Electronic structure of a GaAs quantum well in an electric field

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We apply the stabilization method of quantum chemistry and calculate the energies and widths of resonances of an isolated quantum well in an electric field. We calculate the Stark shifts and tunneling times across the barrier for a single GaAs quantum well. We also test the theories under discussion for the band-edge discontinuities. Our results show a better agreement with recent experimental measurements when we use 57%-43% of the band gap for the band-edge discontinuities of electrons and holes, respectively.

I. INTRODUCTION

Electric fields applied to semiconductor quantum wells induce pronounced effects on the electronic properties of these novel devices.[1] In particular, Mendez and coworkers[2–4] in a series of articles demonstrated that the application of an external electric field, in the range 10–50 kV/cm perpendicular to the layers defining the quantum wells, perceptibly decreases or even completely quenches the luminescence of GaAs-$Ga_{1-x}Al_xAs$ quantum wells. Moreover, the substantial decrease of the lifetime of the photoluminescence decay led them to conclude that the Fowler-Nordhein tunneling of the holes or electrons out of the quantum well (QW) is the mechanism capable of explaining the magnitude of the quenching.[4] A more recent experiment[5] demonstrated that the behavior of the photoluminescence lifetime depends on the width of the well: For sufficiently wide wells (≥ 100 Å) the lifetime increases with the field as a consequence of the decrease of the electron-hole wave-function overlap; in narrow wells (~ 50 Å) the lifetime decreases and even quenches because of the tunneling of electrons or holes through the barriers. The energy-level shifts produced in a single QW has also been measured by electroreflectance technique[6] in a broader range of electric fields (up to 260 kV/cm).

Theoretical attempts to model such systems must include the fact that the bound states for electrons and holes at zero field become resonant states, with certain width, when the field is switched on. The most popular method to calculate the Stark effect is the variational method of Bastard, Mendez, Chang, and Esaki[3] which is a simple bound-state calculation suitable at weak electric fields. Other models have been proposed that are applicable at higher fields.[7,8] In particular, Austin and Jaros solved exactly the Hamiltonian for the envelope functions of electrons or holes within the effective-mass approximation. Nevertheless, some discrepancies exist between the experimental results and the corresponding theoretical predictions. In particular, the disagreement in the energy shifts and the field at which the luminescence peak quenches remains to be explained. In this paper we evaluate those magnitudes by means of the energies and widths of the resonant states of the QW calculated using the stabilization method of quantum chemistry.

The outline of the paper is as follows. In Sec. II we briefly describe the procedure of the stabilization method as applied to this problem. In Sec. III we present the result of our numerical calculation and general conclusions.

II. THE STABILIZATION METHOD

The calculation of the eigenstates of a finite QW subject to a constant electric field is, in principle, an exactly solvable problem. However, in this section we present a conceptually different approach which, from our point of view, gives more physical insight into the process involved.

Similar to previous studies, we reduce the problem to the one-dimensional effective-mass equation. We place the QW of width l and depth V_0 between two infinite barriers separated by a distance L, so in the envelope-function approximation the wave function of a particle confined in the QW is

$$\phi = f_{n,0}(r)\psi(z) \ ,$$

where $f_{n,0}$ is a Bloch state of zero wave vector and band-index n and $\psi(z)$ is the envelope function which obeys the following Schrödinger equation (in a.u.):

$$\begin{aligned} &-\frac{1}{2m^*}\frac{d^2\psi}{dz^2}-(V_0+Fz)\psi=E\psi \ , \quad -L/2\leq z\leq l/2 \ , \\ &-\frac{1}{2m^*}\frac{d^2\psi}{dz^2}-Fz\psi=E\psi \ , \quad |z|\leq l/2 \ , \\ &-\frac{1}{2m^*}\frac{d^2\psi}{dz^2}-(V_0+Fz)\psi=E\psi \ , \quad l/2\leq z\leq L/2 \ , \end{aligned} \tag{1}$$

where F is the electric field applied along the direction of the well z.

The system described by (1) has strictly bound states and can be solved exactly by means of the usual coordinate transformation giving wave functions which are linear combinations of the Airy functions, A_i and B_i. The stabilization method[9,10] exploits the fact that one or several of the eigenenergies of (1) are related to the position of the resonances of the quantum well, and that these resonant eigenenergies are stable with respect to variations of a suitable parameter of (1). In this particular case the parameter which keeps the energy of the resonance stable is the separation L between the infinite barriers. Figure 1 is a plot of the energies of (1) as function of L for fixed values of F and l. As is shown in that figure the plateaus line up at one

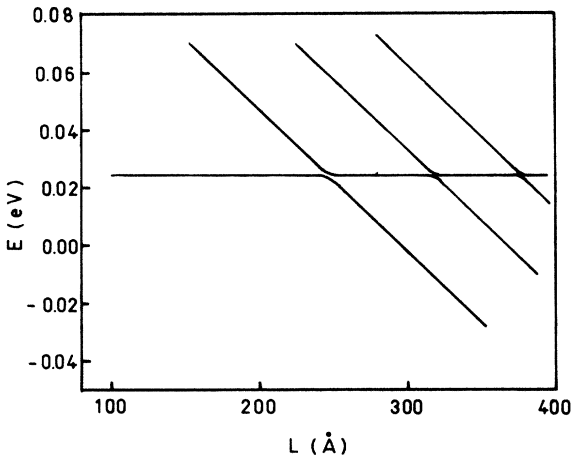

FIG. 1. Stabilization of one eigenvalue, E_{res}, of the Hamiltonian Eq. (1) with $F=100$ kV/cm and $l=37$ Å. We plot the eigenvalues vs the scaling parameter L defined in (1) as the separation between infinite barriers.

particular energy level, the resonance of the quantum well.

The features of Fig. 1 can be explained in terms of wave functions. The resonant level has a corresponding wave function which is mainly concentrated inside the well. Then, as we increase the length L between barriers we can in fact describe the tails of that function better, without causing any appreciable change in the energy level. Figure 2 shows a plot of the resonant function for two lengths L which are in different plateaus. For the larger length, the function has the same exponential decay on the left and a longer tail with oscillations on the right; these oscillations indicate the presence of many k-plane waves in the exact wave function.

The continuum states of the QW behave quite differently; these appear in Fig. 1 as straight lines crossing the resonant level. The wave function associated with one of these states has a definite number of oscillations, and their corresponding energies decrease along the line because the wave function is contained in a box of longer length L. The plotted

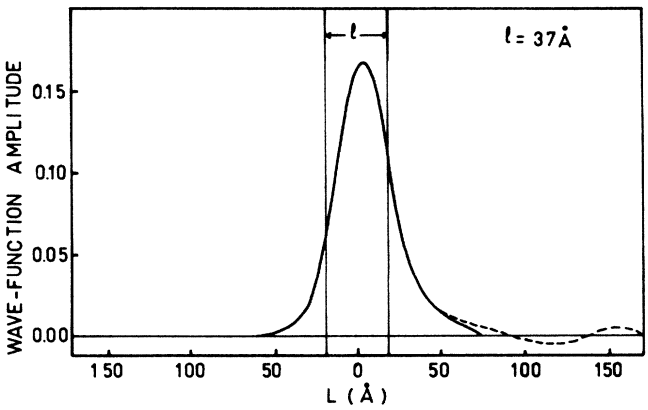

FIG. 2. Comparison of the resonant wave function ψ_{res} for holes in the 37-Å wide quantum well at two different lengths L. Solid line ψ_{res} for $L=150$ Å; dashed line ψ_{res} for $L=340$ Å. The position of the QW is denoted by the two vertical lines separated by l.

lines of energies corresponding to different kinds of states never cross because of the interaction between them.

The energy values and lifetime of the resonant states can be obtained in similar form as has been shown by Simons[11] and Löwdin.[12] The starting points are the curves $E=E(L)$ representing functions of the real scale parameter L. Let us select two specific curves E_1 and E_2 which have an avoided crossing. They can be thought of as solutions from a 2×2 secular problem, whose diagonal elements are $(E_r(L), E_s(L))$, the two "uncoupled" states, and $V(L)$ their interaction. This interaction has a peak at the crossing point $L=L_c$, so there the energies are

$$E=\epsilon\pm V_c \ , \tag{2}$$

where ϵ is half the sum of E_1 and E_2 at L_c and $V_c=V(L_c)$.

In a first approximation we can use (2) to determine the energy of the resonance $E_{res}=\epsilon$, and the lifetime can be evaluated with the usual formula $\tau=\hbar/\Gamma$, where Γ is given by the Fermi golden rule

$$\Gamma=2\pi\rho_c|V_c|^2 \ , \tag{3}$$

where ρ_c is the density of continuum states in the well at $L=L_c$.

III. RESULTS AND DISCUSSION

With the simple model so established we do not consider the many-band structure of electrons and holes and its dependence in k space. This means that we ignore throughout the calculations of the possible admixture of the higher- (lower-) lying states of electrons (holes). This band mixing can appear as a consequence of the spreading in energy of the wave function, and can produce some modification in the lifetimes calculated at high fields. To our knowledge, this fundamental problem has not been solved in the literature and it is under current research.

We have applied the method described in Sec. II to calculate the Stark shifts and lifetime of resonances in isolated QW's of widths 37, 50, and 70 Å, respectively. The different widths studied allowed us to obtain a trend for the lifetime and shifts for electrons and holes and to make a direct comparison with the heavy-hole–electron energy transition recently performed by Alibert *et al.*[6]

The values of V_0 and m^* for electrons and heavy holes used in the calculations are, respectively,

$$\begin{aligned} &m^*=0.067m_0 \ , \quad V_0=572 \text{ meV (electrons)} \ , \\ &m^*=0.45m_0 \ , \quad V_0=100 \text{ meV (holes)} \ , \end{aligned} \tag{4}$$

where m_0 is the free-electron mass. These parameters represent a single QW clad in $Ga_{0.46}Al_{0.54}As$ barriers, and they have been obtained using the 85%-15% rule[13,14] for the conduction- and valence-band discontinuities. In Table I we compare the results obtained with our method with the exact ones (see Ref. 8).

With the parameters chosen in (4), the electrons are practically bound states and accordingly the quenching of the photoluminescence signal should only be determined by the tunneling of the holes. In Fig. 3 (solid lines) we have plotted the tunneling time for holes in wells of width 37 and 70 Å. These results show that for a given field the tunneling time is smaller for a hole in a wider well; this is a natural result because the corresponding energy level is deeper.

TABLE I. Comparison of the exact and approximate resonance parameters at different electric fields F. The values in col. 2 were calculated using the phase shift analysis (see Ref. 8). The values in col. 3 were determined by the stabilization method (see Sec. II).

F (kV/cm)		Exact (eV)	Approx. (eV)
75	E_r	0.025 167	0.025 167
	Γ	1.9×10^{-6}	8.6×10^{-6}
100	E_r	0.024 210 5	0.024 206
	Γ	3.6×10^{-5}	4.1×10^{-5}
150	E_r	0.021 381 6	0.021 170
	Γ	6.4×10^{-4}	6.5×10^{-4}

Moreover, it is also shown in the figure that the difference in lifetime for wells of different width decreases and even vanishes as the applied field is increased. This fact is easily understood if we consider that as the slope in the potential caused by the field becomes larger, the maximum of the wave function for the hole is closer to one side of the QW, and from a certain value of the field onwards, the problem reduces to a hole in a sawtooth potential, the lifetime being independent of the width of the QW.

If we compare the results presented in Fig. 3 with the experimental measurements when a single QW is clearly separated (see Fig. 3 of Ref. 5) they fail to predict the magnitude of the electric field at which the photoluminescence is quenched (~ 85 kV/cm in our calculation).

Very recently, some authors have questioned the validity of the 85%-15% rule for the band-edge discontinuities. For example, Miller, Kleinman, and Gossard[15] have proposed, as more realistic, one corresponding to 57%-43%. This theory modifies the parameters (4) to

$$m^*=0.0665m_0\,,\quad V_0=383\text{ meV (electrons)}\,,$$
$$m^*=0.34m_0\,,\quad V_0=289\text{ meV (holes)}\,. \tag{5}$$

Slight variations of this rule have been proposed by several groups; for example, see the work of Okamura, Misawa, Yoshida, and Gonda.[16] The calculated tunneling times with (5) show that in this case the electrons and not the holes would be responsible for the tunneling. In Fig. 3 the dashed line describes the behavior of the tunneling times for electrons as a function of the electric field in the 37 Å QW. It is apparent that the new theory predicts a substantial increase in the field, which would produce the quenching of the photoluminescence peak. Moreover, that field should be higher due to the band-mixing effect and the spreading of the wave function in k space. These effects are not considered in our calculation, and their inclusion will produce an increased tunneling time.[8]

With respect to the Stark shifts of the energy levels, our results as compared with the variational method[3] deviated slightly as we increased the field. Similar behavior has been obtained by other authors[7,8] using different methods.

The heavy-hole–electron energy transition as a function of the applied electric field can be studied from the energy shifts of electrons and holes. A comparison between the energy shifts for the heavy-hole–electron transition calculated for the two theories that model band-edge discontinuities is showed in Fig. 4. It is possible to appreciate that the new theory predicts lower shifts. This result is closer to the recent measurements done with electroreflectance. The final discrepancy between theory and experiment, about 10%, can be due to the normal incertitude in the adjusted parameters, and experimental errors have to be considered as well.

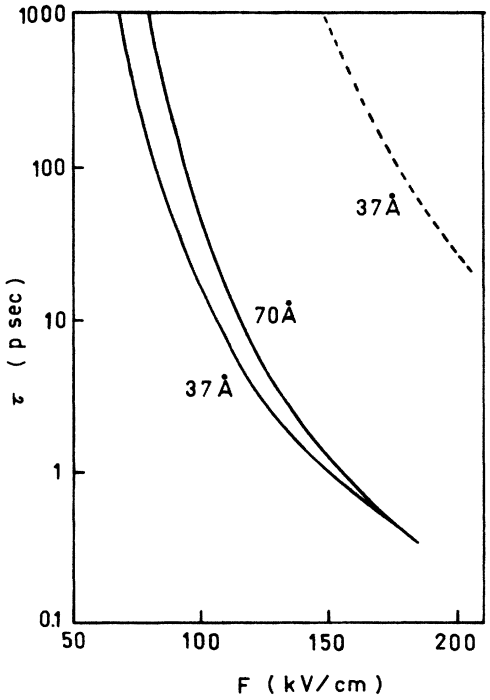

FIG. 3. Calculated tunneling lifetimes as a function of the applied field for 37 and 70 Å wells; the solid lines are the results for the 85%-15% rule; the dashed line is the corresponding one for the QW of width 37 Å using the 57%-43% rule.

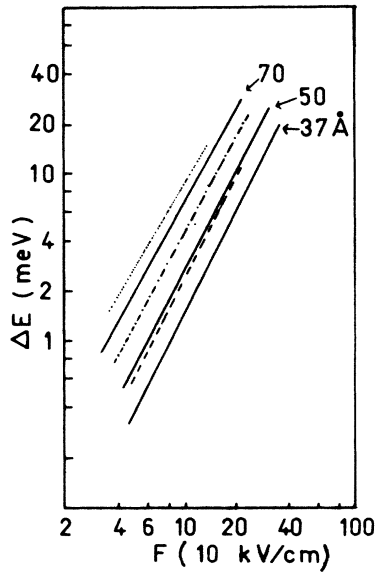

FIG. 4. Theoretically predicted shifts of the heavy-hole–electron transition vs the longitudinal electric field. The solid lines are theoretical values obtained with the 57%-43% rule for the band-edge discontinuities. Dotted, dashed-dotted, and dashed lines are, respectively, the corresponding values for 70-, 50-, and 37-Å-thick single-quantum wells, respectively, obtained with the 85%-15% rule.

In conclusion, we have presented a method based on the stabilization method used in quantum chemistry which is suitable to calculate energy levels and widths of resonances in isolated quantum wells under the influence of electric fields. This method has been applied to study lifetimes of resonances and energy shifts of the heavy-hole–electron transition in order to compare them with recent measurements of those magnitudes done with luminescence and electroreflectance. The two theories currently under discussion about band-edge discontinuities have been used in the calculations. The theory based on the 57%-43% rule for the conduction and valence band discontinuities predicts that the electrons, and not the holes, would be responsible for the quenching; also it predicts a greater magnitude in the field at which the photoluminescence peak is quenched. With respect to the observed shifts for the heavy-hole–electron energy transitions, this theory produces results which are in better agreement with electroreflectance experiments.

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