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Electronic structure of an isolated GaAs-GaAlAs quantum well in a strong electric field

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An exact numerical calculation for an isolated quantum well of a GaAs-GaAlAs system subjected to an external electric field is presented. Resonance positions and widths, and density-of-states profiles are reported for a 30-Å well to demonstrate that the rigorous description of the high-field states as resonances leads to qualitatively new phenomena. In particular, in fields of 4×10^5 V cm^{-1} the effective hole energy shift is reduced to zero and a new antiresonance state emerges from the continuum into the well.

In novel semiconductor devices,[1] carriers are often confined in quantum-well structures and exposed to high electric fields. The existing attempts[2,3] to model the electronic structures of such systems are based on calculations in which the effect of the external field is treated by approximate techniques (i.e., perturbation theory, variational method) appropriate in the weak-field limit. In such calculations, the confined states are viewed as bound states, and the field-induced broadening is ignored. Very recently, Miller *et al.*[3] extended the variational calculations of Bastard, Mendez, Chang, and Esaki[2] for particles in an infinite well, to fields up to 10^5 V cm^{-1}. They also considered an exact solution for an infinite well in terms of resonances described by Airy functions, and concluded that, in the range of fields in question, both methods yield very similar results. This means that the near-quadratic increase of binding energy with field, characteristic of the low-field Stark effect, might also be expected in the high-field limit. In this study, an exact numerical solution is presented for fields of $0-5\times10^5$ V cm^{-1}, and applied to an isolated GaAs-GaAlAs quantum well of finite depth. It is demonstrated that, at experimentally attainable fields (e.g., $1-4\times10^5$ V cm^{-1}), the tunneling widths are in fact quite large, and that qualitatively new phenomena occur which lie outside the scope of the simple bound-state calculations.

Since the chief aim of this paper is to elucidate high-field effects, only the simplest zero-field model Hamiltonian is employed. 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.[2,3] For a particle of charge e (taken here and in the remainder of the paper to be positive) and mass m^*, initially localized in a well of width $2a$ and depth V_0, the Schrödinger equation is

$$\begin{aligned} &-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2}-(V_0+eFx)\psi=0, \quad |x|\le a \ , \\ &-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2}-eFx\psi=0, \quad |x|>a \ , \end{aligned} \tag{1}$$

where F is the electric field applied perpendicular to the interface plane. As in the well-known example of the atomic Stark effect, the applied field causes a shift of the energy levels with respect to their zero-field values, accompanied by a broadening. Since the potential term in (1) tends to $-\infty$ as $x\to+\infty$, the system has strictly no bound states;[4] when F is nonzero the particle can always lower its potential energy by tunneling out of the well; this means that the zero-field bound states are converted into resonances. In moderate fields the Stark states should nevertheless be observable since, as in the atomic case, the tunneling rate should be small compared to the spectroscopic observation time.

The coordinate transformation

$$\begin{aligned} y&=(2eF)^{1/3}x-\frac{2}{(2eF)^{2/3}}(V_0-E) \quad |x|\le a \ , \\ &=(2eF)^{1/3}x+\frac{2E}{(2eF)^{2/3}} \quad |x|>a \ , \end{aligned} \tag{2}$$

allows (1) to be written in the standard form

$$\frac{d^2\psi}{dy^2}+y\psi=0 \ , \tag{3}$$

which has the full solution

$$\begin{aligned} &\psi_1=\mathrm{Ai}(-y), \quad x<-a \ , \\ &\psi_2=C_1\mathrm{Ai}(-y)+C_2\mathrm{Bi}(-y), \quad |x|\le a \ , \\ &\psi_3=C_3\mathrm{Ai}(-y)+C_4\mathrm{Bi}(-y), \quad x>a \ , \end{aligned} \tag{4}$$

where Ai and Bi are Airy functions. The numerical values of the coefficients C_1,C_2,C_3,C_4 can readily be found by matching the values of ψ and its first derivative at the points $x=\pm a$. In the method of phase-shift analysis (previously applied to the hydrogen Stark problem by Damburg and Kolosov[5]) the Stark resonances are characterized by a rapid increase of π in the phase ϕ, where

$$\tan\phi=\frac{C_4}{C_3} \ . \tag{5}$$

The position E_0 and width Γ can be calculated using the Breit-Wigner parametrization

$$\tan\phi=\frac{\Gamma}{2(E_0-E)} \ . \tag{6}$$

(This parametrization is, of course, only approximate for the broad resonances expected at high fields.)

For the numerical calculations, the values of V_0 and m^* appropriate for electrons and heavy holes in GaAs-$Ga_{1-x}Al_xAs$ quantum wells were employed:

$$m^*=0.067m_0, \quad V_0=400 \text{ meV (electrons)} \ ;$$

$$m^*=0.45m_0, \quad V_0=70 \text{ meV (holes)} \ ,$$

where m_0 is the free-electron mass. These parameters and the well width of 30 Å were chosen in order to obtain a direct comparison with the calculations of Bastard *et al.*;[3] this choice corresponds to wells which support only one bound state for both electrons and holes. Figure 1 presents the Stark shifts obtained for applied fields up to 5×10^5 V cm^{-1}. For electrons these can be compared with the variational results.[3] As would be expected, the two calculations are in agreement at low fields; small deviations are found between the variational and exact results at higher fields. The largest deviation found is only about 1% of the total binding energy, so the variational calculations are clearly adequate in this field regime in the case of electrons. For holes the resonance energy plot shows a remarkable feature—at low fields the resonance energy becomes more negative as the applied field is increased, but reaches a minimum for F in the region of 2.5×10^5 V cm^{-1}, and subsequently increases as the field is increased, to the extent that the energy shift becomes positive at very high fields. Similar behavior is also found for electrons, but at much higher field values ($>1.2\times10^6$ V cm^{-1}). The physical significance of the turnaround in energy is not entirely clear, but the same effect has previously been found in a number of Stark-effect calculations, in particular for atomic hydrogen.[6] It is clear that such behavior is highly unlikely to be predicted by a simple variational calculation, thus suggesting that for holes such calculations are valid only up to about 2×10^5 V cm^{-1}. The greater sensitivity of hole states to applied electric fields can be traced back to their smaller binding energy. The onset of the high-intensity regime for a finite well can be roughly defined as $F\geq F_c$, where F_c is the field for which the tunneling barrier to ionization disappears completely; the approximate condition for this to occur is

$$F_c a = -E_0 \ , \tag{7}$$

where E_0 is the zero-field binding energy. F_c thus corresponds to the value of the applied field for which the top of the well is pulled down by the field to the level of the zero-field bound state. This calculation gives $F_c=1.5\times10^6$ V cm^{-1} for electrons and 2.7×10^5 V cm^{-1} for holes; thus in both cases the energy turnaround occurs at fields slightly below F_c. In view of the very high value of F_c for electrons, only the results for holes are presented in the remainder of this paper; it is the field dependence of the hole-binding energy and wave function which would be expected to be dominant; the contribution of the electron states can be satisfactorily predicted using bound-state methods.

For fields close to F_c the ionization rate will be high, and the bound-state assumption of the variational calculation cannot be justified. This is confirmed by studying the resonance widths, which are shown in Fig. 2. The drastic increase in width at high fields means that it is doubtful that the resonance position has any physical meaning for $F\geq F_c$, so it appears unlikely that the energy turnaround effect is in fact experimentally observable. In the context of spectroscopic studies, a more physically meaningful property is the field dependence of the density of states. This cannot be obtained by bound-state methods (which would predict a δ function), but is readily obtainable in the scattering-theory formalism. The change in the density of states is given by[7]

$$\Delta\rho(E)=\frac{2}{\pi}\frac{d\phi(E)}{dE} \ . \tag{8}$$

Since the solutions (4) are based on Airy functions, which describe the behavior of a free charged particle in an electric field, $\Delta\rho$ must be interpreted as the change in the density of states induced by adding the potential well to the free parti-

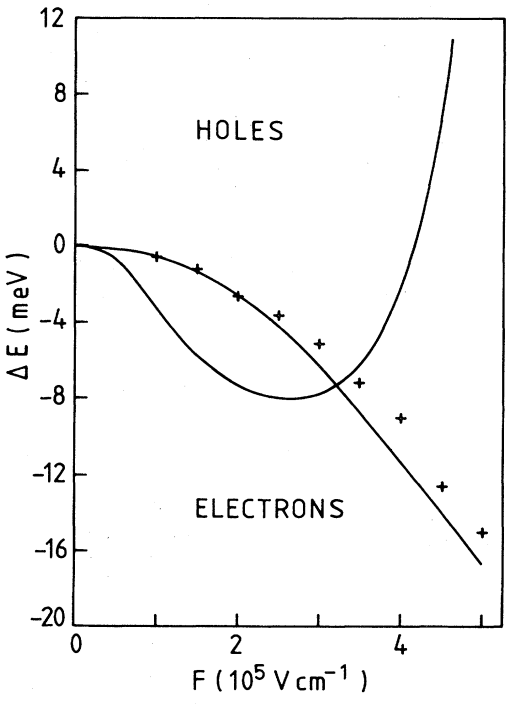

FIG. 1. Calculated energy shifts for electrons and holes. The crosses are the shifts for electrons obtained by Bastard *et al.* (Ref. 3).

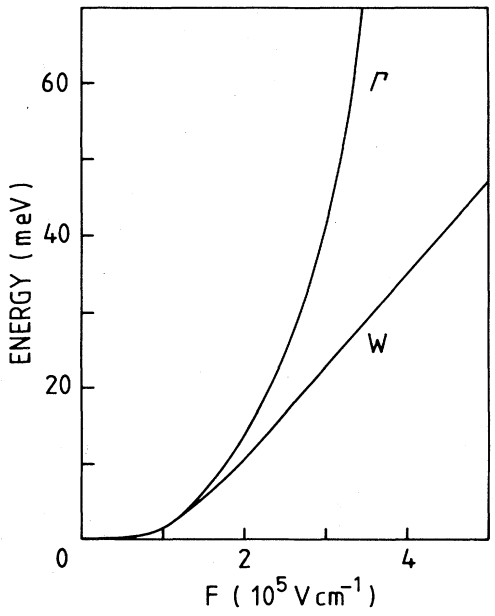

FIG. 2. Resonance width Γ and density-of-states peak width W for holes.

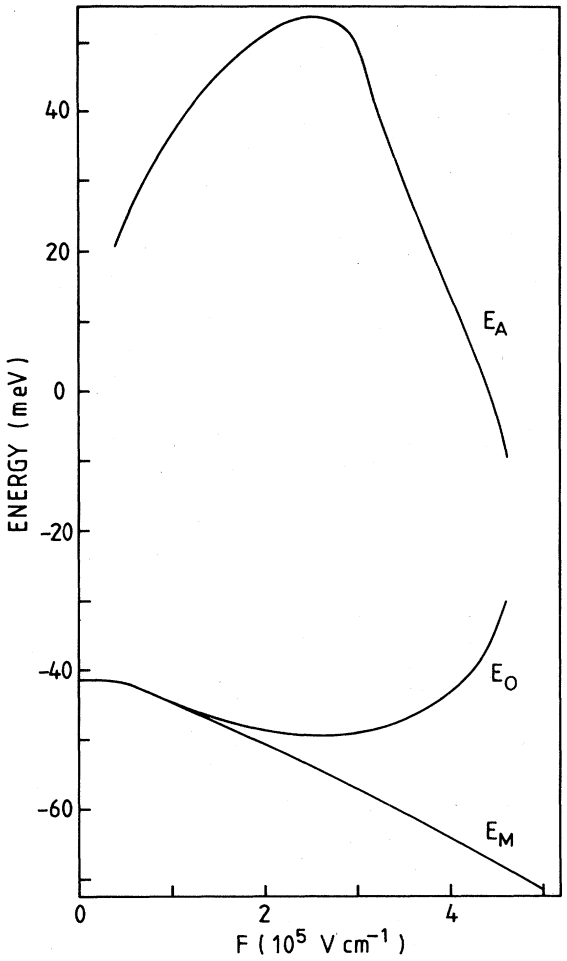

FIG. 3. Resonance and antiresonance energies (E_0, E_A) and position of the density-of-states maximum (E_M) for holes.

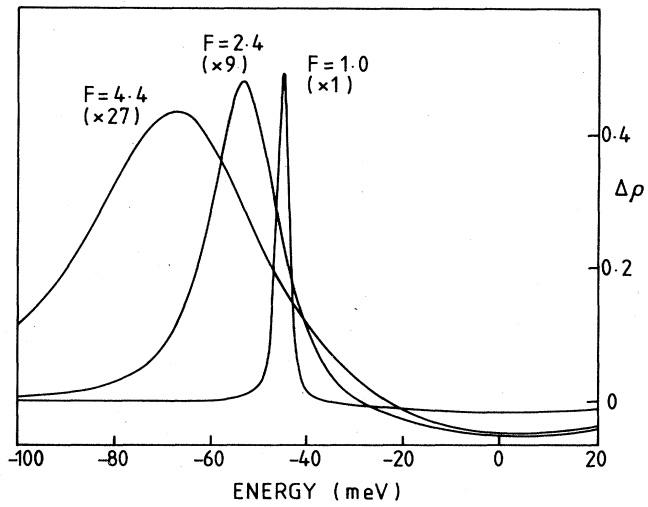

FIG. 4. Plots of $\Delta\rho$ for holes at various field intensities (in units of 10^5 V cm^{-1}). The peak height decreases with increasing field; to compensate for this the curves have been scaled as indicated.

cle system. It follows that a peak in $\Delta\rho$ would be expected to occur at or close to the resonance energy. This explanation is confirmed at low fields but, as shown in Fig. 3, the energy of the peak becomes steadily more negative as the field is increased, in contrast to the behavior of the resonance position. Figure 4 shows some typical $\Delta\rho$ profiles; as the applied field is increased the negative shift of the peak is accompanied by a broadening and a decrease in peak height. In addition, the profiles can be seen to have the characteristic Fano[8] shape, which corresponds to interference between the "resonant" and "background" contributions to $\Delta\rho$.

Further study of the energy dependence of the phase shift reveals an additional interesting feature. The resonance state is characterized by a rapid phase increase of π; at higher energies the phase starts to decrease, and passes through $\pi/2$ from above, apparently tending to zero at high energies. This behavior follows from the fact that ϕ is a continuous function of E; the high-energy phase shift would be expected to tend to zero on physical grounds so at some point, ϕ, having increased at the resonance energy, must pass through a maximum and then decrease. The energy at which ϕ passes through $\pi/2$ from above is readily identifiable from plots of $\tan\phi$; this corresponds to an antiresonance state.[9] The behavior of this feature is also plotted in Fig. 3. At high fields the antiresonance is drawn down into the well and annihilates the resonance in the sense that beyond fields of 4.6×10^5 V cm^{-1} it is no longer meaningful to perform even an approximate Breit-Wigner parametrization, since the phase does not pass through $\pi/2$. A residual peak does, however, persist in the density of states and, perhaps surprisingly, the annihilation of the resonance appears to have very little effect on its general shape.

In conclusion, the results presented here demonstrate that, in shallow wells, new tunneling effects occur at high fields which completely alter the electronic structure. Both the breakdown of the bound-state variational approach and the finite-barrier height are key factors in accounting for the new phenomena; the magnitude of the threshold field and the degree of level broadening strongly reflect the form of the zero-field electronic structure in the well and in the continuum. Although in this study only the simplest possible zero-field Hamiltonian is considered, a rich variety of high-field effects is expected in more complex cases. In particular, recent electronic structure calculations of Jaros, Wong, and Gell[10] have shown that there are a number of well-localized states just above the confining barriers and at secondary minima. Since the effective barrier "seen" by some of these states is very small, such states are expected to be strongly affected by a high electric field. The application of the method described in this paper to more complex quantum-well systems is currently being investigated.

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