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Band-to-Band Transitions in InAs/GaSb Multi-Quantum-Well Structures Using k.p Theory: Effects of Well/Barrier Width and Temperature

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Abstract: We investigated the conduction- and valence-confined energy levels and first band-to-band transition energies of a type-II InAs/GaSb multi-quantum-well at 77 K and room temperature for various well and barrier thicknesses. We calculated the electron and hole confined energies based on Kane's eight-band k.p formalism. We also explored the effect of the barrier width on the wells' interactions, which was negligible for wells with a width wider than 30 nm. Moreover, we proposed a single exponential function to predict the first transition energies without considering the complex approach of k.p theory. Then, we measured the photoluminescence spectra of the manufactured samples, including thin wells (1, 2, and 3 monolayers) and wide barriers (50 nm). Finally, we made comparisons between the theoretical band-to-band transition energies for $k_z = 0$ and experimental results from the photoluminescence spectra for different well thicknesses at 77 and 300 K.

Keywords: InAs/GaSb multi-quantum-well structure; eight-band k.p theory; finite difference method; first transition energy; photoluminescence



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1. Introduction

Currently, there is considerable research interest in zinc-blende III-V semiconductors, such as InAs, InSb, GaAs, and GaSb [1]. Specifically, various high-performance electronic and optoelectronic devices have been realized using antimony-containing III-V compound semiconductor heterostructures. In contrast to the II-VI HgCdTe system, which breaks down its ionic bonds at high temperatures and releases Hg during ion implantation, the III-V semiconductors are chemically stable due to their solid covalent bonds [2]. Among these structures, researchers are attracted to the unique features of InAs/GaSb heterostructures. Very little lattice mismatch (with $\Delta a/a \approx 0.6\%$) between the layers results in a high-quality epitaxially grown material [3]. Because of this, strain is not considered in this model [4]. Some methods and models have explained quantum well (QW) confinement states in the past. For example, Schulman and Chang [5,6] have presented a remarkably detailed description of the confinement states in a QW. They use nearest-neighbor empirical tight-binding models to describe the complex band structures of wells and barriers. Schuurmans and Hooft have described a simple and unified model of conduction- and valence-band confinement states in a quantum well [7]. There have been various studies of type-II QW zinc-blende III-V heterostructures, mainly because of their applications in optoelectronic devices, such as infrared detectors [2,8], mid-infrared (mid-IR) spectroscopy [9,10], and light-emitting diodes [11]. Several semiconductor lasers in the mid-IR range (2–5 μm) have been developed, including inter-band cascade lasers (ICLs), type-II QW lasers, and InAs/GaSb short-period superlattices (SPSLs) [12–14]. In addition to molecular spectroscopy and chemical detection, these lasers may find applications in biomedical and optical communication systems [15,16]. A theoretical analysis of strained

InAs(N)/GaSb/InAs(N) quantum-well heterostructure lasers operating in the mid-IR region has also been performed by Ridene et al. [17]. In addition, several other quantum-size heterostructures have been investigated, including multi-quantum-wells (MQWs) and superlattices (SLs) [12,17–21]. Direct band gaps are found in most optical devices. This type of band gap allows various fascinating physical phenomena to occur at the semiconductor's band edge. To investigate the band structure's energy levels, experimental and theoretical advances have recently been studied for III–V semiconductors [18,19]. Experiments have been conducted with these materials, especially multi-layer structures made of InAs/GaSb [19], to investigate their optical properties, including photoluminescence (PL) spectroscopy [20] and photo-modulated reflectance spectroscopy [21]. Theoretically, several notable attempts have been made to approximate the energy levels of semiconductor materials. The atomistic methods include the Hartree–Fock method [22], the empirical tight-binding method [23], density functional theory (DFT) with local density approximation [24], atomic orbital potential with general gradient approximation [25], and non-atomistic methods, such as the k.p theory [4,18,19,26,27] and effective mass approximation [1]. Because Schrödinger's equation with an energy-dependent effective mass and a nonlinear eigenvalue problem cannot be solved analytically, researchers use numerical methods, such as the transfer matrix method [28], the shooting method [29], the finite element method (FEM) [30,31], and the finite difference method (FDM) [19,26,32]. The k.p theory also helps to calculate energy levels as a semi-empirical theoretical tool. Several research groups theoretically and experimentally studied the optical and topological properties of the band structure for III–V compounds (especially InAs/GaSb) with single QW, MQW, and SL structures [4,19–21,23–26,33]. They investigated the role of the thickness of the well and composition [19,34,35], the magnetic field [36], and the spin–orbit band on the band gap [37], in addition to the temperature [35] for different quantum-sized structures. For example, researchers have also considered higher-order optical transitions in InAs/GaSb SLs [19], which obtained variations in energies for conduction and valence levels versus changing the well width using the eight-band k.p model and optical spectroscopy.

As mentioned, InAs/GaSb (QW, MQW, and SL) structures have been extensively investigated. However, to our knowledge, no general trend in the energies of structures has been identified. In addition, the impact of well/barrier widths on conduction- and valence-confined energies has not been separately considered. As such, we were motivated to consider the structures to achieve more general conclusions about transition energies.

Our work uses the eight-band k.p model and photoluminescence measurements to investigate InAs/GaSb MQW. Using the finite difference method, we discretized MQWs Hamiltonian based on the theoretical energy levels. In addition, we investigated InAs/GaSb MQWs with thin well widths (1–3 MLs) and different barrier thicknesses (5–50 nm) at 77 K and 300 K. During these investigations, we predicted the transition energies of the structures for different well/barrier widths from a single exponential function. The ability to tune an effective band gap by varying layer thicknesses rather than mole composition is one of the more considerable properties of T2SLs [18]. The results of our current work, which include estimating the transition energies, may help predict the energy range of structures with different well/barrier widths, allowing us to design appropriate optoelectronic devices without considering complex k.p theory.

2. Theory

This section provides an overview of Kane's 8×8 k.p method, which relies on the perturbation theory [38]. Initially, we prepared the basics of the eight-band Hamiltonian and introduced the related parameters. In the second part, the foundation of the finite difference method to discretize the Hamiltonian is presented for the sample under investigation. Several previous studies utilized this method to calculate the band structure of InAs/GaSb in bulk, QWs, and SLs [19–21]. Here, we apply and present the eight-band k.p method on InAs/GaSb type-II MQWs. The technique mainly revolves around the band structure's Γ point, and we investigated energy-confined levels. The under-investigated MQW structure

growth direction is [001], which is defined by the z -axis, and the x and y axes are along [100] and [010]. Generally, the electron energy levels can be calculated using the following Schrödinger equation:

$$\hat{H}\psi_j(\mathbf{k}, r) = E\psi_j(\mathbf{k}, r), \quad (1)$$

where $\hat{H}$ is the total Hamiltonian operator, and E is the corresponding energy. The SL (MQW) wave function $\psi_j(\mathbf{k}, r)$ ($j = 1, 2, \dots, 8$) can be expanded as a linear combination of the basis states $u_v(r)$ and envelope function $F_j(\mathbf{k}, r)$ as follows:

$$\psi_j(\mathbf{k}, r) = \sum_{v=1}^8 u_v(r)F_j(\mathbf{k}, r), \quad (2)$$

where r is the in-plane position vector. The wave vector $\mathbf{k}$ is defined as $(k_{\parallel}, k_z)$ and $k_{\parallel} = k_x^2 + k_y^2$, of which k_x and k_y are the wave vector components in the plane of MQW, j is the subband (basis) index, k_z is the SL wave vector along the growth direction (z -axis), $u_v(r)$ are the zone-center basis states, and $F_j(\mathbf{k}, r)$ is the v th component of the j th subband envelope function along the z -axis [39].

The band structure near the high-symmetry extremum points (e.g., Γ , X , L) can be simulated accurately enough to simulate the optoelectronic processes near the semiconductor band gaps using $k \cdot p$ theory. This method uses multi-band envelope functions or effective masses to describe the interaction between bulk bands by considering the general Hamiltonian as perturbed by the $k \cdot p$ term. Increasing the remote bands' effects can also be involved in the theory, and the conduction-band states contribute to the valence-band energies and vice versa. This procedure gives more accurate results than simpler models, such as effective mass approximation for energy levels, and can be readily used for device-level analysis and design.

2.1. The 8×8 $k \cdot p$ Hamiltonian

The complete form of the eight-band Hamiltonian for the bulk zinc-blende semiconductors' Γ point can be expressed as follows [40,41]:

$$H_{8 \times 8} = \begin{pmatrix} T & 0 & \frac{-1}{\sqrt{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{6}}Pk_- & 0 & \frac{-1}{\sqrt{3}}Pk_z & \frac{-1}{\sqrt{3}}Pk_- \\ 0 & T & 0 & \frac{-1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{2}}Pk_- & \frac{-1}{\sqrt{3}}Pk_+ & \frac{1}{\sqrt{3}}Pk_z \\ cc & 0 & U + V & -\bar{S}_- & R & 0 & \frac{1}{\sqrt{2}}\bar{S}_- & -\sqrt{2}R \\ cc & cc & cc & U - V & C & R & \sqrt{2}V & -\sqrt{\frac{3}{2}}\tilde{S}_- \\ cc & cc & cc & cc & U - V & \bar{S}_+ & -\sqrt{\frac{3}{2}}\tilde{S}_+ & -\sqrt{2}V \\ 0 & cc & 0 & cc & cc & U + V & \sqrt{2}R^\dagger & \frac{1}{\sqrt{2}}\bar{S}_+ \\ cc & cc & cc & cc & cc & cc & U - \Delta_0 & 0 \\ cc & cc & cc & cc & cc & cc & cc & U - \Delta_0 \end{pmatrix}, \quad (3)$$

where cc represents the elements' complex conjugate of the matrix's upper half. Additionally,

$$\begin{aligned} k_{\pm} &= k_x \pm ik_y, \quad k_{\parallel}^2 = k_x^2 + k_y^2 \quad \text{and} \quad k_z = -i\frac{\partial}{\partial z}, \\ T &= E_c + \frac{\hbar^2}{2m_0}(\gamma'_0 k_{\parallel}^2 + k_z \gamma'_0 k_z), \\ U &= E_v - \frac{\hbar^2}{2m_0}(\gamma'_1 k_{\parallel}^2 + k_z \gamma'_1 k_z), \\ V &= -\frac{\hbar^2}{2m_0}(\gamma'_2 k_{\parallel}^2 - 2k_z \gamma'_2 k_z), \\ R &= -\frac{\hbar^2}{2m_0}\frac{\sqrt{3}}{2}((\gamma'_3 - \gamma'_2)k_+^2 - (\gamma'_3 - \gamma'_2)k_-^2), \\ \bar{S}_{\pm} &= -\frac{\hbar^2}{2m_0}\sqrt{3}k_{\pm}(\{\gamma'_3, k_z\} + [\kappa', k_z]), \\ \tilde{S}_{\pm} &= -\frac{\hbar^2}{2m_0}\sqrt{3}k_{\pm}(\{\gamma'_3, k_z\} - \frac{1}{3}[\kappa', k_z]), C = \frac{\hbar^2}{m_0}k_-[\kappa', k_z]. \end{aligned} \quad (4)$$

In the above equations, $[\alpha, \beta] = \alpha\beta - \beta\alpha$ and $\{\alpha, \beta\} = \alpha\beta + \beta\alpha$ are the commutator and anticommutator, respectively, for operator α and β . m_0 is the free electron mass, E_g is the band gap between conduction- and valence-band states, and E_c and E_v refer to the conduction and valence band edges, respectively. Δ is the spin–orbit splitting energy and P is the Kane momentum matrix element. $\gamma'_0, \gamma'_1, \gamma'_2, \gamma'_3, \kappa'$ are the modified Luttinger parameters, which describe the coupling to the remote bands. They are related to the original Luttinger parameters of the hole bands, and the $\gamma_0, \gamma_1^L, \gamma_2^L, \gamma_3^L, \kappa$ obtained from experiments correspond to the Dresselhaus definition [42]. The modification of Luttinger parameters is related to the original Luttinger parameters in the following way [38]:

$$\begin{aligned}\gamma'_0 &= \gamma_0 - \frac{E_p}{E_g} \left(\frac{E_g + \frac{2}{3}\Delta_0}{E_g + \Delta_0} \right), \\ \gamma'_1 &= \gamma_1^L - \frac{E_p}{3E_g + \Delta_0}, \\ \gamma'_2 &= \gamma_2^L - \frac{1}{2} \left(\frac{E_p}{3E_g + \Delta_0} \right), \\ \gamma'_3 &= \gamma_3^L - \frac{1}{2} \left(\frac{E_p}{3E_g + \Delta_0} \right), \\ \gamma'_0 &= \frac{m_0}{m'_c} \quad \text{and} \quad \gamma_0 = \frac{m_0}{m_c}.\end{aligned}\tag{5}$$

The E_p is Kane energy, which is defined as $2m_0P^2/\hbar^2$. m_c and m'_c are the effective mass of the conduction band and the corrected effective mass, respectively [38]. The band-structure parameters for InAs and GaSb at 77 K and room temperature are summarized in Table 1. The basic parameters in the simulation need to be renormalized according to Equation (5). We chose the temperatures 77 and 300 K considering the low and high temperatures because the materials' available Luttinger parameters in the literature meant we had to choose these specific temperatures; furthermore, because of our experimental limitations for very low temperatures, we chose 77 K as a low temperature in this study.

Table 1. Material parameters for calculations at 77 and 300 K are adopted from [42–45].

Parameter	77 K		300 K	
	InAs	GaSb	InAs	GaSb
a_0 (Å)	6.0584	6.0954	6.0584	6.0954
E_g (eV)	0.418	0.814	0.359	0.725
Δ_0 (eV)	0.38	0.76	0.38	0.76
E_p (eV)	22.42	22.75	22.19	23.47
m_c/m_0	0.022	0.042	0.019	0.037
γ_1^L	20	11.87	23.8	14.48
γ_2^L	9	4.61	10.7	5.67
γ_3^L	9.16	4.99	10.39	5.6
VBO (eV)	−0.59	0	−0.501	0

The Hamiltonian in Equation (3) is simplified by assuming that the z-axis is the crystal growth direction $\mathbf{k} \equiv (0, 0, k_z)$. All Hamiltonian elements will be position-dependent because of the different material layers in the structures.

2.2. Discretization with FDM

To solve the Schrödinger equation for the unstrained InAs/GaSb MQW structure within the framework of the eight-band k.p model using FDM, the Hamiltonian is discretized in the growth direction. Therefore, it is assumed that the z-component of the wave vector k_z (growth direction of the MQWs) is replaced with the differential form $(-i\partial/\partial z)$, while the x and y components remain constant. Hence, applying the above replacements

yields as shown in Equation (3), one can derive the discretized Hamiltonian as a sum of three terms for each point of the QW structure as follows:

$$H\left(-i\frac{\partial}{\partial z}\right) = H^{(0)}(z_n) - iH^{(1)}(z_n)\frac{\partial}{\partial z} + i\frac{\partial}{\partial z}H^{(2)}(z_n)i\frac{\partial}{\partial z}, \quad (6)$$

where the first term of the above relation is a k_z -independent 8×8 submatrix $H^{(0)}(z_n)$ with no derivative operator, and the second and third terms are 8×8 submatrices $H^{(1)}(z_n)$ and $H^{(2)}(z_n)$ with the first- and second-order derivative operators, respectively. The form of these submatrices is presented in Appendix A. The central difference of FDM is applied to resolve first- and second-order derivative terms. So, the first and second derivatives of the wave function can be written as [46]:

$$\begin{aligned} \frac{\partial \psi_j(z_n)}{\partial z} &= \frac{\psi_j(z_{n+1}) - \psi_j(z_{n-1}))}{2\Delta z_n}, \\ \frac{\partial^2 \psi_j(z_n)}{\partial z^2} &= \frac{\psi_j(z_{n+1}) - 2\psi_j(z_n) + \psi_j(z_{n-1}))}{\Delta z_n^2}. \end{aligned} \quad (7)$$

where n is the mesh indices in the z -direction and Δz is the spacing between two adjacent mesh points ($\Delta z_n \equiv z_{n+1} - z_n$).

Using Equation (7) and the following discretization scheme:

$$\begin{aligned} -i H^{(1)}(z_n) \frac{\partial}{\partial z} \psi_j(z_n) &\approx -i \frac{H^{(1)}(z_{n+1}) + H^{(1)}(z_n)}{4\Delta z_n} \psi_j(z_{n+1}) \\ &+ i \frac{H^{(1)}(z_n) + H^{(1)}(z_{n-1}))}{4\Delta z_n} \psi_j(z_{n-1}), \\ -i \frac{\partial}{\partial z} \left(H^{(2)}(z_n) i \frac{\partial}{\partial z} \psi_j(z_n) \right) &\approx \frac{H^{(2)}(z_{n+1}) + H^{(2)}(z_n)}{2\Delta z_n^2} \psi_j(z_{n+1}) \\ &- \frac{H^{(2)}(z_{n+1}) + 2H^{(2)}(z_n) + H^{(2)}(z_{n-1}))}{2\Delta z_n^2} \psi_j(z_n) \\ &+ \frac{H^{(2)}(z_n) + H^{(2)}(z_{n-1}))}{2\Delta z_n^2} \psi_j(z_{n-1}). \end{aligned} \quad (8)$$

The discretized equation at all grid points can be written as the following matrix:

$$M = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & \cdots & \cdots & M_{10}^* \\ M_{21} & M_{22} & M_{23} & 0 & \cdots & \cdots & 0 \\ 0 & M_{32} & M_{33} & M_{34} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & M_{z_{n-1}z_{n-2}} & M_{z_{n-1}z_{n-1}} & M_{z_{n-1}z_n} \\ M_{z_n z_{n+1}}^* & 0 & \cdots & \cdots & 0 & M_{z_n z_{n-1}} & M_{z_n z_n} \end{bmatrix}, \quad (9)$$

where

$$\begin{aligned} M_{z_n, z_{n-1}} &= -\frac{H^{(2)}(z_n) + H^{(2)}(z_{n-1}))}{2\Delta z_n^2} + i \frac{H^{(1)}(z_n) + H^{(1)}(z_{n-1}))}{4\Delta z_n}, \\ M_{z_n, z_n} &= \frac{H^{(2)}(z_{n+1}) + 2H^{(2)}(z_n) + H^{(2)}(z_{n-1}))}{2\Delta z_n^2} + H^{(0)}(z_n), \\ M_{z_n, z_{n+1}} &= -\frac{H^{(2)}(z_{n+1}) + H^{(2)}(z_n)}{2\Delta z_n^2} - i \frac{H^{(1)}(z_{n+1}) + H^{(1)}(z_n)}{4\Delta z_n}. \end{aligned} \quad (10)$$

The resulting Hamiltonian forms a tridiagonal matrix that contains $n \times n$ elements, and each element consists of an 8×8 matrix. The size of this matrix depends on the number of grid points and must be truncated for a number of the grid points that give convergence eigenvalues (energy levels). By assuming $[k_x, k_y] = [0, 0]$ and discretizing the Hamiltonian, the eigenvalue problem for each point z is written as:

$$M \begin{bmatrix} \psi_1(z_1) \\ \vdots \\ \psi_8(z_1) \\ \psi_1(z_2) \\ \vdots \\ \psi_8(z_2) \\ \vdots \\ \vdots \\ \psi_1(z_{n-1}) \\ \vdots \\ \psi_8(z_{n-1}) \\ \psi_1(z_n) \\ \vdots \\ \psi_8(z_n) \end{bmatrix} = E \begin{bmatrix} \psi_1(z_1) \\ \vdots \\ \psi_8(z_1) \\ \psi_1(z_2) \\ \vdots \\ \psi_8(z_2) \\ \vdots \\ \vdots \\ \psi_1(z_{n-1}) \\ \vdots \\ \psi_8(z_{n-1}) \\ \psi_1(z_n) \\ \vdots \\ \psi_8(z_n) \end{bmatrix} \quad (11)$$

where $\psi_1, \psi_2, \dots, \psi_8$ are the function of z for $k_{\parallel} = 0$. Using this procedure, the resulting Hermitian symmetric Hamiltonian forms a $8n \times 8n$ tridiagonal matrix [47,48]. M_{10}^* and $M_{z_n z_{n+1}}^*$ in Equation (9) denote the boundary conditions. When we encounter a single-quantum-well (SQW) problem, these conditions should be set to zero because the wave functions must vanish far from the well region. This is equivalent to $\psi_j(z_{n+1}) = \psi_j(z_0) = 0$. For an SL or MQW case, it requires that $\psi_j(z_{n+1}) = \exp(ikd)$ and $\psi_j(z_0) = \exp(-ikd)$, where k and d are wave vector along the z -axis and the SL periodicity, respectively. Because these boundary conditions act as the interaction terms between multiple QWs, we have called them interaction terms in the rest of this paper. Our computational model applies the periodic boundary condition in the z (growth) direction.

3. Experimental Section

The schematic diagram of the structure is demonstrated in Figure 1. We grew the 10-period InAs/GaSb type-II MQWs samples by molecular beam epitaxy (MBE). All the MQWs contain (N) ML InAs/50 nm GaSb with $N = 1, 2$, and 3 MLs per period. We grew a 50 nm GaSb buffer layer on a doped GaSb substrate at 500 °C, followed by the MQWs region with 50 nm GaSb barriers. We optically characterized the MQWs samples by PL spectroscopy. For the PL measurements, we used a 532 nm continuous-wave laser as an excitation source and collected the emission using an InSb detector with a detection range of 2.0 to 5.7 nm. The excitation intensity was 566 mW/cm². We used an argon-coated germanium filter to remove the residual pump radiation and any luminescence originating from the GaSb substrate. We amplified the PL signals by using a Stanford lock-in amplifier system.

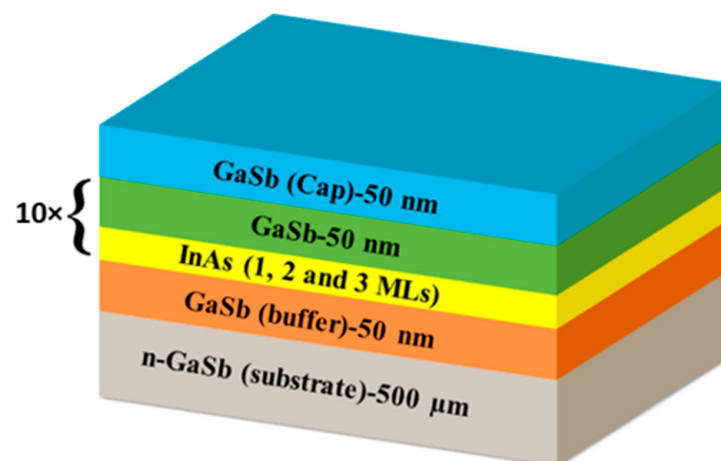


Figure 1. Schematic structure of manufactured InAs/GaSb multi-quantum-wells.

4. Results and Discussion

The results are presented in three subsections. In the first subsection, we demonstrate the simulation outcomes based on the eight-band *k.p* theory, including exploring the effect of the barrier width on the well's interaction, as well as the different well and barrier widths on valence- and conduction-confined energies. In this context, as expressed in the theory section, transforming from SQW to MQW was applied by imposing the periodic boundary conditions in the Hamiltonian (Equation (9)). So, the terms “with interaction” and “without interaction” refer to calculations with and without periodic boundary conditions, respectively. We show the transition energies for different well widths and temperatures in the final part of this subsection. In the second subsection, we present the photoluminescence spectra of the samples for different well widths. Last, we discuss the consistency between the simulations and experimental results.

4.1. Numerical Simulation

As mentioned in the experimental section, the manufactured samples include 10 InAs/GaSb periods sandwiched between the cap and substrate layers. Thus, there are two main differences between the theoretical and experimental models: in the simulations, we assume that (1) the MQW structure has an infinite period of layer, (2) and we ignore the cap and substrate effects on the energy levels. The only boundary condition imposed on the model occurred between the QWs in MQW structures as interaction terms in the Hamiltonian. Figure 2 shows the schematic band diagram of a 1 ML InAs/GaSb quantum well. The corresponding conduction and valence bands are depicted in blue and red colors. The figure demonstrates the type-II nature of the resulting heterostructure. The nominal well thicknesses of the manufactured samples determined that we put $1 \text{ ML} = (a_{\text{InAs}}/2) \sim 0.3 \text{ nm}$ in the calculations, where a_{InAs} is the lattice constant of the InAs. This definition of 1 ML is also used in the literature [49]. To obtain a well convergence for the resulting eigenvalues in discretization with FDM, we selected the number of grid points so that, e.g., for barrier widths of 50 nm, $\Delta z \sim 0.15 \text{ nm}$ was used. Our calculation is based on choosing the band diagram of Figure 2. Accordingly, we selected the GaSb valence band as the origin (zero point) in the simulations.

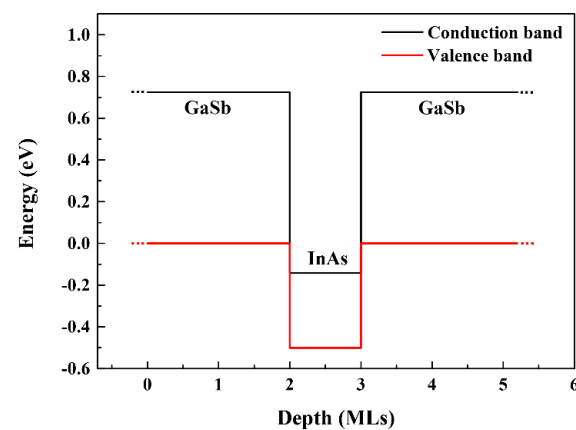


Figure 2. Schematic band diagram of a quantum – well with arbitrary well width.

4.1.1. Effect of the Barrier Width on the Well's Interactions

We investigated the pure effect of different barrier widths on the valence- and conduction-confined energy levels. To do so, we selected the 2 ML InAs/GaSb MQW with varied barrier widths of 7–50 nm and explored the barrier width's effect on the interaction between the wells. Figure 3a demonstrates the variation of the first conduction- (C1) and valence-confined (HH1) energies between wells with and without interaction terms. The figure shows that the difference between conduction (or valence) energies decreases between the two cases. For small barrier widths (7 nm), considering the interaction terms leads to changing the conduction-confined states by as much as 2 meV. However, this difference becomes smaller by increasing the barrier width, reaching zero when the barrier width gets close to 20 nm.

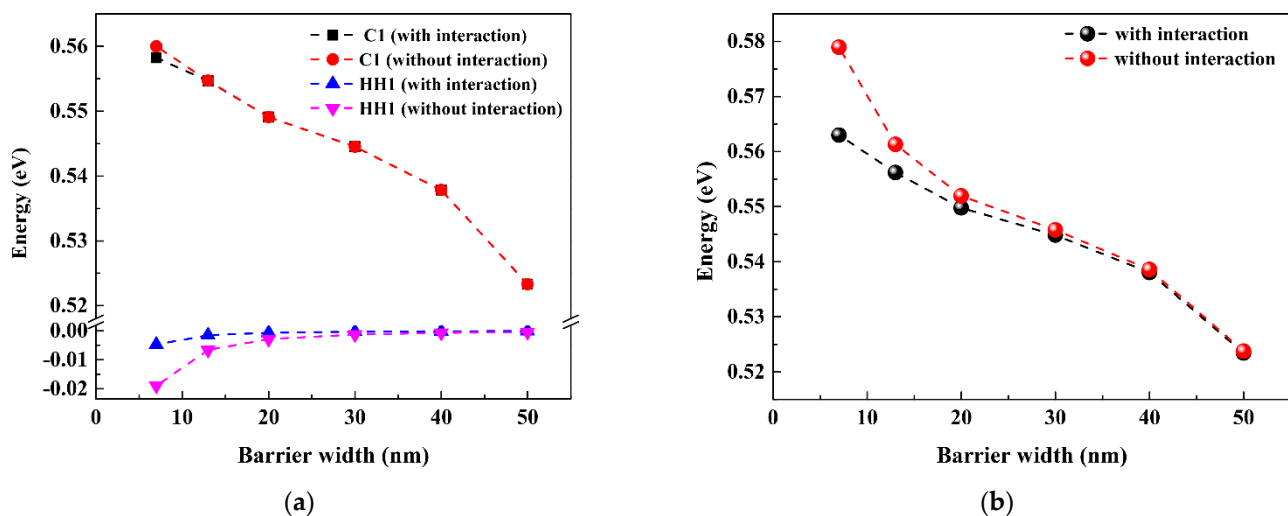


Figure 3. Variation of (a) conduction- and valence-confined energies (C1 and HH1, respectively) and (b) first transition energies for various barrier thicknesses with and without interaction terms.

Consequently, the effect of the interaction on conduction-confined states is negligible for widths wider than 20 nm. On the other hand, the effect of the interaction on valence-confined energies is considerable. For small well widths (7 nm), the difference between the two cases is 14 meV, and increasing the barrier width leads a decreasing difference. When the barrier width reaches 30 nm, the difference is approximately 1 meV and negligible. However, diminishing differences between conduction energies occur much faster compared with valence-confined energies. From these variations, we calculated the first band-to-band transition energies of the 2 ML MQW with and without interactions between the wells, and the results are presented in Figure 3b. The figure shows that the difference between the energies for barrier widths more than 30 nm is less than 1 meV, which is

negligible. As a result, we can consider the MQW problem in this system as an SQW problem for barriers broader than 30 nm. Because our manufactured samples have a 50 nm barrier in this work, we can confidently proceed with the simulation without considering the interaction effects between the wells. Moreover, the computing procedure for SQW is slightly more time-efficient than MQW.

4.1.2. Effect of Barrier Widths on Valence-Band Energy Levels

Here, we consider the effect of barrier widths (5 and 50 nm) on valence-confined energies for different well widths (1–3 MLs). Our results are presented in Figure 4a. As the figure shows, the valence-confined energies, especially for a higher barrier width (50 nm), are very close to the zero point, and the variation of the energies for 1–3 MLs is ~ 0.002 meV. However, selecting the smaller barrier width (5 nm) leads to ~ 2 meV reductions in the energies. The other point is that choosing smaller barrier widths leads to energies far from the zero point. To consider this variation further, we computed the variation in the valence band for a fixed well width (2 ML) and different barrier widths in the range of 5–50 nm; the results are demonstrated in Figure 4b. The figure indicates that, although the variation of the valence-confined energy for wider barrier widths is closer to the zero-point concerning narrower barriers, the minimum valence-confined energy is just 9 meV, which is far from the zero point. Nevertheless, choosing barrier widths wider than 30 nm leads to minimum variations in the valence-confined energies. Consequently, one can suppose the valence-confined energies are a fixed (zero) value for any choice of wide barrier (>30 nm) and well widths of InAs/GaSb MQWs.

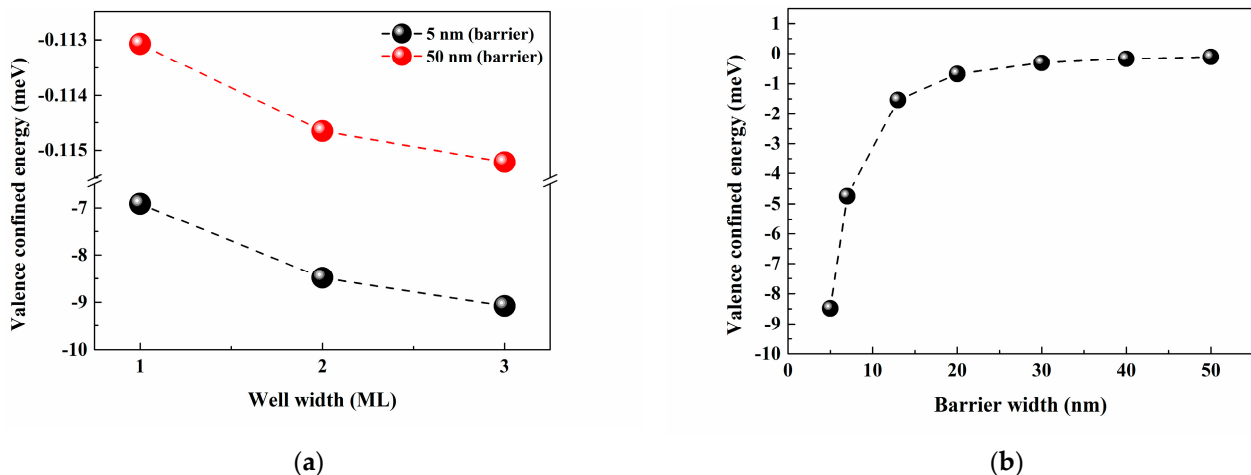


Figure 4. Variations of valence – confined energies for (a) different well and barrier widths and (b) 2 MLs well width and different barrier widths.

Therefore, we conclude that the slight variations in the valence-confined energies and the values close to zero are characteristics of these systems with large barrier widths. This property can be partially confirmed by other works about superlattice structures of InAs/GaSb, such as [19].

4.1.3. Transition Energies for Different Well Widths and Temperatures

The conduction- and valence-confined energy levels for InAs/GaSb QWs of 1, 2, and 3 InAs MLs at 77 K and 300 K temperatures are demonstrated in Figure 5a. The barrier widths were assumed to be 50 nm in all calculations, and the results are presented for the central symmetrical point of the Brillouin zone ($k = 0$). As Figure 5a shows, the conduction confined states for 1, 2, 3, 4, and 5 MLs decrease with increases in the well width for both temperatures. However, as the results show, the energies of the valence-confined states for every well width and temperature do not experience significant changes. Recent simulations show the slow, varying, first valence-confined energies of the InAs/GaSb SL

structure [19]. However, the goal of the work was not to consider the variations in confined states in the structures.

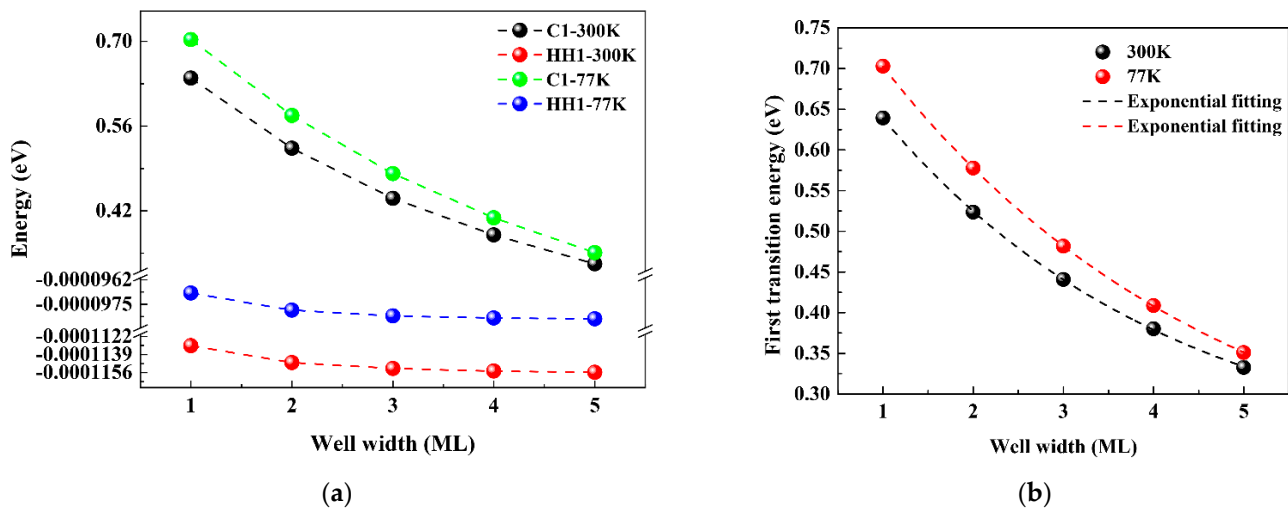


Figure 5. (a) Simulated electron (C1) and heavy-hole (HH1) confined energies and (b) first transition energies for InAs/GaSb multi-quantum-wells for 1 up to 5 MLs of InAs and 50 nm barrier (GaSb) width.

With the descriptions mentioned above, we can assume that we can obtain the first transition energies of the QW structure with just the help of conduction-confined-state energies with no attention to the hole-confined energies. The differences between the first transition energies of 1–5 MLs InAs/GaSb MQW, which are calculated as electron- and heavy-hole-confined states, are depicted in Figure 5b. Our results show that, although the effect of the temperature for a higher well width is lower, the transition energies decrease with increasing well width for both temperatures.

We present theoretical results up to 5 MLs to demonstrate the energy trend for larger well widths. Although k.p theory starts from the Schrödinger equation and, after some cumbersome and time-consuming calculations, leads to the final results, these trends (Figure 5b) show a decaying exponential form and can be very well-fitted (R-square~100%) to a single exponential function. Although this decaying behavior is presented in the literature [19], we found an exponential form with definite values for the exponential function parameters. The resulting exponential function ($A \exp(-w/b) + y_0$, where A , b , and y_0 are constants, and w is the well width) parameters for the two temperatures are summarized in Table 2. With the help of these functions, one can obtain the transition energies of InAs/GaSb type-II SQW or MQW (with high barrier width), without considering the k.p approach. This simple exponential trend may stem from the fact that transition energies, in this case, are obtained mainly from the electron-confined energies due to the constancy of valence-confined energies.

Table 2. Parameters of fitted exponential function as $A \exp(-w/b) + y_0$.

Parameter	77 K	300 K
A	0.703	0.586
b	3.81	3.247
y_0	0.161	0.207

4.2. Experimental Results

In this subsection, we demonstrate the PL spectra of 1, 2, and 3 MLs of well thicknesses. Figure 6a,b shows the normalized PL spectra for 1, 2, and 3 MLs of InAs in InAs/GaSb MQWs. We fitted the spectra to a single Gaussian function to achieve the transition energies for different well thicknesses. Although the fitting function is not completely fitted to

the experimental results because of the existence of some defects or fluctuations in the structures, the high R-square values (~ 1), as well as the negligible difference between the peak point and the fitted energy peak points, allow us to estimate the fitted energy values as the transition energy for each thickness. Moreover, the high PL intensities for the lower temperature (77 K) result in sharp PLs and more noisy spectra at room temperature. This noisy PL behavior at room temperatures is related to the very low-intensity amplitude of the PL at room temperature, relative to the low-temperature spectra. The amplitude of PL at room temperature is about 10^4 times weaker than the corresponding spectrum for 77 K. Because of this low amplitude and the finite sensitivity of the used detector, the resulting PL spectra have such fluctuations.

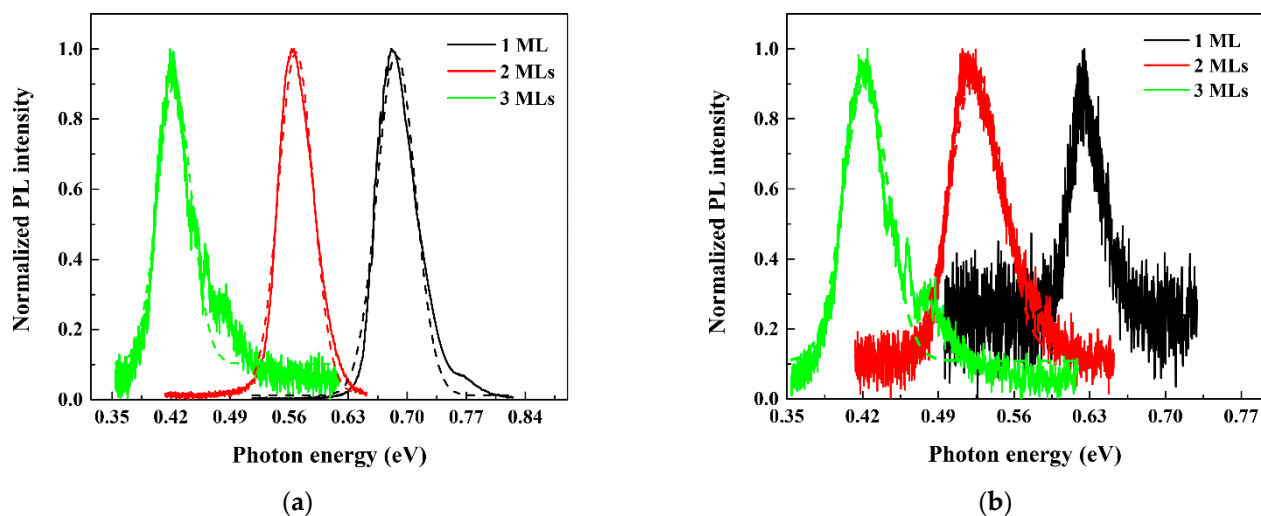


Figure 6. Normalized PL intensities of 1, 2, and 3 MLs of InAs/GaSb MQW for (a) 77 K and (b) 300 K.

4.3. Comparisons of Theoretical and Experimental Results

In this subsection, we compare the theoretical and experimental results of the first transition for different well widths. The calculated and experimental results for the first transition energies of 1, 2, and 3 MLs of InAs/GaSb MQW are demonstrated in Figure 7a,b for 300 and 77 K. The difference between experimental and theoretical energies for 1 MLs and 77 K is 16 meV ($\sim 2.3\%$), for 2 MLs it is 9 meV ($\sim 1.6\%$), and for 3 MLs it is 57 meV ($\sim 12\%$). These differences for 300 K are 13 meV ($\sim 2.1\%$), 1 meV ($\sim 0.2\%$), and 18 meV ($\sim 4.1\%$), for 1, 2, and 3 MLs, respectively. These results show that apart from the 3 MLs case, the maximum deviation between theoretical and experimental results is about 2.3%. Although this difference is negligible, the possible reasons for that can be explained as follows: the MQWs width may have some thickness fluctuations, leading to differences in the well thicknesses and resulting in different energy levels.

In the case of 3 MLs well width, we observed a relatively large mismatching (maximum 57 meV) between theoretical and experimental results. As seen in Figure 6a,b, for the 3 MLs case, some fluctuation occurs primarily at the right shoulder of the PL spectra. These fluctuations can stem from the absorption peaks of some elements in the air (specifically H_2O). The literature shows that [50] the absorption spectrum of H_2O has a remarkable peak of around 0.41 eV (3 μm). Unfortunately, this peak is in the transition energy range of 3 MLs. Therefore, the water absorption peak overlaps the transition peak, meaning we cannot distinguish the exact peak point of the 3 MLs transition energy.

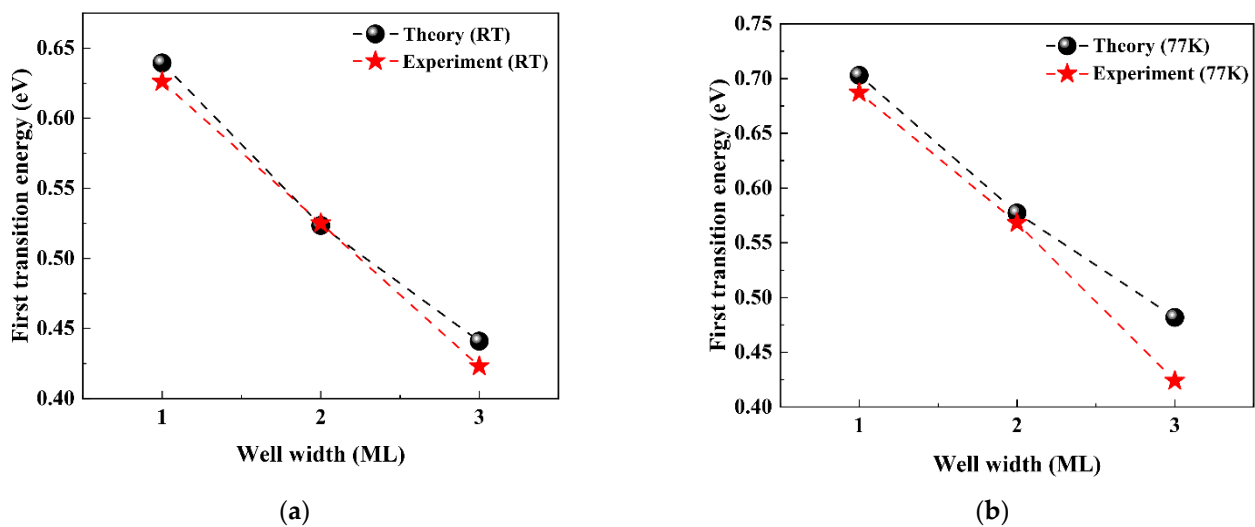


Figure 7. Theoretical and experimental results of first transition energies for 1, 2, and 3 MLs of InAs/GaSb MQW for (a) 300 K and (b) 77 K.

Furthermore, we investigated the PL spectra of 3 MLs for different temperatures in the 60–300 K range. The results are illustrated in Figure 8a, and the variations in the peak energies are demonstrated in Figure 8b. As the figure shows, increasing the temperature leads to decreasing energy levels. However, the peak energy difference between 60 K and 300 K is just about 5 meV, meaning that it has a very small value relative to the temperature dependencies of the energy levels of other InAs/GaSb structures. Moreover, our efforts to fit these variations to the well-known Varshni equation [51] (with various constant values) were unsuccessful, mainly because of the slight decrease in the peak energy. Therefore, the temperature dependence of the peak energy strengthens our previous conjecture about the overlapping of the 3 MLs spectrum with air molecules' absorption.

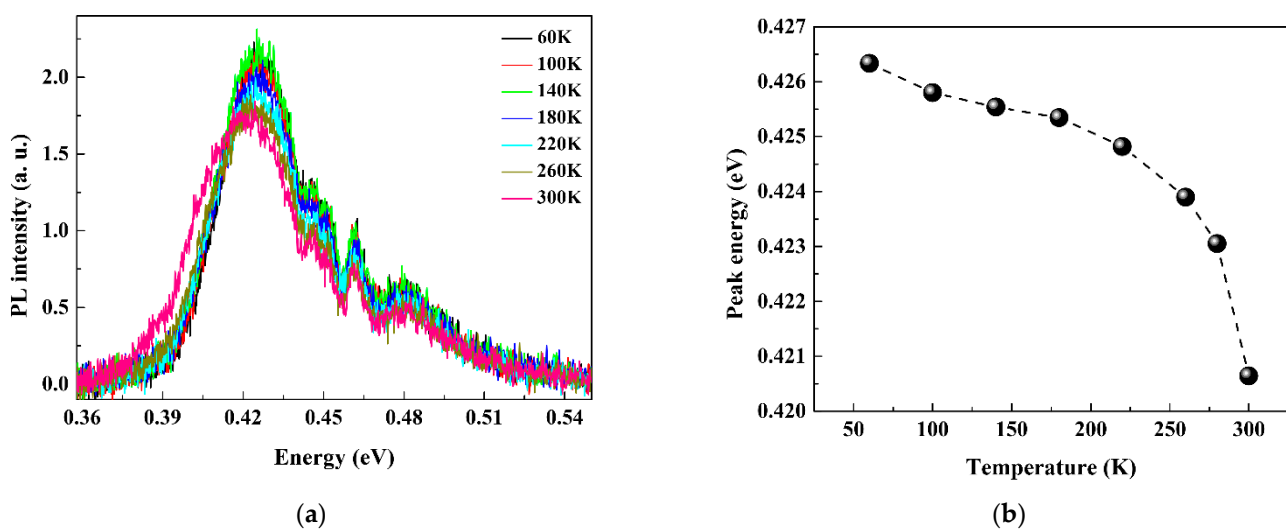


Figure 8. (a) PL spectra for different temperatures range of 60–300 K; (b) variation in peak point of PL spectra for different temperatures.

With the results mentioned above, it seems that the difference between the experimental results of 77 and 300 K for 3 MLs stems from the fact that the actual PL spectrum of the 3 MLs overlapped with the air elements' absorption spectra. To overcome this issue, the PL measurement apparatus should be embedded in the large vacuum chamber to eliminate any air molecules; however, this was impossible in our measurement configuration.

5. Conclusions

We applied the eight-band k.p theory to InAs/GaSb type-II multi-quantum-well structures with various well widths and barriers at two temperatures and observed the variations in conduction- and valence-confined energies. With and without considering the boundary conditions in the Hamiltonian, we considered the effect of the wells' interactions for different well and barrier widths. Our results showed that the valence-confined states for different well widths displayed a negligible difference for different wells (5–50 nm) and wide barrier widths (30 nm). Our results lead us to using only electron-confined energy states to compute the transition energy. The effect of the well's interaction with the first transition energy showed that one could consider the InAs/GaSb MQW structure as a single-quantum-well system for barriers broader than 30 nm. We proposed an exponential function for achieving these systems' first transition energies without considering the eight-band theory procedure. Therefore, we confirmed the consistency of the theoretical and experimental results for 1 and 2 MLs at 77 and 300 K.

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Appendix A

The final form of the $H^{(0)}$, $H^{(1)}$, and $H^{(2)}$ matrices are as follows:

$$H^{(0)} = \begin{pmatrix} E_c(z_n) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_c(z_n) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_v(z_n) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_v(z_n) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_v(z_n) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_v(z_n) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\Delta_0(z_n) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\Delta_0(z_n) \end{pmatrix}, \quad (\text{A1})$$

$$H^{(1)} = \begin{pmatrix} 0 & 0 & 0 & \sqrt{\frac{2}{3}}P & 0 & 0 & \frac{-1}{\sqrt{3}}P & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}}P & 0 & 0 & \frac{1}{\sqrt{3}}P \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}P & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}}P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{-1}{\sqrt{3}}P & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}}P & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (A2)$$

and

$$H^{(2)} = \frac{\hbar^2}{2m_0} \begin{pmatrix} \gamma'_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \gamma'_0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & (-\gamma'_1 + 2\gamma'_2) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & (-\gamma'_1 - 2\gamma'_2) & 0 & 0 & \frac{4m_0\sqrt{2}\gamma'_2}{\hbar^2} & 0 \\ 0 & 0 & 0 & 0 & (-\gamma'_1 - 2\gamma'_2) & 0 & 0 & \frac{-4m_0\sqrt{2}\gamma'_2}{\hbar^2} \\ 0 & 0 & 0 & 0 & 0 & (-\gamma'_1 + 2\gamma'_2) & 0 & 0 \\ 0 & 0 & 0 & \frac{4m_0\sqrt{2}\gamma'_2}{\hbar^2} & 0 & 0 & \frac{-2m_0\gamma'_1}{\hbar^2} & 0 \\ 0 & 0 & 0 & 0 & \frac{-4m_0\sqrt{2}\gamma'_2}{\hbar^2} & 0 & 0 & \frac{-2m_0\gamma'_1}{\hbar^2} \end{pmatrix}. \quad (A3)$$

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