Corrections to the Expression for Gain in GaAs

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Abstract—There have been many papers on the subject of theoretical gain calculations. However, in comparing the expressions for gain derived in various papers, we have found that a number of inconsistencies exist among several publications. These inconsistencies have propagated through the literature and continue to do so. This letter is specifically devoted to explaining how these inconsistencies originated such that they will not be repeated in future work on the subject.

I. INTRODUCTION

PREDICTING the gain in bulk semiconductors and quantum well material as a function of injection current and/or carrier density is of great importance to the proper design and optimization of semiconductor lasers. Consequently, many publications have been devoted to theoretical gain calculations throughout the years, providing a firm basis for studying and understanding the properties of gain in semiconductors (for example, see [1]–[10]). However, in comparing the expressions for gain in a few specific publications [5]–[10], we have observed some inconsistencies. These inconsistencies are apparent in Table I, where we provide a list of prefactors that need to be included in the cited equations of [5]–[10] to make them consistent with the work of others (for example, [2]–[4]). The purpose of the present letter is to explain how these inconsistencies originated such that they will not be repeated in future work on the subject. In addition to this, we would like to point out a 30 percent correction to the magnitude of the transition matrix element that was experimentally determined over 10 years ago, but which is still being neglected by most authors including [1]–[10].

Most of the inconsistencies listed in Table I can be traced back to the expression used for the transition matrix element in the cited publications. In Section II, we provide a general discussion of the matrix element, including spin degeneracy considerations, the procedure typically used in estimating the magnitude of the momentum matrix element, as well as the enhancement of the matrix element in quantum well structures. In Section III, we write down the correct expression for gain and spontaneous emission in semiconductors within the framework of Fermi's Golden Rule, for comparison purposes. We then conclude in Section IV.

TABLE I
PREFACTORS THAT SHOULD BE INCLUDED IN THE CITED EQUATIONS OF VARIOUS PUBLICATIONS

Reference	Prefactor*	Referred Equation
[5]	2	(3.2.33)
	2 x 1.5 (heavy hole)	(9.4.2)
[6]	$\frac{1}{\pi}$	(2)
	$2\left(\frac{1}{4\pi\varepsilon_0}, \text{c.g.s.}\right)$	(3)
	1.5 (heavy hole)	(4)
	$\frac{1}{4\pi^2\hbar^2}$	(7)
[7]	$(v_g)^{-1}$	(6)
	$(\pi L_z)^{-1}$	(7)
	$2\left(\frac{1}{4\pi\varepsilon_0}\right)\left(\frac{\hbar c n}{E}\right)$	(8)
	1.5 (heavy hole)	(8)'
	$\frac{1}{4\pi^2\hbar^2}$	(10)
[8]	2	(2)
[9]	2x1.5 (heavy hole)	(7)
	0.5	(12)
[10]	0.5x1.5 (heavy hole)	(2)

* A factor of 1.27 should be multiplied to all.

II. THE INTERBAND TRANSITION MATRIX ELEMENT

A. Spin Degeneracy

Within the framework of Fermi's Golden Rule, the two major components of gain calculations are the electron and hole density of states (DOS), and the transition matrix element describing the interaction between the conduction and valence band states. The factor of two needed for spin degeneracy can be accounted for in either the DOS or the matrix element. However, it has become customary with some authors [5]–[10] to use the expression for the matrix element derived by Casey and Panish ($1.33m_0 E_g$) [1], without considering how the spin degeneracy was dealt with in obtaining the original expression.

The derivation by Casey and Panish used a no k-selection rule model which included a factor of two for *both* valence and conduction band DOS's. However, transitions between states of opposite spin are not allowed. They corrected for this by adding a factor of $1/2$ to their matrix element to obtain $1.33m_0 E_g$. In gain calculations involv-

ing k-selection rules, a reduced DOS is used which accounts properly for the spin degeneracy with a single factor of two. It is therefore a mistake to use the matrix element of Casey and Panish in this case, without first removing the factor of $1/2$. Most of the correction factors of 2 that appear in Table I are due to this error.

B. Magnitude of the Momentum Matrix Element

The method used to determine the magnitude of the momentum matrix element comes from the theory of Kane [11]. In simple terms, an expression is derived in his $k \cdot p$ theory which describes the curvature of the conduction band in terms of, among other things, the transition momentum matrix element. However, the expression is most commonly used in reverse to determine the magnitude of momentum matrix element from the measured value of the electron effective mass (which is a measure of the conduction band curvature). This is the typical approach used by Casey and Panish and others. Below we will describe this method in more detail and then discuss known corrections to the presented model that have been reported in the literature [12]–[14].

The matrix element can be modeled as a constant near $k^2 = 0$, where k is the wave vector of the electron. It is common to approximate the matrix element by using Kane's $k \cdot p$ approach [11]. By diagonalizing the 8×8 interaction matrix which results from considering a four-band model (which only includes the conduction band and the three valence bands, neglecting all higher and lower bands), four double roots of the secular equation can be solved to yield the four band energies as a function of k. For small values of k^2, the energy of the upper state, i.e., the conduction band is given by

$$E_c = \frac{\hbar^2 k^2}{2m_0} + \frac{P^2 k^2}{3} \left(\frac{2}{E_g} + \frac{1}{E_g + \Delta} \right) \qquad (1)$$

where

$$P = -i \frac{\hbar}{m_0} \langle S | P_z | Z \rangle = -i \frac{\hbar}{m_0} M, \qquad (2)$$

m_0 is the free electron mass, E_g is the direct band gap, M is the transition matrix element between conduction $\langle S |$ and valence $| Z \rangle$ states, and Δ represents the spin-orbital splitting energy of the valence band, experimentally determined to be equal to 0.341 eV [15]. The energy dispersion of (1) as a function of k^2 is a straight line with the inverse of the slope being defined as an effective mass, as shown in Fig. 1, where we use m^* as the energy dispersion of the conduction band due to the 8×8 interaction [that is, (1)]. The approach taken by Casey and Panish (and many others) is to equate m^* with the measured effective mass of the conduction band. However, the true curvature of the conduction band is affected not only by the four bands taken into account in Kane's theory, but also by higher and lower bands. The true effective mass m_c yields a curve shown by the solid line in Fig. 1, where we see that m_c is larger than m^*. The experimental work
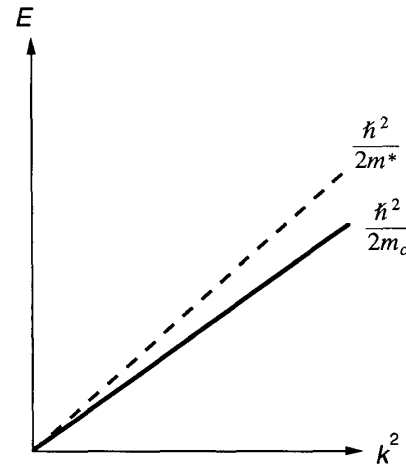

Fig. 1. The energy dispersion as a function of k^2. The dashed line with the slope of $\hbar^2/(2m^*)$ is the energy dispersion of the conduction band due to the 8×8 interaction matrix. However, the true curvature of the conduction band is affected not only by the four bands taken into account in Kane's theory, but also by higher and lower bands. The true effective mass m_c yields a curve shown by the solid line where we see that m^* is smaller than m_c.

of Chadi [12] and, shortly afterwards, Hermann and Weisbuch [13], [14] can be used to estimate m^*. It is found that $m^* = 0.053m_0$ as opposed to the measured $m_c = 0.0665m_0$. The momentum matrix element can be expressed in terms of m^* using (1) and (2) as

$$|M_{avg}|^2 = \frac{m_0}{6} \left(\frac{m_0}{m^*} - 1 \right) \frac{E_g (E_g + \Delta)}{\left(E_g + \frac{2}{3} \Delta \right)} \qquad (3)$$

where the average denotes the fact that (2) is the momentum matrix element for optical transitions when the light is polarized along the z-direction. For unpolarized light (or equivalently, for electron k vectors randomly distributed), we need to average over orthogonal directions resulting in a factor of $1/3$ which has been included above [11], [16]. Using the above quoted value of m^* we obtain $3.38m_0 E_g$, or an increase of 1.27 over that obtained without considering the effects of other bands on the curvature of the conduction band [17]. Thus, in Table I, all expressions for the matrix element in the quoted references should be multiplied by 1.27 (in addition to the factor of two mentioned earlier) *except* for [8], which analyzes the InGaAsP system. The factor of 1.27 contribution from higher bands is specific to GaAs. For higher band contributions in other systems, see [13] and [14]. Regarding spin degeneracy, the above expression for the matrix element assumes that *one* factor of two will be included in the expression for the DOS.

It should be noted that the measured absorption is higher than the calculated one, even if the correction factor of 1.27 is included [1]. This is thought to be due to the Coulomb interaction between electrons and holes [18]. Actually, the excitonic effect changes the shape of the ab-

sorption spectrum from the simple one-particle picture. In high injection cases such as lasers, the Coulomb interaction is screened due to the presence of many charged carriers [19].

C. The Matrix Element in Quantum Well Structures

The factor of $1/3$ included in (3) is a result of averaging the matrix element over orthogonal directions as mentioned. For gain calculations, the averaging is over all electron k vector directions (for a fixed electric field polarization). For spontaneous emission calculations, the averaging is over all polarizations of the emitted radiation (for a fixed electron k vector) [16]. Either case yields a factor of $1/3$ in the final expression. However, in a quantum well, the matrix element used in gain calculations is only averaged over a *restricted* set of k vector directions for a given electric field polarization. Thus, the factor of $1/3$ needs to be modified [2], [16], [20].

It has been shown that for *gain calculations*, the momentum matrix element for a TE-polarized wave in a quantum well laser configuration provides a factor of $3/2$ enhancement over the bulk momentum matrix element (the factor of $1/3$ becomes $1/2$) for heavy-hole transitions near the band edge [2], [20]. The expression can be written as a function of the energy of the electron above the band edge for the heavy-hole transition as [2]

$$|M_{QW}|^2 = \frac{3}{4}|M_{avg}|^2 \left[1 + \frac{E_z}{E_c - E_{g,B}} \right] \qquad (4)$$

where E_z is the quantized electron energy relative to the conduction band edge of GaAs, $E_{g,B}$, and E_c is the total energy of the electron. Thus, the matrix element becomes energy dependent, *decreasing* for increasing electron energies in the case of heavy-hole transitions [20].

Some recent papers [5], [9], [10] dealing with gain in quantum wells have ignored the above enhancement effect and used simply the bulk value of Casey and Panish, while others [6], [7] have actually used a wrong expression for the enhancement. In addition, the enhancement is different for the light-hole and heavy-hole transitions. Thus, when summing over both bands, different expressions should be used for each. All of these factors are important to consider, especially when making comparisons between quantum well and bulk material [10], because the gain scales directly with the matrix element.

The above enhancement in the matrix element is unique to gain and absorption calculations. When considering *total* spontaneous emission output (as is necessary for calculating the total radiative carrier recombination), we need to consider the radiation emitted into all polarization directions, regardless of whether or not the k vector directions of the electrons are restricted. Therefore, the factor of $1/3$ remains valid in (3), even in a quantum well structure, for *spontaneous emission* calculations. This point has been mentioned in [4] and treated in detail in [16]. The implication is that if the radiative component of the current is properly calculated by using the integrated spontaneous emission rate, while *also* using the quantum well

matrix element given by (4), one will overestimate the radiative current by approximately a factor of $3/2$ [6], [7].

III. Expressions for Gain and Spontaneous Emission

A. Gain

Referring to Table I, we find that factors of 2, 1.27, and $3/2$ are explained by the above discussions. Factors of $(4\pi\epsilon_0)^{-1}$ are assumed to be due to some authors use of cgs units instead of MKS units [6], [7] (although it is not explicitly mentioned). When including intraband scattering of the electrons, the Lorentzian line shape used should include a factor of $1/\pi$ for proper normalization. This possibly explains the correction factor of $1/\pi$ needed in [6] and [7]. However, other inconsistencies are harder to explain (specifically in [7]). Furthermore, there are probably additional references which should be added to Table I that we have not found. Therefore, we have decided to write down the expression for gain (in the framework of Fermi's Golden Rule) for easy comparison to the literature.

For simplicity and purposes of illustration, we assume k-selection rules without consideration of the intraband relaxation time of the electrons (which is considered in a density matrix approach [2]-[4]). If no k-selection rules are assumed (or a mix of the two), then the electron and hole DOS are included separately and are typically modified from the traditional parabolic band model to account for band tail states which might arise due to heavy doping of the material [1]. However, when k-selection rules apply as in the case of undoped active regions, the DOS is always given by a reduced DOS for bulk or quantum well material. The reduced DOS is given by using the reduced effective mass $m_r = m_e m_h/(m_e + m_h)$ in the standard DOS expression. The correct expression for the gain for bulk or quantum well material can be written in MKS units as

$$g(E) = \left[\left(\frac{2\pi}{\hbar} \right) \left(\frac{e}{m_0} \right)^2 \left(\frac{2\hbar\omega/\epsilon V}{4\omega^2} \right) |M|^2 V \rho_{red}(E) \right]$$
$$\cdot \left[\frac{n}{c} \right] [f_c(1 - f_v) - f_v(1 - f_c)] \qquad (5)$$
$$= \left(\frac{\pi e^2 \hbar}{\epsilon_0 n \, c \, m_0^2 E} \right) |M|^2 \rho_{red}(E) (f_c - f_v). \qquad (6)$$

In (5), we have grouped meaningful terms together, and $|M|^2 = |M_{avg}|^2$ or $|M_{QW}|^2$. The term in large brackets is an expression for Fermi's Golden Rule which expresses the probability per unit time for transitions occurring from a filled state to an empty state. The second term is brackets converts the probability per unit time into probability per unit length. The third term in brackets represents the probability that the initial state is filled and the final state is empty (the two terms represent the stimulated emission minus the absorption). The Fermi–Dirac function f_v is defined as the *electron* occupation probability (it is occasionally defined as the hole occupation probability [5],

[8], [9], in which case f_v above should be replaced by 1 $- f_v$).

The expression for Fermi's Golden Rule is obtained by assuming an $A \cdot p$ interaction Hamiltonian and hence uses the *momentum* matrix element (as opposed to the dipole matrix element, $e^2 |x|^2$ commonly used in a density matrix approach [the two matrix elements are fundamentally related by $e^2 M^2 = m_0^2 \omega^2 e^2 |x|^2$]). The third term in the expression is the magnitude squared of the vector potential for one photon (found by relating the electric field to the energy density of a single photon in a given volume). A factor of four exists in the denominator of this term because only one of the two cosine harmonics leads to a non-zero matrix element. The volume V cancels out of the final equation converting the *number* of final states to a *density* of final states.

B. Spontaneous Emission

The expression for the spontaneous emission rate is useful in calculating the current required to provide a given gain found in (6). Many authors use the simple bimolecular recombination expression ($J = qBnp$) to obtain the radiative current from the carrier densities (which can be found from the quasi-Fermi levels used to specify the gain). However, this expression holds only for the case of no k-selection rules where the conduction and valence bands are integrated independently. For the case of k-selection, one must find the radiative component of the current density by evaluating the spontaneous emission rate integrated over all energies. The spontaneous emission rate per unit energy at a given energy ($R_{sp}(E)$ has units of per unit time per unit volume per unit energy) is given by

$$R_{sp}(E) = \left(\frac{2\pi}{\hbar}\right)\left(\frac{e}{m_0}\right)^2 \left(\frac{2\hbar\omega/\epsilon}{4\omega^2}\right) |M_{avg}|^2 \rho_{red}(E)$$

$$\cdot D(E) \cdot f_c (1 - f_v) \qquad (7)$$

where $D(E)$ is the optical mode density, in the material with a refractive index of n, given by

$$D(E) = \frac{n^3 E^2}{\pi^2 \hbar^3 c^3}. \qquad (8)$$

From this we have, by assuming the current is injected vertically,

$$J = qd \int R_{sp}(E) \, dE \qquad (9)$$

where d is the thickness of the active region (for a quantum well, d is the well width). It should be noted that the use of (7) in (9) will yield the proper magnitude of radiative current even if relaxation broadening is taken into account [4]. Thus, a double integration is not necessary in (9) when considering relaxation broadening effects (contrary to that implied by [6] and [7]).

IV. CONCLUSION

The inconsistencies between various publications indicated in Table I, are, we hope, resolved in this letter. Our general approach has been to point out some potentially confusing key features of gain and spontaneous emission calculations, which at the same time serve to explain why some of the inconsistencies presented in Table I exist in the literature. To summarize these, we pointed out that a factor of 1.27 should be included in the momentum matrix element in calculating optical transitions from valence to conduction band in GaAs when Kane's model is adopted. As well, careful attention should be paid to the inclusion of the spin degeneracy: if the spin degeneracy of 2 is counted in the reduced density of states, the momentum matrix element should be taken as $3.38m_0E_g$ (including 1.27 correction), as opposed to $1.33m_0E_g$ in Casey and Panish. Quantum well enhancement of the matrix element should also be included in *gain* calculations of quantum well material, but should not be included in *spontaneous emission* calculations. Incorrectly including it will lead to an overestimation of the radiative current by a factor of approximately $3/2$. Correct expressions for the gain and spontaneous emission were also presented for comparison to the literature.

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