Effects of uniaxial stress on hole subbands in semiconductor quantum wells. I. Theory

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The valence subbands and the corresponding wave functions in semiconductor quantum wells under uniaxial stress are analyzed by solving a 4×4 Luttinger-Kohn Hamiltonian together with a 4×4 strain Hamiltonian in the spin $J=\frac{3}{2}$ basis. Appropriate boundary conditions are obtained by integrating the total Hamiltonian across the interfaces of the quantum wells and, if a proper unitary transformation is made, yield eight linear equations that determine the eigenenergies and eigenfunctions. The results of our general formalism can be greatly simplified for some special cases which are used as examples in order to explore the underlying physics. The causes of the valence-band mixing, the effect of the valence-band warping, and the behavior of the hole effective masses under uniaxial stress are discussed. The numerical results are presented in a paper to follow.

I. INTRODUCTION

A general formalism for space quantization of the energy spectrum for the valence band in semiconductor films has been proposed by Nedorezov.[1] He started from the Luttinger-Kohn Hamiltonian[2] in the spin $J=\frac{3}{2}$ basis by neglecting spin-orbit interaction, and imposed the zero boundary conditions that are valid for describing free carriers confined to an infinitely deep well. The subband structure of the valence band and the corresponding effective mass of the hole were derived analytically. Recently, Fasolino and Altarelli[3] adopted Nedorezov's formalism to study the subband structure and Landau levels in heterostructures by neglecting the warping of the valence band. By including the warping of the valence band, Lee and Vassell[4] found that the hole subbands differ significantly from those reported by Fasolino and Altarelli.[3] In the spirit of Ref. 3, Chang[5] studied the problem of the enhancement of optical nonlinearity in p-type semiconductor quantum wells due to spatial confinement and stress. It is well known that as a result of spatial confinement in a quantum well, the degeneracy of the light- and heavy-hole valence-band energies is lifted at $k=0$, where $\mathbf{k}$ is the wave vector describing the relative electron-hole motion parallel to the interface of the quantum well. Excitons, when generated in such an environment, exhibit two series of discrete energy levels corresponding to electrons bound to either the light hole (LH) or heavy hole (HH).[6,7] Allowed transitions across the band gap occur between energy levels with the same quantum number, n ($\Delta n=0$), and have been observed in the absorption, photoluminescence excitation (PLE), and other spectra which probe the higher transitions of the quantum well.[7] However, normally "forbidden" transitions [parity allowed (Δn even) and parity forbidden (Δn odd)] have also been reported in the literature[8] and interpreted as a result of the valence-band mixing.[9] In the Luttinger-Kohn formalism for the valence band, all off-diagonal elements in the Hamiltonian are zero at the Brillouin-zone center, $k=0$. Thus parity disallowed transitions can only be attributed to direct transitions between eigenstates from zone center (i.e., $k\neq0$). However, if uniaxial stress or tension is applied parallel to the plane of the quantum wells, the off-diagonal elements of the total Hamiltonian, which is a sum of the Luttinger-Kohn Hamiltonian and the strain Hamiltonian, can be nonzero, even at $k=0$. That is, the uniaxial stress itself can "induce" valence-band mixing.[10-12] If the stress is applied perpendicular to the quantum-well layers, then there is no additional mixing due to this external perturbation.[10-12]

From the above discussions we realize that (1) the LH and HH subbands can be precisely identified by monitoring the stress dependence, and (2) the valence-band mixing occurs when the quantum wells are under stress parallel to the interfaces or when k is away from zone center (i.e., $k\neq0$). Therefore the main purpose of this paper is to examine the effects of the uniaxial stress on quantum wells at arbitrary k in the Luttinger-Kohn Hamiltonian for the valence band. In Sec. II, a theoretical model is presented for calculating the eigenenergies and the corresponding eigenfunctions of the total Hamiltonian. Finally, in Sec. III a discussion of our theoretical analysis is given. Detailed numerical results of the hole subbands, wave functions, and hole effective mass as functions of stress, well thickness, barrier height, and k are reported in the paper to follow.[13]

II. THEORY

The total Hamiltonian describing the energy spectrum for the valence band in a quantum well in the presence of uniaxial stress can be written as[5,14]

$$H=H_h+H_\varepsilon\ , \tag{1}$$

where H_h and H_ε represent the Luttinger-Kohn Hamiltonian for the hole states and the strain Hamiltonian introduced by the uniaxial stress via

$$-H_h=\frac{\hbar^2}{m_0}\left(\tfrac{1}{2}\gamma_1K^2-\gamma_2[(J_x^2-\tfrac{1}{3}J^2)k_x^2+\text{c.p.}]\right.$$
$$\left.-2\gamma_3(\{J_x,J_y\}k_xk_y+\text{c.p.})\right)+V_h(z) \tag{2}$$

and

$$H_\varepsilon = D_d(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})+\tfrac{2}{3}D_u[(J_x^2-\tfrac{1}{3}J^2)\varepsilon_{xx}+\text{c.p.}] + \tfrac{4}{3}D_u'(\{J_x,J_y\}\varepsilon_{xy}+\text{c.p.}) , \quad (3)$$

where m_0 is the free-electron mass, D_d, D_u, and D_u' are deformation potentials for the valence bands, ε_{ij} are components of the strain tensor, J_i are the angular momentum matrices corresponding to a spin $-\frac{3}{2}$ state, c.p. indicates cyclic permutation of indices and $\{a,b\} \equiv \frac{1}{2}(ab+ba)$. Here, k_x, k_y, and k_z are components of the wave vector of a hole along the x, y, and z axes, respectively, and

$$K^2 \equiv k_x^2+k_y^2+k_z^2 .$$

The hole is confined in the z direction by a square-well potential, $V_h(z)$, with a well width L and a potential barrier height V_0. We assume that the Luttinger-Kohn parameters γ_1, γ_2, and γ_3 vary with z as

$$\gamma_i = \begin{cases} \gamma_{iw} & \text{if } |z| \le L/2 , \quad i=1,2,3 \\ \gamma_{ib} & \text{if } |z| > L/2 , \quad i=1,2,3 , \end{cases} \quad (4)$$

where the subindices w and b refer to well and barrier, respectively. When we adopt effective units

$$R = \frac{\hbar^2}{m_0 a_0^2}, \quad a_0 = \frac{\hbar^2}{m_0 e^2} \quad (5)$$

for energy and length, respectively, the total Hamiltonian can be written as the 4×4 matrix

$$H = \begin{bmatrix} P+Q & R & -S & 0 \\ R^* & P-Q & 0 & S \\ -S^* & 0 & P-Q & R \\ 0 & S^* & R^* & P+Q \end{bmatrix} \quad (6)$$

with

$$P \pm Q = [\tfrac{1}{2}(\gamma_1 \pm \gamma_2)k^2 + \tfrac{1}{2}(\gamma_1 \mp 2\gamma_2)k_z^2] + \{D_d(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}) \pm \tfrac{2}{3}D_u[\varepsilon_{zz}-\tfrac{1}{2}(\varepsilon_{xx}+\varepsilon_{yy})]\} + V_h(z) , \quad (7)$$

$$R = \frac{\sqrt{3}}{2}[\gamma_2(k_x^2-k_y^2) - i2\gamma_3 k_x k_y] + \left[\frac{D_u}{\sqrt{3}}(\varepsilon_{yy}-\varepsilon_{xx}) + i\frac{2}{\sqrt{3}}D_u'\varepsilon_{xy} \right] , \quad (8)$$

$$S = [i\gamma_3\sqrt{3}(k_x - ik_y)k_z] - \left[\frac{2}{\sqrt{3}}D_u'(\varepsilon_{yz}+i\varepsilon_{zx}) \right] , \quad (9)$$

where $k^2 \equiv k_x^2+k_y^2$. As proposed by Broido and Sham,[15] this 4×4 total Hamiltonian can be reduced to two 2×2 matrices by using the unitary transformation,

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\varphi} & 0 & 0 & -e^{i\varphi} \\ 0 & e^{-i\eta} & -e^{i\eta} & 0 \\ 0 & e^{-i\eta} & e^{i\eta} & 0 \\ e^{-i\varphi} & 0 & 0 & e^{i\varphi} \end{bmatrix} , \quad (10)$$

with

$$\varphi = \frac{\pi}{4} + \tfrac{1}{2}(\alpha+\beta) , \qquad \eta = \frac{\pi}{4} - \tfrac{1}{2}(\alpha-\beta) , \quad (11)$$

where

$$\tan\alpha = \frac{\sqrt{3}\gamma_3 k_x k_y - \frac{2}{\sqrt{3}}D_u'\varepsilon_{xy}}{\frac{\sqrt{3}}{2}\gamma_2(k_x^2-k_y^2) + \frac{D_u}{\sqrt{3}}(\varepsilon_{yy}-\varepsilon_{xx})} , \qquad \tan\beta = \frac{\sqrt{3}\gamma_3 k_x k_z - \frac{2}{\sqrt{3}}D_u'\varepsilon_{zx}}{\frac{2}{\sqrt{3}}D_u'\varepsilon_{yz} + \gamma_3\sqrt{3}k_y k_z} . \quad (12)$$

Note that, in order to assure that U is unitary, we require that φ and η be real. By examining Eq. (12), we notice that if ε_{zx} and ε_{yz} are nonzero, β may become complex because k_z may be complex; therefore, φ and η are complex, implying that U is not unitary. However, if $\varepsilon_{zx}=\varepsilon_{zy}=0$, $\tan\beta$ becomes real because k_x and k_y are real; thus U is unitary. Throughout this paper, we limit our discussions to the assumptions that ε_{zx} and ε_{yz} are zero. If the uniaxial stress X is parallel to the [001], [100], or [110] direction, the assumptions $\varepsilon_{zx}=\varepsilon_{yz}=0$ are fulfilled. We rewrite Eq. (9) as

$$S = i\gamma_3\sqrt{3}k_- k_z , \quad |S| = (\gamma_3\sqrt{3}k)k_z \quad (9')$$

and $\tan\beta$ in Eq. (12) as $\tan\beta = k_x/k_y = \cot\theta$ where θ is the polar angle of $\mathbf{k}$. The wave equation

$$H\Psi = E\Psi \quad (13)$$

that we intend to solve is transformed into

$$H'\Psi' - E\Psi' = 0 \quad (14)$$

with

$$H' = UHU^+$$

and

$$\Psi' = U\Psi , \quad (15)$$

where Ψ is the eigenfunction and E is the corresponding eigenvalue. Equation (14) can be written explicitly as

$$\begin{bmatrix} P+Q-E & |R|-i|S| & 0 & 0 \\ |R|+i|S| & P-Q-E & 0 & 0 \\ 0 & 0 & P-Q-E & |R|-i|S| \\ 0 & 0 & |R|+i|S| & P+Q-E \end{bmatrix} \begin{bmatrix} \Psi_1' \\ \Psi_2' \\ \Psi_3' \\ \Psi_4' \end{bmatrix} = 0 . \quad (16)$$

The secular equation of Eq. (15), taken with Eqs. (7), (8), and (9′), gives

$$k_z^2=(4\Gamma_+\Gamma_-)^{-1}[B\pm(B^2-16\Gamma_+\Gamma_-C)^{1/2}]\ , \tag{17}$$

where

$$B=(6\gamma_3^2-\gamma_1^2-2\gamma_2^2)k^2+2\gamma_1(E'-\eta)-4\gamma_2\delta\ ,$$
$$C=(A_+-E')(A_--E')-|R|^2\ ,$$
$$\Gamma_\pm=(\gamma_1\pm2\gamma_2)/2\ ,$$

with

$$E'=E-V_h(z)\ ,$$
$$|R|^2=\left[\frac{\sqrt{3}}{2}\gamma_2k^2\cos2\theta+\nu\right]^2+\left[\frac{\sqrt{3}}{2}\gamma_3k^2\sin2\theta-\xi\right]^2\ ,$$
$$A_\pm=\tfrac{1}{2}(\gamma_1\pm\gamma_2)k^2+\eta\pm\delta\ ,$$
$$\nu=D_u(\varepsilon_{yy}-\varepsilon_{xx})/\sqrt{3}\ , \tag{18}$$
$$\xi=2D_u'\varepsilon_{xy}/\sqrt{3}\ ,$$
$$\eta=D_d(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})\ ,$$
$$\delta=2D_u[\varepsilon_{zz}-\tfrac{1}{2}(\varepsilon_{xx}+\varepsilon_{yy})]/3\ .$$

Equation (17) yields four roots for k_z: $\bar{q}_1$, $-\bar{q}_1$, $\bar{q}_2$, and $-\bar{q}_2$. Subscripts 1 and 2 refer to the plus and minus signs, respectively, in Eq. (17) for k_z^2. The wave functions Ψ_1' and Ψ_2' have the following mathematical form:

$$\begin{bmatrix}\Psi_1'(z)\\ \Psi_2'(z)\end{bmatrix}=N_u\begin{bmatrix}-\Lambda(\bar{q}_1)C_{21}e^{i\bar{q}_1z}-\Lambda(-\bar{q}_2)C_{22}e^{-i\bar{q}_1z}-\Lambda(\bar{q}_2)C_{23}e^{i\bar{q}_2z}-\Lambda(-\bar{q}_2)C_{24}e^{-i\bar{q}_2z}\\ C_{21}e^{i\bar{q}_1z}+C_{22}e^{-i\bar{q}_1z}+C_{23}e^{i\bar{q}_2z}+C_{24}e^{i\bar{q}_2z}\end{bmatrix}\ , \tag{19}$$

where

$$\Lambda(\bar{q}_j)=[(|R|-i|S|)/(P+Q-E)]_{k_z=q_j}\ ,$$

N_u is a normalization constant, and C_{2j}, $j=1,2,3,4$, are known constants which must be determined by appropriate boundary conditions. If $|z|\le L/2$ we set

$$V_h(z)=0,\quad \gamma_i=\gamma_{iw},\quad \bar{q}_1=q_1\ ,$$
$$\bar{q}_2=q_2,\quad \text{and}\quad C_{2j}=W_{2j}$$

to represent the wave functions in the well. If $|z|>L/2$, we choose

$$V_h(z)=V_0,\quad \gamma_i=\gamma_{ib},\quad \bar{q}_1=-i\kappa_1\ ,$$
$$\bar{q}_2=-i\kappa_2,\quad \text{and}\quad C_{2j}=B_{2j}$$

to represent the wave functions in the barrier. The wave functions Ψ_3' and Ψ_4' for the lower block of the new total Hamiltonian can be obtained by using the replacement of $\gamma_2\to-\gamma_2$, $\delta\to-\delta$, and $\nu\to-\nu$ for k_z [see Eqs. (16)–(18)]. We have

$$\begin{bmatrix}\Psi_3'(z)\\ \Psi_4'(z)\end{bmatrix}=N_L\begin{bmatrix}-\Lambda(\bar{q}_1)C_{41}e^{i\bar{q}_1z}-\Lambda(-\bar{q}_1)C_{42}e^{-i\bar{q}_1z}-\Lambda(\bar{q}_2)C_{43}e^{i\bar{q}_2z}-\Lambda(-\bar{q}_2)C_{44}e^{-i\bar{q}_2z}\\ C_{41}e^{i\bar{q}_1z}+C_{42}e^{-i\bar{q}_1z}+C_{43}e^{i\bar{q}_2z}+C_{44}e^{-i\bar{q}_2z}\end{bmatrix}\ , \tag{20}$$

where

$$\Lambda(\bar{q}_j)=[(|R|-i|S|)/(P+Q-E)]_{k_z=\bar{q}_j}\ ,$$

N_L is a normalization constant, and $C_{4j}=W_{4j}$ ($C_{4j}=B_{4j}$) if $|z|\le L/2$ ($|z|>L/2$) for the well region (barrier regions).

The boundary conditions are obtained from Eq. (16) by using the operator $k_z=-i\partial_z$ and integrating across the interfaces at $z=\pm L/2$. Let z_w and z_b be the values of z near the interfaces in the well and barrier regions, respectively. Then we have the following boundary conditions:

$$\left[\Gamma_{+w}\frac{\partial\Psi_2'}{\partial z}-\sqrt{3}\gamma_{3w}k\Psi_1'(z)\right]_{z=z_w}=\left[\Gamma_{+b}\frac{\partial\Psi_2'}{\partial z}-\sqrt{3}\gamma_{3b}k\Psi_1'(z)\right]_{z=z_b}\ , \tag{21}$$

$$\left[\Gamma_{-w}\frac{\partial\Psi_1'}{\partial z}+\sqrt{3}\gamma_{3w}k\Psi_2'(z)\right]_{z=z_w}=\left[\Gamma_{-b}\frac{\partial\Psi_1'}{\partial z}+\sqrt{3}\gamma_{3b}k\Psi_2'(z)\right]_{z=z_b}\ , \tag{22}$$

where $\Gamma_{\pm w}=(\gamma_{1w}\pm2\gamma_{2w})/2$ and $\Gamma_{\pm b}=(\gamma_{1b}\pm2\gamma_{2b})/2$ [γ_{iw} and γ_{ib} are defined in Eq. (4)]. Furthermore, we assume that

$$\Psi_j'(z_w)=\Psi_j'(z_b),\quad j=1,2\ . \tag{23}$$

Since $\Psi_j(z)$ has to be convergent when $z\to\pm\infty$ in the barrier regions, we require that

$$C_{21}=B_{21}=0,\quad C_{23}=B_{23}=0\quad \text{if}\quad z\to+\infty$$

and

$$C_{22}=B_{22}=0,\quad C_{24}=B_{24}=0 \quad \text{if } z\to-\infty \ . \tag{24}$$

The boundary conditions for Ψ_3' and Ψ_4' can be obtained similarly, by defining the following notation:

$$C_j=\cos q_jL/2,\quad S_j=\sin q_jL/2\ ,$$

$$\Lambda_{rw}(q_j)=|R|/\Delta(q_j)\ ,$$

and

$$\Lambda_{sw}(q_j)=-\sqrt{3}\gamma_{3w}kq_j/\Delta(q_j)$$

for the well region, and

$$b_j=e^{-\kappa_jL/2},\quad \Lambda_{rb}(\kappa_j)=|R|/\Delta(-i\kappa_j)\ ,$$

and

$$\Lambda_{sb}(\kappa_j)=\sqrt{3}\gamma_{3b}k\kappa_j/\Delta(-i\kappa_j)$$

for the barrier regions, where

$$\Delta(\bar{q}_j)=(P+Q-E)_{k_z=\bar{q}_j}$$

has been defined in Eq. (7). We get eight equations from Eqs. (21)–(24) at $z=\pm L/2$ and they are written in matrix form as shown in Eq. (25) at right, where $P=\sqrt{3}k(\gamma_{3b}-\gamma_{3w})$ is adopted and the following transformations are used:

$$W_{21}=\tfrac{1}{2}(W_{21}'+iW_{22}'),\quad W_{22}=\tfrac{1}{2}(W_{21}'-iW_{22}')\ ,$$

$$W_{23}=\tfrac{1}{2}(W_{23}'+iW_{24}'),\quad W_{24}=\tfrac{1}{2}(W_{23}'-iW_{24}')\ ,$$

$$B_{21}=\tfrac{1}{2}(B_{21}'+B_{22}'),\quad B_{22}=\tfrac{1}{2}(B_{21}'-B_{22}')\ ,$$

$$B_{23}=\tfrac{1}{2}(B_{23}'+B_{24}'),\ \text{and}\ B_{24}=\tfrac{1}{2}(B_{23}'-B_{24}')\ .$$

Equation (25) is used to describe the energy spectrum $E(\mathbf{k})$ and the corresponding eigenvectors $\Psi_1'(z)$ and $\Psi_2'(z)$ when holes are confined in a finite potential well with a barrier height V_0 and a well width L to which stress is applied. For the eigenvector $\Psi_3'(z)$ and $\Psi_4'(z)$, we need only replace γ_2 with $-\gamma_2$, δ with $-\delta$, and ν with $-\nu$, for k_z in Eqs. (17) and (18) and W_{2j}' with W_{4j}', B_{2j}' with B_{4j}', in Eq. (25). The original eigenvector Ψ as defined in Eq. (13) can now be obtained by using Eq. (15):

$$\begin{bmatrix}\Psi_1(z)\\ \Psi_2(z)\\ \Psi_3(z)\\ \Psi_4(z)\end{bmatrix}=\frac{1}{2}\begin{bmatrix}[\Psi_4'(z)+\Psi_1'(z)]e^{i\varphi}\\ [\Psi_3'(z)+\Psi_2'(z)]e^{i\eta}\\ [\Psi_3'(z)-\Psi_2'(z)]e^{-i\eta}\\ [\Psi_4'(z)-\Psi_1'(z)]e^{-i\varphi}\end{bmatrix} \tag{26}$$

where the normalization condition

$$\int_{-\infty}^{\infty} dz\,\Psi^{+}\Psi=1$$

requires that

$$\begin{bmatrix}
-\Lambda_{rw}(q_1)C_1 & \Lambda_{sw}(q_1)C_1 & -\Lambda_{rw}(q_2)C_2 & \Lambda_{sw}(q_2)C_2 & \Lambda_{rb}(\kappa_1) & \Lambda_{sb}(\kappa_1) & \Lambda_{rb}(\kappa_2) & \Lambda_{sb}(\kappa_2)\\
\Lambda_{sw}(q_1)S_1 & \Lambda_{rw}(q_1)S_1 & -\Lambda_{sw}(q_2)S_2 & \Lambda_{rw}(q_2)S_2 & -\Lambda_{sb}(\kappa_1) & -\Lambda_{rb}(\kappa_1) & \Lambda_{sb}(\kappa_2) & -\Lambda_{rb}(\kappa_2)\\
C_1 & 0 & C_2 & 0 & -1 & 0 & -1 & 0\\
0 & -S_1 & 0 & -S_2 & 0 & 1 & 0 & 1\\
0 & -q_1\Gamma_{+w}C_1 & 0 & -q_2\Gamma_{+w}C_2 & -P\Lambda_{rb}(\kappa_1) & -\kappa_1\Gamma_{+b}-P\Lambda_{sb}(\kappa_1) & -P\Lambda_{rb}(\kappa_2) & -\kappa_2\Gamma_{+b}-P\Lambda_{sb}(\kappa_2)\\
-q_1\Gamma_{+w}S_1 & 0 & -q_2\Gamma_{+w}S_2 & 0 & \kappa_1\Gamma_{+b}+P\Lambda_{sb}(\kappa_1) & P\Lambda_{rb}(\kappa_1) & \kappa_2\Gamma_{+b}+P\Lambda_{sb}(\kappa_2) & P\Lambda_{rb}(\kappa_2)\\
q_1\Gamma_{-w}\Lambda_{sw}(q_1)C_1 & q_1\Gamma_{-w}\Lambda_{rw}(q_1)C_1 & q_2\Gamma_{-w}\Lambda_{sw}(q_2)C_2 & q_2\Gamma_{-w}\Lambda_{rw}(q_2)C_2 & -P+\kappa_1\Gamma_{-b}\Lambda_{sb}(\kappa_1) & \kappa_1\Gamma_{-b}\Lambda_{rb}(\kappa_1) & -P+\kappa_2\Gamma_{-b}\Lambda_{sb}(\kappa_2) & \kappa_2\Gamma_{-b}\Lambda_{rb}(\kappa_2)\\
q_1\Gamma_{-w}\Lambda_{rw}(q_1)S_1 & -q_1\Gamma_{-w}\Lambda_{sw}(q_1)S_1 & q_2\Gamma_{-w}\Lambda_{rw}(q_2)S_2 & -q_2\Gamma_{-w}\Lambda_{sw}(q_2)S_2 & -\kappa_1\Gamma_{-b}\Lambda_{rb}(\kappa_1) & P-\kappa_1\Gamma_{-b}\Lambda_{sb}(\kappa_1) & -\kappa_2\Gamma_{-b}\Lambda_{rb}(\kappa_2) & P-\kappa_2\Gamma_{-b}\Lambda_{sb}(\kappa_2)
\end{bmatrix}
\begin{bmatrix}W_{21}'\\ W_{22}'\\ W_{23}'\\ W_{24}'\\ \dfrac{B_{21}'b_2}{2}\\ \dfrac{B_{22}'b_2}{2}\\ \dfrac{B_{23}'b_2}{2}\\ \dfrac{B_{24}'b_2}{2}\end{bmatrix}=0 \tag{25}$$

$$\int_{-\infty}^{\infty} dz(\Psi_1^*\Psi_1+\Psi_2^*\Psi_2)=\int_{-\infty}^{\infty} dz(\Psi_3^*\Psi_3+\Psi_4^*\Psi_4)=1 \tag{27}$$

and serves to determine the normalization constants N_U and N_L in Eqs. (19) and (20). The probability density and the effective mass are defined as $\rho_j(z)=|\Psi_j(z)|^2$ with $j=1,2,3,4$ and $m^*=(\partial_k^2 E)^{-1}$, respectively.

The magnitudes of the physical quantities δ, η, ξ, and ν [Eq. (18)] in the strain matrix elements depend on the direction of the applied uniaxial stress of magnitude X and are listed below.

1. X applied parallel to [100]:

$$\eta=D_d(S_{11}+2S_{12})X,\quad \delta=-\tfrac{1}{3}D_u(S_{11}-S_{12})X\ ,$$
$$\nu=\sqrt{3}\delta,\quad \xi=0\ .$$

2. X applied parallel to [001]:

$$\eta=D_d(S_{11}+2S_{12})X\ ,\quad \delta=\tfrac{2}{3}D_u(S_{11}-S_{12})X\ ,$$
$$\nu=\xi=0\ .$$

3. X applied parallel to [110]:

$$\eta=\tfrac{1}{2}D_d(S_{11}+3S_{12})X,\quad \delta=-\tfrac{1}{3}D_u(S_{11}-S_{12})X\ ,$$
$$\nu=0,\quad \xi=\frac{1}{2\sqrt{3}}D_u'S_{44}\ .$$

Here S_{ij} is the compliance tensor.

To summarize this section, the general formalism for holes confined in a quantum well under stress has been completed by solving a 4×4 total Hamiltonian with appropriate boundary conditions. Even though our results are valid only as long as $\varepsilon_{zx}=\varepsilon_{yz}=0$, they cover the directions where stress can be applied experimentally.

III. DISCUSSION

In this section, we discuss a special case (X applied parallel to [100], $V_0=\infty$ for the infinite potential well) which might give us some physical implications.

When V_0 is infinite, κ_1 and κ_2 obtained from Eq. (17) become infinite; therefore, b_1 and b_2 are infinitesimal and Eq. (25) reduces to

$$\begin{bmatrix} -\Lambda_r(q_1)C_1 & \Lambda_s(q_1)C_1 & -\Lambda_r(q_2)C_2 & \Lambda_s(q_2)C_2 \\ \Lambda_s(q_1)S_1 & \Lambda_r(q_1)S_2 & \Lambda_s(q_2)S_2 & \Lambda_r(q_2)S_2 \\ C_1 & 0 & C_2 & 0 \\ 0 & -S_1 & 0 & -S_2 \end{bmatrix}\begin{bmatrix} W_{21}' \\ W_{22}' \\ W_{23}' \\ W_{24}' \end{bmatrix}=0 \tag{28}$$

with

$$q_{1,2}=(4\Gamma_+\Gamma_-)^{1/2}[B\pm(B^2-16\Gamma_+\Gamma_-C)^{1/2}]^{1/2}\ , \tag{29}$$

where q_i are positively defined and the subscripts 1 and 2 in q refer to plus and minus signs, respectively. The secular equation obtained from Eq. (28) gives

$$(\Delta_1\Delta_2'+\Delta_1'\Delta_2-2|R|^2)\sin q_1L\,\sin q_2L =(6\gamma_3^2k^2q_1q_2)(1-\cos q_1L\,\cos q_2L)\ , \tag{30}$$

where

$$\Delta_i=P+Q(q_i)-E\ ,\quad \Delta_i'=P-Q(q_i)-E,\quad i=1,2 \tag{31}$$

and $P\pm Q(q_i)$ are shown in Eq. (7). The numerical results for the energy spectra $E(k)$ without stress (i.e., $\delta=0$) have been reported in the literature.[3-5] At $k=0$, Eq. (30) yields

$$E_n=\Gamma_\mp\left[\frac{n\pi}{L}\right]^2+\eta\pm\delta,\quad n=1,2,3,\ldots \tag{32}$$

where the upper (lower) sign refers to the heavy (light) hole. Equation (32) indicates that (1) if η and δ are positive under stress $X<0$, E_n for the heavy hole linearly increases faster than E_n for the light hole as $|-X|$ increases, and (2) E_n for the heavy hole runs across E_n for the light hole at

$$X=\left[3\gamma_2\left[\frac{n\pi}{L}\right]^2\right]\Big/[2D_u(S_{11}-S_{12})]<0$$

because $\Gamma_-<\Gamma_+$. Thus, when X is parallel to [001], there is no anticrossing in E_n for the light and heavy holes. This occurs because in this direction of the stress, and at $k=0$, $|R|=|S|=0$, so that Eq. (16) is decoupled. Therefore the wave functions Ψ_1' and Ψ_2' (Ψ_4' and Ψ_3') represent pure states of the heavy and light hole, respectively, i.e., there is no valence-band mixing.

The effective masses of the heavy hole and light hole are given by

$$m_n^*=[\partial_k^2E_n(k)]^{-1}\quad\text{at}\quad k\to0 \tag{33}$$

where

$$[\partial_k^2E_n(k)]_{k\to0}=\gamma_1\pm\gamma_2\mp\frac{3\gamma_3^2}{\gamma_2-Y_n}+\frac{6\gamma_3^2(\Gamma_\mp\pm2Y_n)[(-1)^{n+1}+\cos\theta_n]}{(\gamma_2-Y_n)^2\theta_n\sin\theta_n} \tag{34}$$

with

$$Y_n=\delta L^2/n^2\pi^2$$

and

$$\theta_n = n\pi[(\Gamma_\mp \pm 2Y_n)/\Gamma_\pm]^{1/2} . \quad (35)$$

Without stress ($Y_n = 0$) and without warping of the valence band ($\gamma_2 = \gamma_3$), Eqs. (33)–(35) reproduce the same result as calculated by Fasolino and Altarelli,[3] and confirm that m_n^* for the heavy and light holes are independent of well width, L. However, if stress is applied to the system ($Y_n \neq 0$), m_n^* is a function of L and δ. Equations (33)–(35) indicate that (1) when $Y_n = \gamma_2$, i.e., $X = -3\gamma_2 n^2\pi^2/L^2 D_u(S_{11} - S_{12})$, m_n^* becomes zero because the curvature of $E_n(0)$ is infinite, and (2) $[\partial_k E_n(k)]_{k=0}$ may become zero for certain Y_n, implying, m_n^* is $\pm\infty$. The effective mass m_n^* has strong dependences on δ and L.

By examining the upper block of Eq. (16), we notice that $\Psi_1'(z)$ and $\Psi_2'(z)$ are coupled as long as $|R|^2 + |S|^2$ is nonzero and composed of four components: $e^{\pm iq_1 z}$ and $e^{\pm iq_2 z}$ in the well region. We call the first components heavy-hole-like and the second components light-hole-like. Whether $\Psi_1'(z)$ is heavy-hole-like or light-hole-like depends on the amplitude of each of the components which are governed by Eq. (25). In this case, valence bands are mixed and $E_n(k)$ considered for heavy hole and light hole as a function of stress X is expected to show an anticrossing; this is in contrast to the case where $|R|^2 + |S|^2$ is zero, as discussed earlier (in the case of X parallel to [001]). It is interesting to notice also that, at $k = 0$, Eq. (25) can be decoupled into two 4×4 matrix equations by letting $\Lambda_{sw} = \Lambda_{sb} = 0$ and $P = 0$. One of these two matrix equations describes the eigenvalues with the even wave functions, and the other one the eigenvalues with odd wave functions. Detailed discussion of these two decoupled matrix equations is presented elsewhere.[12] Finally, it is worth mentioning that, if $|R|^2 + |S|^2$ is zero, Eq. (16) yields

$$E = A_\pm - \frac{\Gamma_\mp |R|^2}{3\gamma_3^2 k^2} \quad (k \neq 0) ,$$

which are the trivial solutions of Eq. (25) and therefore must be discarded because they do not provide any information about the quantum size effects.

In order to compare out theoretical prediction with some of the experimental results, and to show the full implications of the formalism in Sec. III, we solve Eq. (25) numerically for finite potential barriers, V_0, and various well widths, L. Since there is no guarantee that k_z^2 in Eq. (17) is real if k and stress are nonzero, we have to treat k_z as complex values. All these results, including effective-mass studies, are reported in a paper to follow.[13]

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