Stark ladders in periodically Si-δ-doped GaAs

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We study theoretically the electronic structure of periodically Si δ-doped GaAs subject to a homogeneous electric field applied along the growth direction. The space-charge potential due to δ doping is obtained by means of the Thomas-Fermi approach. Analyzing the change in the density of states in the superlattice introduced in the electric field, we observe a set of equally-spaced sharp peaks corresponding to Stark-ladder resonances. Intrinsic broadening of resonances turns out to be smaller than the level spacing in the whole range of the electric field we consider. We use the inverse participation ratio to evaluate the spatial extent of electron wave functions, and we find that the Stark-ladder spectrum is related to a strong-localization regime at high field.

I. INTRODUCTION

During recent years, much work has been devoted to investigating the occurrence of Stark ladders in the electronic energy spectrum of quantum-well superlattices placed in an electric field along the growth direction.[1–6] These ladders do not comprise infinitely sharp levels, as was proposed originally, but rather they are resonant levels whose lifetimes are finite. The spacing between the energy levels in each ladder is eFa, where F is the magnitude of the electric field, and the electron states are localized and spatially shifted relative to one another by integer multiples of the superlattice period a. Recent experiments seem to firmly establish the existence of a ladder structure in quantum-well superlattices.[7–11] Epitaxial-growth techniques are currently used to prepare δ-doped semiconductor structures, in which a sheet of impurity atoms is localized within a few monolayers of the crystal. Impurity atoms usually supply electrons and give rise to strong confinement by the space-charge potential. In periodically δ-doped structures, the overlap of electron wave functions of adjacent potential wells causes the formation of subbands, as observed experimentally by optical[12] and Shubnikov–de Haas[13] measurements in Si-δ-doped GaAs. As far as we know, however, field effects on the subband structure and the possible occurrence of Stark ladders in periodically δ-doped structures have not been reported in the literature.

In the present work we investigate theoretically the electron dynamics and the density of states (DOS) in periodically Si-δ-doped GaAs subject to an external, static electric field parallel to the growth axis. We shall show that Stark-ladder resonances are clearly revealed in the DOS, hence suggesting that this structure should also be observable experimentally in periodically δ-doped GaAs, as was the case in quantum-well superlattices. Some practical considerations, mainly related to loss of quantum coherence by disorder, are raised at the end of the paper.

II. THE MODEL

The system we study in this work is a superlattice made of Si-δ-doped GaAs, with the following parameters, which we take from the samples grown by Egues *et al.*[13] by molecular beam epitaxy: the superlattice unit cell is a 500–Å slab of GaAs with a Si-δ-doped layer embedded in its center. We assume that there exists a uniform p-type background doping with $N_A = 1 \times 10^{15}\,\mathrm{cm}^{-3}$ acceptors per unit volume, and that the doping layer consists of a continuous positive slab of thickness $d = 50$ Å with $N_D = 3 \times 10^{12}\,\mathrm{cm}^{-2}$ ionized donors per unit area. The whole superlattice consists of ten unit cells sandwiched between two 1 000-Å buffer layers of GaAs. The doping periods $a = 500$ Å is intermediate between two limiting cases discussed by Degani.[14] This author found by self-consistent calculations that for large periods ($a \sim 1\,000$Å) the system behaves as a single doping layer, whereas for short periods ($a \sim 200$ Å) a superlattice is formed due to strong coupling between adjacent wells. Therefore, our study acquires additional importance to assess the effect of moderate coupling on the electronic structure.

The first step in the calculation is to compute the potential energy $V(x)$ in the unit cell. This we accomplish by means of the Thomas-Fermi (TF) semiclassical model. The TF formulation is equivalent to a self-consistent formulation in a wide range of doping concentrations,[15] and it has been previously applied to periodic structures in the absence of field by Egues *et al.*[13] The nonlinear TF differential equation reads

$$\frac{d^2V(x)}{dx^2} = -\frac{8}{3\pi}\left[\epsilon_F - V(x)\right]^{3/2} + \frac{8\pi}{d}N_D\theta\left(x+\frac{d}{2}\right)\theta\left(x-\frac{d}{2}\right) - 8\pi N_A\theta\left(x+\frac{a}{2}\right)\theta\left(x-\frac{a}{2}\right), \tag{1}$$

where ϵ_F denotes the Fermi energy. Distances and energies are measured in units of the effective Bohr radius a* (= 100 Å) and effective Rydberg, Ry* (= 5.8 meV), respectively. The boundary conditions for this equation are those of the superlattice, given by

$$\left(\frac{dV(x)}{dx}\right)_0 = \left(\frac{dV(x)}{dx}\right)_{a/2} = 0. \tag{2}$$

We assume the validity of the effective-mass approximation. Thus, once the potential $V(x)$ is found from (1), the electron dynamics along x inside the unit cell, in the presence of a homogeneous applied electric field F perpendicular to the doping layers, is obtained from the following one-dimensional Schrödinger equation

$$-\frac{d^2\psi(x)}{dx^2}+[eFx+V(x)]\,\psi(x)=E\psi(x). \tag{3}$$

The origin of the spatial coordinate is set at the left edge of the system, and energies are measured from the potential value at that edge. In what follows, we restrict ourselves to electron energies in the range $0 < E < eFL$.

In the case of zero-field structures, the Bloch theorem holds and formation of subbands occurs. The dispersion relation inside allowed subbands and energy gaps may be found using the numerical method previously given by Méndez *et al.*[16] However, an applied electric field breaks the translational symmetry of the potential and the computation of the electronic structure requires a different approach. Consider an electron of energy E impinging from the left on the structure. Since we shall only deal with electron energies $E < eFL$, the electron will be reflected with probability unity. Therefore, the reflection amplitude r can be expressed as follows

$$r=e^{2i\Phi(E)}, \tag{4}$$

where the phase shift $\Phi(E)$ is real. Levinson's theorem relates this phase shift and the change[17] in the density of states $\Delta\rho(E)$ due to the finite potential through the equation[18]

$$\Delta\rho(E)=\frac{1}{2\pi}\frac{d\Phi(E)}{dE}. \tag{5}$$

The reflection amplitude is calculated by solving the Schrödinger equation (3), assuming that the wave function for $x < 0$ is a superposition of incoming and outgoing plane waves of the form $\psi(x) = \exp(i\sqrt{E}\,x) + r\exp(-i\sqrt{E}\,x)$, while for $x > L$ it decays exponentially as $\psi(x) = C\exp(-\sqrt{eFL-E}\,x)$.

III. RESULTS AND DISCUSSION

The TF potential $V(x)$ in the unit cell is plotted in Fig. 1(a), choosing the origin of x at the middle of the cell for clarity; this potential is symmetric around the center of the cell.[19] Figure 1(b) shows the dispersion relation $E(\kappa)$ inside allowed subbands along the growth direction in periodically δ-doped GaAs, in the absence of external fields. Here κ denotes the crystal momentum along that direction. There exist three subbands below the top of the potential for the impurity concentration we consider. The two lowest subbands are only slightly broadened and become almost nondispersive. This indicates that adjacent wells are only weakly coupled when the doping period is $a = 500$ Å. On the other hand, the third subband is clearly dispersive, as would be expected from the V-shape form of the potential (the higher the energy, the smaller the distance between adjacent wells). Also note that gaps above the Fermi energy are very narrow.

The applied external electric field modifies the energy spectrum of the system. The change in the DOS as a function of the electron energy exhibits a set of pronounced peaks separated equidistantly, as shown in Fig. 2 for two values of the applied electric field (the DOS is expressed in arbitrary units because we are mainly interested in the position and width of these peaks). In the method of phase-shift analysis, Stark resonances are characterized by a rapid increase of π in the phase $\Phi(E)$; consequently, the change in the DOS presents sharp peaks. The number of pronounced peaks equals the number of layers in the superlattice examined, which indicates the occurrence of a well-defined Stark-ladder structure in the energy spectrum. There exists more than one Stark ladder, each one evolving from a different zero-field subband. Therefore, ladders may be labeled by the band index n ($n = 1$ denotes the lowest subband, and so on). For instance, the pronounced peaks of Fig. 2(a) correspond to $n = 3$ whereas those shown in Fig. 2(b) correspond to $n = 2$. It is also worth mentioning the occurrence of subsidiary peaks when the electric field is increased; this point will be discussed later.

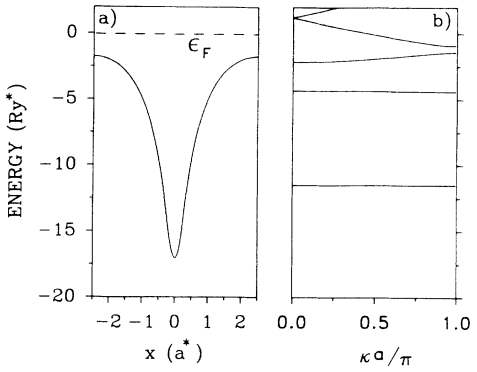

FIG. 1. (a) TF potential due to a single δ-doped layer obtained by solving the corresponding TF equation. (b) Subband structure, on the same energy scale, of periodically δ-doped GaAs along the growth direction, where κ is the crystal momentum in that direction.

The spacing between consecutive Stark levels is almost the same for a fixed value of the electric field. We realize that the average level spacing is of the form $\Delta = eFa$ in a wide range of electric fields. As pointed out by Ritze *et al.*[3] in the case of $Ga_{1-x}Al_xAs$-based quantum-well superlattices, the position of the peaks arises from the interplay between two interactions, namely, the coupling

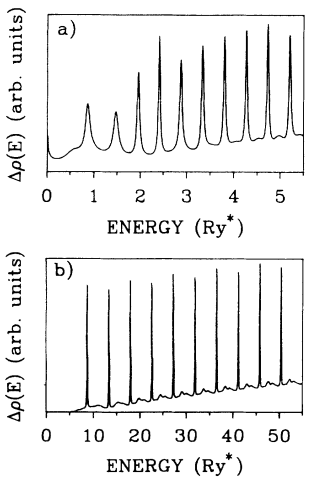

FIG. 2. Change in the DOS versus electron energy for two different values of the applied electric field: (a) $F = 0.5$ kV/cm and (b) $F = 5.0$ kV/cm.

between different wells and the coupling with the applied electric field. This causes a sublinear dependence of the Stark level spacing Δ as a function of the applied electric field in the low-field range, as they observed in thinner barriers. In the periodically δ-doped GaAs we are dealing with, the coupling between adjacent wells is relatively weak, as we mentioned earlier, and the interaction with the electric field dominates. Therefore, the Stark level spacing Δ is linear in the whole range of electric fields, even at low fields. We would like to stress that our system is finite and thus it lacks perfect periodicity. Finite-size effects should be appreciable at low fields, when the interaction between wells becomes important. This effect is apparent in Fig. 2(a), where one observes that (i) the two lower-lying Stark levels are broader and lower, (ii) the spacing between them is somewhat larger than the predicted value eFa, and (iii) subsidiary peaks only appear between higher-lying levels. The absence of a perfect periodic pattern in the DOS indicates that Stark-ladder states are rather localized; only states localized at the outermost wells (giving rise to lower- and higher-lying resonances) experience the missing spatial periodicity. We will give later further evidence of localization.

With increasing field, the peaks corresponding to the same Stark ladder shift and become broader and lower. In general, the shapes of Stark-ladder resonances are fitted by Lorentzian curves. In our computations, all the widths turn out to be much smaller than the spacing Δ in the whole range of electric fields. The position of the peaks, E_{nk} (n is the ladder index and $k = 0, 1, \ldots, 9$ runs over the peaks), depends linearly on the applied electric field, except for lower resonances at very low fields. The energy of Stark levels for a not very low field is approximately given by

$$E_{nk} = (k + 5/2)eFa + E_n^0, \tag{6}$$

where E_n^0 is roughly the energy of the n subband. The factor $5/2$ comes from the fact that the first δ-doped layer is placed at $x = (5/2)a$. We actually found that extrapolation to $F \to 0$ of each resonance belonging to the same ladder yields slightly different values of E_n^0. This is to be expected because the width of the zero-field subband, from which the corresponding Stark ladder evolves, is actually nonzero. For those ladders shown in Fig. 2, the mean values are $E_3^0 = -0.06\,\mathrm{Ry}^*$ and $E_2^0 = -1.9\,\mathrm{Ry}^*$, in good agreement with the center of the third and the second subbands, respectively, measured from the top of the TF potential[19] (see Fig. 1). Zhao[20] has recently studied a two-band, tight-binding Hamiltonian and demonstrated that field-independent terms also involve interband coupling. In our system this contribution seems to be negligible, so we are led to the conclusion that coupling between different bands may be neglected as a first approximation.

At zero field electronic states are delocalized and form bands. This picture holds even when a very low electric field is applied. However, as the field increases the states of each well are shifted and quantum coherence is then reduced. Because of the decreasing coherence, localization of the electron wave function occurs, with quantum states confined in individual wells. This result is clearly seen in Fig. 3(a), showing a localized electron wave function confined in the sixth well due to an applied electric field ($F = 5\,\mathrm{kV/cm}$). The electron energy is $31.887\,\mathrm{Ry}^*$, corresponding to the sixth pronounced peak in Fig. 2(c), that is, this state belongs to the second Stark ladder. A detailed view of the change in the DOS in this energy range appears in Fig. 4(a). Notice that the energy level is below barrier (i.e., below the local maximum of the potential after applying the electric field) so that, in fact, it is a tunneling state. High spatial localization means high lifetime and, consequently, the level width is small, as observed in Fig. 4(a). On the other hand, the subsidiary peaks are broader, thus corresponding to more extended states. These broad peaks are due to above-barrier states, as shown in Fig. 3(b). The energy of this less localized state is $33.750\,\mathrm{Ry}^*$, and it coincides with the position of the broad resonance inmediately above the pronounced peak in Fig. 4(a). Similar conclusions have previously been reached by Ritze *et al.*[3] in regard to below- and above-barrier states in quantum-well superlattices.

The degree of localization may be evaluated by means of the inverse participation ratio (IPR), as introduced by Bell and Dean.[21] The IPR measures the volume occupied by the electron wave function: the smaller the IPR, the more extended the electron state. The IPR has been successfully used to study localization of Stark-ladder states in tight-binding Hamiltonians by Leo and MacKinnon[1] and in GaAs-AlAs superlattices by Degani.[4] We have evaluated the IPR as a function of the electron energy, for fixed field, in periodically δ-doped GaAs, as shown in Fig. 4(b) for $F = 5\,\mathrm{kV/cm}$. A comparison between Figs. 4(a) and (b) demonstrates that a pronounced peak in the change of the DOS, corresponding to Stark-ladder

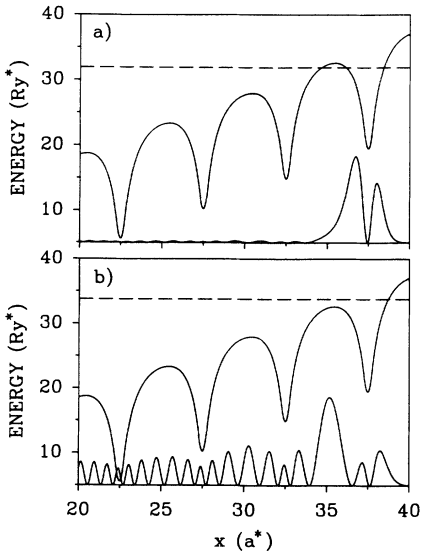

FIG. 3. Squared electron wave functions for an applied electric field $F = 5\,\mathrm{kV/cm}$: (a) a state belonging the second Stark ladder localized in the sixth well with energy $31.887\,\mathrm{Ry}^*$ and (b) above-barrier state with energy $33.750\,\mathrm{Ry}^*$. The potential profile of the structure subject to the electric field is also shown, and the dashed line indicates the energy of the state.

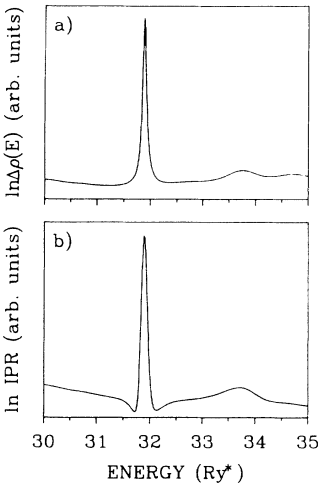

FIG. 4. (a) Change in the DOS and (b) IPR as a function of the electron energy for an applied electric field $F = 5\,\mathrm{kV/cm}$.

states, yields a sharp peak in the IPR, implying that those states are strongly localized. However, a subsidiary peak, corresponding to above-barrier states, yields a minor increase in the IPR, reflecting the fact that those states are rather delocalized. Therefore, we may state that the IPR confirms the results we discussed above.

IV. CONCLUDING REMARKS

We have numerically investigated the change in the DOS introduced by periodically Si-δ-doped GaAs in an electric field applied perpendicular to the layers. The space-charge potential due to the layer of impurity atoms has been calculated by means of the semiclassical Thomas-Fermi model, which yields very good results in a wide range of donor concentrations. The change in the DOS exhibits a set of equidistant pronounced peaks, demonstrating the occurrence of well-defined Stark ladders in the energy spectrum. The corresponding electron wave functions are localized in a single potential well, indicating loss in the quantum coherence due to the misfit of quasilocal levels. Electronic states are pushed upward and become broader as the electric field is increased, hence giving rise to the so-called above-barrier states. The IPR clearly shows that these states are less localized than Stark-ladder states.

As a major point, we have found that the average Stark level spacing is always larger than the level width. The physical relevance of this result is evident since one requires well-separated levels for experimental observation. However, the level width refers to the *intrinsic* broadening predicted by scattering theory; there are many scattering mechanisms not included in our model (electron-phonon interactions, scattering by disorder), which could result in broadening. The experience gained in connection with quantum-well superlattices suggests that the temperature should be kept low to reduce electron-phonon interaction, making easier the observation of Stark ladders. In the case of periodical δ doping, broadening due to scattering by disorder might be more dramatic than in quantum-well superlattices. The random distribution of donors in the δ-doped layers as well as fluctuations in their thickness may lead to a strong reduction of phase coherence. Therefore, experimental work is necessary to elucidate whether the molecular-beam-epitaxy techniques now available can fabricate samples with the required large coherence length. We hope that our results will encourage experimental effort in that direction.

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