Tunneling transitions in a complex valence band in a semiconductor

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A study is made of the tunneling of holes between the light and heavy subbands of the degenerate valence band (described by an isotropic Luttinger Hamiltonian) of a Ge-type semiconductor in a static electric field E. The transition probabilities and the flux densities are found for the tunneling of holes between subbands, and the results of numerical calculations are presented. It is found that the effective tunneling region in momentum space is a torus at the center of the Brillouin zone, with axis along E and linear dimensions of the order of $(2m^*\hbar eE)^{1/3}$ ($1/m^*$ is the difference between the reciprocals of the effective masses of light and heavy holes, and e is the charge of a hole). In this region the tunneling probability is close to unity.

A strong electric field causes tunneling transitions of electrons between different energy bands in a semiconductor. However, studies of these transitions have dealt mainly with the tunneling of electrons between the valence and conduction bands,[1–5] which leads to an increase in the total number of free change carriers in the semiconductor.

In the present study we consider the tunneling of holes between subbands of the degenerate valence band of a germanium-type semiconductor. This tunneling does not change the total number of free charge carriers but leads only to a redistribution among subbands. This redistribution must be taken into account in streaming effects, in producing inverted hole distributions in semiconductors, and in other phenomena pertaining to the hot-carrier region.

In studying tunneling within a degenerate band one cannot use the methods developed for studying band-to-band tunneling, as these methods rely on the smallness of the tunneling probability due to the finite gap width.

Let us consider the case when the valence band is fourfold degenerate at the point $\mathbf{p} = 0$ in momentum space, neglecting the presence of the three corresponding twofold degenerate subbands split off by the spin-orbit interaction. In this case the behavior of the holes in the vicinity of $\mathbf{p} = 0$ is described to good accuracy by the Schrödinger equation with the isotropic Luttinger Hamiltonian[6] for particles with spin 3/2:

$$i\hbar\frac{\partial\psi}{\partial t}=\hat{H}\psi, \quad \hat{H}=\hat{H}_0-e\mathbf{E}\mathbf{r}, \tag{1}$$

$$\hat{H}_0=\frac{1}{m_0}\left[\frac{\hat{\mathbf{p}}^2}{2}\left(\gamma_1+\frac{5}{2}\gamma\right)-\gamma(\hat{\mathbf{J}}\hat{\mathbf{p}})^2\right],$$

where $\hat{H}_0$ is the Luttinger Hamiltonian, e is the hole charge, $\mathbf{E}$ is the electric field, m_0 is the free-electron mass, $\hat{\mathbf{p}}$ is the momentum operator, $\hat{\mathbf{J}}$ is the spin-3/2 operator, and γ_1 and γ are dimensionless parameters which are well known from experiment for many semiconductors. They are related to the effective masses m_l and m_h of the light and heavy holes, respectively, by

$$m_l=m_0/(\gamma_1+2\gamma), \quad m_h=m_0/(\gamma_1-2\gamma). \tag{2}$$

For Ge these parameters are $\gamma_1 = 13.35$ and $\gamma = 5.11$. The rest of the notation ($\hbar,t,\mathbf{r}$) is standard.

For definiteness let us use a coordinate system with x axis directed along $\mathbf{E}$. The other axes will be chosen later. We shall work in the representation of the operators $\hat{H}_0$ and $\hat{\mathbf{p}}$. The coordinate parts of their eigenfunctions are de Broglie waves corresponding to the eigenvalues $\mathbf{p}$ and $\varepsilon_\lambda(p)$ ($\lambda = l$ for light holes, $\lambda = h$ for heavy holes). The choice of the spinor parts of the eigenfunctions is dictated by the following considerations. In the absence of electric field the projection of the spin onto the direction of the momentum J_p is conserved. The value of this projection (the helicity) is different in the light-hole ($J_p = \pm 1/2$) and heavy-hole ($J_p = \pm 3/2$) subbands. The electric field, by changing the value of p_x, alters the direction of the momentum and thereby, by virtue of the spin inertia, induces transitions between J_p states, including transitions between subbands. In a uniform electric field the transitions between subbands conserve the hole momentum (they are vertical transitions) but change the average hole coordinate by $\Delta x = \Delta\varepsilon(p)/eE$, where $\Delta\varepsilon(p) = \varepsilon_l(p) - \varepsilon_h(p)$. The rate of change of the momentum direction is greatest in the region $p_x \sim p_\perp$ ($p_\perp$ is the value of the momentum component perpendicular to the field $\mathbf{E}$). In this region there are also relatively intense transitions between subbands. If the rate of change of the momentum direction is small, then the hole spin is able to follow the change, and spin flips and transitions between subbands do not occur (this is the case of adiabatically slow change in the direction of $\mathbf{p}$). The state with $p_\perp = 0$ is a special case. For this state J_x is an integral of motion, and therefore transitions between subbands do not occur. For motion near $p_x = 0$ the momentum direction changes appreciably over a time $\Delta t \sim p_\perp/eE$, during which $p_x \sim p$. This is the effective time over which the perturbation that causes transitions

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between J_p states acts on the system. Their probability is relatively large if $\Delta t \gtrsim \hbar/\Delta\varepsilon(p)$. Eliminating Δt from these relations, we obtain $p_\perp \gtrsim p^*$, where

$$p^* = (2m^*\hbar eE)^{1/3}, \quad \frac{1}{m^*} = \frac{1}{m_l} - \frac{1}{m_h}. \tag{3}$$

On the other hand, the probability of subband-to-subband transitions is also small at large $p_\perp$, because here the potential barrier through which the tunneling occurs is high and wide. According to Ref. 3, the corresponding transparency factor is

$$D(p_\perp) \propto \exp\left[-{}^4/_3 (p_\perp/p^*)^3\right], \quad p_\perp > p^*.$$

Consequently, the effective tunneling region in momentum space at fixed **E** is a torus at the center of the Brillouin zone, with axis along **E** and linear dimensions of the order of p^*. At fixed $p_\perp$ the tunneling probability vanishes for $E \to \infty$ because the time Δt spent by a hole in the effective region goes to zero and there is insufficient time for the spin state to change.

The description of the hole behavior in the J_p representation, though transparent, is not very convenient, since the electric field mixes all four of its states, making it necessary to solve a system of four differential equations. Here, however, we are interested only in subband-to-subband transitions without reference to the sign of the spin projection J_p and do not care about spin flips within a subband. We shall show that this problem reduces to the study of transitions between two types of states, described by two equations. Since the proposed method is applicable to a wide range of problems, let us elaborate it in some detail.

The total Hamiltonian $\hat{H}$ is invariant with respect to reflections in a plane with normal **n** along **p**$\times$**E**. The corresponding reflection operator $\hat{T}_n$, which commutes with $\hat{H}$, can be represented as a product of the operators for inversion and rotation about **n** by an angle π:

$$\hat{T}_n = i \exp\left[i\pi \mathbf{J}\times\mathbf{n}\right]. \tag{4}$$

The coordinate part of this operator for states with $p_n = 0$ is the identity transformation. The eigenvalues of $\hat{T}_n$, which determine the parity of the state with respect to reflection in the given plane, are $\alpha = \pm 1$, while the eigenfunctions $\psi^{(\pm 1)}$ (with allowance for the definiteness of the energy) is a linear combination of states with spin projections $J_p = \pm 1/2$ for the light holes and $J_p = \pm 3/2$ for the heavy holes. It follows directly from (4) that these functions are simultaneously linear combinations of the eigenstates J_n with eigenvalues 3/2 and $-1/2$ for $\psi^{(1)}$ and $-3/2$ and 1/2 for $\psi^{(-1)}$. For convenience we take the direction of the normal **n** to be the z axis. In this coordinate system the orthonormal eigenfunctions common to the operators $\hat{\mathbf{p}}$, $\hat{H}_0$, and $\hat{T}_n$ are of the form

$$\psi_l^{(1)} = \frac{1}{2}\left(\frac{p_-}{p}\right)^{3/2} \begin{vmatrix} 1 \\ 0 \\ -3^{1/2}p_+^2/p^2 \\ 0 \end{vmatrix} f(\mathbf{r}),$$

$$\psi_l^{(-1)} = \frac{1}{2}\left(\frac{p_+}{p}\right)^{3/2} \begin{vmatrix} 0 \\ -3^{1/2}p_-^2/p^2 \\ 0 \\ 1 \end{vmatrix} f(\mathbf{r}),$$

$$\psi_h^{(1)} = \frac{1}{2}\left(\frac{p_+}{p}\right)^{3/2} \begin{vmatrix} 3^{1/2}p_-^2/p^2 \\ 0 \\ 1 \\ 0 \end{vmatrix} f(\mathbf{r}),$$

$$\psi_h^{(-1)} = \frac{1}{2}\left(\frac{p_-}{p}\right)^{3/2} \begin{vmatrix} 0 \\ 1 \\ 0 \\ 3^{1/2}p_+^2/p^2 \end{vmatrix} f(\mathbf{r}), \tag{5}$$

where

$$p_\pm = p_x \pm ip_y, \quad f(\mathbf{r}) = (2\pi\hbar)^{-3/2} \exp(i\mathbf{pr}/\hbar).$$

In these states the average value of the hole spin projection onto any direction is equal to zero. The states $\psi_\lambda^{(1)}$ and $\psi_\lambda^{(-1)}$ have opposite signs of the average values of J_n^3 and can be obtained from each other by the conjugation operation (the product of the inversion and time-reversal operations). Transitions between states of different parity do not occur under **E**. Moreover, we have excluded from consideration the uninteresting spin flips within a subband and reduced to two the number of states coupled by **E**. The nonzero matrix elements of the coordinate x (and their conjugates) in the representation of eigenfunctions (5) are

$$\langle \alpha, \lambda, \mathbf{p} | x | \alpha, \lambda, \mathbf{p}' \rangle = -i\hbar \frac{\partial}{\partial p_x'} \delta^{(3)}(\mathbf{p}-\mathbf{p}');$$

$$\langle 1, l, \mathbf{p} | x | 1, h, \mathbf{p}' \rangle = -\langle -1, l, \mathbf{p} | x | -1, h, \mathbf{p}' \rangle^*$$

$$= -\frac{\sqrt{3}}{2} \hbar \frac{p_y p_+}{p^3} \delta^{(3)}(\mathbf{p}-\mathbf{p}'). \tag{6}$$

With allowance for the conservation of integrals of motion $\mathbf{p}_\perp$ and α, we seek a solution to Eq. (1) of the form

$$\psi^{(\alpha)}(\mathbf{p}_\perp, \mathbf{r}, t)$$

$$= \sum_{p_x} \left[C_l^{(\alpha)}(\mathbf{p}, t)\psi_l^{(\alpha)}(\mathbf{p}, \mathbf{r}) + C_h^{(\alpha)}(\mathbf{p}, t)\psi_h^{(\alpha)}(\mathbf{p}, \mathbf{r})\right]. \tag{7}$$

The expansion coefficients $C_\lambda^{(\alpha)}(\mathbf{p}, t)$ with $\alpha = 1$ satisfy the equations

$$\left[\varepsilon_l(\mathbf{p}) - i\hbar eE\frac{\partial}{\partial p_x}\right] C_l^{(1)}(\mathbf{p}, t) + \frac{\sqrt{3}}{2}\frac{\hbar eE p_y p_+}{p^3} C_h^{(1)}(\mathbf{p}, t)$$

$$= i\hbar \frac{\partial}{\partial t} C_l^{(1)}(\mathbf{p}, t), \tag{8}$$

$$\frac{\sqrt{3}}{2}\frac{\hbar e E p_y p_-}{p^3}C_l^{(1)}(\mathbf{p},t)+\left[\varepsilon_h(\mathbf{p})-i\hbar eE\frac{\partial}{\partial p_x}\right]C_h^{(1)}(\mathbf{p},t)$$

$$=i\hbar\frac{\partial}{\partial t}C_h^{(1)}(\mathbf{p},t). \quad (9)$$

The equations for the states with $\alpha = -1$ are obtained from (8) and (9) by the substitution $t\to -t$ and $\mathbf{E}\to -\mathbf{E}$ and by the operation of complex conjugation.

Suppose at the initial time $t = t_0$ a hole is located in the light band in the state $\mathbf{p} = \mathbf{p}_0$, $\alpha = 1$, i.e.,

$$C_l^{(1)}(\mathbf{p},t_0)=\delta^{(3)}(\mathbf{p}-\mathbf{p}_0),\quad C_h^{(\alpha)}(\mathbf{p},t_0)=C_l^{(-1)}(\mathbf{p},t_0)=0. \quad (10)$$

Since the hole momentum changes in accordance with the law $\mathbf{p} = \mathbf{p}_0 + e\mathbf{E}(t - t_0)$ and the parity of the hole state is conserved, the solution of the system of equations (8) and (9) can be written

$$C_\lambda^{(1)}(\mathbf{p},t)=\delta^3(\mathbf{p}-\mathbf{p}_0-e\mathbf{E}(t-t_0))\exp\left[\frac{i}{\hbar eE}\int_0^{p_x}\varepsilon_\lambda(\mathbf{p})\,dp_x\right]a_\lambda(\mathbf{p}). \quad (11)$$

Substituting (11) into (8) and (9) and introducing the dimensionless variables

$$\xi=p_x/p_\perp,\quad \tilde{\gamma}=(p_\perp/p^*)^3, \quad (12)$$

we obtain a system of two ordinary differential equations

$$\frac{d}{d\xi}a_l(\xi)-\frac{\sqrt{3}}{2}\frac{(1-i\xi)}{(1+\xi^2)^{3/2}}\exp\left[i\tilde{\gamma}\xi\left(1+\frac{\xi^2}{3}\right)\right]a_h(\xi)=0, \quad (13)$$

$$\frac{d}{d\xi}a_h(\xi)+\frac{\sqrt{3}}{2}\frac{(1+i\xi)}{(1+\xi^2)^{3/2}}\exp\left[-i\tilde{\gamma}\xi\left(1+\frac{\xi^2}{3}\right)\right]a_l(\xi)=0 \quad (14)$$

with boundary conditions

$$a_l(\xi_0)=1,\quad a_h(\xi_0)=0. \quad (15)$$

Equations describing the evolution of the holes in the state with parity $\alpha = -1$ are obtained from (13) and (14) by the substitutions $l\leftrightarrows h, \tilde{\gamma}\to -\tilde{\gamma}$. We shall therefore carry out our study for positive and negative $\tilde{\gamma}$ with allowance for this interpretation of the solutions.

Figure 1 shows the results of a numerical calculation of the probability of a hole tunneling from the light subband to the heavy subband as a function of the initial value p_x^0, for a final value $p_x\to\infty$ and for $\tilde{\gamma}=0.5$ and $\tilde{\gamma}=1$ ($\alpha = 1$) and $\tilde{\gamma}= -0.2$ ($\alpha = -1$). Figure 2 shows the transverse-momentum dependence of the total probability $D(\tilde{\gamma}) = |a_h(+\infty)|^2$ of a hole tunneling from the light subband to the heavy subband in moving from $p_x^0 = -\infty$ to

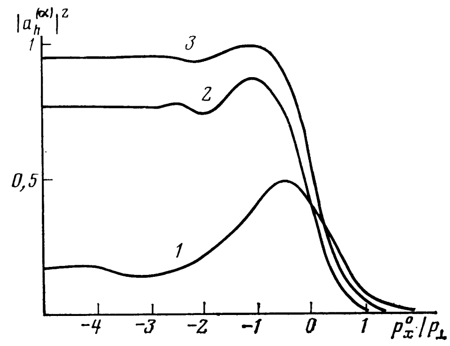

FIG. 1. Probability of finding a hole in the heavy band at $p_x = \infty$ as a function of the initial value p_x^0 for $\tilde{\gamma} = -0.2$ (curve 1), $\tilde{\gamma} = 1$ (curve 2), and $\tilde{\gamma} = 0.5$ (curve 3).

$p_x = \infty$. We see from equations (13) and (14) that if $a_l = f_l(\xi)$ and $a_h = f_h(\xi)$ are solutions of these equations, then $a_l = f_h^*(\xi)$ and $a_h = -f_l^*(\xi)$ are also solutions. Consequently, the probability of the transition $|\alpha,l,\mathbf{p}\rangle\to|\alpha,h,\mathbf{p}'\rangle$ is equal to the probability of the transition $|\alpha,h,\mathbf{p}\rangle\to|\alpha,l,\mathbf{p}'\rangle$. The invariance of $\hat{H}$ and $\hat{T}_h$ with respect to the reversal and reflection in the xz plane implies equal probabilities for the transitions:

$$|\alpha, h, p_x, p_y\rangle\to|\alpha, l, p_x', p_y\rangle,$$

$$|\alpha, l, -p_x', p_y\rangle\to|\alpha, h, -p_x, p_y\rangle.$$

Consequently, the probabilities for the tunneling of a hole from one subband to another in moving from $p_x^0 = -\infty$ to p_x are described by the curves in Fig. 1 with the substitution $p_x^0\to p_x$. We note that the curves shown in dimensionless variables in Figs. 1 and 2 are identical for all semiconductors described by the isotropic Luttinger model, and are therefore universal.

Let us find approximate expressions for $D(\tilde{\gamma})$ for $|\tilde{\gamma}|\ll 1$ and $|\tilde{\gamma}|\gg 1$. For $\tilde{\gamma}=0$ the solutions of Eqs. (13), (14) with boundary conditions (15) are of the form ($\xi_0\to -\infty$)

$$a_l(\xi)=\frac{\xi-i/2}{\xi+i}\left(\frac{\xi+i}{\xi-i}\right)^{1/4},\quad a_h(\xi)=\frac{i\sqrt{3}}{2(\xi+i)}\left(\frac{\xi+i}{\xi-i}\right)^{1/4}. \quad (16)$$

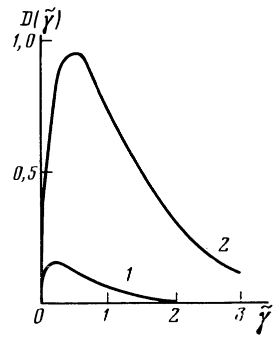

FIG. 2. Total probability for the tunneling of a hole into the heavy band in moving from $p_x = -\infty$ to $p_x = +\infty$ as a function of $\tilde{\gamma}$ (curve 1 is for odd states, curve 2 for even).

Using (16) to find a first approximation in $\tilde{\gamma}$, we obtain

$$D(\tilde{\gamma}) \approx \frac{9}{4}\left(\frac{\tilde{\gamma}}{3}\right)^{2/3} \Gamma^2\left(\frac{2}{3}\right), \quad |\tilde{\gamma}| \ll 1, \tag{17}$$

where $\Gamma(x)$ is the gamma function. For $|\tilde{\gamma}| \gg 1$ the functions $a_\lambda(\xi)$ are not very different, but their derivatives oscillate rapidly. Using boundary conditions (15) as the zeroth approximation in $|\tilde{\gamma}|^{-1}$, we obtain

$$D(\tilde{\gamma}) \approx \frac{3}{4}\left|\int_{-\infty}^{+\infty} \frac{1-ix}{(1+x^2)^{3/4}} \exp\left[i\tilde{\gamma}x\left(1+\frac{x^2}{3}\right)\right] dx\right|^2. \tag{18}$$

Evaluating the integral in (18) by the saddle-point method[7] (we note that the saddle point coincides with a branch point), we finally get

$$D(\tilde{\gamma}) \approx \begin{cases} {}^3/_4 |\tilde{\gamma}|^{-1/2} \Gamma^2({}^5/_4)\, e^{4\tilde{\gamma}/3}, & \tilde{\gamma} \ll -1 \\ 3\tilde{\gamma}^{1/2} \Gamma^2({}^3/_4)\, e^{-4\tilde{\gamma}/3}, & \tilde{\gamma} \gg 1 \end{cases}. \tag{19}$$

Let us now estimate the tunneling flux of holes between subbands, making some simplifying assumptions. Let us suppose that in the effective tunneling region with dimensions p^* the hole distribution function varies slowly and is equal to $W_\lambda^{(\alpha)}$. In order to exclude the effect of scattering on the tunneling, we shall assume that the relaxation time τ of the hole distribution function is longer than the time required for the holes to traverse the region p^*, i.e., $\tau \gg [\hbar m^*/(eE)^2]^{1/3}$. In this case the number of holes which tunnel from the heavy to the light subband per unit time in a unit volume of the semiconductor is

$$\left(\frac{dn}{dt}\right)_T = \frac{2}{3}\frac{\pi e (p^*)^2}{(2\pi\hbar)^3}\left\{ (W_h^{(1)} - W_l^{(1)}) \int_0^\infty D(\tilde{\gamma}) \frac{d\tilde{\gamma}}{\tilde{\gamma}^{1/3}} + (W_h^{(-1)} - W_l^{(-1)}) \int_0^\infty D(-\tilde{\gamma}) \frac{d\tilde{\gamma}}{\tilde{\gamma}^{1/3}} \right\}. \tag{20}$$

The first integral in (20) is approximately equal to 1.8, and the second to 0.21. Over a time τ, $(dn/dt)_T\tau$ holes appear in the light subband. This quantity is a measure of the deviation of the population of the light subband from its equilibrium value. In Ge, for example, with $W_h^{(\alpha)} - W_l^{(\alpha)} \sim 1$, $\tau \sim 10^{-11}$ sec, and $E \approx 300$ V/cm we have $\tau(dn/dt)_T \sim 10^{16}$ cm^{-3}. This rather large value indicates that the subband-to-subband tunneling must be taken into account in considering effects which are governed by hot charge carriers.

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