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Author(s)	Zhu, JX; Wang, ZD; Gong, CD
Citation	Journal Of Applied Physics, 1996, v. 80 n. 4, p. 2291-2295
Issued Date	1996
URL	http://hdl.handle.net/10722/42437
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Resonant tunneling of holes in double-barrier structures in the presence of an in-plane magnetic field

Jian-Xin Zhu

Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China and Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong

Z. D. Wang^{a)}

Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong

Chang-De Gong

Center of Theoretical Physics, Chinese Center of Advanced Science and Technology (World Laboratory), P. O. Box 8730, Beijing 100080, People's Republic of China and Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China

(Received 10 October 1995; accepted for publication 14 May 1996)

Using the asymptotic transfer-matrix method, we investigate the resonant tunneling of holes in double-barrier semiconductor structures in the presence of an in-plane magnetic field. The transmission coefficients including ll (light to light hole), hl (light to heavy hole), hh (heavy to heavy hole), and lh (heavy to light hole) are calculated as a function of energy. As in the case of nonzero parallel wave vectors, the mixing of hole tunneling can also occur due to the in-plane magnetic field. Moreover, as has been observed by resonant magnetotunneling spectroscopy, we also find that the different resonances have quite different magnetic-field dependences. © 1996 American Institute of Physics. [S0021-8979(96)05316-9]

I. INTRODUCTION

Since the publication of the pioneering work by Tsu and Esaki,¹ much interest²⁻⁵ has been devoted to the study of resonant tunneling in semiconductor heterostructures, which is motivated by both device application and basic quantum mechanical aspects. However, to the best of our knowledge, extensive efforts have only been focused on the resonant tunneling of electrons, considerably less known is the resonant tunneling of holes. Hole tunneling in heterostructures is also of interest because of the degeneracy at the top of the valence band, which may admit the mixing and tunneling through the structure via different light-hole and heavy-hole channels. Mendez *et al.*⁶ observed resonant tunneling of holes through GaAs-AlAs heterostructures. Theoretically, a method for studying hole resonant tunneling was proposed by Xia in Ref. 7, where the author integrates numerically a set of differential equations followed by application of the Adams predictor once and corrector twice method to obtain transfer matrices. The mixing effect of heavy and light holes in the process of tunneling at nonzero in-plane wave vector is shown, which does not exist in the electronic resonant tunneling. Using a transfer matrix method, Wessel and Altarelli⁸ also found that for the nonvanishing in-plane wave vector, mixing of light hole and heavy hole states occurs. They further noted that interesting structure in the line shape occurs because of interference of different channels. Recently, Hayden *et al.*⁹ and Eaves *et al.*¹⁰ described a novel magnetotunneling spectroscopy technique. The resulting shift in the voltage positions of the resonant in current-voltage (*I-V*) curves reveals strong mixing between light- and heavy-hole states in the presence of an in-plane magnetic

field. In this paper, based on a four-band description of hole subbands, we establish a 4×4 transfer matrix and generalize the asymptotic transfer-matrix method¹¹ to study the resonant tunneling of holes in semiconductor double-barrier structures in the presence of an in-plane magnetic field. Due to the magnetic field, tunneling holes can acquire an effective parallel wave vector. Therefore, even when the parallel canonical momentum is zero, heavy and light holes can be mixed by the magnetic field in the process of tunneling. In addition, for our typical structure, in which one quasibound light-hole and two heavy-hole quasibound states exist, we find that the resonance position associated with the light-hole quasibound state almost does not shift with the increase of magnetic field, the resonance position associated with the first low-lying heavy-hole quasibound state shifts little while that associated with the second low-lying quasibound state shifts appreciably, which is in reasonable agreement with the experimental observation.

The paper is organized as follows: In Sec. II, we give the wave functions in the bulk material and the boundary conditions at each potential step, and generalize the asymptotic transfer-matrix method to compute the transmission coefficient. In Sec. III we discuss the transmission coefficients as a function of energy for a typical double-barrier structure and at a variety of situations; a brief summary is given in Sec. IV.

II. THEORETICAL METHOD

The holes in semiconductor heterostructures such as GaAs and Ge can be described by the four-band Luttinger effective-mass Hamiltonian¹²

^{a)}To whom all correspondences should be addressed; Electronic mail: zwang@hkucc.hku.hk

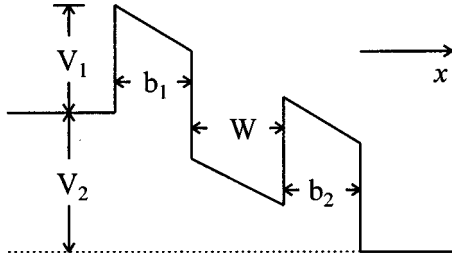


FIG. 1. Potential barrier region for hole tunneling.

$$H_L = \frac{\hbar^2}{m_0} \left[\left(\gamma_1 + \frac{5\gamma_2}{2} \right) \frac{\hat{\mathbf{k}}^2}{2} - \gamma_2 (\hat{k}_x^2 \hat{J}_x^2 + \hat{k}_y^2 \hat{J}_y^2 + \hat{k}_z^2 \hat{J}_z^2) \right. \\ \left. - 2\gamma_3 \{ \hat{k}_x \hat{k}_y \} \{ \hat{J}_x \hat{J}_y \} + \{ \hat{k}_y \hat{k}_z \} \{ \hat{J}_y \hat{J}_z \} + \{ \hat{k}_z \hat{k}_x \} \{ \hat{J}_z \hat{J}_x \} \right] \\ + \frac{eq}{\hbar c} (\hat{J}_x^3 B_x + \hat{J}_y^3 B_y + \hat{J}_z^3 B_z) + \frac{e\kappa}{\hbar c} \hat{\mathbf{J}} \cdot \mathbf{B}, \quad (1)$$

where m_0 is the mass of a free electron, γ_1 , γ_2 , γ_3 , κ , and q are Luttinger parameters, \mathbf{J} is the orbital angular momentum of $\frac{3}{2}$, $\hat{k}_\alpha = (\hat{p}_\alpha + eA_\alpha/c)/\hbar$, ($\alpha = x, y, z$), with \hat{p}_α the canonical momentum, and $\{\dots\}$ abbreviates the relation between two operators, e.g., \hat{O}_1 and \hat{O}_2 ,

$$\{ \hat{O}_1 \hat{O}_2 \} = (\hat{O}_1 \hat{O}_2 + \hat{O}_2 \hat{O}_1) / 2. \quad (2)$$

The vector potential \mathbf{A} gives the magnetic field by $\mathbf{B} = \nabla \times \mathbf{A}$. Here the hole energy is counted as positive.

As shown in Fig. 1, we choose the x -axis perpendicular to the interfaces of the double-barrier structure. The magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$ is applied parallel to the z -axis, and the vector potential is then of the form $\mathbf{A} = (0, Bx, 0)$ in the Landau gauge. As usual, we assume that $k_z = 0$, $q = 0$, and the system Hamiltonian in the matrix form can be disconnected into two 2×2 submatrices

$$H_1 = \begin{bmatrix} P_+ + 3\kappa\hbar\omega_c/2 & Q \\ Q^* & P_- - \kappa\hbar\omega_c/2 \end{bmatrix} + V_p(x), \quad (3a)$$

$$H_2 = \begin{bmatrix} P_- + \kappa\hbar\omega_c/2 & Q \\ Q^* & P_+ - 3\kappa\hbar\omega_c/2 \end{bmatrix} + V_p(x), \quad (3b)$$

where $\omega_c = eB/m_0c$ is the cyclotron frequency, $V_p(x)$ is the potential function describing the variation of valence band edge along the x -axis, and

$$P_\pm = \frac{\hbar^2}{2m_0} (\gamma_1 \pm \gamma_2) (\hat{k}_x^2 + \hat{k}_y^2), \quad (4a)$$

$$Q = -\frac{\sqrt{3}\hbar^2}{2m_0} [\gamma_2 (\hat{k}_x^2 - \hat{k}_y^2) - 2i\gamma_3 \{ \hat{k}_x \hat{k}_y \}]. \quad (4b)$$

Notice that the two components of the wave vector, \hat{k}_x and \hat{k}_y , do not commute with each other in the presence of a magnetic field. However, if we divide the system into a large number of sublayers, the vector potential and band edge potential inside each sublayer can be regarded as constants. The wave vector operators \hat{k}_x and \hat{k}_y inside each sublayer will

commute with each other, and then $\{ \hat{k}_x \hat{k}_y \} = \hat{k}_x \hat{k}_y = \hat{k}_y \hat{k}_x$. This treatment is somewhat similar to the path integral method in quantum mechanics.

In the following we are concerned with the subspace corresponding to Eq. (3a); Eq. (3b) can be treated similarly.¹³ Inside the l th sublayer, the equation for eigenenergies is written as

$$\begin{bmatrix} E - V_p^l - P_+ - 3\kappa\hbar\omega_c/2 & -Q \\ -Q^* & E - V_p^l - P_- + \kappa\hbar\omega_c/2 \end{bmatrix} \begin{bmatrix} F_1^l \\ F_2^l \end{bmatrix} = 0, \quad (5)$$

where F_1^l and F_2^l are the envelope functions in the sublayer. Here we have omitted the superscript l on P_\pm and Q .

In view of the translational invariance of the system along the y -axis and k_y is a good quantum number in each sublayer, we find the general solution to Eq. (5) to be

$$F_1^l = \sum_{j=1}^4 A_j^l \exp[i\tau_j^l(x-x_l) + ik_y y], \quad (6a)$$

$$F_2^l = \sum_{j=1}^4 \beta_j^l A_j^l \exp[i\tau_j^l(x-x_l) + ik_y y], \quad (6b)$$

where

$$\tau_1^l = -i \left[\frac{b + (b^2 - 4av)^{1/2}}{2a} \right]^{1/2}, \quad (7a)$$

$$\tau_2^l = -\tau_1^l, \quad (7b)$$

$$\tau_3^l = -i \left[\frac{b - (b^2 - 4av)^{1/2}}{2a} \right]^{1/2}, \quad (7c)$$

$$\tau_4^l = -\tau_3^l. \quad (7d)$$

The parameters involved in Eqs. (6) and (7) are given as

$$a = \gamma_1^2/4 - \gamma_2^2, \quad (8a)$$

$$b = [2a - 3(\gamma_3^2 - \gamma_2^2)]k_y^2 - \left(\frac{m_0}{\hbar^2} \right) [\gamma_1(E - V_p^l) + (\gamma_1/2 - \gamma_2)\kappa\hbar\omega_c], \quad (8b)$$

$$v = ak_y^4 + \left(\frac{m_0}{\hbar^2} \right) [(\gamma_1/2 - \gamma_2)\kappa\hbar\omega_c - \gamma_1(E - V_p^l)]k_y^2 + \left(\frac{m_0}{\hbar^2} \right)^2 [(E - V_p^l)^2 - (E - V_p^l)\kappa\hbar\omega_c - 3(\kappa\hbar\omega_c)^2/4], \quad (8c)$$

and

$$\beta_j^l = \frac{(2m_0/\hbar^2)(E - V_p^l - 3\kappa\hbar\omega_c/2) - (\gamma_1 + \gamma_2)[(\tau_j^l)^2 + k_y^2]}{\sqrt{3}\{\gamma_2[(\tau_j^l)^2 - k_y^2] - 2i\gamma_3\tau_j^l k_y\}}, \quad (j = 1, 2, 3, 4). \quad (9)$$

Now the parallel wave vector could be written as $k_y = k_{y_0} + eBx_l/\hbar c$ with x_l the position of the l th sublayer.

It was argued by Altarelli¹⁴ that if the Hamiltonian of a system, composed of two kinds of materials, is of the form

$$H_{jj'} = \sum_{\alpha, \beta=x,y} D_{jj'}^{\alpha, \beta} k_\alpha k_\beta + \sum_{\alpha=x,y} \mathcal{S}_{jj'}^\alpha k_\alpha + E_j \delta_{jj'}, \quad (j, j' = 1, 2, \dots, J), \quad (10)$$

the general boundary conditions at the interface of two consecutive sublayers are then as follows

$$F_j, \text{ continuous } (j = 1, 2, \dots, J), \quad (11a)$$

$$\sum_{j'=1}^J \left[(D_{jj'}^{xy} + D_{jj'}^{yx}) k_y - 2i D_{jj'}^{xx} \frac{\partial}{\partial x} \right] F_{j'}, \quad (11b)$$

continuous $(j = 1, 2, \dots, J)$.

For the system considered here, the counterparts of Eq. (11) at the interface between two consecutive sublayers read

$$F_1^l(x_{l+1} - 0^+) = F_1^{l+1}(x_{l+1} + 0^+), \quad (12a)$$

$$F_2^l(x_{l+1} - 0^+) = F_2^{l+1}(x_{l+1} + 0^+), \quad (12b)$$

$$\left[(\gamma_1 + \gamma_2) \frac{\partial}{\partial x} F_1^l - \sqrt{3} \left(\gamma_3 k_y + \gamma_2 \frac{\partial}{\partial x} \right) F_2^l \right]_{x=x_{l+1}-0^+} = \left[(\gamma_1 + \gamma_2) \frac{\partial}{\partial x} F_1^{l+1} - \sqrt{3} \left(\gamma_3 k_y + \gamma_2 \frac{\partial}{\partial x} \right) F_2^{l+1} \right]_{x=x_{l+1}+0^+}, \quad (12c)$$

$$\left[(\gamma_1 - \gamma_2) \frac{\partial}{\partial x} F_2^l + \sqrt{3} \left(\gamma_3 k_y - \gamma_2 \frac{\partial}{\partial x} \right) F_1^l \right]_{x=x_{l+1}-0^+} = \left[(\gamma_1 - \gamma_2) \frac{\partial}{\partial x} F_2^{l+1} + \sqrt{3} \left(\gamma_3 k_y - \gamma_2 \frac{\partial}{\partial x} \right) F_1^{l+1} \right]_{x=x_{l+1}+0^+}. \quad (12d)$$

Matching the wavefunction Eq. (6) and its slope according to Eq. (12), we can obtain the transfer matrix \mathbf{t}_l , which connects the amplitudes of the wavefunction of the l th sublayer to those of the $(l+1)$ th sublayer, and the system transfer matrix $\mathbf{M} = \prod_{l=1}^N \mathbf{t}_l$, which connects the amplitudes of the wavefunction at the left-hand side (LHS) of the system to those at the right-hand side (RHS).

In the spherical approximation $\gamma_3 = \gamma_2$, one yields the x -component of the wave vector on the both emitter and collector of the system, where the magnetic field is absent,

$$\tau_1^{L(R)} = \tau_l^{L(R)} = \left[\frac{2m_l}{\hbar^2} (E - V_p^{L(R)}) - k_y^2 \right]^{1/2}, \quad (13a)$$

$$\tau_2^{L(R)} = -\tau_l^{L(R)}, \quad (13b)$$

$$\tau_3^{L(R)} = \tau_h^{L(R)} = \left[\frac{2m_h}{\hbar^2} (E - V_p^{L(R)}) - k_y^2 \right]^{1/2}, \quad (13c)$$

$$\tau_4^{L(R)} = -\tau_h^{L(R)}, \quad (13d)$$

where $m_l = m_0/(\gamma_1 + 2\gamma_2)$, and $m_h = m_0/(\gamma_1 - 2\gamma_2)$. Equation (13) shows clearly that there are generally four independent hole states: light hole states with longitudinal wave vectors $\tau_l, -\tau_l$, and heavy hole states with longitudinal wave vectors $\tau_h, -\tau_h$.

Once given the transfer matrix \mathbf{M} , the transmission amplitudes T and reflection amplitudes R can be calculated as

$$\begin{aligned} T_{ll} &= \frac{M_{33}}{M_{11}M_{33} - M_{13}M_{31}}, & T_{hl} &= -\frac{M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \\ T_{hh} &= \frac{M_{11}}{M_{11}M_{33} - M_{13}M_{31}}, & T_{lh} &= -\frac{M_{13}}{M_{11}M_{33} - M_{13}M_{31}}, \\ R_{ll} &= \frac{M_{21}M_{33} - M_{23}M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, & R_{hl} &= \frac{M_{41}M_{33} - M_{43}M_{31}}{M_{11}M_{33} - M_{13}M_{31}}, \\ R_{hh} &= \frac{M_{11}M_{43} - M_{13}M_{41}}{M_{11}M_{33} - M_{13}M_{31}}, & R_{lh} &= \frac{M_{11}M_{23} - M_{13}M_{21}}{M_{11}M_{33} - M_{13}M_{31}}, \end{aligned} \quad (14)$$

where T_{ll} represents the transmission amplitude from light hole to light hole, T_{hl} the amplitude of heavy hole outgoing on the collector from an incident light hole at the emitter, and so forth.

III. RESULTS AND DISCUSSIONS

In the following, we would like to calculate the transmission probability of holes through GaAs/Ga_{1- δ} Al _{δ} As double-barrier structures in the presence or absence of an in-plane magnetic field. According to the formula given in Ref. 15

$$\varepsilon_g = 1519.2 + 1247\delta \text{ (meV)}, \quad (16)$$

where δ is the concentration of Al in Ga_{1- δ} Al _{δ} As. The band offset used is the empirical ‘‘60% rule’’ for the band gap discontinuity between the conduction and valence bands. If we take $\delta = 0.2$, the conduction- and valence- band discontinuity are

$$V_s = 249.4 \times 60\% = 149.64 \text{ (meV)},$$

and

$$V_p = 249.4 \times 40\% = 99.76 \text{ (meV)},$$

respectively. In the spherical approximation, which neglects the warping of the bulk valence bands altogether, the effective-mass parameters γ_2 and γ_3 are replaced by a suitable average $\bar{\gamma} = (3\gamma_2 + 2\gamma_3)/5$.¹⁶ We thus have $\gamma_1 = 6.85$, $\bar{\gamma} = 2.58$ for GaAs and $\gamma_1' = 6.17$, $\gamma_2' = \gamma_3' = \bar{\gamma}' = 2.27$ for Ga_{0.8}Al_{0.2}As.¹⁷ In addition, the structure parameters $b_1 = b_2 = W = 40 \text{ \AA}$ and the Luttinger parameter $\kappa = 1.2$ are taken in our calculation.

Figure 2 shows the transmission coefficients of the light and heavy holes $(T^*T)_{ll}$, $(T^*T)_{hh}$ as a function of energy E in the absence of electromagnetic field, $\mathcal{E} = B = 0$, and at zero parallel component of the canonical momentum $p_y = 0$. The resonant peaks corresponding to the light and heavy holes are seen clearly, and there is no mixing effect between

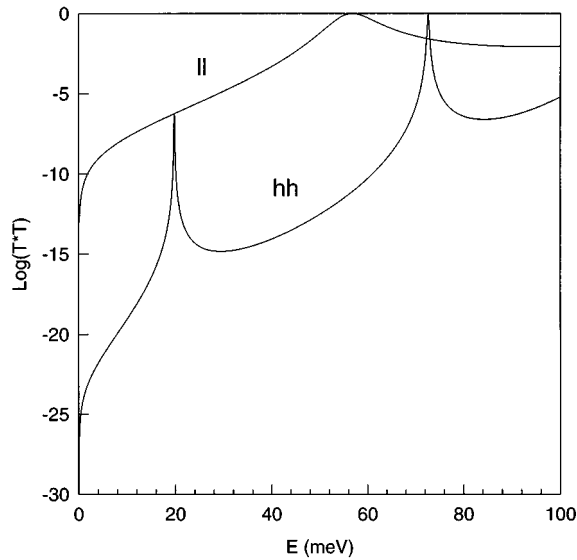


FIG. 2. Transmission coefficients $(T^*T)_{II}$ and $(T^*T)_{hh}$ as a function of incident energy E , calculated with the parameters given in the context and $\mathcal{E}=0$, $B=0$, and $p_y=0$.

light and heavy holes in the process of tunneling. Since the light and heavy holes have different effective mass, there is a different number of quasi-bound states for them. At the structure parameters were taken, one light-hole and two heavy-hole quasibound states exist within the range of barrier energy. Figures 3(a) and 3(b) show, respectively, the transmission coefficients versus the energy, $(T^*T)_{II}$, $(T^*T)_{hl}$, and $(T^*T)_{hh}$, $(T^*T)_{lh}$, at $\mathcal{E}=0$, $p_y=0$ but $B=2$ T. All three peaks appear in each curve. Evidently, the mixing of light- and heavy-hole states occur due to the large magnetic field. Moreover, the influence of the quasibound state associated with light holes on the heavy-heavy and heavy-light hole tunneling is weaker than that of the quasi-

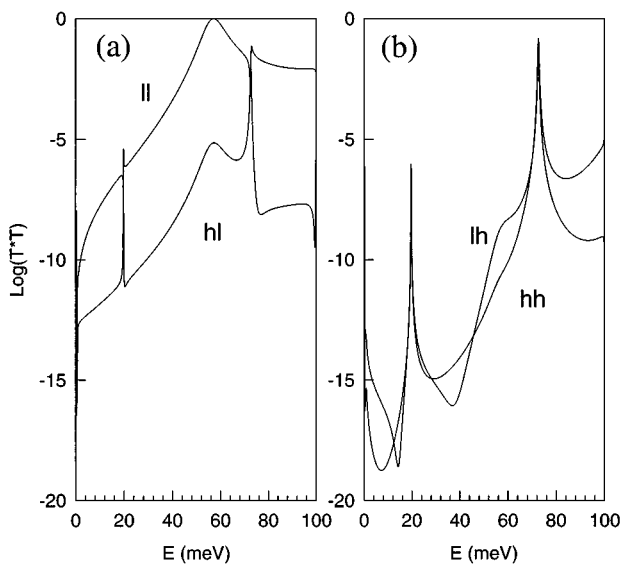


FIG. 3. Transmission coefficients: (a) $(T^*T)_{II}$ and $(T^*T)_{hl}$; and (b) $(T^*T)_{hh}$ and $(T^*T)_{lh}$, as a function of incident energy E , calculated with the parameters given in the context and at $\mathcal{E}=0$, $p_y=0$ but $B=2$ T.

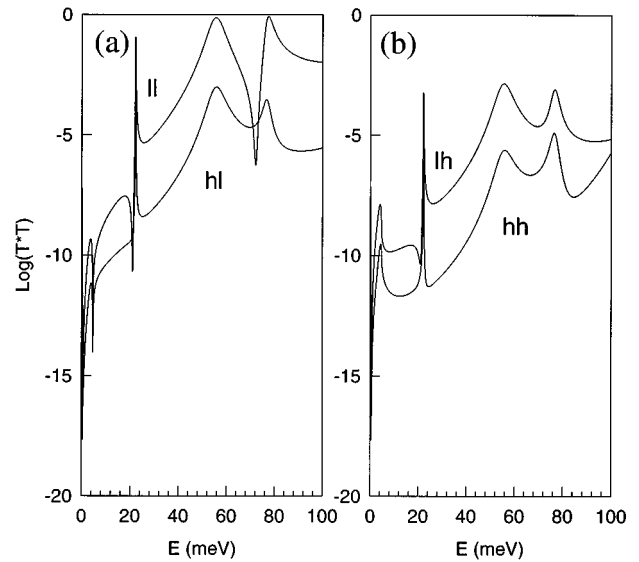


FIG. 4. Same as Fig. 3 but at $B=0$ and $p_y/\hbar=0.01 \text{ \AA}^{-1}$.

bound states associated with heavy holes on the light-light and light-heavy hole tunneling. In addition, we also calculate the transmission versus the energy at a higher magnetic field $B=10$ T ($\mathcal{E}=0$ and $p_y=0$). The resonance line shapes are almost the same as those shown in Fig. 3 and we thus do not intend to plot these transmission coefficient curves. However, we find that the different resonances have quite different magnetic-field dependences. The resonance position associated with the low-lying light-hole quasibound state almost does not shift with the increase of magnetic field, the resonance position associated with the first low-lying heavy-hole quasibound state shifts little while that associated with the second low-lying quasibound state shifts appreciably. For the double barrier structure studied by Hayden *et al.*⁹ and Eaves *et al.*,¹⁰ two light-hole and three heavy-hole quasibound states exist. They found that the first low-lying light-hole and heavy-hole resonances shift very little, whereas the second low-lying heavy-hole resonances shift appreciably in opposite sense. Therefore, our results are in reasonable agreement with the experimental observation for the low-lying quasibound states. In Figs. 4(a) and 4(b), the transmission characteristics are plotted at $\mathcal{E}=0$ and $B=0$ but $p_y/\hbar=0.01 \text{ \AA}^{-1}$. In this case of nonzero p_y , the energy E must be greater than $E_{th1}=p_y^2/2m_h=0.65$ meV for heavy-hole propagating channel to be opened and it must be greater than $E_{th2}=p_y^2/2m_l=4.62$ meV for the light-hole propagating channel to be opened. Thus the dips at $E=0.65$ meV in all of the transmission coefficient curves and those at $E=4.62$ meV in II and hl curves are meaningless, and the transmission probability $T_{hh}^*T_{lh}$ from heavy-hole channel to light-hole channel within the energy range $E_{th1}<E<E_{th2}$ should be interpreted as the strength of the evanescent light-hole channel. This phenomenon is quite similar to the electron transport through a quasi-one-dimensional multichannel quantum wire, where a dip appears whenever the Fermi energy approaches the bottom of a transverse subband.¹⁸

IV. SUMMARY

By means of the asymptotic transfer method, we have calculated the transmission coefficients of the hole resonant tunneling as a function of energy in the presence of an in-plane magnetic field. The results show that the mixing of hole tunneling can also occur due to the large magnetic field, which plays the role of an effective parallel wave vector. Moreover, as has been observed by resonant magnetotunneling spectroscopy, we also find that the different resonances have quite different magnetic-field dependences. It is noteworthy to point out that the resonant tunneling of holes in such more complex situations as in the presence of the voltage bias can also be studied by the asymptotic transfer method.

ACKNOWLEDGMENTS

We would like to thank G. Qin, B.-G. Wang, and H. X. Tang for invaluable help. J.-X. Zhu is grateful to the Robert Black College of the University of Hong Kong for an offer of the Wang Gungwu Scholarship.

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