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Intersubband optical transition matrix elements for hole states in semiconductor quantum wells

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Abstract. Intersubband optical transition matrix elements between quantized hole states in semiconductor quantum wells, calculated from the 4×4 Hamiltonian, are derived, taking into account the position dependence of Luttinger γ parameters. Furthermore, the transition matrix elements between states obtained within the axial approximation, from the 2×2 Hamiltonian, are also derived. Numerical calculations indicate the importance of taking the position dependence of Luttinger parameters into account for bound–free transitions.

1. Introduction

Intersubband transitions in semiconductor quantum well (QW) structures have attracted considerable research attention, related to the possibility of making infrared photodetectors and similar devices. While the normally polarized, in-plane incident radiation can always induce these transitions, the technically more favourable case of normally incident, hence in-plane-polarized, radiation is different. In n-type QWs such transitions are allowed only between states arising from ‘tilted’ indirect valleys, e.g. [1]. In p-type QWs, however, the normally incident radiation can also induce transitions, regardless of the fact that the valence band top is at the Brillouin zone centre, e.g. [2, 3]. This is sometimes ascribed to p-like character of hole wavefunctions, in contrast to the s-like character of electronic wavefunctions, but in fact it stems from the contribution of bands other than those included in the zero-order ‘envelope times Bloch’ description of the wavefunctions (this actually applies for any polarization of the incident radiation). In the case of interband transitions it turns out that these first-order corrections may be safely ignored when calculating optical transition matrix elements. For intersubband transitions, however, they usually happen to be very important, giving the main part of the matrix elements. When dealing with electron states, for instance, discarding the wavefunctions’ ‘fine structure’ would result in values of $A \cdot p$ matrix elements lower by a factor of m^* (electron effective mass in free electron mass units) than their real values. Similarly, assuming that hole wavefunctions include only the envelopes multiplying Bloch states, the latter written in terms of $(|X\rangle, |Y\rangle, |Z\rangle)$, $(|\uparrow\rangle, |\downarrow\rangle)$ states, would clearly result in zero values of matrix elements for the in-plane polarized light, while they are really finite. The objective is then to find the light–matter interaction operator that would act on the envelope wavefunctions only, instead of applying the $A \cdot p$ operator to the full detailed wavefunctions.

Intersubband transition matrix elements between hole quantized states, as calculated from the 4×4 Hamiltonian, have been derived in [4, 5] taking into account the higher-order

corrections to the wavefunctions. The split-off band was here ignored, which is justified for GaAs/AlAs-based structures in the energy range of interest, $\hbar\omega \sim 0.1$ eV. The position dependence of Luttinger γ parameters (because they vary with the material composition), however, was not taken into account. In this paper we shall first describe an alternative, more simple way than that used in [4, 5] to find matrix elements for the intersubband transitions, allowing for γ parameters to be position dependent as well. The method relies on the fact that the wavefunctions' 'fine structure' is already contained, via the corresponding sum rules, in the 'effective' Hamiltonian itself (the term 'effective' denotes the conventional Hamiltonian that acts on the envelope functions only). We then derive the expressions for matrix elements that use the wavefunctions found within the block-diagonalized form of the Hamiltonian in conjunction with the axial approximation.

2. Hole states calculated from the 4×4 Hamiltonian

The Hamiltonian matrix describing heavy and light holes in a bulk semiconductor (hence with constant values of Luttinger γ parameters) is given in [6], and its operator form to be used for hole state quantization is obtained by substituting the corresponding momentum components with momentum operators. In case of QWs, therefore, $\hbar k_z \rightarrow \hat{p}_z$ (however, in the text below, the hat symbol over the operator is omitted). To include the position dependence of γ parameters we first make a Hermitian generalization of the conventional bulk Hamiltonian [6]. This is done in analogy to the case of electrons, where the kinetic energy part $p^2/m^* \rightarrow p(1/m^*)p$ to remain Hermitian if $m^* = m^*(z)$. Thus, in the conventional form, given in [6], we substitute $\gamma_i p_z^2 \rightarrow p_z \gamma_i p_z$ ($i = 1, 2$) and $2\gamma_3 p_z p_{x,y} \rightarrow p_{x,y}(\gamma_3 p_z + p_z \gamma_3)$ to get

$$2m_0 H = p(\gamma_1 + \frac{5}{2}\gamma_2)pI_4 - 2(\gamma_2 p_x^2 J_x^2 + \gamma_2 p_y^2 J_y^2 + p_z \gamma_2 p_z J_z^2) - 2[2\gamma_3 p_x p_y J_{xy} + (\gamma_3 p_z + p_z \gamma_3)(p_x J_{xz} + p_y J_{yz})] \quad (1)$$

where $J_{ij} = (J_i J_j + J_j J_i)/2$, $J_{x,y,z}$ are the spin- $\frac{3}{2}$ matrices, I_4 the 4×4 unity matrix, energy is measured from the valence band top downwards, and the momentum components $p_{x,y,z}$ are used instead of the wavevector components $k_{x,y,z}$ for convenience. The z -axis is chosen as perpendicular to the QW plane, so in studying the hole state quantization in QWs p_z is the operator $-i\hbar d/dz$, and $p_{x,y} = \hbar k_{x,y}$ are hole momentum components in the QW plane. The detailed form of the Hamiltonian depends on the 'phase convention' for $J_{x,y}$ matrices, and also on basis state ordering. Some references, e.g. [7], use the real J_y , imaginary J_x , and others, e.g. [8], the real J_x , imaginary J_y convention. Certainly, either choice leads to the same results for physical quantities. In this paper we use the latter choice, and order the basis states $|j, m_j\rangle$ as $|\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, -\frac{1}{2}\rangle, |\frac{3}{2}, \frac{1}{2}\rangle$, and $|\frac{3}{2}, -\frac{3}{2}\rangle$, just as in [8]. Their amplitudes, the envelope function components, are denoted as f_1, f_2, f_3, f_4 , respectively. The Hamiltonian, for the case of [001]-grown QWs, is then given by

$$H = \begin{bmatrix} P + Q + U & R & -S & 0 \\ R^\dagger & P - Q + U & 0 & S \\ -S^\dagger & 0 & P - Q + U & R \\ 0 & S^\dagger & R^\dagger & P + Q + U \end{bmatrix} \quad (2)$$

where the z -dependent potential $U = U(z)$ has been added to the diagonal elements, and [8]

$$P = \frac{1}{2m_0}[\gamma_1(p_x^2 + p_y^2) + p_z \gamma_1 p_z] \quad (3)$$

$$Q = \frac{1}{2m_0}[\gamma_2(p_x^2 + p_y^2) - 2p_z\gamma_2p_z] \quad (4)$$

$$R = -\frac{\sqrt{3}}{4m_0}[(\gamma_2 + \gamma_3)(p_x - ip_y)^2 + (\gamma_2 - \gamma_3)(p_x + ip_y)^2] \quad (5)$$

$$S = \frac{\sqrt{3}}{2m_0}(\gamma_3p_z + p_z\gamma_3)(p_x - ip_y) \quad (6)$$

The Hamiltonian of this form, although not explicitly stated, has in fact been implicitly assumed in deriving the boundary conditions for the wavefunction components at the interface between two different semiconductors, e.g. [7], where the γ parameters change abruptly. It is also important to note that these boundary conditions, obtained in the conventional manner, i.e. by integration of the Hamiltonian in the vicinity of the interface, coincide with those obtained from the requirement for current continuity (the expressions for hole current density are given in [9]).

In the presence of an electromagnetic field, described by a magnetic vector potential $A(\mathbf{r}, t)$ the Hamiltonian (2) changes so that $p_{x,y,z} \rightarrow p_{x,y,z} - eA_{x,y,z}$. While this has been commonly used in the case of a static magnetic field, it is equally true when dealing with the electromagnetic field of a light wave. Now, denoting by H_A the Hamiltonian in the presence of the perturbation $A(\mathbf{r}, t)$, the interaction (i.e. perturbation) Hamiltonian H_{int} is clearly equal to the difference of H_A and the unperturbed Hamiltonian (2). Thus, after very simple algebra, and neglecting terms proportional to $A_i A_j$, $i, j = x, y, z$, as well as derivatives of $A_{x,y,z}$, we find

$$H_{int} = \frac{1}{2m_0} \begin{bmatrix} a & d & -c & 0 \\ d^\dagger & b & 0 & c \\ -c^\dagger & 0 & b & d \\ 0 & c^\dagger & d^\dagger & a \end{bmatrix} \quad (7)$$

where

$$a = -2(\gamma_1 + \gamma_2)(A_x p_x + A_y p_y) - [(\gamma_1 - 2\gamma_2)p_z + p_z(\gamma_1 - 2\gamma_2)]A_z \quad (8)$$

$$b = -2(\gamma_1 - \gamma_2)(A_x p_x + A_y p_y) - [(\gamma_1 + 2\gamma_2)p_z + p_z(\gamma_1 + 2\gamma_2)]A_z \quad (9)$$

$$c = -\sqrt{3}[(\gamma_3 p_z + p_z \gamma_3)(A_x - iA_y) + 2\gamma_3(p_x - ip_y)A_z] \quad (10)$$

$$d = 2\sqrt{3}[\gamma_2(A_x p_x - A_y p_y) - i\gamma_3(A_x p_y + A_y p_x)] \quad (11)$$

The interaction Hamiltonian (7) acts on the state vector of length four with the z -dependent envelope function components, $V = [f_{3/2}, f_{-1/2}, f_{1/2}, f_{-3/2}]^T$, to give the transition matrix element as

$$M_{fi} = V_f^\dagger \cdot H_{int} \cdot V_i \quad (12)$$

where the subscripts i and f denote the initial and final hole states, and the integration over z is implicitly assumed. In calculating absorption, this matrix element squared is to be integrated over p_x and p_y , and summation over the initial and final quantized states performed, subject to the energy and momentum conservation rules.

If the Luttinger γ parameters are assumed to be z independent, this result coincides with that of [4], obtained in a different way, as discussed above. In addition, we may note that the interaction Hamiltonian can also be written as (or found from)

$$H_{int} = ev \cdot A = \frac{ie}{\hbar}[H, \mathbf{r}] \cdot A \quad (13)$$

where v denotes the velocity operator [10, 11], also a 4×4 matrix, elements of which are themselves vectors, and $[\dots, \dots]$ is the commutator. Generally, this form of the interaction operator is quite important, not only for the case of holes, because it applies if the potential in the Schrödinger equation is either local or nonlocal, while the conventional $\mathbf{A} \cdot \mathbf{p}$ form fails for nonlocal potentials [12]. Finally, we may note that the described method of finding the interaction Hamiltonian is also applicable for intersubband transitions between electronic quantized states [13].

3. Hole states calculated from the block diagonal Hamiltonian and the axial approximation

It is well known that the Hamiltonian (2) can be block diagonalized into two uncoupled 2×2 blocks by introducing the unitary transform matrix [8]

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\varphi} & 0 & 0 & -e^{i\varphi} \\ 0 & e^{-i\eta} & -e^{i\eta} & 0 \\ 0 & e^{-i\eta} & e^{i\eta} & 0 \\ e^{-i\varphi} & 0 & 0 & e^{i\varphi} \end{bmatrix} \quad (14)$$

where φ and η are chosen so that UHU^\dagger is block diagonal. Although there is no relation between the two, the block diagonalization is commonly used together with the axial approximation, which amounts to neglecting the difference between γ_2 and γ_3 in the off-diagonal terms of (2). However, since φ and η take fixed values ($\varphi = 3\pi/4 - 3\theta/2$, $\eta = -\pi/4 + \theta/2$, $\theta = \tan^{-1}(p_x/p_y)$), independent of the γ parameters if the axial approximation is employed, e.g. [14], it is used throughout this section. The advantage of this approach is that the initial 4×4 problem splits into two uncoupled 2×2 problems, i.e.

$$H_U \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \begin{bmatrix} P + Q + U & \tilde{R} \\ \tilde{R}^\dagger & P - Q + U \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = E \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} \quad (15)$$

and

$$H_L \begin{bmatrix} F_3 \\ F_4 \end{bmatrix} = \begin{bmatrix} P - Q + U & \tilde{R} \\ \tilde{R}^\dagger & P + Q + U \end{bmatrix} \begin{bmatrix} F_3 \\ F_4 \end{bmatrix} = E \begin{bmatrix} F_3 \\ F_4 \end{bmatrix} \quad (16)$$

with

$$\tilde{R} = |R| - i|S| = \frac{\sqrt{3}}{2m_0} [\bar{\gamma} p_t^2 - i p_t (\bar{\gamma} p_z + p_z \bar{\gamma})] \quad (17)$$

where $p_t^2 = p_x^2 + p_y^2$ is the in-QW-plane hole momentum and $\bar{\gamma}$ the arithmetic average of γ_2 and γ_3 used in the off-diagonal elements of (2). If the potential $U(z)$ of the QW structure is symmetric then the upper H_U and the lower H_L block of the Hamiltonian give identical, i.e. degenerate eigenenergies (Kramers degeneracy), but if $U(z) \neq U(-z)$ the degeneracy is lifted, e.g. [9]. The axial approximation works very well in the case of [001]- (and also [111]-) grown QWs, e.g. [14], and should be attractive for use in calculation of QWs optical properties.

To evaluate the transition matrix elements, and eventually absorption, if the wavefunctions $[F_1, F_2]^T$ and possibly $[F_3, F_4]^T$ have been found from the block-diagonal form of the Hamiltonian (15), (16), one can in principle back-transform the F -envelopes of (15, 16) to the f -envelopes (amplitudes of $|j, m_j\rangle$ states) by the unitary transform matrix U (14), i.e. make

$$V_U = U^\dagger \cdot [F_1, F_2, 0, 0]^T \quad (18)$$

and

$$V_L = U^\dagger \cdot [0, 0, F_3, F_4]^T \quad (19)$$

and then proceed as described in section 2 (this means, *inter alia*, integration over p_x and p_y in-plane momentum components). The question, however, arises on whether it is possible to give an appropriate 2×2 interaction Hamiltonian, in analogy to the one given by equation (7), that would directly use the envelope functions calculated within the block-diagonal representation, in order to find the transition matrix elements. This would in turn require a single integration over p_t in calculating the absorption. Furthermore, if the potential $U(z)$ is symmetric and degenerate pairs of states occur, is it enough to actually evaluate and use only $[F_1, F_2]$, but not $[F_3, F_4]$, envelope functions? The same global structure of the basic (2) and the interaction (7) Hamiltonians suggests that this could be done. However, the structure of elements of the two matrices is quite different, and it may easily be checked that the unitary transform (14) does not block diagonalize the interaction Hamiltonian, except when the polarization of the light wave is perpendicular (i.e. if only A_z is nonzero). Furthermore, there is no unitary transform that would block diagonalize the basic and the interaction Hamiltonians simultaneously, and hence there is no 2×2 interaction Hamiltonian that would act only on eigenstates of the upper, or only of the lower, Hamiltonian block. Stated differently, although the eigenstates of H_U and H_L are fully independent in the unperturbed QW (and thus 'upper' and 'lower' holes exist, in analogy to spin-up and spin-down electrons), light can induce transitions between the upper and lower hole states, provided it has the in-plane component of polarization. The transition matrix elements have therefore, at least temporarily, to be evaluated within the 4×4 system, even though the quantized states are found within the 2×2 blocks of the Hamiltonian.

To proceed, then, we start from two states $[F_1^i, F_2^i, 0, 0]^T$ and $[0, 0, F_3^i, F_4^i]^T$ as the two independent initial states, and the corresponding two final hole states (superscript f), and use them, via (18) and (19), in equation (12) to find the four transition matrix elements M_{UU} , M_{LU} , M_{UL} , and M_{LL} , the first subscript denoting the type of the final, the second of the initial state. As noted above, in asymmetric QWs these transitions correspond to different energies, and in symmetric QWs all the four would occur at the same energy. These matrix elements turn out to depend explicitly on the in-plane hole momentum components p_x and p_y , not just p_t which would be in the spirit of the axial approximation, and also on all the three components of A . However, with $p_x + ip_y = p_t \exp(i\theta)$, and defining $A_x + iA_y = A_t \exp(i\delta)$, the 'in-plane' terms in matrix elements take the form of either $A_t p_t \sin(\Delta)$ or $A_t p_t \cos(\Delta)$, where $\Delta = \delta - \theta$ is the angle between the in-plane momentum of the particular hole state undergoing transition and the in-plane component of the light polarization vector. Both the initial and the final state have the same in-plane momentum vector, since it is the conserved quantity in the transition. Now, in a QW structure at thermal equilibrium, or at least not departing much from it, we may justifiably assume that the initial hole states will be uniformly distributed in respect to their in-plane momentum orientation, i.e. the angle Δ , in the range $(0, 2\pi)$. Since it is the modulus of M_{ij} squared that is of interest in absorption, it is this quantity that has to be averaged over Δ . Thus, using $\overline{\cos(\Delta)} = 0$, $\overline{\cos^2(\Delta)} = \frac{1}{2}$, and the same for the sine function, we get the expressions for the direction-averaged matrix elements squared:

$$\overline{M_{UU}^2} = \frac{1}{2} |2(\gamma_{11}^{(+)} + \gamma_{22}^{(-)} + \sqrt{3}\overline{\gamma}_{12} + \sqrt{3}\overline{\gamma}_{21})p_t - i\sqrt{3}(\Pi_{12} - \Pi_{21})|^2 A_t^2 + |\Pi_{11}^{(-)} + \Pi_{22}^{(+)} - i2\sqrt{3}p_t(\overline{\gamma}_{12} - \overline{\gamma}_{21})|^2 A_t^2 \quad (20)$$

$$\overline{M_{UL}^2} = \frac{3}{2} |\Pi_{31} - \Pi_{42} + i2p_t(\overline{\gamma}_{31} - \overline{\gamma}_{42})|^2 A_t^2 \quad (21)$$

$$\overline{M_{LU}^2} = \frac{3}{2} |\Pi_{13} - \Pi_{24} - i2p_t(\overline{\gamma}_{13} - \overline{\gamma}_{24})|^2 A_t^2 \quad (22)$$

$$\begin{aligned} \overline{M_{LL}^2} = & \frac{1}{2} |2(\gamma_{44}^{(+)} + \gamma_{33}^{(-)} + \sqrt{3}\overline{\gamma}_{34} + \sqrt{3}\overline{\gamma}_{43})p_t - i\sqrt{3}(\Pi_{34} - \Pi_{43})|^2 A_t^2 \\ & + |\Pi_{44}^{(-)} + \Pi_{33}^{(+)} - i2\sqrt{3}p_t(\overline{\gamma}_{34} - \overline{\gamma}_{43})|^2 A_z^2 \end{aligned} \quad (23)$$

where e.g. $\gamma_{11}^{(+)} = \langle F_1^f | \gamma^{(+)} | F_1^i \rangle$, $\Pi_{12} = \langle F_1^f | \Pi | F_2^i \rangle$, etc are the 'partial' matrix elements of the operators

$$\gamma^{(\pm)} = \gamma_1(z) \pm \gamma_2(z) \quad (24)$$

$$\overline{\gamma} = \frac{\gamma_2(z) + \gamma_3(z)}{2} \quad (25)$$

$$\Pi^{(\pm)} = (\gamma_1 \bullet 2\gamma_2)p_z + p_z(\gamma_1 \pm 2\gamma_2) \quad (26)$$

$$\Pi = \overline{\gamma}p_z + p_z\overline{\gamma} \quad (27)$$

calculated with the corresponding wavefunction components of the upper [F_1, F_2] and the lower [F_3, F_4] Hamiltonian block, both for final (f) and initial (i) quantized hole states. As noted above, in the case of asymmetric QWs there is no Kramers degeneracy, and the four matrix elements calculated at a specified value of p_t correspond to different transition energies, or, conversely, if required at a specified transition energy they should be calculated at appropriate different p_t values. In such a case there is no relation between the upper and lower block eigenfunctions, and both have to be calculated from (15) and (16). To calculate the absorption, finally, the integration over $2\pi p_t dp_t$ has to be done, which is a significant saving when compared with the integration over $dp_x dp_y$ when the axial approximation is not employed.

The final problem that we address is the important case of symmetric QWs, where the upper and the lower block produce degenerate energy states, but the wavefunctions are certainly different. All the four matrix elements (20)–(23), calculated at a specified p_t value, now contribute to the transition rate at the same energy. Furthermore, there is a simple relation between the eigenfunctions of the upper and the lower block so that, as we show below, it is enough to actually evaluate only F_1 and F_2 envelopes for the purpose of the matrix elements and the absorption calculation.

To find the relation between the [F_1, F_2] and [F_3, F_4] eigenfunctions, we first note that sets of equations (15) and (16) are differential equations with real coefficients, and whether the solutions (eigenfunctions) will be real or complex depends on the boundary conditions. Thus, bound states will have real eigenfunctions, and those of free states, interesting for the bound-free transitions, will be complex. Furthermore, the individual F_i do not have definite parity even if the potential $U(z)$ is symmetric, due to the mixed-parity \tilde{R} term. Now we Fourier transform (with the kernel $\exp(iKz)$) both sets of equations. The derivative terms become $dF(z)/dz \rightarrow iKF(K)$ and $d^2F(z)/dz^2 \rightarrow -K^2F(K)$, and the product $U(z)F(z)$ turns into the convolution $\int U(K')F(K-K') dK'$. Now, if (and only if) $U(z)$ is symmetric its Fourier transform is real, and one can see that the complex conjugate of one set will coincide (because $U(K) = U^*(K)$) with the other set upon substitution $F_1(K) \rightarrow F_4^*(K)$ and $F_2(K) \rightarrow F_3^*(K)$ at the same energy. Were the potential $U(z)$ asymmetric, $U(K)$ would be complex, the two sets of equations would not be simply related, and indeed the degeneracy would be lifted. This is an alternative demonstration that degeneracy appears only in symmetric potentials, that does not directly invoke the time reversal operator. In the symmetric case, with the Fourier transforms of degenerate state eigenfunctions satisfying $[F_3(K), F_4(K)] = [F_2^*(K), F_1^*(K)]$, in real space we have

$$F_3(z) = F_2^*(-z) \quad F_4(z) = F_1^*(-z). \quad (28)$$

Using this property one can show after some algebra that $|M_{UU}|^2 = |M_{LL}|^2$ and $|M_{UL}|^2 = |M_{LU}|^2$, as expected, so only the two of them, say M_{UU} and M_{UL} , should be really calculated. Now, while the evaluation of M_{UU} requires the explicit use of $F_1(z)$ and $F_2(z)$ only, the expression for M_{UL} may be further transformed in the same fashion, making use of equation (28), to get

$$\overline{M_{UL}^2} = \frac{3}{2} |\Pi_{21} - \Pi_{12} + i2p_l(\overline{v_{21}} - \overline{v_{12}})|^2 A_i^2 \quad (29)$$

where the overbar in the subscript means that the particular 'partial' matrix element is to be evaluated with unconjugated but transposed ($z \rightarrow -z$ about the origin in the QW centre) corresponding wavefunction component for the final state, e.g. $\Pi_{12} = \int F_1^f(-z)\Pi F_2^i(z) dz$.

Therefore, for symmetric QWs considered within the axial approximation in the block-diagonal representation it is enough to find only F_1 and F_2 envelopes to evaluate the effective transition matrix element squared

$$|M_{eff}^2| = 2(|M_{UU}|^2 + |M_{UL}|^2) \quad (30)$$

making use of equations (20) and (29). In calculating the absorption it should be integrated over $2\pi p_l dp_l$, with only the upper block hole states included; the existence of the lower block states is implicitly taken account of in the matrix element itself.

There is an additional point to note, related to equation (28) and the expressions derived by using it. For bound states of the upper and the lower block it is easily checked that equation (28) holds true. The case of free states is slightly more complicated, related to the degeneracy, within each block, that appears in the continuum. In bulk and superlattices, choosing plane waves (in the latter case modulated by superlattice Bloch functions) as the independent degenerate solutions for the upper block, equation (28) would work quite well, producing the lower block states of the same, i.e. plane-wave-like, type. Generally, however, the degenerate solutions, in whatever form they are obtained, may be combined to give the wavefunctions of the form required for a particular problem. For example, for a quantum well one may construct scattering states of the upper, and also of the lower block. Starting from the upper-block scattering states, it is obvious that application of equation (28) will not deliver any proper scattering states at all, and definitely not those of the lower block (assuming that this form of free-state wavefunctions is desired for the lower block, too). Nevertheless, it may be shown that $[F_3, F_4]$ obtained from equation (28) may be expressed in terms of the lower-block scattering states (or vice versa) through a unitary transform, which is the reason that the expressions derived by using equation (28) are valid for free states as well.

4. Numerical examples and discussion

The application of the relations derived above to the design of a p-doped quantum well infrared detector will be considered in a future publication. Here we present just a few sample calculations of transition matrix elements in order to explore the influence of the position dependence of Luttinger parameters. For this purpose we have chosen a 4 nm wide GaAs well embedded in $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ bulk. Values of Luttinger parameters in GaAs are taken as $\gamma_1 = 6.85$, $\gamma_2 = 2.1$, $\gamma_3 = 2.9$, and in AlAs as $\gamma_1 = 3.45$, $\gamma_2 = 0.68$, $\gamma_3 = 1.29$, after [15], and linear interpolation is used for the alloy. The valence band discontinuity at the interface is $U_0 = 0.15$ eV. This quantum well has bound states at -120 meV (hh), -83 meV (lh) and -40 meV (hh), measured from the well top at reference zero energy. Relative error in the effective transition matrix element squared between the lowest two states, if the position dependence of Luttinger parameters is neglected, amounts to 2–10%, depending on

the hole in-plane momentum. Thus, it would average out to a few per cent in absorption, making the correction not too important. For other transitions the error is somewhat larger, but the matrix elements themselves are smaller. In this system, therefore, the position dependence of Luttinger parameters, due to its small variation, does not produce any major effect on bound-bound transitions. The situation is different for transitions to the continuum (bound-free). Errors occurring in evaluation of the matrix element squared from the lowest (hh) bound state to continuum states, if the Luttinger parameters are taken as constant, are as large as 20–80%, again depending on the in-plane momentum. In the case of bound-free transitions, therefore, considering the position dependence of Luttinger parameters is essential. Physically, this is quite an expected result: the stronger the confinement to one material, the less important is the spatial dependence of γ parameters. Although not related to this position dependence, it is also interesting to note that the ratio of matrix elements for ‘block-conserving’ ($|M_{UV}|^2$) and ‘block-flip’ transitions ($|M_{UZ}|^2$) is equal to one for zero in-plane momentum, and as it increases this ratio may vary between roughly 0.2 and 20. This is quite different from the situation with ‘spin-flip’ transitions between electronic states.

5. Conclusion

The matrix elements for the intersubband optical transitions between the quantized hole states in semiconductor quantum wells, calculated from the 4×4 Hamiltonian, are derived by a method alternative to that of [4], and taking into account the position dependence of Luttinger γ parameters. Furthermore, the expressions for the transition matrix elements are also derived for the case where the hole states are calculated within the axial approximation from the 2×2 block-diagonalized Hamiltonian. It is found from numerical calculations that considering the position dependence of Luttinger parameters is important mostly for bound-free transitions.

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