I-V characteristics of 1D-0D-1D double-barrier structures and persistence of fine structure at high temperatures

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A theoretical investigation of coupled quantum-wire–quantum-dot–quantum-wire resonant-tunneling diodes is presented, with particular emphasis on the basic mechanisms producing the fine structure in the current-voltage characteristics. The possibility of having two different types of fine structure is remarked upon, and an explanation is proposed for the relative lack of thermal smearing observed in certain devices that could be important for the use of low-dimensional devices at high temperatures. The I-V curves are calculated numerically for two typical structures and very good agreement with experiments is obtained.

I. INTRODUCTION

Three-dimensionally confined structures, namely, quantum dots, have been fabricated in recent years by means of both etching techniques[1,2] and the use of split gates,[3,4] opening the way for the possibility of studying systems containing very few electrons (typically 1–5 in etched structures and 1–50 in gated devices). The marked feature of quantum dots is the character of their spectra which, for isolated dots, takes the form of sets of individual levels. Various experimental techniques have been used to investigate the properties of such structures, among which transport measurements have proven very successful in highlighting the zero-dimensional (0D) nature of quantum dots. In this paper we shall focus our attention on etched structures, though we believe that most of the arguments will also apply to gated devices.

A typical structure for studying transport properties of quantum dots consists of a GaAs-$Al_xGa_{1-x}As$ double-barrier structure that is etched vertically to nanometer dimensions, yielding a quantum dot "sandwiched" between two quantum wires (1D-0D-1D resonant diode), one acting as an emitter and the other one as a collector.

The discrete nature of the quantum-dot spectrum is revealed in transport measurements by the appearance of a steplike fine structure in the I-V curve superimposed on the broader peak typical of the current-voltage characteristics of quantum wells,[1,2,5] which sparked hopes of using quantum dots for new devices based on a resonant tunneling logic. The sharpness of these steps is fundamental for such devices to exhibit multistable logic behavior; their thermal robustness also becomes a very important feature if such devices are to operate at high temperature.

Evidence of tunneling through 0D states was observed by Reed *et al.*[1] in their measurements of the I-V curves of 1D-0D-1D cylindrical resonant diodes. At low temperature (1 K) a series of upward steps in the current was clearly detected. As the temperature was raised, the sharpness of the fine structure progressively deteriorated until it was completely lost by about 35 K [see Fig. 4(b)]. In more recent experiments by Ramdane, Faini, and Launois,[2] Faini *et al.*,[6] and Faini,[7] in the same type of structures used by Reed *et al.*,[1] both upward and downward steps of 0D origin were observed at low T, and the latter persisted almost unchanged up to 77 K [see Fig. 3(d)], and beyond.

Several papers[5,8–10] have pointed out the competition between two mechanisms in a quantum dot, namely, size quantization and charging effects, each producing a discrete spectrum and manifesting in the same fashion experimentally. While the appearance of upward steps is well understood theoretically[5,9,11,12] in terms of the single-particle aspect of 1D-0D-1D resonant tunneling,[7,9,11] downward steps have received little attention and their thermal properties, to the best of our knowledge, have never been addressed. Studies of the electrostatic effects in a quantum dot are also available in the literature,[9,10,13] however, quantitative calculations of I-V curves of 1D-0D-1D structures including the electrostatic interaction inside a dot have, as far as we know, never been performed.

To fill this gap we have modeled the electrostatic interaction inside a quantum dot by means of a Hubbard-like Hamiltonian, which has been inserted into a transfer-matrix framework that enables us to calculate the I-V curve of a quantum-wire–quantum-dot–quantum-wire structure. The effects of a finite temperature are also included, enabling us to give an explanation of the observed thermal robustness of downward steps[7] and to suggest designing criteria to obtain devices showing 0D features at room temperature.

II. QUALITATIVE ASPECTS AND METHOD

The system under consideration is a cylindrical structure formed of two quantum wires and a quantum dot. The wire exhibits a spectrum of 1D subbands filled up to the Fermi energy, while the dot has a fully discrete spectrum, see Fig. 1. The study of the quantum-dot spectrum is simplified by the fact that, in all experimental situations, its dimension along the growth direction, i.e., the separation between the barriers (Fig. 1), is about ten times smaller than the lateral size of the cylindrical pillar.

Longitudinal quantization produces such a large energy difference that all but the energy levels resulting from the lowest longitudinal quantization are irrelevant in this work. We will return to this point later in the paper.

The lateral confining potential in the wires and dot is essentially the same, and results from the pinning of the Fermi level at the surface at about midgap.[1,2,11,12] While the quantum-wire regions are doped to ensure the presence of electrons in the conduction band, the region around the quantum dot is kept undoped to avoid contamination of the $Al_xGa_{1-x}As$ barriers. As previously reported,[11,12] the nonuniformity in the doping concentration gives rise to large upward band bending around the quantum dot. Due to the band bending around the dot, at zero applied voltage the quantum-dot states are well above the Fermi energy in the emitter and so no electrons can tunnel.

The application of an external voltage moves the states in the quantum dot towards the Fermi energy in the emitter. The potential barrier to the well gives rise to a large threshold voltage[1,11,16] before the lowest dot level is aligned with the Fermi energy and electrons from the emitter wire can tunnel. As the voltage is further increased the higher quantum-dot states will follow suit.

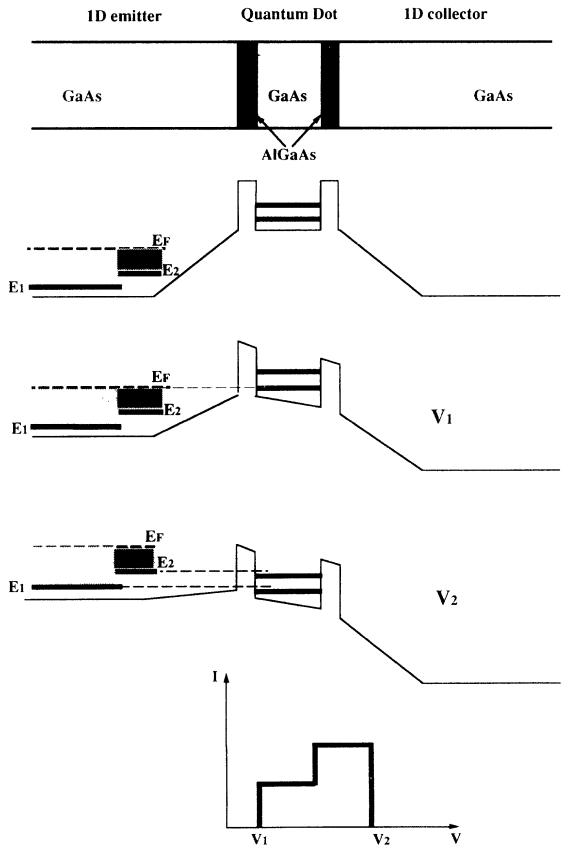

FIG. 1. Top: schematic view of the 1D-0D-1D resonant diodes. Bottom: opening and closing of channels when dot levels and emitter subbands are equally spaced; the dot states are shown at threshold voltage and in proximity to the subbands' bottoms. The expected I-V curve is shown: as all the channels close for the same voltage, the negative-differential resistance region does not show steplike structure.

As in the case of large-area quantum wells, the effects of surface roughness and changes in the confining potential along the structure have little consequence on the tunneling process because the variations that they produce are smooth on the length scale of a typical electronic wavelength. One can, therefore, assume that the tunneling process takes place in a "lateral state" conserving regime, i.e., the electrons from the lowest emitter subband tunnel only through the lowest dot state, those from the second subband tunnel via the second dot state, and so on, as a detailed calculation by Bryant[12] confirms. In other words, the transverse nature of the subband wave function ensures that there is little cross coupling between wire and dot states arising from different subbands. Thus, we can consider the contribution from tunneling via each subband independently. There will be, therefore, step increases in the current as each tunneling channel associated with a subband opens. This is shown schematically in Fig. 1.

For higher voltages, the lowest quantum-dot level will eventually reach the bottom of the lowest subband in the emitter and resonant tunneling from the lowest subband will no longer be possible. There will then be a step decrease in the current as that channel closes. There will be similar step decreases in the current for each subband at the voltage corresponding to the alignment of the dot level with the appropriate subband. We would expect, therefore, the I-V characteristic to consist of the superposition of these upward and downward steps.

The lateral confining potential in the emitter and dot is essentially the same; a single-particle picture would, therefore, predict similar energy separations both in the quantum wires and dot. The channel opening occurs at voltages determined by the alignment of the dot levels with the Fermi level. The channel closure, however, occurs through alignment of the subband minima and the dot levels. If the dot-energy level separation is essentially the same as in the wires, *all* the channels will close simultaneously giving rise to a large but structureless drop in the current (as shown in Fig. 1). Only if the dot-energy levels are different from those in the wire will a downward staircase be seen (Fig. 2). In practical terms, one can assume the energy spacing in the two regions to be different if such a difference is not swamped by the width of the resonant levels inside the dot. There is, in fact, experimental evidence for both types of fine structures[1,6] [Figs. 3(d) and 4(b)].

It is important to note that the above analysis suggests quite different thermal behavior for the opening and closing of the channels. The opening of a channel is related to the states in the emitter that are at the Fermi level. As the temperature is raised, the I-V structure resulting from channel opening will acquire a finite width, reflecting the thermal occupation of the states around the Fermi level in the emitter. The step increase in the current will be washed out when the thermal smearing ($\approx kT$) is of the same order as the dot-energy splittings, i.e., when

$$kT \approx E_{n+1} - E_n \ . \tag{1}$$

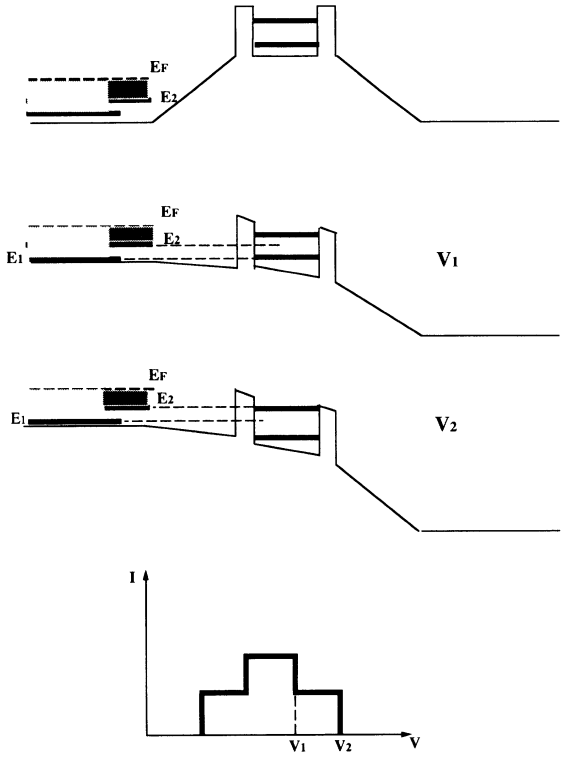

FIG. 2. The energy separation of the dot states is bigger than the subbands splitting in the emitter, and this results in the downward steps in the negative-differential resistance region of the I-V curve. Note that in the vicinity of channel closing the electrons that tunnel resonantly are far away from the Fermi energy.

On the other hand, the closure of a channel is related to those states lying at the bottom of a subband. These are several meV below the Fermi energy (see Fig. 2), so that they will only be affected by thermal smearing at much higher temperatures, i.e., when

$$kT \approx E_f - E_n \ . \tag{2}$$

In a typical device structure[1,2,6,11] we would expect that $E_n - E_{n+1} \approx 5$ meV while $E_f - E_n \approx 20$ meV. This would give typical maximum temperatures for the observation of channel opening (upward staircase in the I-V curve) as 30 and 200 K for the channel closings (downward staircase on the I-V).

This has very important consequences for the design of high-temperature operation of quantum-dot devices. It is now seen that it is essential to optimize the *differences* between the energy levels in the dot and the wires. This is a very different requirement from optimizing the energy separation within the dot. The structural parameters are not directly relevant to the former since, in the etched structure, it is the lateral potential which governs the separation and this is the same for wire and dot. However, the confinement within the dot can give rise to a large Coulombic term, which as we shall show, can produce the required effect.

As already pointed out in several works,[1,2,8,12,14] the confining potential in etched structures is smooth and can be assumed to be parabolic without lack of accuracy. With this assumption, one finds for the single-particle energy spacing,

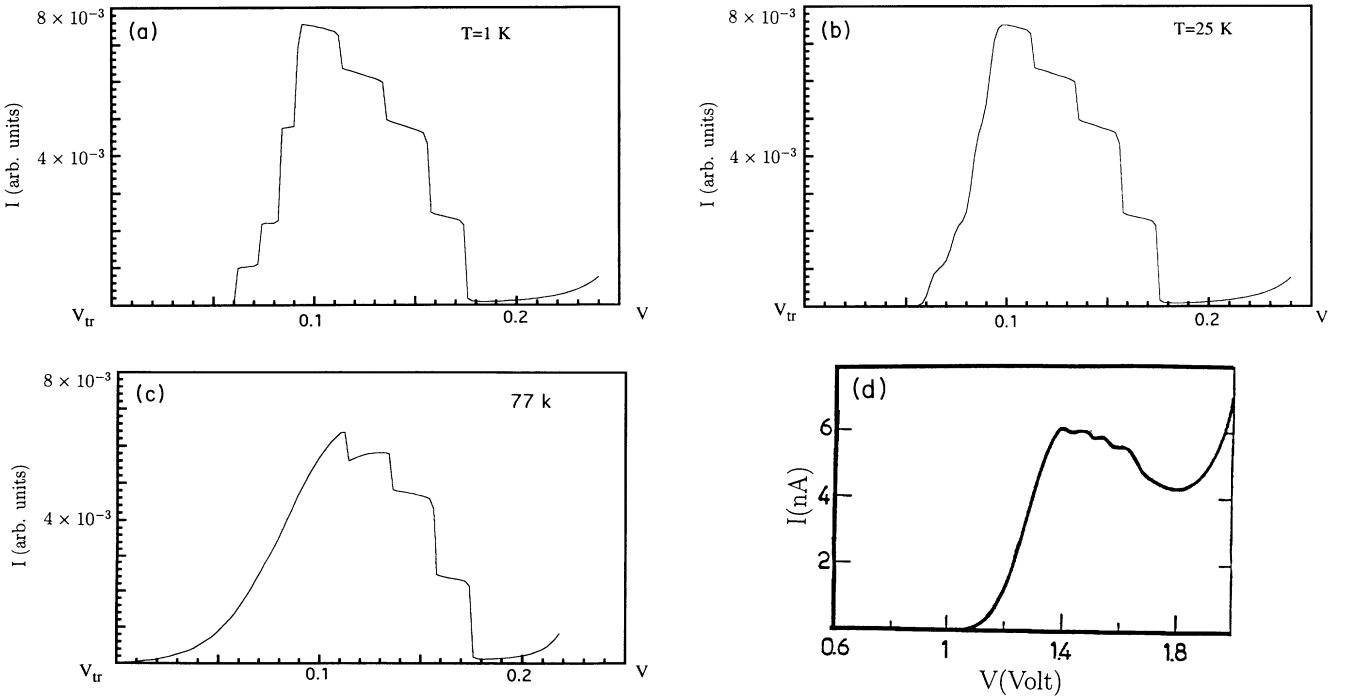

FIG. 3. Calculated I-V curve at 1 K for the double-barrier structure of Faini *et al.*; (b) the temperature is raised to 25 K: the upward steps are almost lost while the downward ones show no change; (c) I-V curve at 77 K showing very good agreement with (d) the experimental curve at 77 K. All calculated curves are shown from threshold voltage.

$$\Delta E = \frac{\hbar\sqrt{2\Delta V}}{R\sqrt{m}} , \tag{3}$$

i.e., the energy that characterizes the parabolic confinement scales with the inverse of the radius R of the cylindrical diode; here m is the electron effective mass and ΔV is the lateral confining potential ($\approx E_{\text{gap}}/2$).

To estimate the electrostatic interaction inside the dot, we can take as a first approximation the extension r of the electron wave functions by recalling that, for a parabolic potential,

$$\tfrac{1}{2}m\omega^2\langle r\rangle^2 = \tfrac{1}{2}E_n , \tag{4}$$

where E_n is the energy of the nth harmonic oscillator state. Taking $\langle r\rangle$ from Eq. (4) as the average separation between two electrons in the dot, one finds for the Coulomb interaction,[15]

$$U \approx \frac{e^2(2m\Delta V)^{1/4}}{4\pi\varepsilon\sqrt{\hbar R}} , \tag{5}$$

where the symbols in Eqs. (4) and (5) have their usual meaning. The average separation of two electrons in the dot so calculated assumes that the wave functions have negligible spread in the longitudinal direction, since the size along the growth direction is about ten times smaller than $\langle r\rangle$.

For GaAs the two energies are approximately equal (at 5 meV) for $R \cong 90$ nm. Thus, for devices where the radius is significantly less than 90 nm, we would expect size quantization to dominate. These devices would be characterized by upward steps with poor high-temperature resolution. In contrast, devices with R larger than or of the order of 90 nm, there would be a significant contribution to the level spacing from Coulombic effects within the dot. This should enable the more thermally robust downward staircase to be obtained.

A convenient way of accounting for the electrostatic repulsion is to use a Hubbard-type interaction. This results in an enhancement of the energy spacing between the Nth and $(N+1)$th level, in a Hartree-Fock sense, from $(E_{n+1}-E_n)$ as given by an independent-particle picture to $(E_{n+1}-E_n)+NU$, where U is the average electrostatic interaction of two electrons inside the quantum dot. Such an approximation should give a fairly faithful account of the principal effects of electrostatic interaction in a confined region, as it has proven to do, for example, in explaining the enhanced period of Aharonov-Bohm oscillations of the conductance of quantum dots.[10]

Assuming a parabolic confining potential, the Hubbard Hamiltonian for a quantum dot becomes

$$H = \frac{1}{2m}\sum_i (p_{xi}^2 + p_{yi}^2) + \tfrac{1}{2}m\omega^2 \sum_i (x_i^2 + y_i^2) + \tfrac{1}{2}N(N-1)U , \tag{6}$$

where m is the effective mass, ω characterizes the strength of the parabolic confinement, N is the total number of electrons in the dot, and U is the average electrostatic interaction.

This Hamiltonian can also be viewed as resulting from an approximation to the Coulombic interaction within the dot. It has already been pointed out that due to the confinement the Coulomb interaction can be approximated by simpler analytically tractable forms, which can give exactly solvable model Hamiltonians.[8] The present Hamiltonian arises when the in-plane Coulomb interaction is approximated by a constant rather than by a parabolic term. As in the case of the Johnson-Payne model,[8] one should primarily consider U in Eq. (6) as a fitting pa-

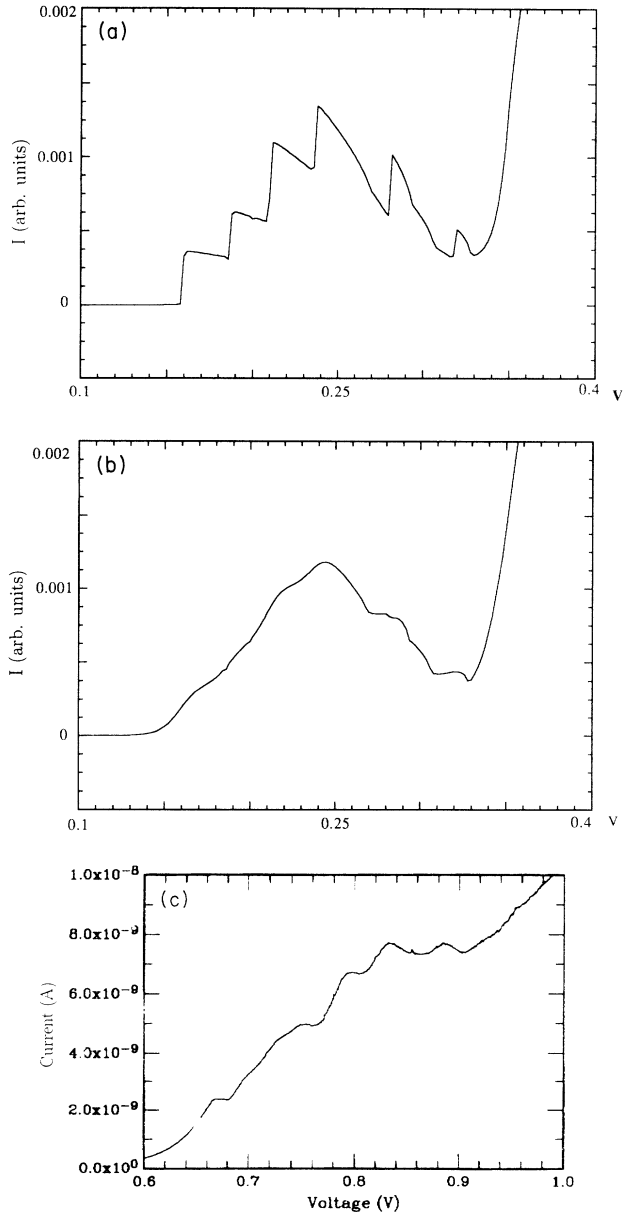

FIG. 4. (a) Calculated and (c) experimental I-V characteristics of the devices by Reed *et al.* at 1 K: see how the total number of fine structures is again correctly reproduced by our calculations. These fine structures are mainly produced by channel opening so that they disappear rather quickly as the temperature is raised as shown in (b) ($T=30$ K). Note, however, how the two downward steps survive at high temperature in (b).

rameter to best account for the effects of confinement, surface charges, finite size along the growth direction, etc., that nontrivially modify the Coulombic interaction inside the quantum dot. It can be seen from Fig. 1 in Ref. 8 that a constant is at least as good an approximation as a parabolic potential for typical dot dimensions.

The approach we follow to calculate the I-V curve consists of embedding Hamiltonian (6) in an effective-mass, transfer-matrix framework. That is, the system consists of a double-barrier-defined quantum dot within a quantum wire. The states in the wire and dot are calculated for the transverse and longitudinal potential along the wire-dot-wire system for a given applied potential[11] using the transfer-matrix method. Such a calculation also provides us with the wave function of each occupied electron state inside the dot. The expression for N is obtained by integrating over the occupied electron wave functions inside the dot:

$$N=\sum_n \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{En}^{+\infty} dE\, f(E) \times \int_{-a/2}^{+a/2} dz |\psi_{E,n}(x,y,z)|^2 , \tag{7}$$

where the E_n are the energies of the subbands in the emitter, $f(E)$ is the Fermi-Dirac distribution function, and a is the width of the quantum dot in the growth direction. The sum over the subbands also accounts for the degeneracy of each subband. Equation (7) shows that N is both a function of temperature through the Fermi-Dirac factor and the external bias through voltage-induced changes in the wave functions and occupancy of the dot. Each time N is calculated one finds a new position of the energy levels in the quantum dots, so that the whole procedure is iterated to self-consistency. Once self-consistency is achieved, the transmission coefficients for electron tunneling through the dot are calculated and summed to give the current. Repeating the procedure for all values of the applied voltage we obtain the I-V curve. A more detailed account of our method will be presented in future work.

III. RESULTS

The calculations presented here have been designed to model two experimental structures. In the device described by Reed *et al.*[1] R was 50 nm. From the discussion above, we would expect that size quantization would dominate over electrostatic effects. In the Faini *et al.*[7] diodes the radius was 100 nm, so that the electrostatic effect would be slightly more pronounced than size quantization. Furthermore, Faini *et al.*[6] used 85-Å barriers whereas Reed *et al.*[1] employed 40-Å barriers, so that in the former case the electron confinement and hence the electrostatic repulsion inside the dot could be expected to be more effective. Su, Goldman, and Cunningham[15] obtained the same conclusion by means of a time-dependent analysis of resonant tunneling in double-barrier structures.

Our calculations are shown in Fig. 3 for the structure of Faini *et al.*[6] In these calculations the value of U given by Eq. (5) was 5 meV and the size confinement was also about 5 meV. One can see [Fig. 3(a)] that, as expected, at low temperature both upward and downward steps are present. As the temperature is raised, however, the upward steps are rapidly lost and have virtually disappeared by 25 K [Fig. 3(b)], while the downward steps survive with little changes to 77 K. The experimental results at 77 K are shown in Fig. 3(d) for comparison. The downward staircase is clearly seen while the upward staircase has disappeared altogether. Comparison of Figs. 3(c) and 3(d) shows that our calculations correctly reproduce the number of fine structures observed experimentally. The difference in the voltage scale of the structure between theory and experiment reflects primarily the difficulty in modeling the voltage drop in the collector and has nothing to do with the physics of the dot. In addition there is a smooth background current present in the experimental device.[12]

The calculations have been repeated for the device structure measured by Reed *et al.*[1] Here size quantization is about 11 meV while the electrostatic repulsion from formula (5) yields a value of about 7 meV, but due to the thin barriers used, the electrostatic repulsion inside the dot is expected to be considerably reduced (Su, Goldman, and Cunningham[15]). For this reason we have chosen a value of U of 3 meV for the structures of Reed *et al.*[1] Our calculation at 1 K is shown in Fig. 4(a). This reproduces the fine structures observed experimentally, Fig. 4(c). Confirming our expectations, the I-V curve is dominated by upward steps. In the experiment, the upward steps are seen to disappear quickly with increasing temperature (Fig. 3, Ref. 1), while the two downward steps are still visible at the highest temperature in agreement with the theoretical development shown in Figs. 4(a) and 4(b). The use of the larger value (7 meV) for U simply scales the structure on the voltage axis without changing the physical interpretation or temperature behavior.

IV. DISCUSSION AND CONCLUSIONS

It is clear from the previous section that the Hubbard transfer-matrix method gives a good account of the transport properties. The model as it stands, however, does omit some processes.

For the structures considered here, the size quantization along the growth direction can be neglected because the energy scale it produces is much larger than the lateral one. Furthermore, for narrow quantum wells, the linewidths of the higher longitudinal states are very broad because of their position near the top of the well (if they are bound at all), which makes the observation of fine features in transport due to these states unlikely.[12] This argument effectively rules out the possibility of obtaining fine structure from the longitudinal quantization, even if one could etch the lateral dimensions so that lateral and longitudinal confinement were comparable. However, in the case of wide quantum wells where quantum confinement could be similar in all directions, channel-closing fine structure could be produced by longitudinal states being moved below the emitter band bot-

tom in the way described in Sec. II. Their thermal properties would then be similar to those described in Fig. 3. However, wide quantum wells would have a fine-energy structure, so the resulting critical temperature would still be low.

We have taken no account of inelastic processes. In particular, the occurrence of the downward steps requires that the filling of the dot states be negligible once they move below the relevant subband energy. This is to be expected in the structures considered above because the states are separated by less than the optical phonon energies available,[16] so the inelastic scattering rate into the level from the higher occupied states will be low.[16] The corollary is that optical phonon energy then provides a natural upper bound to the state separation one could have and maintain the channel-closing structure.

Taken together, these two limitations would suggest that the structural values for an etched pillar would be in the region of $R \sim 80-100$ nm to give a maximum difference between dot and wire levels and, hence, optimally separated fine structure. For a doping level as in the above devices this structure would then survive to a temperature of ~ 300 K. In addition, the thickness of the barriers has to be about the size of the Bohr radius[15] (~ 100 Å in GaAs) to have efficient confinement and strong Coulomb repulsion in the dot. A further reduction in the lateral radius would produce a larger electrostatic repulsion, but size quantization would increase even more and would eventually push all the emitter subbands above the Fermi energy. In these conditions the device would be "pinched off" and no current would flow.

The maximum temperature at which downward steps are observable is determined mainly by the energy separation between the Fermi level and the 1D subbands in the emitter. Such separation can be controlled by changing the doping level in the structure so that, in principle, one could tune a device to show sharp downward steps within a large range of temperatures. For example, in the structure by Faini *et al.*,[6] the barriers and the lateral radius are suitably dimensioned to show electrostatic effects, while the doping concentration is quite low. An increase of the latter by a factor of 2 or more should be technologically feasible; no major changes to the electrostatics would be expected, while the lowest subbands would be about 25 meV below the Fermi energy. In these conditions the downward steps due to the lowest subbands should survive up to room temperature.

V. SUMMARY

In this paper we have studied the I-V characteristics of 1D-0D-1D resonant diodes. We have implemented a technique to calculate I-V curves of 1D-0D-1D resonant diodes that accounts for size confinement as well as Coulomb repulsion inside the dot. Based on the transfer-matrix technique and the Hubbard Hamiltonian, such a method can account for the effects of finite temperature. (The presence of a magnetic field can also be investigated and will be reported later.)

We have pointed out, both qualitatively and via direct calculations of the I-V curves, that in principle fine structure can be observed in the negative- as well as in the positive-differential resistance regions. The presence of a sizable electrostatic repulsion in the quantum dot is a key ingredient to observe downward steps, hence the geometrical features of the device have to be carefully chosen. The importance of downward steps lies in their robustness against thermal smearing, which makes them the prime candidate to develop devices based on 0D features.

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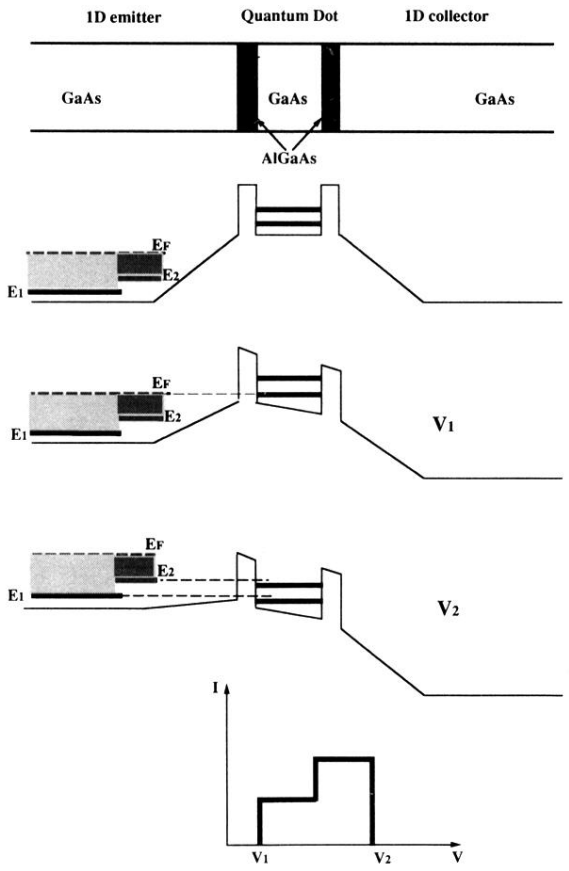

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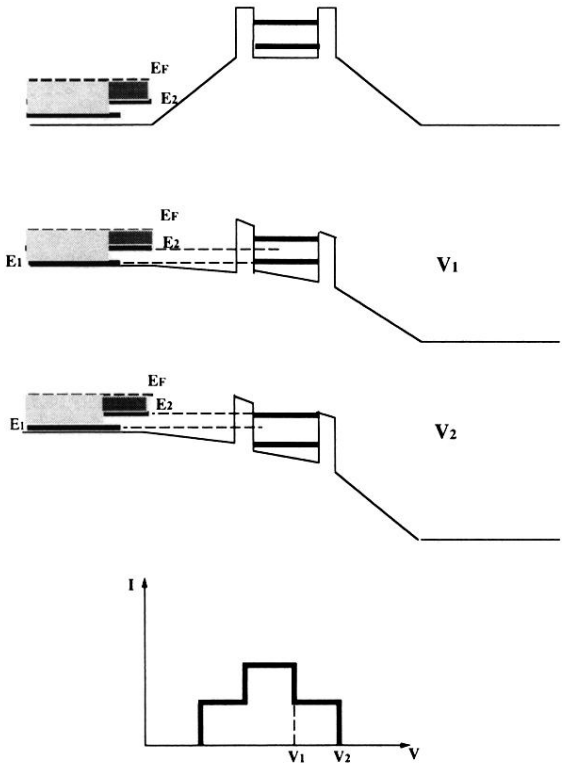

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