Mapping the electronic wave functions by determining current-voltage curves

A. Nogueira and A. Latgé*
Instituto de Física, Universidade Federal Fluminense, Avenida Litorânea sn, 24210-340 Niterói Rio de Janeiro, Brazil
(Received 25 June 1997)

Resonant tunneling in double-barrier heterostructures in the presence of impurity planes is studied within the Green-function formalism following the diagram technique for nonequilibrium processes proposed by Keldysh [Sov. Phys. JETP **20**, 1018 (1965)]. A simple one-band tight-binding Hamiltonian is adopted in the theoretical framework. The effects of an isoelectronic impurity plane, localized in the well region of a GaAs-$Ga_{1-x}Al_xAs$ double-barrier heterostructure, on the resonant curves of the current are analyzed as a function of the impurity plane position. The theoretical results show that the evolution of the resonant bias, corresponding to the resonant peaks due to transport through quantum-well quasibound states, reflects the behavior of the spatial variation of the associated electronic wave function. This indicates unambiguously that transport measurements can be performed for a mapping of wave functions in quantum-well systems. [S0163-1829(98)08103-X]

I. INTRODUCTION

Double-barrier heterostructures have been studied extensively due to the resonant tunneling phenomenon exhibited in these systems, which presents numerous applications in ultrahigh-speed electronic devices. On the other hand, intentional impurity profiles on semiconductor nanostructures can be used to monitor a great number of their physical properties. Resonant tunneling through charged impurities has been reported in many experimental works.[1–4] Dellow *et al.*[1] reported current curves exhibiting resonant peaks at voltages below the calculated resonant threshold. These features have been attributed to the presence of a favorable carrier path due to an ionized donor in the well region. Also resonant tunneling through two impurities in short lateral barriers of a GaAs metal-semiconductor transistor has been observed by Savchenko *et al.*[5] It manifests itself as a peak in the current curve rather than the steplike feature observed in the resonant tunneling through one single impurity.

Concerning neutral impurity layers, the effects of a defect layer located in the barrier regions of double-barrier quantum-well diodes, on the tunneling currents have been analyzed theoretically.[6] An enhancement of the peak current intensity and the peak to valley ratio were found for certain positions of the defect layer. From the experimental point of view, a series of samples has been prepared by Marzin and Gérard[7] each with an isoeletronic impurity plane located at the well regions of a $Ga_{0.71}As$-$GaAl_{0.29}As$ multiple-well system. They were able to measure the spatial variation of the probability densities in the first few electron states of a quantum well from an optical determination of the energies of the bound states as a function of the position of the highly localized perturbation. They doped the reference system with In and Al monolayers and the optical transition energies were determined from photoluminescence excitation spectroscopy. They were thus able to present an experimental probe of the quantum-well electronic eigenstates. A similar experimental approach was reported by Hsieh, Miller, and Chiang[8] to determine the envelope function corresponding to the surface state of Ag in the (111) direction.

In the present work we are concerned with the study of the tunneling current through a GaAs-$Ga_{1-x}Al_xAs$ double-barrier heterostructure taking into account a quite localized perturbation generated by the insertion of a monolayer (ML) planar probe, located at the well region. We have followed the nonequilibrium Green-function formalism proposed by Keldysh[9] and described the system by a single-band tight-binding Hamiltonian.[10,11] The choice of this simple Hamiltonian can be justified by the fact that the charge carriers involved in the electronic transport have energies close to the band edges. The planar probe is taken to be isoelectronic to the system and we analyze the possibility of mapping the spatial density of the electronic wave functions from resonant tunneling calculations. Since the study of electronic properties is also suitable for the present discussion, we also present some results concerning the density of electronic states in the well region of the double-barrier system.

II. THEORY

Double-barrier heterostructures can be described by a simple one-band tight-binding Hamiltonian with only nearest-neighbor interactions. The matrix elements are given by $H_{ij}^{\alpha\beta}=\langle \alpha i|H|\beta j\rangle$, where the indices α and β denote the planes and i and j the localization of the sites in the planes. Assuming that the system can be described by a simple cubic lattice and taking into account the translational symmetry of the planes in the interface direction, a Fourier transform is done, reducing the three-dimensional (3D) problem to a one-dimensional one with renormalized energies that depend on the in-plane wave vector $(k_x;k_y)$ by

$$\mathcal{E}_j^k=\mathcal{E}_j+2V_j[\cos(k_xa)+\cos(k_ya)], \tag{1}$$

with $\mathcal{E}_j$ being the site energy ($\mathcal{E}_w$ and $\mathcal{E}_b$ for the well and barrier sites, respectively) and V_j the hopping elements that assume the values V_w, V_b, and $V_{w,b}$ depending upon the atomic enviroment. The height of the barrier potential is given by $\Delta E=(\mathcal{E}_w-\mathcal{E}_b)+2(V_w-V_b)$. The electronic density of states corresponding to the 3D double-barrier system can be derived by performing a convolution between one- and two-dimensional electronic densities of states in a stan-

dard way. The effect of an applied electric field is considered in the diagonal energies of the Hamiltonian making a linear interpolation between the two barriers. This implies a neglect of the heterostructure band bending due to charge accumulation that is present in real quantum-well structures. By assuming a single plane with a different energy value in our theoretical microscopic description we are able to generate a very thin localized well or barrier potential, with intensity given by ΔE_i, in a particular position of the quantum well.

In addition to the usual advanced and retarded Green functions of the usual theories, two other correlation functions are defined in the Keldysh formalism[9]

$$G_{i,j}^{+-}(\omega)=i\int \langle c_j^{\dagger}(t)c_i(0)\rangle e^{i\omega t}dt,$$

$$G_{i,j}^{-+}(\omega)=-i\int \langle c_i(0)c_j^{\dagger}(t)\rangle e^{i\omega t}dt, \tag{2}$$

where the statistical mean values are taken on a nonequilibrium stationary state of the system, which corresponds to a situation where there is a current flowing in the heterostructure due to the external potential. By following the standard procedure usually adopted in the Keldysh scheme, the full system is decoupled in two equilibrium ones [right (R) and left (L)] and the associated Green functions are obtained. Renormalized dressed Green functions for the nonequilibrium case can be derived, via a Dyson equation, by linking the two subsystems with the perturbed Hamiltonian. The average current induced in the system is given by

$$\langle J\rangle=\frac{2eT}{\hbar}\int_{-\infty}^{\infty}d\omega[G_{0,1}^{+-}(\omega)-G_{1,0}^{-+}(\omega)], \tag{3}$$

which can be written in terms of the density of states of the two equilibrium subsystems $\rho_{R,L}(\hbar\omega)$ as

$$\langle J\rangle=\frac{4\pi eV^2}{\hbar}\int_{\mu_R}^{\mu_L}\frac{\rho_L(\hbar\omega)\rho_R(\hbar\omega)}{|\Lambda(\hbar\omega)|^2}d(\hbar\omega), \tag{4}$$

where

$$|\Lambda|^2=(1-g_{LL}^{A}g_{RR}^{A}V^2)(1-g_{LL}^{R}g_{RR}^{R}V^2), \tag{5}$$

with $g_{LL(RR)}^{A(R)}$ corresponding to the advanced (retarded) Green function of the left (right) subsystem. We have considered $\mu_R<\mu_L$, μ_L and μ_R being the chemical potentials of the injector and collector located on the left- and right-hand sides of the system, respectively. In the following we will refer to the left chemical potential uniquely as the Fermi energy.

In the present description, the well and barrier lengths N_w and N_b defining a particular double-barrier heterostructure are determined by the number of iterative steps considered in a continued-fraction scheme adopted to solve the Dyson equations. In following this microscopic model we have used the GaAs electronic effective mass $m^*=0.067m_0$, m_0 being the free electron mass, and a lattice constant $a=2.82$ Å. The electronic concentration at the injector is determined by assuming a three-dimensional free-electron gas. In the present discussion, we consider small doping of the order of $1.0\times10^{18}/\mathrm{cm}^{-3}$ considering Fermi energies equal to 50, 65, and 75 meV. The value of the impurity-plane energy was chosen so as to generate a barrier (or a well) corresponding to the same potential height of the GaAs-$Ga_{1-x}Al_xAs$ double-barrier heterostructure, i.e., $\Delta E_i=\Delta E$. The substitution of this isoelectronic defect plane defines a localized perturbation on the reference system. In that sense, it can be represented by a δ function at a particular z_i position of the quantum well; following a first-order perturbation theory, it is easy to show that the first-order z_i dependence of the energy is given by $\Delta\epsilon_{z_i}=\Delta E_i|\psi(z_i)|^2$, with $|\psi(z_i)|^2$ being the probability density envelope function of the unperturbed system.

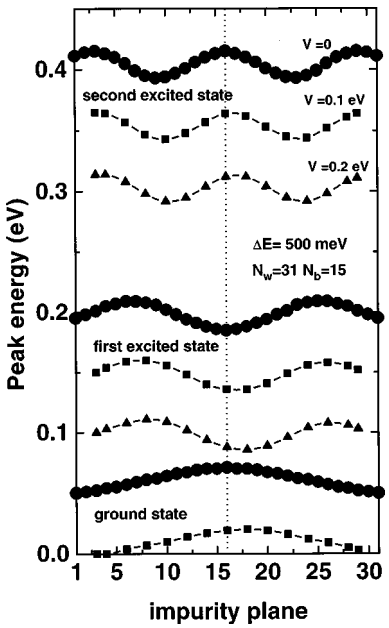

FIG. 1. Energies associated with the peaks of the electronic density of states of GaAs-$Ga_{1-x}Al_xAs$ heterostructure as functions of the impurity-layer position. The peak energies are related to the quantum-well quasibound states. Full circles are for zero bias, whereas full squares and triangles are the results for V = 0.1 and 0.2 eV, respectively.

III. RESULTS AND CONCLUSIONS

A simple and illustrative way of getting information about the main physical properties of an electron in a quantum-well system is the determination of the density of electronic states. By deriving the density of states of distinct heterostructures, each one with an impurity-plane probe located at a different position, it is possible to determine the electronic distribution inside the well region. This is illustrated in Fig. 1, where we have plotted the energies corresponding to the first peaks of the density of states of distinct ''doped'' heterostructures as functions of the impurity-plane position. These peaks are associated with the quantum-well quasibound electronic states. Results concerning the equilibrium situation (zero applied bias) are represented by full circles in the figure. They clearly exhibit the expected symmetry of the related states since the density of states of the whole junction has a mirror symmetry with respect to the center of the quantum-well region. It is worth noting, however, the lack of symmetry as a finite bias is applied, since in that case the electronic cloud is shifted towards one of the barriers as a

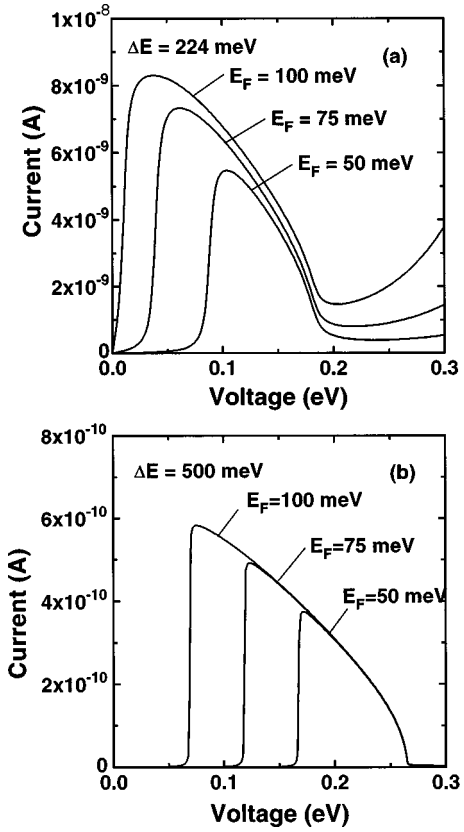

FIG. 2. Characteristic curves of current versus voltage for a GaAs-$Ga_{1-x}Al_xAs$ double-barrier heterostructure composed of $N_w = N_b = 15$ atoms (42 Å), with a barrier potential of (a) 224 meV and (b) 500 meV for different values of the Fermi level.

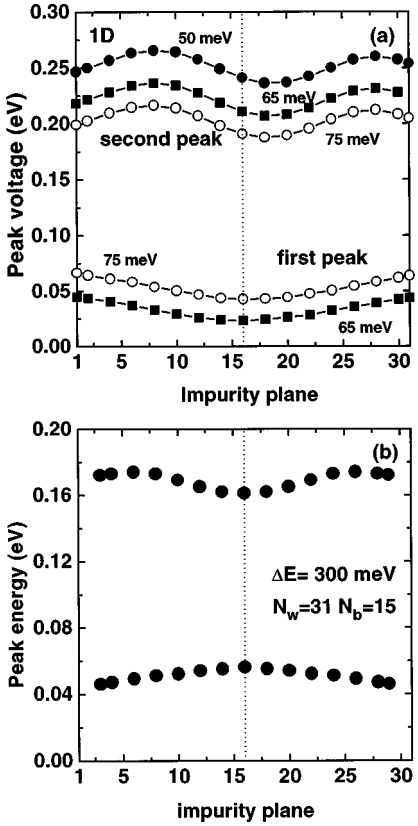

FIG. 3. (a) Peak voltage and (b) peak energy as functions of the impurity-plane position for a double-barrier GaAs-$Ga_{1-x}Al_xAs$ system with $N_w = 31$ and $N_b = 15$ atoms and for $\Delta E = \Delta E_i = 300$ meV. Results for different Fermi energy values are presented in (a). Both results are obtained via a one-dimensional description of the heterostructure.

consequence of the triangular potential shape generated by the applied electric field. The localized potential defined by the impurity plane acts as a small perturbation and can be used to provide information concerning the spatial electronic distribution in the quantum-well region.

In regard to transport properties, let us consider a simple double-barrier heterostructure. Characteristic curves of current versus voltage are presented in Fig. 2 corresponding to a one-dimensional modeled GaAs-$Ga_{1-x}Al_xAs$ heterostructure with $N_w = N_b = 15$ planes, barrier potentials of $\Delta E = 224$ and 500 meV, and for three Fermi energy values. As the emitter electronic concentration is reduced the resonant peak is shifted to higher energies and the resonant tunneling voltage range is also reduced. On the other hand, as the barrier potential increases the tunneling takes place at higher voltage values due to an increase of the electronic confinement and the current intensity is clearly reduced, as expected. In a three-dimensional description of the GaAs-$Ga_{1-x}Al_xAs$ heterostructure, different shapes for the current curves are expected due to the additional requirement of momentum conservation. In fact, the 3D resonant curves exhibit the qualitative features of characteristic experimental curves. It is worth noticing, however, that as impurity and phonons scattering effects are not taken into account in the model, the theoretical results cannot present a perfect quantitative agreement with measurements. However, the main electronic (quasibound states) and transport (resonant tunneling) properties manifest themselves in both 1D and 3D models.

As the formation of the quantum-well bound states is affected by local perturbations, we have calculated the current as a function of the applied voltage, taking into account substituted impurity monolayers in different positions of the reference double-barrier system. The results clearly show a dependence of the resonant voltage on the position of the impurity plane, indicating the possibility of monitoring the resonant voltage and the performance of a tunneling diode. A detailed study of the dependence of the resonant voltage on the position of the impurity plane is required to understand properly the role played by the defect monolayer on the resonant tunneling. Results for the resonant voltage (peak voltage) as functions of the defect-layer position are shown in Fig. 3(a) for a one-dimensional modeled GaAs-$Ga_{1-x}Al_xAs$ double-barrier heterostructure with $N_w = 31$ and $N_b = 15$ atoms, barrier potentials $\Delta E = 300$ meV, and for three values of the Fermi energy. We assume that the impurity creates a localized potential barrier also equal to 300 meV. The two resonant peaks are related to the ground (first peak) and the first excited state (second peak) of the quantum well. Notice that for $E_F = 50$ eV we have displayed only the results related to the second resonant peak. It is worth noticing that the evolution of the resonance voltages exhibits a spatial dependence behavior related to the wave function describing the electron motion inside the quantum well and moreover, as expected, it presents deviations from the symmetry behavior of the quantum-well states, which is characteristic of the effects of an applied voltage on the electron wave function of

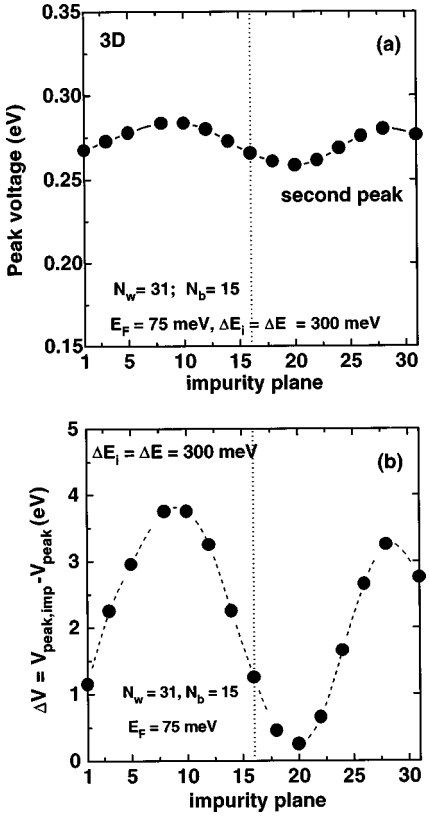

FIG. 4. (a) Evolution of the resonant voltage associated with the second quasibound state and (b) shift of the peak voltage related to the reference system, as functions of the impurity-plane position for a double-barrier GaAs-$Ga_{1-x}Al_xAs$ system with N_w and N_b equal to 31 and 15 planes, respectively. The barriers of the heterostructure and the localized defect potential are considered to be equal to 300 meV. Both results are obtained via a three-dimensional description of the heterostructure.

double-barrier systems. Figure 3(b) shows the results for the energy of the quasibound quantum-well states for the same system, obtained from the electronic density of states, which are related to the probability density of the envelope wave functions.

Figure 4(a) illustrates the same behavior of the resonant tunneling as a function of the position of the impurity layer, following a three-dimensional description for the GaAs-$Ga_{1-x}Al_xAs$ heterostructure and taking into account only the results for the second resonant peak (second excited state). A comparison between the resonant voltages obtained for the doped systems and the reference one, ΔV, is shown in Fig. 4(b) for the same case. For the case where the position of the impurity plane coincides with a node of the electronic wave function, we know from the density of states that no shifts in energy are expected for the position of the corresponding quasibound quantum-well state when compared to the situation in which there is no impurity plane. However, one must not forget that in the calculation we are dealing with, there is an applied electric field that distorts the heterostructure and reflects itself in the electron motion inside the wells. For this reason again we note a lack of symmetry in

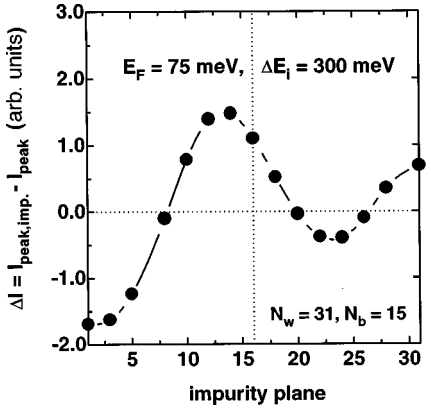

FIG. 5. Shift of the resonant current concerning the first excited state for different positions of the defect-plane potential for a double-barrier GaAs-$Ga_{1-x}Al_xAs$ system (same parameters as in Fig. 4, and following a three-dimensional description).

Fig. 4(b) and also a clear difference between the values of ΔV when the defect plane is located at the interfaces of the well and the barriers. This is not the case in Marzin and Gérard's measurements[7] which are concerned with optical data in the absence of an applied field.

Tunneling currents obtained for different doped systems are compared with the original one concerned with the undoped system by displaying the shifts of the current peaks from the normal tunneling device ΔI for the same heterostructure as a function of the impurity layer position. The results are shown in Fig. 5. Notice that for this particular choice of geometry an increase of the peak current is obtained for a large range of impurity plane positions, mainly next to the central well region. This fact indicates unambiguously that the tunneling performance of a diode can be artificially monitored by adding an impurity plane during the growth process of the nanostructure.

In summary, we have presented a study of resonant tunneling in double-barrier heterostructures in the presence of isoelectronic monolayers at different positions inside the well. We have followed a theoretical description based on Keldysh's nonequilibrium Green functions, which are adequate to describe transport properties. We have neglected effect suchs as band bendings due to charge accumulation and have considered a linear interpolation to describe the potential profile induced by the applied voltage. The real-space microscopic description of the system can be understood as an appropriate formalism in which, for instance, substituted impurity planes are easily incorporated in the theoretical treatment. Moreover, we have shown that transport measurements can also be used to allow a mapping of the electronic wave functions inside different heterostructures.

ACKNOWLEDGMENTS

We are grateful to P. Shultz and S. S. Makler for helpful discussions. This work was partially supported by Conselho Nacional de Desenvolvimento Cientifico e Tecnólogico, Brazil.

*Electronic address: latge@if.uff.br

[1] M. W. Dellow, P. H. Beton, C. J. G. M. Langerak, T. J. Foster, P. C. Main, L. Eaves, M. Henini, S. P. Beaumont, and C. D. W. Wilkinson, Phys. Rev. Lett. **68**, 1754 (1992).

[2] A. K. Geim, P. C. Main, N. La Scala, Jr., L. Eaves, T. J. Foster, P. H. Beton, J. W. Sakai, F. W. Sheard, M. Henini, G. Hill, and M. A. Pate, Phys. Rev. Lett. **72**, 2061 (1994).

[3] A. K. Geim, T. J. Foster, A. Nogaret, N. Mori, P. J. McDonnel, N. La Scala, Jr., P. C. Main, and L. Eaves, Phys. Rev. B **50**, 8074 (1994).

[4] E. Wolak, K. L. Lear, P. M. Pitner, E. S. Hellman, B. G. Park, T. Weil, J. S. Harris, Jr., and D. Thomas, Appl. Phys. Lett. **53**, 201 (1988).

[5] A. K. Savchenko, V. V. Kuznetsov, A. Woolfe, D. R. Mace, M. Pepper, D. A. Ritchie, and G. A. C. Jones, Phys. Rev. B **52**, R17 021 (1995).

[6] M. A. Davidovich and T. Gornsztejn, Solid State Commun. **92**, 213 (1994).

[7] J. Y. Marzin and J. M. Gérard, Phys. Rev. Lett. **62**, 2172 (1989).

[8] T. C. Hsieh, T. Miller, and T. C. Chiang, Phys. Rev. Lett. **55**, 2483 (1985).

[9] L. V. Keldysh, Zh. Éksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys. JETP **20**, 1018 (1965)].

[10] E. V. Anda and A. Latgé, Phys. Rev. B **50**, 8559 (1994); P. L. Pernas, F. Flores, and E. V. Anda, *ibid.* **47**, 4779 (1993).

[11] P. A. Schultz and C. E. T. G. da Silva, Phys. Rev. B **38**, 10 718 (1988); P. A. Schultz, *ibid.* **44**, 8323 (1991); P. A. Schultz, D. S. Galv$\widetilde{ao}$, and M. J. Caldas, *ibid.* **44**, 6073 (1991).