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Electronic structure and transport properties of GaAs-GaAlAs superlattices in high perpendicular electric fields

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We present a study of the effect of high ($\sim 1\times10^5$ V/cm) perpendicular electric fields on the electronic structure of a GaAs-$Ga_{0.7}Al_{0.3}As$ superlattice represented by five quantum wells separated by 70-Å barriers. An exact solution is obtained by using the transfer-matrix technique to match the Airy functions at the interfaces. The method of phase-shift analysis is employed to evaluate the energy levels, the width of the Stark resonances, the real-space wave functions, and the time of flight associated with the field-induced phenomena. Wells of 50- and 70-Å width are used to elucidate the relationship between level depth and field. The quantum states above the semiclassical confining barrier, which have so far been represented by a continuum, are correctly accounted for. These states are mainly localized in the barrier material. It is shown that the real-space localization and bandwidth of these states are significantly altered by the external field. In particular, we evaluate the time delay for electrons above the barrier due to the field-induced change in the density of states, which is related to the presence of the above higher-lying confined states and which would be observed in current–voltage measurements.

I. BACKGROUND

The electronic structure and transport properties of quantum-well and superlattice systems are topics of great current interest and importance. The spatial variation of the band structure and the existence of quantum-confined states in these systems have been exploited in a number of novel devices (see, for example, Refs. 1–5 and references therein). This interest in device applications has stimulated a number of calculations on perpendicular electron transport in quantum-well and superlattice systems (Refs. 6–8 and others). These calculations were performed for zero-field conditions. An important feature of many of the proposed devices is, however, that very high electric fields are applied to the quantum-well structures; frequently, the energy of interaction of the carriers with the applied field is greater than their binding energy. Under these circumstances nonlinear and nonperturbative field effects can become significant, and an appropriate theoretical treatment is required. Ideally, a large-scale calculation, in which the band structure of the superlattice components would be taken into account and the effect of the applied field introduced in a self-consistent manner, would be performed. Results of this type are not currently available for the following reasons: (1) The electric field breaks the translational symmetry of the lattice, and so the usual methods of band theory are not directly applicable. (2) There are mathematical and computational problems associated with the use of the unbounded operator $-Fz$.[9] For example, performing a real-space calculation with "box" boundary conditions can lead to an unphysical "pile-up" of states at one end of the structure. An alternative approach to electric field effects, which has been extensively employed in the literature, is the envelope-function effective-mass approximation; this leads to a one-dimensional Schrödinger equation for the envelope function in the z (growth) direction whose exact or approximate zero-field solutions provide a suitable starting point for most transport studies. Approximate solutions, valid for weak external electrical fields, were obtained within a variational scheme by Bastard *et al.*[10] and Miller *et al.*[11,12] In the case of strong fields, however, the use of the exact Airy-function solutions is more appropriate. This method has been employed by a number of workers.[11–17] In general, these calculations have been concerned with corrections to energy levels and have ignored the extensive field-induced tunneling that occurs in these structures when the bound states become field-induced resonances.

In particular, we were first to introduce into the problem the method of phase-shift analysis, which is familiar in other applications of quantum theory and yields a variety of observables, such as the density of states, lifetimes, and the time of flight. We have evaluated such quantities for a few typical isolated and double quantum-well GaAs-GaAlAs systems with a view to elucidating some of the conceptual novelties this approach offers.[18–21]

In this paper we study the effect of high perpendicular electric fields on the electronic structure of a GaAs-GaAlAs superlattice consisting of five GaAs wells. In our analysis we also include the states lying above the confining barrier. Such states can be approximately accounted for by the envelope-function effective-mass model used here as a zero-field starting point. Only the states derived from the lowest minimum of the conduction (bulk) band of GaAs and GaAlAs are involved. The states above the semiclassical confining

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barrier may play an important role in vertical transport problems because they have been shown to have wide bandwidth and exhibit localization in the barrier material. We will show that the external field can modify their character and that they contribute to the change in the state density in the hot-electron range of energies and, consequently, to the current–voltage characteristics.

In addition to the states derived from the lowest minimum, there is a rich variety of localized states associated with the secondary bulk minima at the X and L points.[22–25] Although these states are highly relevant in hot-electron transport problems, they lie outside the scope of the treatment employed in the present study. However, it might be worth pointing out that a quantitative understanding of these states, both theoretical and experimental, is now available and may serve as a basis for simpler models.[26] The latter is already apparent from the work of Jaros *et al.*,[23] Wong *et al.*,[27] and Ninno *et al.*,[25] who presented the momentum space wave functions of these states and showed that, with the exception of very narrow wells, the higher states are well localized in momentum space and therefore clearly separable from the equally well localized (at Γ, i.e., $k = 0$) states that lie deep in the well. The difficulty of implementing a scheme that includes states of different bulk momentum character in the present context lies in the requirement that the phase of the rapidly varying components of the individual states must be correctly accounted for. This presents technical difficulties in the phase-shift method, which relies on the matching of the envelope functions at the interface.

The results presented here are complementary to the recent low-field calculations of McIlroy[17] who considered the effect of an external electric field on a GaAs multi-quantum-well system. We are not aware of any other comparable theoretical work on superlattices in the literature.

Experimentally, electric field effects have been studied by spectroscopic and photocurrent methods.[11,12,16,28–34] The main results of these experiments are the following:

(1) The confined states in GaAs-GaAlAs quantum wells undergo a Stark shift. At low fields the shifts are quadratic in the field for an isolated quantum well, as predicted by perturbation theory.[10] Anomalous Stark shifts are predicted to occur only at very high fields.[18] The experimental and calculated level shifts are generally in good agreement.[12,19] For narrow wells, some discrepancies between experiment and theory are found. This is presumed to indicate a breakdown of the envelope-function effective-mass approximation.

(2) Electron-hole recombination transitions and the corresponding photocurrent peaks are substantially broadened and the broadening increases with field; this can be accounted for by a sharp decrease in the nonradiative lifetime of the carriers due to field-induced tunneling out of the well. The radiative recombination lifetime undergoes a simultaneous increase because of field-induced spatial separation of the electrons and holes. The overall lifetime is generally dominated by the effect of tunneling.

(3) Exciton transitions remain observable at high fields because of carrier confinement in the wells. The observed spectroscopic and photocurrent peaks decrease in integrated intensity as the field-induced tunneling increases.

The problem of vertical transport (see Ref. 15 for a recent review) in superlattices, where adjacent wells are in "contact" because of the spatial overlap of the confined wave functions, has not been frequently studied, and the spectroscopic information available for isolated quantum wells is missing. However, the work of Bastard *et al.*[10] indicates that the tunneling effects that occur in multi-quantum-well structures may play an even more important role in superlattices. The present study is an attempt to identify the key qualitative features peculiar to the superlattice system in the energy range up to and above the confining barrier. It is also the first attempt to introduce into the picture the states lying above the confining barrier and demonstrate their behavior in an external field. Recently, Babiker and Ridley[35] have demonstrated the importance of these states in electron–phonon interactions in superlattices, and Song *et al.*[36] have studied the corresponding radiative recombination rates.

II. CALCULATION AND RESULTS

A. Introduction

We have performed calculations on quantum-well systems with various numbers (N) of wells. Inspection of the results shows that "superlattice" features (i.e., states localized in the barrier) can be observed for $N = 3$ and, in some instances, even for $N = 2$. It is thus apparent that superlattices can be modeled by using relatively small values of N. The majority of the results presented here are for structures with $N = 5$.

It is appropriate to reconsider the values used for the valence and conduction-band offsets in our previous work.[18–21] Recent experimental work (for example, Refs. 37–39) suggests that the ratio of the conduction and valence-band offsets is in the vicinity of 60:40, rather than the previously accepted ratio of 85:15. It should be noted that changing the values of the offsets used in our calculations does not affect the qualitative nature of the phenomena predicted (i.e., the occurrence of anomalous high-field Stark shifts, extensive tunneling out of the wells, and the effects of above-barrier states). Certain quantitative predictions do of course depend on the choice of offsets; in particular, electron- rather than hole-dominated tunneling is predicted when the 60:40 offsets are used,[12] although the Stark shifts are remarkably insensitive to the offset choice. The results presented here were obtained by using the currently accepted values of the offsets. As well as consistency with experiment, concentrating on electrons rather than holes has the additional advantage that the conduction band of III–V semiconductors is known to conform more closely to the effective-mass approximation than does the valence band.

B. Method

We consider GaAs-$Ga_{1-x}Al_xAs$ structures with $x \approx 0.3$. The structure studied is shown in Fig. 1. Comparison of the results of single-well calculations with experiment have shown that reasonable agreement is obtained for well widths $\geqslant 50$ Å.[11,12,19,29] By considering a superlattice of 70-Å

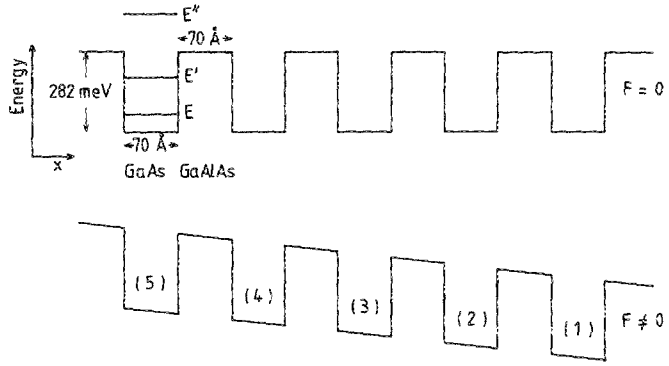

FIG. 1. Quantum-well structure used in the calculations. The effective mass used is $m^* = 0.067m_0$. The numbering of the wells is used in the discussion of wave-function localization. The energy levels associated with each well taken in isolation are indicated. The well depth is -282 meV.

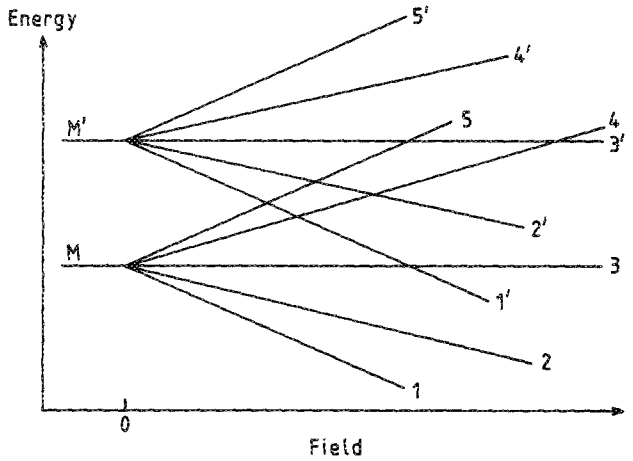

FIG. 2. Schematic diagram of the predicted weak-field Stark splittings of the "minibands" M and M' of a five-well structure. The state labeling corresponds to the localization properties of the wave functions.

wells, direct experimental predictions should thus be obtainable.

The method of calculation is as described previously[18–21]; the solutions of the one-dimensional Schrödinger equation for the envelope function $\psi(z)$ (in scaled atomic units),

$$-\frac{1}{2}\frac{d^2\psi}{dz^2} + (V_0 - E)\psi - Fz\psi = 0, \qquad (1)$$

with the potential V_0 of Fig. 1, can be obtained as linear combinations of Airy functions; the coefficients of the Airy functions are obtained by the transfer-matrix technique. Application of the method of phase-shift analysis allows the positions and widths of the Stark resonances to be found; differentiation of the phase shift allows the change in the density of states $\Delta\rho$ to be calculated. In these calculations the electric field is taken to be perpendicular to the well plane. Parallel transport in these structures is also an important topic,[40] but is not considered in the present work.

C. General results

An isolated quantum well with the chosen parameters supports two bound states, as illustrated in Fig. 1. For the $N = 5$ system, tunneling between the wells gives rise to a closely spaced set of five levels in the vicinity of each $N = 1$ state; these sets are the precursors of minibands in larger, truly periodic, structures. The effect of a weak electric field on each "miniband" can be predicted from a simple 5×5 matrix calculation. The resulting (linear) Stark pattern is illustrated schematically in Fig. 2. As in the double-well system,[21] the zero-field states are delocalized. Turning on the field localizes the states, as indicated in Fig. 2.

Figure 3 shows the resonance positions obtained from the Airy-function calculations. Figure 4 shows some typical resonance wave functions and Fig. 5 some typical change of density-of-states plots. The main features of these results are the following:

(1) Linear Stark shifts are obtained up to $F \approx 2\times10^5$ V cm^{-1}; deviations from linear behavior are found at higher fields. The states 3 and 3′ can be seen to have energies that are virtually independent of field in this region. This is due to the localization of the wave function in the central well.

(2) Strong coupling between the confined states and the continuum is indicated by the variation of state width with field. In general, the width of each state increases with field, although some oscillatory behavior is observed. (This is associated with the interaction between resonance and above-barrier states, described in more detail in the next section.) The extent of the field-induced broadening is a sensitive function of the zero-field binding energy, since the tunneling probability increases strongly as binding energy decreases. For the M states ($E_0 \approx -225$ meV) the resonances have widths of only a few tenths of an meV for $F = 3\times10^5$ V cm^{-1}; by contrast, the M' states ($E_0 \approx -75$ meV) are broadened by around 50 meV at the same field. These figures should be compared with the upper (M') miniband widths of $\sim$20 meV obtained from large-scale zero-field superlattice calculations.

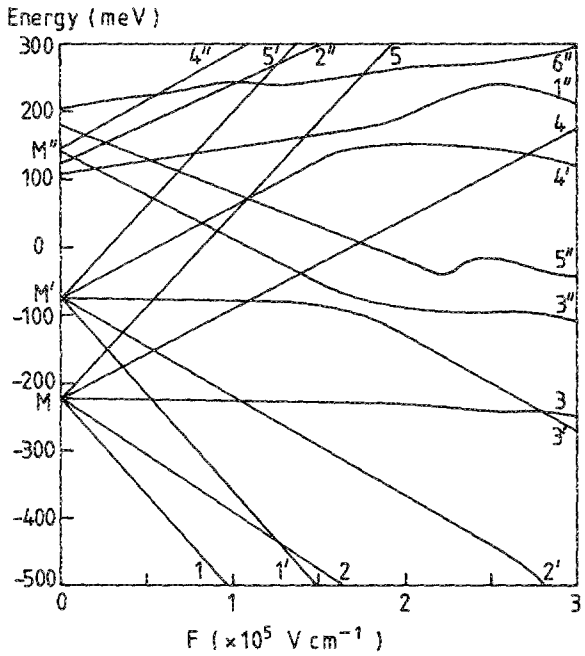

FIG. 3. Positions of resonances and above-barrier states as a function of electric field.

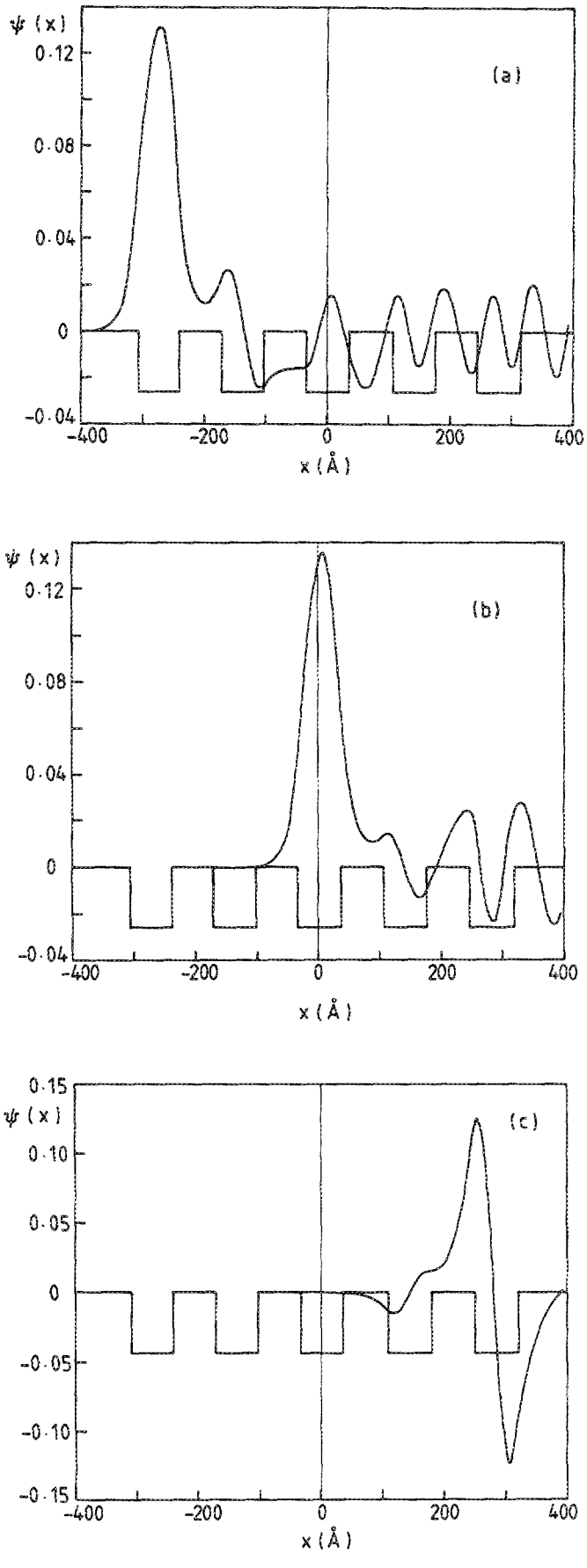

FIG. 4. Examples of normalized resonance wave functions; the positions of the wells and barriers are shown. (a) State 5, $E = 52$ meV, $F = 10^5$ V cm^{-1}. (b) State 3, $E = -229$ meV, $F = 1.2\times10^5$ V cm^{-1}. (c) State 1′, $E = -131$ meV, $F = 2\times10^4$ V cm^{-1}.

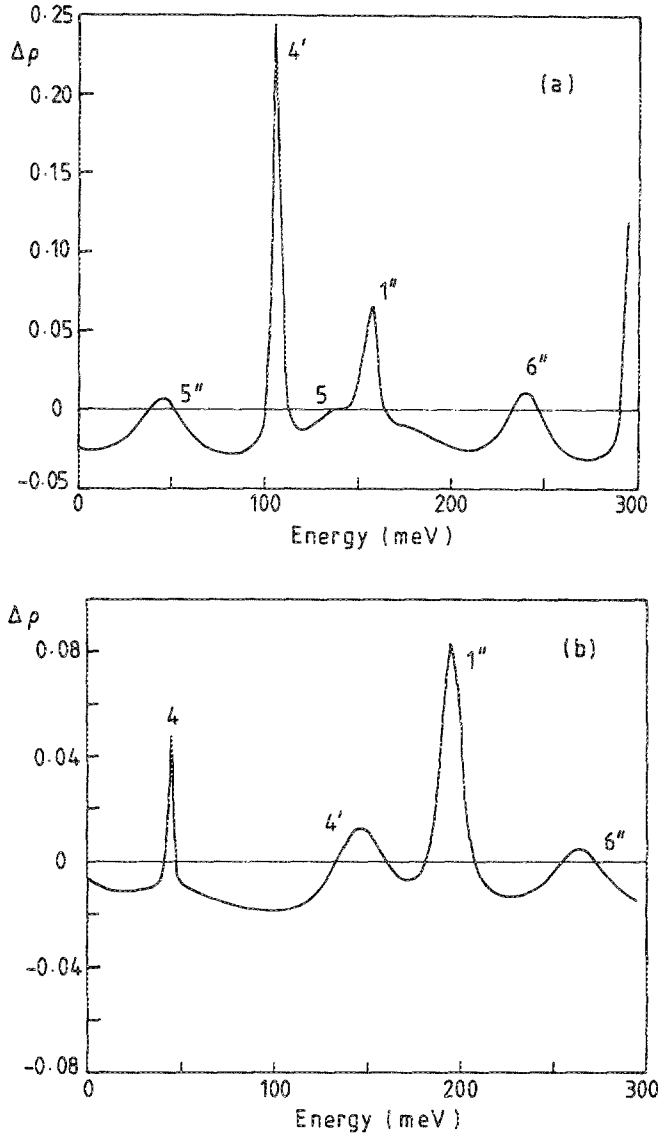

FIG. 5. Density of states in the region 0–300 meV. (1) $F = 1.36\times10^5$ V cm^{-1}. (b) $F = 2\times10^5$ V cm^{-1}.

Taking a more extreme case, we have calculated resonance positions and widths for a structure in which the well width is reduced to 50 Å and the upper miniband occurs only 8 meV below the top of the well; these states are broadened by ~ 5 meV at $F = 4\times10^4$ V cm^{-1}, increasing to $\sim 5\times10^2$ meV at $F = 3\times10^5$ V cm^{-1}. This illustrates the point made in previous work[18] that weakly bound states are particularly liable to show anomalous field effects.

The sharp increase of width with field observed for all states implies very rapid electron tunneling out of the structure at high fields. It should be noted that the present calculation gives a steady-state description of tunneling. In experiments where a wave packet is incident on a superlattice, the detailed dynamics will depend on the shape of the wave packet.[41,42]

(3) As was found for $N = 2$,[21] wave function localization effects can also cause high-energy resonances to have smaller widths than low-energy resonances in the same miniband. This occurs because high-energy states are spatially localized far from the tunneling barrier.

(4) The density-of-states plots for the superlattice show the shift, broadening, and decrease in area found experimentally and in previous calculations.[18,20]

The breakdown of a simple bound-state treatment is apparent from these results (strong coupling to the continuum is also indicated by the field dependence of the positions of the above-barrier states discussed in the next section). At the same time, near-linear energy shifts, as predicted from the bound-state model, are obtained even at high fields. This paradox can be resolved by inspection of typical real-space wave-function plots (Fig. 4). Each resonance state can be seen to have a large peak in one well, with oscillatory behavior outside. The *net* charge deposited outside the well into the oscillatory tail of the wave function is surprisingly small. Thus if the field undergoes an increase ΔF, the off-diagonal matrix elements of ΔFz are small; essentially, the resonances do not "see" each other. This also explains the observed remarkable stability of excitons in quantum wells exposed to strong electric fields, which would seem to be incompatible with the calculated field-induced wave-function tails and density-of-states fluctuations.

D. Above-barrier states and implications for transport and spectroscopic properties

Above-barrier confined states, derived from the lowest conduction-band minimum, are found in both envelope-function[43] and large-scale[22–27] calculations; the latter work revealed the momentum-space wave-function characteristics of these states. The implications of the existence of such states for transport properties have not been fully explored. However, it is well known that if the above-barrier density of states is not flat, oscillatory structure in current–voltage curves would be expected, by analogy to the well-known below-barrier resonant-tunneling phenomenon.[44–47]

In the present calculation we have studied the field dependence of a group of above-barrier states. These states are identified from subsidiary maxima in the change of the density of states computed from the phase shifts. (This is in contrast to the "antiresonance" states described previously,[18,21] which are associated with density-of-states minima.) Some examples of these features can be seen in Fig. 5, and the field dependence of the energies of these states is shown in Fig. 3. Inspection of the wave functions (examples are shown in Fig. 6) shows that they all have some degree of localization in the GaAlAs barriers, although the localization is much less clear cut than for the resonances. Mixing between resonance and above-barrier states and changes in wave-function localization properties occur at the avoided crossings shown in Fig. 3.

Unlike the resonances, the above-barrier states are broad, having widths of tens or even hundreds of meV at low fields. These states of course have nonzero widths in the absence of a field (large-scale zero-field calculations on truly periodic structures with 70-Å wells and 70-Å barriers give widths of ~ 100 meV; for details see Ref. 27); the field induces additional broadening and restructures the density of states.

The oscillations in the density of states in Fig. 5 are associated with both resonance states that have been Stark

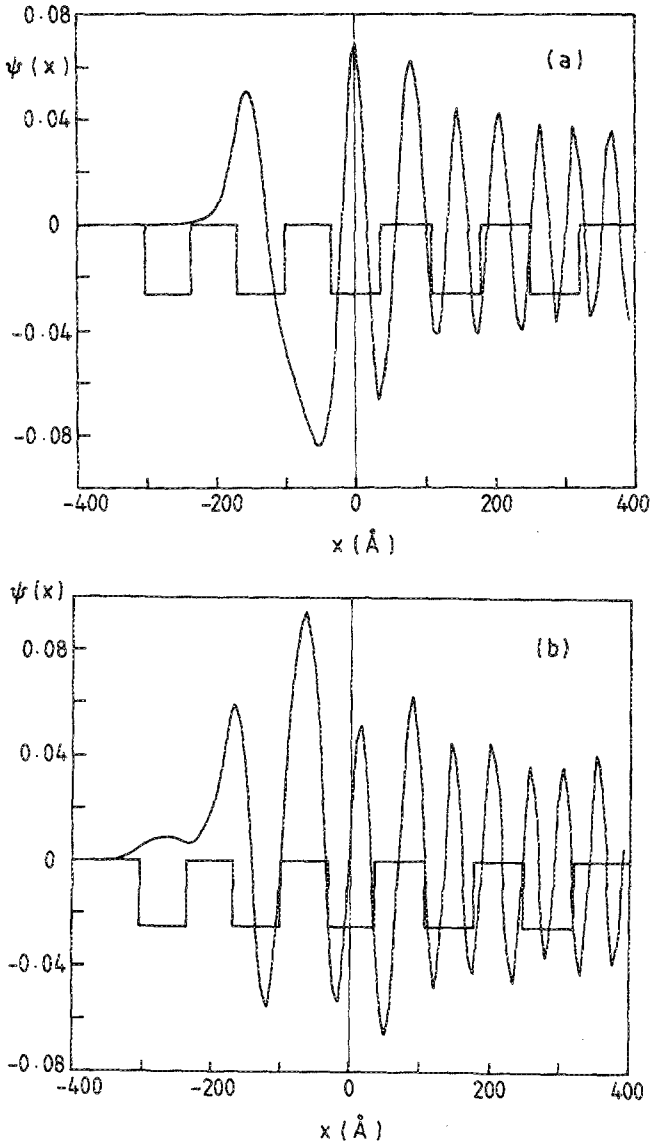

FIG. 6. Examples of normalized wave functions of above-barrier states. (a) State 1″, $E = 149$ meV, $F = 1.5\times10^5$ V cm^{-1}. (b) State 6″, $E = 255$ meV, $F = 1.8\times10^5$ V cm^{-1}.

shifted upwards and above-barrier states. Note also that two states initially above the barrier are drawn into the wells at high fields. The ability of a structure to transmit electrons is clearly affected by the presence of both the resonance and the above-barrier states. The time delay introduced by the structure is related to the phase shift ϕ by

$$\Delta t = \frac{d\phi}{dE}. \tag{2}$$

Calculation of the time delay as a function of voltage for electrons of a given energy is of particular interest. Typical results are shown in Fig. 7. Such results can be used directly to analyze hot-electron spectrometer data that are currently used to assess hot-electron transistors (see, for example, Ref. 48 and references therein). Indeed, our predictions indicate that the results of experimental studies on vertical transport in superlattices must be carefully analyzed in order to account for the contribution of the Γ-related above-barrier states described above, which will hybridize with X-related

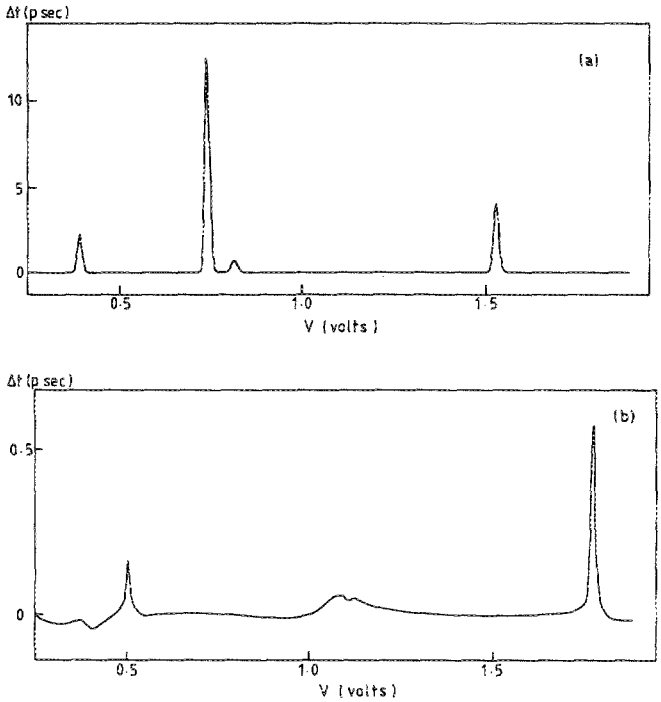

FIG. 7. Time delay as a function of voltage for electrons of energy. (a) 100 meV. (b) 150 meV.

states in the manner predicted by Ninno *et al.*[25] and, more recently, by Gell *et al.*[26]

As well as affecting transport properties, the existence of the above-barrier confined states and their field dependence would be expected to affect the spectroscopic properties of superlattices. The number and strength of the transitions observed will vary as a function of field; particularly strong intensity variations would be expected to occur in the vicinity of avoided crossings.

III. CONCLUSIONS

In this paper we have studied the effects of perpendicular electric fields on a model superlattice structure. Our calculations recover a number of features that resemble those reported for isolated wells, such as anomalous Stark shifts, resonance width broadening, and tunneling out of the well. Several new effects, peculiar to the superlattice structure, have also been obtained. In particular:

(1) Both the well states and the above-barrier states contribute to the transport properties of the system. The existence of confined states in the hot-electron region leads to oscillatory current–voltage behavior, negative differential resistance, and the possibility of current amplification and oscillation under appropriate conditions. Above-barrier states can also be drawn into the wells and thus contribute to "ordinary" resonant tunneling.

(2) An important feature in perturbed superlattice systems is the differing spatial localization of electrons of different energy. This suggests that carrier capture or excitation will be preferentially connected with certain spatial regions of the structure in question and that the occurrence of differential stability effects will depend on the applied field, as well as on the structural geometry.

ACKNOWLEDGMENTS

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