Theory of hole resonant tunneling in quantum-well structures

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A method of studying the hole resonant tunneling in quantum wells is proposed. Because of the band-mixing effect at $k_{\parallel}\neq 0$, the heavy and light holes can transform into each other in the process of tunneling. The transmission coefficients including *h-h* (heavy to heavy hole), *h-l* (heavy to light hole), *l-l* (light to light hole), and *l-h* are calculated as functions of hole energies, parallel wave vectors $k_{\parallel}$, and electric-field bias. The resonant energies are consistent with the energies of bound states in the same quantum well. After the difference in the effective-mass parameters in the two materials is taken into account, the theoretical results are in agreement with those of the experiments. The theoretical method developed in the paper is applicable to the study of various kinds of tunneling transmission and subband structure problems in superlattices.

I. INTRODUCTION

Resonant tunneling is a special effect in quantum wells, which was noted by Tsu and Esaki[1] early in 1973, when the concept of superlattices had just been proposed. Resonant tunneling may lead to a negative-resistance region in the current-voltage curve and hence has good prospects for wide applications. It has been investigated extensively experimentally[2] and theoretically,[3-5] but up to the present, almost all the research efforts have focused on resonant tunneling of electrons. Recently hole resonant tunneling has been observed in GaAs-AlAs heterojunctions experimentally,[6] yet no adequate theoretical treatment for a hole resonant tunneling appears to be available. In Ref. 6 hole tunneling resonant energies are calculated by the theory of electronic resonant tunneling on the assumption that the heavy and light holes have the effective masses $0.6m_0$ and $0.1m_0$, respectively, and there is no coupling between them. The results are not in agreement with the experiments. As noted in Ref. 6, nonparabolicity and band mixing effects are probably the main reasons for the discrepancies. An additional possible cause is the external electric field, which may modify significantly the hole states especially at high voltages.

In this paper we propose a theoretical method for studying hole resonant tunneling. The method takes account of the band nonparabolicity, the band mixing, the electric-field bias effects, and the difference of the effective-mass parameters in the two materials, etc. Certain phenomena, which do not exist in the electronic resonant tunneling, are discovered; for instance, the heavy hole and light hole may transform into each other during tunneling and the spin degeneracies of the resonant energies are removed by the application of an electric field bias.

II. THEORETICAL METHOD

The effective-mass Hamiltonian of superlattices can be written as

$$H=H_L+V(z)\ , \tag{1}$$

where $V(z)$ is the effective potential of the superlattice,

$$H_L=\frac{1}{2}\begin{vmatrix} P_1 & Q & R & 0 \\ Q^* & P_2 & 0 & R \\ R^* & 0 & P_2 & -Q \\ 0 & R^* & -Q^* & P_1 \end{vmatrix}\ , \tag{2}$$

$$\begin{aligned} P_1&=(\gamma_1+\gamma_2)p_{\parallel}^2+(\gamma_1-2\gamma_2)p_z^2\ ,\\ P_2&=(\gamma_1-\gamma_2)p_{\parallel}^2+(\gamma_1+2\gamma_2)p_z^2\ ,\\ Q&=-i2\sqrt{3}\gamma_3p_z(p_x-ip_y)\ ,\\ R&=\sqrt{3}[\gamma_2(p_x^2-p_y^2)-i2\gamma_3p_xp_y]\ , \end{aligned} \tag{3}$$

where $p_{\parallel},p_z$ are the momentum operators, and $\gamma_1,\gamma_2,\gamma_3$ are the Luttinger parameters.[7]

In order to simplify the calculation of transfer matrices we first transform the Hamiltonian (2) by an unitary transformation, to two independent (2×2)-dimensional matrices,[8] which represent two spin-degenerate states of holes, respectively. Thus the problem of calculating a (8×8)-dimensional transfer matrix is simplified to a problem of calculating two (4×4)-dimensional transfer matrices separately:

$$U^+HU=\frac{1}{2}\begin{vmatrix} P_1 & i\,|Q\,|p_z-|R\,| & 0 & 0 \\ -i\,|Q\,|p_z-|R\,| & P_2 & 0 & 0 \\ 0 & 0 & P_2 & -i\,|Q\,|p_z+|R\,| \\ 0 & 0 & i\,|Q\,|p_z+|R\,| & P_1 \end{vmatrix}\ . \tag{4}$$

In following we shall confine ourselves to the subspace corresponding to the upper left 2×2 matrix of (4), namely,

$$H_1=\frac{1}{2}\begin{vmatrix} P_1 & i\,|Q\,|p_z-|R\,| \\ -i\,|Q\,|p_z-|R\,| & P_2 \end{vmatrix} . \quad (5)$$

The potential barrier region is illustrated in Fig. 1. At the left side of the potential barrier region $V(z)$ is assumed to be zero, then the wave functions of holes are of the form

$$\psi=\begin{bmatrix} a \\ b \end{bmatrix} e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel+ik_z z} . \quad (6)$$

Substituting (6) in the effective mass equation we obtain the eigen energies of holes,

$$E=\tfrac{1}{2}\gamma_1 k^2\pm[\gamma_2^2k^4+3(\gamma_3^2-\gamma_2^2)(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{1/2} , \quad (7)$$

where the signs $\pm$ correspond to the light and heavy holes, respectively. As the holes enter into the potential barrier region, where $V(z)$ is not a constant (see Fig. 1), the hole wave functions become

$$\psi=\begin{bmatrix} U_1(z) \\ U_2(z) \end{bmatrix} e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel} , \quad (8)$$

where $\mathbf{k}_\parallel$ is still a good quantum number. After the holes pass through the potential barrier region and arrive at the right side, where $V(z)=-V_2$ is a constant again, the hole wave functions assume the form given by (6), but in which k_z is replaced by k_z'. The k_z' satisfy the following eigenenergy equation:

$$E=-V_2+\tfrac{1}{2}\gamma_1 k'^2 \pm[\gamma_2^2k'^4+3(\gamma_3^2-\gamma_2^2)(k_x^2k_y^2+k_y^2k_z'^2+k_z'^2k_x^2)]^{1/2} . \quad (9)$$

When the energy E and parallel wave vector $\mathbf{k}_\parallel$ are fixed, there are generally four independent hole states at the left-hand side of the potential barrier region: The heavy states ψ_{h,k_h}, $\psi_{h,-k_h}$ with perpendicular wave vectors $k_h,-k_h$ and the light-hole states $\psi_{l,k_l}\psi_{l,-k_l}$ with perpendicular $k_l,-k_l$:

$$\psi=\alpha\psi_{h,k_h}+\beta\psi_{h,-k_h}+\gamma\psi_{l,k_l}+\delta\psi_{l,-k_l} . \quad (10)$$

Similarly at the right-hand side we have

$$\psi'=\alpha'\psi_{h,k_n'}+\beta'\psi_{h,-k_h'}+\gamma'\psi_{l,k_l'}+\delta'\psi_{l,-k_l'} . \quad (11)$$

The coefficients $(\alpha,\beta,\gamma,\delta)$ and $(\alpha',\beta',\gamma',\delta')$ are connected by a transfer matrix M,

$$\begin{bmatrix}\alpha\\ \beta\\ \gamma\\ \delta\end{bmatrix}=\begin{bmatrix}M\end{bmatrix}\begin{bmatrix}\alpha'\\ \beta'\\ \gamma'\\ \delta'\end{bmatrix} . \quad (12)$$

The usual method of calculating the transfer matrices[3–5] will be very complicated when it is applied to this hole problem. We have developed an effective method for investigating hole resonant tunneling, the method is equally applicable to electronic resonant tunneling. Our method consists essentially of numerically integrating the set of differential equations, thus we just apply the Adams predictor once and corrector twice method to calculate transfer matrices. We proceed as follows.

(1) Suppose that the holes move from left to right through the potential barrier region (see Fig. 1). To start with, we calculate the hole wave functions at the right end, where $V(z)=-V_2$(constant) from the Hamiltonian (5). We obtain the heavy-hole wave function $\psi_{h,k_n'}$ and the light-hole wave function $\psi_{l,k_l'}$. For given energy E and parallel wave vector $\mathbf{k}_\parallel$, the perpendicular wave vector k_z is to be obtained from the eigenenergy Eq. (9). In the isotropic approximation $\gamma_3=\gamma_2$, we get simply

$$k_z=\left[\frac{2(E+V_2)}{\gamma_1\pm 2\gamma_2}-k_\parallel^2\right]^{1/2} , \quad (13)$$

where the $\pm$ signs correspond to light and heavy holes, respectively.

(2) Substituting the hole wave functions in the potential barrier region (8) into the Hamiltonian (5) we obtain the equation of motion of holes,

$$U_1''=\frac{1}{\gamma_1-2\gamma_2}\{(\gamma_1+\gamma_2)k_\parallel^2U_1-|R\,|U_2+|Q\,|U_2' -2[E-V(z)]U_1\} ,$$
$$U_2''=\frac{1}{\gamma_1+2\gamma_2}\{(\gamma_1-\gamma_2)k_\parallel^2U_2-|R\,|U_1-|Q\,|U_1' -2[E-V(z)]U_2\} . \quad (14)$$

The boundary conditions at the right boundary can be determined from $\psi_{h,k_n'}$ or $\psi_{l,k_l'}$. Then we integrate the set of differential equations (14) from right to left by the Adams method, and obtain the values of wave functions

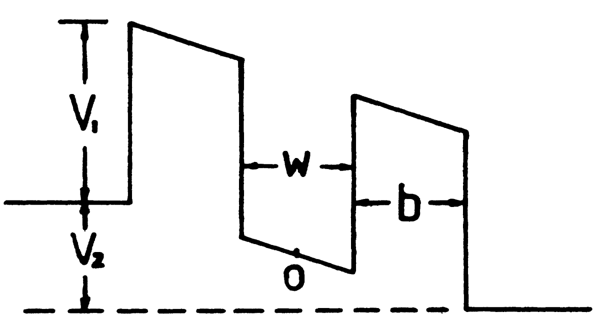

FIG. 1. Potential barrier region for hole tunneling.

and their derivatives U_1, U_1', U_2, U_2' at the left boundary of the barrier region.

(3) The hole wave function on the left of the barrier can be generally expressed as a linear combination of $\psi_{h,k_h}, \psi_{h,-k_h}, \psi_{l,k_l}$, and $\psi_{l,-k_l}$ [see Eq. (10)], their linear coefficients α, β, γ, and δ are determined by

$$\begin{aligned} &a_{h,k_h}\alpha + a_{h-k_h}\beta + a_{lk_l}\gamma + a_{l-k_l}\delta = U_1 \ , \\ &b_{hk_h}\alpha + b_{h-k_h}\beta + b_{lk_l}\gamma + b_{l-k_l}\delta = U_2 \ , \\ &ik_h a_{hk_h}\alpha - ik_h a_{h-k_h}\beta + ik_l a_{lk_l}\gamma - ik_l a_{l-k_l}\delta = U_1' \ , \\ &ik_h b_{hk_h}\alpha - ik_h b_{h-k_h}\beta + ik_l b_{lk_l}\gamma - ik_l b_{l-k_l}\delta = U_2' \ , \end{aligned} \tag{15}$$

where (a_{hk_h}, b_{hk_h}) and (a_{lk_l}, b_{lk_l}) are the coefficients in the wave functions (6) of the heavy and light holes, respectively.

(4) If it is a heavy hole at the right end ($k_z > 0$), the transfer matrix equation (12) will be

$$\begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = [M] \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \tag{16}$$

From (16) we obtain

$$M_{11} = \alpha, \quad M_{21} = \beta, \quad M_{31} = \gamma, \quad M_{41} = \delta \ . \tag{17}$$

If it is a light hole at the right end ($k_z > 0$), in the similar way we obtain

$$M_{13} = \alpha, \quad M_{23} = \beta, \quad M_{33} = \gamma, \quad M_{43} = \delta \ . \tag{18}$$

(5) Knowing the transfer matrix M, the transmission amplitudes T and reflection amplitudes R [1] can be calculated from Eq. (12),

$$T_{hh} = \frac{M_{33}}{M_{11}M_{33} - M_{13}M_{31}}, \quad T_{hl} = \frac{-M_{31}}{M_{11}M_{33} - M_{13}M_{31}} \ , \tag{19}$$

$$\begin{aligned} &T_{ll} = \frac{M_{11}}{M_{11}M_{33} - M_{13}M_{31}}, \quad T_{lh} = \frac{-M_{13}}{M_{11}M_{33} - M_{13}M_{31}} \ , \\ &R_{hh} = \frac{M_{21}M_{33} - M_{23}M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \quad R_{hl} = \frac{M_{41}M_{33} - M_{43}M_{31}}{M_{11}M_{33} - M_{13}M_{31}} \ , \\ &R_{ll} = \frac{M_{11}M_{43} - M_{13}M_{41}}{M_{11}M_{33} - M_{13}M_{31}}, \quad R_{lh} = \frac{M_{11}M_{23} - M_{13}M_{21}}{M_{11}M_{33} - M_{13}M_{31}} \ , \end{aligned} \tag{20}$$

where T_{hh} represents the transmission amplitude T from heavy hole to heavy hole, T_{hl} represents T from heavy hole to light hole, that is, the amplitude of light hole coming out at the right end from an incident heavy hole on the left, etc.

(6) From the second Hamiltonian of (4) we can use the same method to obtain the transmission amplitudes T and reflection amplitudes R for the holes spin degenerate to the above.

III. CALCULATION RESULTS

In order to check the efficiency of the Adams method in dealing with this kind of problem, we calculate the resonant energies of heavy and light holes with effective masses $0.6m_0$ and $0.1m_0$, respectively, in the case of $k_\parallel = 0$ so that there is no coupling between the heavy and light holes. The results are in agreement with those of Ref. 6 completely.

The parameters in the calculation are the same as in Ref. 6: $w = 50$ Å, $V_1 = 550$ meV. In Ref. 6 the width of the potential barrier is taken as $b = 50$ Å so that the width of resonant peaks are very narrow (see Fig. 1 of Ref. 6). The width of the resonant peaks is related to the width of the subbands in the k_z direction, which decreases as the width of the potential barrier increases. Calculations show that if the width of potential barrier b is reduced, the resonant peaks will broaden, but their positions remain basically unchanged. In the following we shall take $b = 20$ Å.

To simplify the calculation we take the isotropic approximation $\gamma_3 = \gamma_2$. The effective mass parameters γ_1 and γ_2 are determined from the experimental values of the effective masses of heavy and light holes m_h^*, m_l^* (Ref. 9) by

$$\begin{aligned} &\gamma_1 = \frac{1}{2}\left[\frac{1}{m_l^*} + \frac{1}{m_h^*}\right] , \\ &\gamma_2 = \frac{1}{4}\left[\frac{1}{m_l^*} - \frac{1}{m_h^*}\right] . \end{aligned} \tag{21}$$

The effective mass parameters used in this paper are listed in Table I. In Table I the first group of parameters are the same as that of Ref. 6 taking the average effective masses of GaAs and AlAs, the second group takes account of the difference of effective masses in the two materials.

A. Resonant tunneling energies as function of $k_\parallel$

Taking the first group of effective mass parameters in Table I and the electric field $F = 0$ we calculate the resonant tunneling energies as functions of $k_\parallel$. The results are shown in Fig. 2. The dashed lines in Fig. 2 represent

$$E = \tfrac{1}{2}(\gamma_1 \pm 2\gamma_2)k_\parallel^2 \ , \tag{22}$$

TABLE I. Effective-mass parameters of GaAs-AlAs quantum well.

	γ_1	γ_2	m_h^*	m_l^*
GaAs	5.833	2.083	0.600	0.100
AlAs	5.833	2.083	0.600	0.100
GaAs	6.800	2.347	0.475	0.087
AlAs	3.991	1.338	0.760	0.150

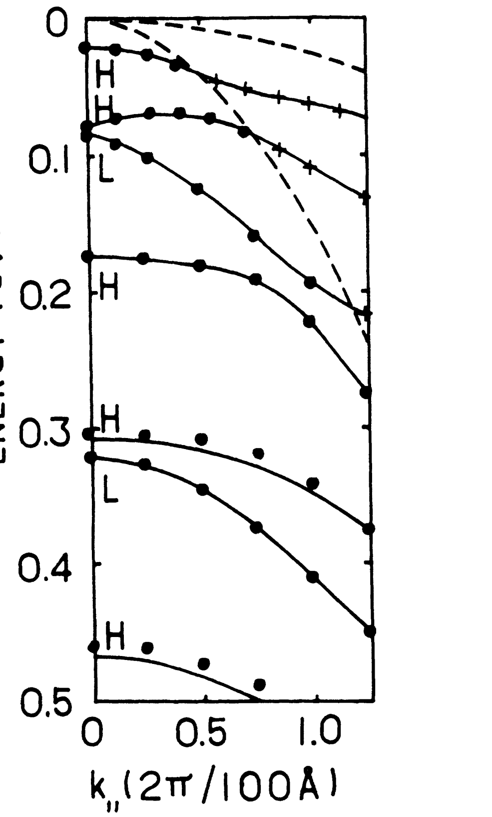

FIG. 2. Resonant energies and subband energies as functions of $k_{\parallel}$, calculated with the first group of effective mass parameters and at electric field $F=0$. The solid lines are subband energies, ● and + are resonant energies.

respectively. In the region above the upper dashed line $E=\frac{1}{2}(\gamma_1-2\gamma_2)k_{\parallel}^2$ the kinetic energies of the heavy and light holes in the $k_{\parallel}$ direction exceed the total energies E; hence, in the k_z direction they can only exist as a form of evanescent wave and cannot go through the barriers. In the range between the two dashed lines the kinetic energy of the heavy hole in the $k_{\parallel}$ direction is smaller than the total energy so that it is a traveling wave in the k_z direction, but the light hole is still an evanescent wave. The resonant energies in this range (represented by + in Fig. 2) are obtained from T_{hh} and T_{hl} (T_{ll} and T_{lh} have no meaning). The T_{hl} are calculated by replacing the traveling wave state of the light hole by the appropriate evanescent wave function. The symbols H and L in Fig. 2 represent the heavy and light hole properties of resonant peaks at $k_{\parallel}=0$. At $k_{\parallel}=0$ there is no coupling between the heavy and light holes; therefore, the T_{hl} and T_{lh} are all zero. At $k_{\parallel}\neq 0$ the T_{hl} and T_{lh} no longer vanish; this indicates that in the tunneling process there is mixing of the heavy and light holes, the heavy hole can transform into light hole, and vice versa. The solid lines in Fig. 2 are the energies of bound states in the corresponding superlattice calculated by the plane wave expansion method.[10] From Fig. 2 we see that the two sets of energies are in agreement.

B. Variation of resonant energies with electric fields

Figure 3 gives the resonant energies and subband structures calculated with the first group of effective mass parameters in the applied electric field $F=4$ mV/Å. From Fig. 3 we see that in the electric field as $k_{\parallel}\neq 0$ the two degenerate states split, it indicates that their transfer properties are different. In Fig. 3 the zero of energy is placed at the centre of the potential well (0 point in Fig. 1); thus only holes with the energies $|E|>\frac{1}{2}V_2=\frac{1}{2}F(w+2b)$ can tunnel through. The resonant energies (absolute values) in Fig. 3 are all larger than $E=\frac{1}{2}V_2$, represented by the dashed line. The solid lines in Fig. 3 are the energies of bound states calculated in the quasistationary state approximation.[11] Comparing Figs. 3 and 2 we find that the subband structures with and without applied electric field are clearly different at $|E|<\frac{1}{2}V_2$, but are basically the same at $|E|>\frac{1}{2}V_2$. It is due to this fact that we can determine the subband structures in the quantum well from the experimental resonant peak positions in the current-voltage curve.

C. Effect of the difference of effective-mass parameters in two materials

Taking the second group of effective-mass parameters in Table I, we calculate the resonant energies and find that they are appreciably different from those calculated with the first group of parameters. The resonant energies

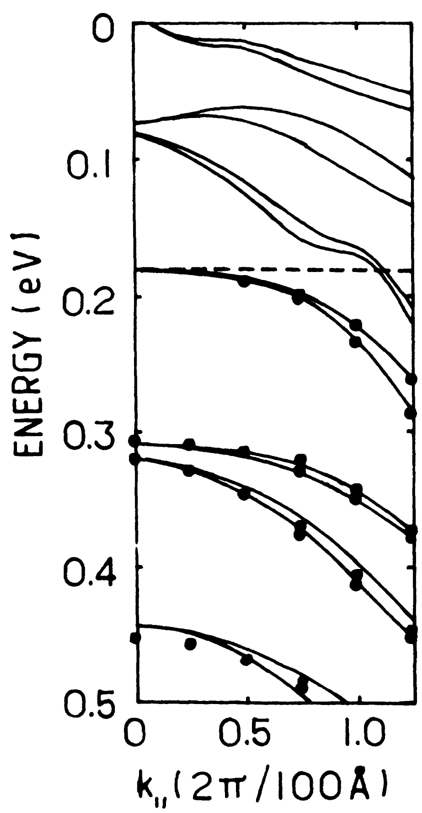

FIG. 3. Same as Fig. 2 but at $F=4$ mV/Å.

TABLE II. Comparison of resonant energies at $k_{\parallel}=0$ (in units of meV).

<table>
<tr><th></th><th>HH1</th><th>HH2</th><th>LH1</th><th>HH3</th><th>LH2</th><th>HH4</th><th>HH5</th></tr>
<tr><td>First parameters</td><td>20</td><td>78</td><td>83</td><td>172</td><td>318</td><td>302</td><td>458</td></tr>
<tr><td>Second parameters</td><td>26</td><td>100</td><td>104</td><td>220</td><td>372</td><td>376</td><td>574</td></tr>
<tr><td>Expt. (Ref. 6)</td><td></td><td colspan="2">100</td><td>215</td><td colspan="2">335</td><td>558</td></tr>
</table>

calculated with the two groups of parameters and the experimental values[6] are given in Table II. From Table II we see that after the difference of effective-mass parameters in the two materials is taken into account the calculation results are in agreement with the experiment. The resonant energies of HH2,LH1 and LH2,HH4 are very close, which may lead to some strong resonant peaks observed in the experiment.

D. Variation of transmission coefficients with energies

Figure 4 shows the transmission coefficients of the heavy and light hole $(T^*T)_{hh},(T^*T)_{ll}$ as functions of energy E at $F=0$ and $k_{\parallel}=0$. The resonant peaks corresponding the heavy and light hole are seen clearly in the figure, since for $k_{\parallel}=0$ there is no mixing between the heavy and light holes. The width of the second resonant peak of the light hole is large, which corresponds to a wide k_z subband of the superlattice (about 80 meV).

Figures 5 and 6 show the $(T^*T)_{hh},(T^*T)_{hl}$ and $(T^*T)_{ll},(T^*T)_{lh}$, respectively, as functions of E at $F=0$ and $k_{\parallel}=0.3(2\pi/70\ \text{Å})$. From Fig. 5 we see that $(T^*T)_{hh}$ and $(T^*T)_{hl}$ contain almost all the resonant peaks of the heavy and light holes; this means a strong mixing between them. One peak is an exception, namely, the fourth peak appears in the *hh* curve, but not in the *hl* curve. Similarly, in Fig. 6 the fourth peak only appears in the *lh* curve, but not in the *ll* curve. It indicates that this peak derives from a heavy-hole resonance. Besides, the fifth peak is only seen in the *lh* curve, and not in the *ll* curve; thus it is also a heavy-hole resonance.

E. Tunneling current

Since at $k_{\parallel}\neq 0$, there are various transmission probabilities of T_{hh}, T_{hl}, T_{ll}, and T_{lh}, the tunneling current should include all the contributions from these transmission coefficients. As an extension to the formula for the electronic tunneling current,[1] the formula for hole tunneling current should have the following form:

$$J=\frac{e}{2\pi^2\hbar}\int_0^{\infty}k_{\parallel}dk_{\parallel}\left[\sum_{i,j}\int_{E_{\parallel,i}}^{\infty}dE[f(E)-f(E')]T_{ij}^*T_{ij}(E,k_{\parallel})\right],\quad i,j=h,l\ . \tag{23}$$

For typical hole densities, at the low temperature limit, the effective hole kinetic energy is only about 5 meV, so that $k_{\parallel}$ for the tunneling holes can be considered as virtually zero. Therefore in Table II the comparison of the experimental resonant energies and the calculated energies at $k_{\parallel}=0$ is reasonable at low temperature, but at high temperature the effect of $k_{\parallel}\neq 0$ should be considered.

IV. SUMMARY

(1) In this paper we have developed a theoretical method for studying hole resonant tunneling. It is a numerical integration method, using Adams predictor once and corrector twice method to integrate the set of equations of hole motion in the potential barrier region, and

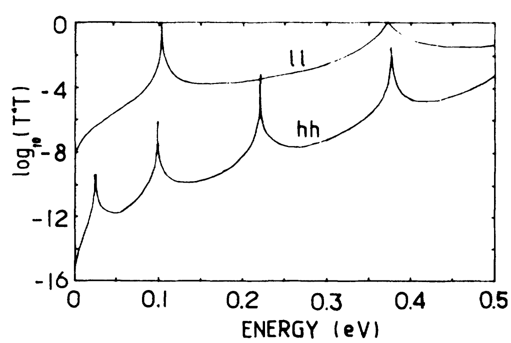

FIG. 4. Transmission coefficient $(T^*T)_{hh}$ and $(T^*T)_{ll}$ as functions of energy, calculated with the second group of parameters and at $F=0$ and $k_{\parallel}=0$.

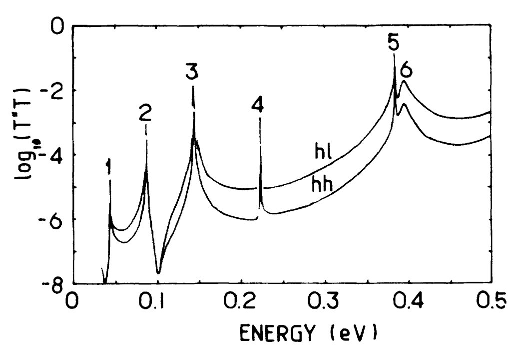

FIG. 5. Transmission coefficients $(T^*T)_{hh}$ and $(T^*T)_{hl}$ as functions of energy, calculated with the second group of parameters and at $F=0$ and $k_{\parallel}=0.3(2\pi/L)$.

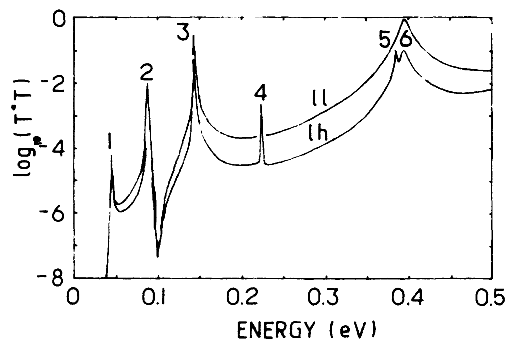

FIG. 6. Transmission coefficients $(T^*T)_{ll}$ and $(T^*T)_{lh}$ as functions of energy, calculated with the second group of parameters and at $F=0$ and $k_{\parallel}=0.3(2\pi/L)$.

obtaining thereby the transfer matrices and the transmission coefficients.

(2) With this method we have investigated hole resonant tunneling, taking account of the nonparabolicity of subbands, the mixing of the heavy and light holes, and effects of applied electric field bias, etc. The transmission coefficients $(T^*T)_{hh}, (T^*T)_{hl}, (T^*T)_{ll}, (T^*T)_{lh}$ and resonant energies of the heavy and light holes are obtained as functions of the parallel wave vectors $k_{\parallel}$ and electric field F. It is found that when $k_{\parallel}\neq 0$ the transmission coefficients $(T^*T)_{hl}$ and $(T^*T)_{lh}$ are not equal to zero. This means that heavy hole can be transformed into light hole in the process of tunneling, and vice versa. When $k_{\parallel}\neq 0$ and $F\neq 0$, the two spin-degenerate states of holes split. These phenomena do not exist in the electronic resonant tunneling. Taking account of the difference of the effective-mass parameters in the two materials, we have calculated the resonant energies of holes, which are in agreement with experiments.[6]

(3) The method proposed by us is also applicable to the study of the subband structures of superlattices, especially to those cases involving different effective-mass parameters in the two materials, or superlattices of types II and III.

ACKNOWLEDGMENT

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