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Electric field induced shifts and lifetimes in GaAs-GaAlAs quantum wells

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We have performed an exact numerical calculation for an isolated GaAs quantum well system subjected to an external electric field. This calculation predicts both the shifts and widths of the Stark resonances. The shift predictions are in agreement with recent experimental results and the width calculations allow the observed decrease in luminescence lifetime with field to be interpreted in terms of the field-induced tunneling of the carriers.

Recent experimental studies[1,2] of the effects of electric fields on GaAs quantum well systems have enabled both the field-induced level shifts[1] and the field dependence of the photoluminescence lifetime[2] to be obtained. In this letter the theoretical interpretation of these results is considered within the framework of an exact numerical solution of the Schrödinger equation[3] for an isolated quantum well system subjected to an electric field. This calculation provides a unified approach to the prediction of Stark shifts and widths and the observed decrease in luminescence lifetime with increasing field strength is accounted for in terms of field-induced quantum mechanical tunneling.

Previous theoretical calculations[4,5] of electric field effects on quantum well systems have treated the effect of the external field on the electronic structure by approximate techniques (in particular the variation method) appropriate in the weak-field limit. In these calculations the confined states are viewed as bound states and their field-induced broadening is ignored. Such calculations correctly predict the quadratic variation of the Stark shift with field at moderate field intensities. However, the bound state model fails to account for the decrease in the luminescence lifetime[2] with field and a more detailed calculation is required.

In the envelope function approximation the rapidly varying Bloch component of the wave function is ignored and the problem reduces to the one-dimensional effective mass equation familiar from previous studies.[4,5] For a particle of charge e and mass m^*, initially localized in an isolated well of width $2a$ and depth V_0, the Schrödinger equation is

$$\begin{aligned} -\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} - (V_0 + eFx)\psi = E\psi \qquad & |x| \leqslant a \\ -\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} - eFx\psi = E\psi \qquad & |x| > a, \end{aligned} \tag{1}$$

where F is the electric field applied perpendicular to the interface plane. The exact solutions of (1) can be obtained as linear combinations of Airy functions; application of the method of phase shift analysis to the solutions enables the Stark resonance positions and widths to be calculated. It was found[3] that for moderate fields both the variational and exact calculations predict a quadratic dependence of the Stark shift on the field; this shift can be explained by perturbation theory. The quadratic Stark shift of the ground state $|0\rangle$ of a quantum system is given by

$$\Delta E = e^2F^2 \sum_{k \neq 0} \frac{|\langle k|x|0\rangle|^2}{E_0 - E_k}, \tag{2}$$

where the states $|k\rangle$ are the excited states of the system. An increase in the well depth increases the binding energy E and thus decreases ΔE; an increase in well width increases the spatial extent of the ground state wave function and thus the matrix elements $\langle k|x|0\rangle$. At high fields the variational bound state formalism breaks down and the predictions of the two calculations differ considerably. The exact calculation predicts a decrease in the effective energy shift at high fields and the emergence of new antiresonance states from the continuum into the well.

Figure 1 gives a comparison of the predictions of the

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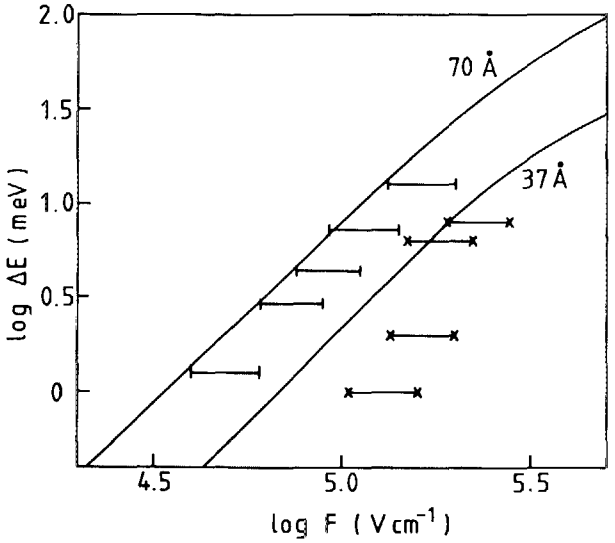

FIG. 1. Comparison of calculated and experimental[1] Stark shifts for ≈ 70 Å and ≈ 37 Å wells. In the calculation the well depth was taken as 100 meV and the hole effective mass as $0.45m_e$ in order to facilitate a comparison with the calculated shifts of Ref. 1. However, the results obtained in the quadratic regime as illustrated are not particularly sensitive to the assumed well depth. The horizontal bars extend between the "experimental" and "scaled" fields of Ref. (1): (|————|) 70 Å data; (*X*————*X*) 37 Å data.

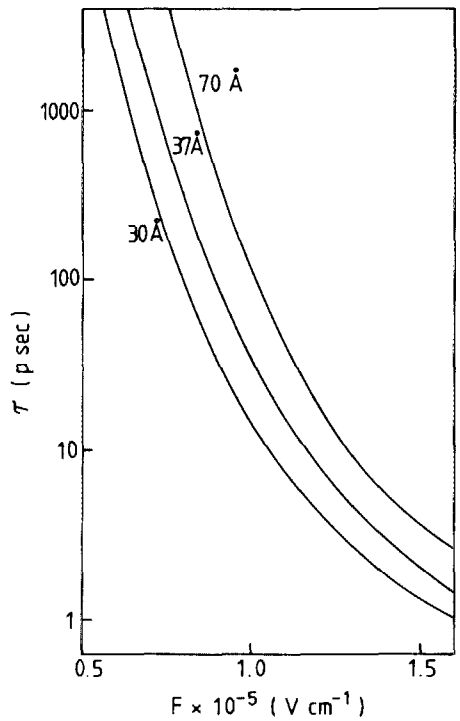

FIG. 2. Calculated tunneling lifetimes as a function of applied field for 30 Å, 37 Å, and 70 Å wells; the other parameters used in the calculation are the same as for Fig. 1.

present calculation and the experimental results[1] obtained for ≈ 37 Å and ≈ 70 Å wells. The calculations represent only the hole energy shift; because of the shallower well depth for holes this is the major contribution to the total Stark shift. For the wider well the calculated and experimental shifts are in good agreement given the large uncertainties in the determination of the experimental electric field values. However, the figure shows that the shifts predicted for the ≈ 37 Å well are much too high, except for the highest field values. One possible source of this discrepancy is suggested by the results of more detailed (zero field) calculations[6] which go beyond the envelope function approximation employed here (and in all previous Stark shift calculations). These large calculations show that in narrow wells the wave function of the confined state is more extended in k space. Consequently the matrix element in (2) should be written as

$$\langle \phi_{n,\mathbf{k}} | x | \sum_{n'\mathbf{k}'} A_{n',\mathbf{k}'} \phi_{n',\mathbf{k}'} \rangle,$$

where $\phi_{n,\mathbf{k}}$ is a Bloch function associated with band n and reduced wave vector $\mathbf{k}$. Since the characteristic value for $\mathbf{k}'$ of most of the terms on the right-hand side of this matrix element is different from $\mathbf{k}$ on the left, the value of the matrix element is substantially reduced. (This quenching of the matrix element is familiar from studies of the breakdown of the effective mass approximation for impurities in semiconductors[7] and leads to a systematic error on ΔE as calculated here which is greatest for narrow wells.) As the field strength increases, the quantum state is broadened into a resonance by the interaction with the field. This energy broadening, which is accompanied by spreading of the wave function in k space, increases rapidly with field and dominates at high field. Since the field-induced broadening is fully represented in the present calculation, it is not surprising that our high-field Stark shifts agree with experiment.

From the calculated resonance width Γ it is possible to obtain the corresponding lifetime τ; the variation of lifetime with field for quantum wells of various widths is illustrated in Fig. 2. The mechanism of state decay is field-induced tunneling out of the well and, as would be expected, this effect is greatest for narrow wells, where the particle binding energy is low. The luminescence of optically pumped quantum well systems is caused by the recombination of electron-hole pairs; nonradiative processes compete with radiative recombination and the experimental lifetime τ_e is related to the radiative and nonradiative lifetimes by

$$1/\tau_e = 1/\tau_r + 1/\tau_{nr}. \tag{3}$$

The experimental lifetime measurements[2] (performed on ≈ 30 Å wells) demonstrate that luminescence lifetime, peak luminescence intensity, and integrated luminescence all decrease when the field is increased. Theoretical considerations suggest that τ_r should increase with field. In the envelope function approximation the wave function of a particle confined in a quantum well is

$$\psi = f(x)\phi_{n,0}(r), \tag{4}$$

where $\phi_{n,0}(r)$ is a Bloch state of zero wave vector and band index n. Since $f(x)$ is a slowly varying function, the transition probability for recombination can be factorized as

$$|\langle f_e(x)|f_h(x)\rangle|^2 \; |\langle \phi_{n',0}|\mathbf{p}\cdot\mathbf{A}|\phi_{n,0}\rangle|^2. \tag{5}$$

Under the influence of the electric field the maxima of the electron and hole wave functions are shifted in opposite directions and thus the overlap $|\langle f_e(x)|f_h(x)\rangle|^2$ decreases, leading to a decrease in the transition probability and an increase in the radiative lifetime. However, the magnitude of this effect [as previously estimated from the variational solutions of (1)[4]] is much too small to account for the observed rate of

luminescence quenching. The calculation described here suggests additional field-dependent effect on the radiative lifetime. The energy broadening of the confined quantum well hole states into resonances also implies the above-mentioned spreading of the wave function in k space and thus a decrease in its $k = 0$ component which will in turn reduce the transition probability (Ref. 7). This reduction is expected to be greatest for narrow quantum wells. The model adopted in the present study is too crude to provide a quantitative estimate of this effect, since the details of the band structure at the top of the valence band are ignored. Such details may be quite important because the applied field can make quantum well valence states associated with different n and $\mathbf{k}$ quasi-degenerate. Since the admixture of a higher lying state $|n',\mathbf{k}'\rangle$ with the state $|n,\mathbf{k}\rangle$ is proportional to $(E_{n,\mathbf{k}} - E_{n,\mathbf{k}'})^{-1}$, we might expect the transition probability to be a sensitive function of the field-induced broadening.

The results presented here predict a rapid decrease of the hole lifetime with increasing applied field due to the tunneling of carriers out of the quantum wells. The decrease in the observed luminescence lifetime follows from Eq. (4), provided that the change in nonradiative lifetime is the dominant effect. This seems likely in view of the predicted exponential dependence in Fig. 2 of the hole lifetime on field strength. The increase of τ_r with field explains the decrease in luminescence intensity. Comparison of Fig. 2 with the experimental results[2] shows that the nonradiative lifetimes are underestimated in our calculation. (The experimentally measured overall lifetimes are in the range 50–300 ps.) This is well in keeping with our remarks concerning the spreading of the zero field hole wave function in k space. By adopting the envelope function effective mass Hamiltonian to represent the zero field solution, we have introduced a systematic error which increases with decreasing well width and which may underestimate the lifetime by as much as an order of magnitude. In the limit of very strong fields our method[3] of determining the resonance width leads to a further overestimate of the broadening effect due to tunneling.

An additional effect found in the experimental measurements is an increase in luminescence lifetime with increased carrier number density. This has been interpreted in terms of exciton polarization.[2] The present calculations suggest that an alternative explanation of this effect may be found in the tunneling of free carriers out of their respective wells. The resulting charge separation sets up an electric field which opposes the applied field, so the "effective field" experienced by the system is smaller at high carrier number densities.

In conclusion, we have presented an exact numerical solution of the Schrödinger equation for the quantum well Stark resonance problem which predicts the origin and magnitudes of level shifts and provides an adequate explanation of the observed lifetimes. Our calculation has a conceptual advantage over previous work[4,5] in that it goes beyond the limit of validity of bound state calculations and provides a unified approach to Stark shifts and widths.

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Metalorganic growth of epitaxial films of CdTe and HgCdTe on sapphire substrates

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Specular epitaxial films of CdTe have been grown on (0001) sapphire substrates by the metalorganic chemical vapor deposition technique. The films grow with the (111)*A* orientation and exhibit narrow x-ray linewidths. Secondary ion mass spectrometry profiles indicate negligible diffusion of aluminum from the substrates. Epitaxial films of HgCdTe have been grown on top of the CdTe layers. Initial Hall measurements are encouraging for an all metalorganic chemical vapor deposition process for depositing HgCdTe on sapphire substrates.

Epitaxial films of HgCdTe are needed for the active elements in infrared detection systems. Conventionally, HgCdTe is grown on CdTe substrates which have the attractive properties of a close lattice match with HgCdTe and of immunity from autodoping of the HgCdTe films. However, CdTe substrates are expensive, fragile, not available in large areas, and are of lower crystalline quality compared to commonly available substrates such as Si, GaAs, Al_2O_3(sapphire), or InSb. Therefore, an alternative substrate material is desired. An attractive candidate is sapphire because of its

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