E_{n'}^{(2)}$ differ from the first-order gaps, $E_n^{(1)}-E_{n'}^{(1)}$.

The rather surprising result of the approximate equivalence of equations (7) and (17) has the following origin. For a filled band, the applied field produces two distinct effects, a polarization of the valence electrons similar to an ordinary atomic polarizability, and a Zener tunneling leading to conductivity. Both these effects are contained in the interband term $X_{nn'}$ of equation (1). Since the Bloch functions are not localized in space, and consequently not in energy, this term does not distinguish between the virtual transitions associated with polarization and the energy-conserving transitions associated with Zener tunneling. The energy eigenfunction treatment which we have given does separate these two effects and shows that the matrix elements between states of equal energy are very little affected by the WANNIER–ADAMS transformation.

The WANNIER–ADAMS treatment could be carried out to arbitrary order, removing the interband coupling to any desired order in the field. A succession of integrations by parts would show that the Zener tunneling effect remains substantially unaltered.

3. EVALUATION OF THE TUNNELING PROBABILITY

We follow the procedure of FRANZ[9] and KELDYSH[12] and evaluate the integral of equation (7) by a technique similar to the method of stationary phase. The path of integration in equation (7) can be deformed into the complex plane to pass through the point which makes the maximum contribution to the integral, namely the point $k_x = q$ for which

$$E_n^{(1)}(q) = E_{n'}^{(1)}(q) \tag{18}$$

Equation (18) is satisfied for a branch point in the complex plane where the conduction and valence bands join. KELDYSH has derived the behavior of E and X in the vicinity of this branch point by using some very general properties of the solutions of second-order differential equations. We feel that it is useful to derive his results more explicitly by using a particular model. The model we use is that of two bands "interacting" via the $k \cdot p$ perturbation. InSb is a good example of a material for which this approximation applies.[15]

The two-band Hamiltonian is:

$$H = \begin{pmatrix} E_G+\hbar^2k^2/2m & (\hbar/m)kp \\ (\hbar/m)kp & \hbar^2k^2/2m \end{pmatrix} \tag{19}$$

The band gap is E_G, the zero of energy is the top of the valence band, and the bands "repel" each other via the momentum matrix element p, which may be taken to be real and positive.

The solutions of equation (19) are:

$$E_\pm = \frac{E_G}{2}+\frac{\hbar^2k^2}{2m}\pm\frac{\eta}{2} \tag{20}$$

$$\eta = \sqrt{E_G^2+\frac{4\hbar^2k^2p^2}{m^2}} \tag{21}$$

where + refers to the conduction band and − refers to the valence band. We can calculate the effective masses at the band edge to be:

$$\frac{1}{m_+} = \frac{2p^2}{m^2E_G}\pm\frac{1}{m} \tag{22}$$

(We use the convention that effective masses are positive quantities. The two-band approximation is valid only in cases where equation (22) gives positive masses for both bands.) If we define a reduced mass, m_r, by:

$$\frac{1}{m_r} = \frac{1}{m_+}+\frac{1}{m_-} \tag{23}$$

we can express p in terms of m_r as follows:

$$p = \frac{m}{2}\sqrt{\frac{E_G}{m_r}} \tag{24}$$

Rewriting equation (21) with the use of equation (24), we have:

$$\eta = \sqrt{E_G^2+E_G\hbar^2k^2m_r^{-1}} \tag{25}$$

Equations (20) and (25) show clearly that the

conduction and valence bands are two sheets joined at the branch points, q:

$$q = \pm i\sqrt{\frac{m_r E_G}{\hbar^2} + k_z^2 + k_y^2} \tag{26}$$

(For our purposes we regard only k_x as being a complex variable.) If u refers to the cell-periodic functions for $k = 0$, then the functions U which diagonalize H of equation (19) are given by:

$$U_c = \frac{1}{\sqrt{(2\eta)}}\{(\eta+E_G)^{\frac{1}{2}}u_c + (\eta-E_G)^{\frac{1}{2}}u_v\} \tag{27}$$

$$U_v = \frac{1}{\sqrt{(2\eta)}}\{(\eta-E_G)^{\frac{1}{2}}u_c - (\eta+E_G)^{\frac{1}{2}}u_v\}$$

Using these expressions, we can calculate $X_{nn'}$ as given by equation (3):

$$X_{cv} = i\hbar E_G^{\frac{1}{2}}/2m_r^{\frac{1}{2}}\eta^2 \tag{28}$$

$$X_{cc} = X_{vv} = 0 \tag{29}$$

$$E_c - E_v = \eta \tag{30}$$

$$\int_0^{k_x} \eta\, dk_x = \frac{k_x\eta}{2} + \frac{\sqrt{(m_r E_G)}}{\hbar}\left\{E_G + \frac{\hbar^2}{m_r}(k_z^2+k_y^2)\right\}\times \log\left[\frac{\eta+\hbar k_x\sqrt{(E_G/m_r)}}{\{E_G^2+E_G\hbar^2(k_z^2+k_y^2)m_r^{-1}\}^{\frac{1}{2}}}\right] \tag{31}$$

The maximum contribution to the integral of equation (7) comes from the vicinity of the point q for which $\eta = 0$. We deform the contour of integration in the k_x plane to pass by this point, as shown in Fig. 1. The factor X_{cv} has a pole at q. The contribution to the integral from the semicircle, $\int_{sc}$, is:

$$\int_{sc} = \frac{\pi\sqrt{(E_G m_r)}}{4\hbar q\kappa} F \exp\left[\frac{i}{F}\int_0^q \eta\, dk_x\right] \tag{32}$$

The horizontal integral in the neighborhood of q will also contribute to the value of the integral. To calculate this contribution, we make an expansion

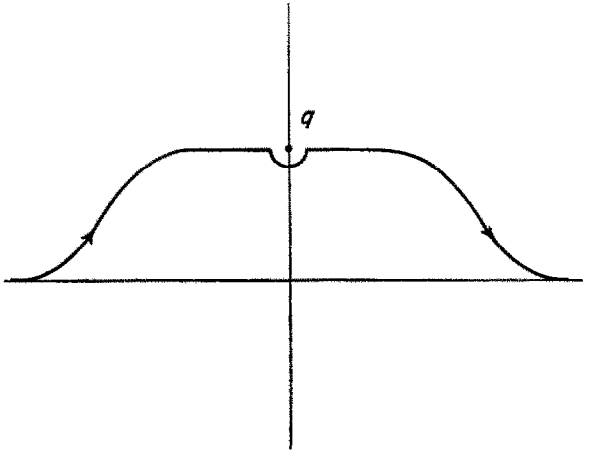

FIG. 1. Contour of integration for equation (33).

of η as a function of k about q:

$$\sigma = k - q \tag{33}$$

$$\eta = (\sqrt{2})\hbar\sqrt{\frac{E_G}{m_r}}\sqrt{(\sigma q)} + \ldots \tag{34}$$

$$\int_0^\sigma \eta\, dk = \frac{2(\sqrt{2})\hbar}{3}\sqrt{\frac{E_G}{m_r}}q^{\frac{1}{2}}\sigma^{\frac{3}{2}} + \ldots \tag{35}$$

We substitute the leading terms of these expansions in equation (7) and extend the limits of integration to $\pm\infty$. These approximations are justified for small F. The integral over the horizontal portion

of the contour in the vicinity of q, $\int_{hor}$ then becomes:

$$\int_{hor} = \frac{\pi\sqrt{(E_G m_r)}F}{12\hbar q\kappa} \exp\left\{\frac{i}{F}\int_0^q \eta\, dk_x\right\} \quad (36)$$

Combining the two contributions to the integral of equation (7) and evaluating equation (31) for $k_x = q$, we find:

$$M_{nn'}^{(1)} = \frac{\pi\sqrt{(m_r E_G)}F}{3\hbar q\kappa} \exp\left\{\frac{-\pi\hbar|q^2|E_G^{\frac{1}{2}}}{4Fm_r^{\frac{1}{2}}}\right\} \quad (37)$$

To compute the rate of Zener tunneling per cm^3, we multiply the transition probability per electron, w, by the number of electrons per cc, $2\kappa(2\pi)^{-3}\, dk_y\, dk_z$ and integrate k_y and k_z over the filled band. (We are including a factor of 2 for spin.) The result is:

$$n = \frac{FE_G m_r}{36\pi\hbar^3}\int \frac{1}{|q|^2}\exp\left\{\frac{-\pi\hbar|q|^2E_G^{\frac{1}{2}}}{2Fm_r^{\frac{1}{2}}}\right\} dk_y dk_z \quad (38)$$

n is the number of electrons per sec per cm^3 leaking from the valence band to the conduction band. Transforming to circular coördinates and replacing q^2 by $E_G m_r/\hbar^2$ in the denominator (an approximation valid for small F), we obtain:

$$n = \frac{F^2 m_r^{\frac{1}{2}}}{18\pi\hbar^2 E_G^{\frac{1}{2}}}\exp\left\{\frac{-\pi m_r^{\frac{1}{2}}E_G^{\frac{1}{2}}}{2\hbar F}\right\} \quad (39)$$

The fact that the quantity κ does not appear in the final result lends credence to the assumption that the calculation for a general field direction proceeds as we have outlined it. Our treatment is rigorous only when κ is a principal vector of the reciprocal lattice, as we have already noted. KELDYSH also justifies his derivation in this way.

4. DISCUSSION

Equation (39) is very similar to equation (19) in KELDYSH's paper.[12] If we compare the two results for InSb, for which the approximations made here should apply, equation (39) gives a value of n which is a factor 72 smaller than KELDYSH's result. Of this factor 72, a factor 9 is due to a numerical error in the evaluation of the contour integral leading to $|M_{nn'}|^2$, a factor 2 is of uncertain origin, and a factor 4 is due to a different method of counting the valence electrons. KELDYSH multiplies his density of states by a factor equal to the number of valence electrons in the unit cell (8 for InSb). Our view is that this factor should be 2, since this is the number of electrons in the light mass band. Only these electrons have an appreciable probability of tunneling into the conduction band.

We find that KELDYSH's constant γ, which he leaves unspecified, should be set equal to zero for the case considered here.*

KELDYSH's result is derived more generally than our own. We find an isotropic mass, m_r, whereas KELDYSH finds an anisotropic mass. Results analogous to equations (32) and (36) can, in fact, be derived quite generally by KELDYSH's method. However, the evaluation of the exponential factor which involves the integral

$$\int_0^q \eta\, dk_x$$

cannot be done in general by using equation (25) (or its generalization to an anisotropic effective mass). Correct evaluation of this integral requires an accurate knowledge of the band structure from $k_x = 0$ to $k_x = q$. KELDYSH's expansion about the branch point, q, will not be sufficiently accurate for this purpose in the general case.

To give some idea of the magnitude of the Zener effect, we evaluate equation (39) for InSb with a field of 5×10^4 V/cm. The parameters we use are $E_G = 0{\cdot}23$ eV, $m_r = 0{\cdot}0065\, m_0$. (The reduced mass is appropriate to an electron and a *light* hole.) The exponential pre-factor has the value:

$$\frac{F^2 m_r^{\frac{1}{2}}}{18\pi\hbar^2 E_G^{\frac{1}{2}}} = 4\times10^{29} \text{ per cc sec}$$

* *Note added in proof:* We have assumed $X_{cc} = X_{vv} = 0$. For a material like InSb which lacks inversion symmetry this is not correct. The wave functions at $k = 0$ may possess dipole moments which lead to a first order stark shift in the energy bands as indicated in equation (2). This term is included in equation (7) and may be shown to lead to KELDYSH's constant, γ. Estimates of γ indicate that it will make only a small correction to equation (39).

and the exponent is

$$\frac{\pi m_r^{\frac{1}{2}} E_G^{\frac{3}{2}}}{2\hbar F} = 10{\cdot}2$$

which yields

$$n = 1{\cdot}4 \times 10^{25} \text{ per cm}^3 \text{ sec.}$$

If the field extends over 10^{-4} cm, the current would then be $j = 220$ A/cm^2. These values are purely for illustrative purposes. In an actual junction the field will not be constant, and equation (39) must be integrated over the junction. If the field is not substantially constant over a region for which the potential varies by one band gap, the derivation leading to equation (39) is not valid.

We can use equation (13) to estimate what error the neglect of polarization corrections to the energy bands has introduced into our calculations. With the help of equation (28) we compute that for $F = 5 \times 10^4$ cm/sec

$$\Delta E_G = 0{\cdot}006 E_G$$

$$\Delta \frac{1}{m_r} = -0{\cdot}06 \frac{1}{m_r}$$

The correction to the effective mass is larger than the band-gap correction, but neither is a big effect for this field. Since the corrections go as F^2, they quite rapidly become important for higher fields.

In our treatment of Zener tunneling we have considered only the conduction band and the light mass valence band. Actually InSb also has a heavy mass valence band degenerate at $k = 0$ with the light mass band. (The most exact description of the bands is even more complicated.[15]) The coupling between the two degenerate bands can be ignored only in the semiclassical limit which corresponds to weak fields. We expect this approximation to break down for fields of the same order as those calculated above.

FRANZ[9] has considered the effect of the coulomb attraction between electron and hole on the Zener current. He finds the effect expressible as a multiplicative factor, f_{eh}, which should multiply the right-hand side of equation (39). FRANZ gives:

$$f_{eh} = \exp\left\{\frac{\sqrt{(2m^*)}e^2}{4\hbar\epsilon\sqrt{(E_G)}}\right\} \tag{40}$$

where ϵ is the dielectric constant (16 for InSb). This factor is almost exactly unity for InSb.

For other III–V materials with minima at $k = 0$, the simple two-band theory is not as accurate as for InSb, because the p-like valence band lowered by spin-orbit interaction has an important influence on the conduction-band mass. It should not be too difficult to insert a more accurate expression for η in equations (32) and (36) to obtain useful numerical results in these cases.

In the case of germanium, the indirect band gap poses additional problems. For low fields, transitions from the valence band to the (111) conduction band minimum will involve phonons to insure k conservation. This point has been discussed by KELDYSH[12]. For high fields and reverse bias, Zener transitions to the $k = 0$ minimum will be most likely, but here, too, the simple two-band theory is invalidated by the spin-orbit split-off band.

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APPENDIX

The meaning of the energy eigenfunctions $q_n(k)$ of equation (4) is more readily appreciated if they are expressed in the familiar r representation:

$$q_n(k) \to Q_n(r) = \kappa^{-\frac{1}{2}} \int e^{ik\cdot r} u_{nk}(r) \times$$

$$\times \exp\left\{\frac{i}{F}\int_0^{k_x} [E - E_n(k')]\, dk_x'\right\} dk_x. \tag{A.1}$$

Equation (A.1) becomes more revealing if it is evaluated approximately by the method of steepest descents.[16] We write the integrand in the form

Integrand $= e^f$

$$f = ik \cdot r + (i/F) \int_0^{k_x} [E - E_n(k')]\, dk_x' + \ln u_{nk}(r) \tag{A.2}$$

The function f is then written as a Taylor series about the point of stationary phase k_{xs}

$$f = f(k_{xs}) + \frac{(k - k_{xs})^2}{2} f''(k_{xs}) + \cdots \tag{A.3}$$

$$f'(k_{xs}) = 0, \tag{A.4}$$

where equation (A.4) determines the point of stationary phase. The integral then has the value (asymptotic in $1/F$):

$$Q_n(r) = \kappa^{-\frac{1}{2}} [-2\pi/f''(k_{xs})]^{\frac{1}{2}} e^{f(k_{xs})}. \tag{A.5}$$

Equations (A.2) and (A.4) then give the following conditions for k_{xs}, $f''(k_{xs})$

$$E - E_n(k_{xs}) + Fx - iF\left(\frac{\partial}{\partial k_x} \ln u_n\right)_{k_{xs}} = 0. \tag{A.6}$$

$$f''(k_{xs}) = -\frac{i}{F}\left(\frac{\partial E}{\partial k_x}\right)_{k_{xs}} + i\left(\frac{\partial^2}{\partial k_x^2} \ln u_n\right)_{k_{xs}} \tag{A.7}$$

The terms involving u_n in equation (A.6) and (A.7) can be ignored in the limit of small F, giving the result:

$$Q_n(r) = \kappa^{-\frac{1}{2}} \left[-2\pi i F \Big/ \frac{\partial E_n}{\partial k_x}\right]_{k_{xs}}^{\frac{1}{2}} u_n(k_{xs}, r) \exp\left\{\frac{i}{F} \int_0^{k_{xs}} [E - E_n(k_x') + Fx]\, dk_x' + i(k_{y0} y + k_{z0} z)\right\} \tag{A.8}$$

$$E - E_n(k_{xs}) + Fx = 0. \tag{A.9}$$

As before, k_{y0} and k_{z0} are constants of the motion.

The integral in the exponent of equation (A.8) can be given a more familiar form by a change of variables $k_x \to x$ where k_x and x are related by an equation of the same form as equation (A.9):

$$E - E_n(k_x) + Fx = 0 \tag{A.10}$$

An integration by parts then yields

$$Q_n(r) = \kappa^{-\frac{1}{2}} \left[2\pi F \Big/ \frac{\partial E_n}{\partial k_x}\right]_{k_{xs}}^{\frac{1}{2}} u_n(k_{xs}, r) \times \exp i\left\{\int_{x_0}^{x} k_x\, dx + k_{y0} y + k_{z0} z\right\} \tag{A.11}$$

where x_0 corresponds to $k_x = 0$ in equation (A.10) and we have discarded an unimportant phase factor. The "stationary phase" relationship of equation (A.9) is the "classical" relationship between position and k-vector.

In the limit of low fields the classical requirement of defining position and k-vector at the same time can be satisfied. Equations (A.10) and (A.11) show that the phase of the wave function accumulates along the classical trajectory in the standard manner of a WKB function.

The transformation of variables from k_x to x given by equation (A.10) can also be used to clarify the meaning of equations (7) and (37). Equation (7) may be written:

$$M_{nn'} = -(F/\kappa) X_{nn'}(k) \exp i\left\{\int_{x_0'}^{x'} \bar{k}_x\, dx' - \int_{x_0}^{x} k_x\, dx\right\} \tag{A.12}$$

where x' and x_0' obey a relation analogous to equation (A.10) with $E_{n'}$ replacing E_n. Equation (37) was derived from equation (7) by the method of steepest descents. The point of steepest descent k_σ as given by equation (30):

$$E_c(k_\sigma) = E_v(k_\sigma)$$

is the same as the condition

$$x_\sigma = x'_\sigma \tag{A.13}$$

$$M_{nn'} \sim \exp i\left\{\int_{x_0'}^{x_\sigma} \bar{k}_x\, dx' + \int_{x_\sigma}^{x_0} k_x\, dx\right\} \tag{A.14}$$

Equation (A.14) gives the exponential factor in equation (A.12) evaluated for $x = x'$. The exponent in equation (A.14) is the integral of an imaginary k vector from one band edge to the other where the k vector is determined from equation (A.10) with E_n on one side of the branch point, $E_n = E_{n'}$, and by the analogous equation with $E_{n'}$ on the other. The imaginary k vector leads to attenuation in the manner typical of barrier penetration.