Hysteresis Effects on Quantum Wires: Do They Exist or Not?

Flávio ARISTONE

Departamento de Física, Universidade Federal de Mato Grosso do Sul,
Caixa Postal 549, 79070900 Campo Grande - MS, Brazil

José SANCHEZ-DEHESA

Universidad Autónoma de Madrid, FMC, Cantoblanco, 28049 Madrid, Spain

(Received 9 November 2000)

We present a self-consistent calculation for an arbitrary profile of quantum wires based on the simultaneous solution of the Schrödinger and Poisson equations. In our description, the Fermi energy level is maintained constant. Numerical results are discussed for rectangular quantum wires, which are supposed to be obtained from permanent plastic deformation of $\delta-$ doped samples. We are able to discuss very rigorously the conditions under which bi-stability exists in quantum wires. Hysteresis effects occur if and only if exchange-correlation term of energy is taken into account.

Semiconductor devices, especially those named heterostructures, are very attractive systems to study the quantum behavior of nature. Quantum-mechanical effects are particularly important for designing new classes of devices for specific applications. As a general rule, the final goal is to obtain smaller devices (for best integration) able to operate at higher frequencies for transmission of more information (and lower prices). Three steps are fundamental in the engineering of complex semiconductor devices before testing: to model, to grow, and to process.

Heterostructures are complex devices of different semiconductor films for which the typical widths are of the order of some atomic layers. The reality of growing these structures opened new and enthusiastic possibilities in physics (basic and applied), as well as in micro- and nano-electronics. Results are very clear: direct applications to different fields of science and new high-technology products. The benefits of these artificial man-made crystals are easy to find anywhere: see for example Refs. [1–5]

We want to study complex structures in which carriers (electrons) are restricted to move in one-dimension (1D), different from the usual three-dimensional (3D) bulk materials, due to confinement effects. In particular, we intend to analyze what are called quantum wires (QW), in which only one dimension remains unconfined for the electrons movement. Quantum wires have a great potential for many applications in microelectronics, such as novel opto-electronics devices and transistors. They can be obtained in two manners: either from a growth profile [6] or from a technologic process on a sample [7].

Firstly, we describe the electrostatic potential for a rectangular quantum wire of charge. Then, we introduce the potential term due to accumulation of attracted charges that leads to the self-consistent Schrödinger-Poisson system of equations in which we take into account the Fermi energy as constant. Finally, we introduce the exchange correlation energy in our formalism and discuss the physical implications of that term. When the exchange correlation is neglected, no hysteresis effect is observed, even for a very asymmetric wire shape. However, we observe bi-stability when exchange correlation is taken into account, even for absolutely symmetric cases such as square quantum wires.

The electrostatic potential for (fixed) positive charges can be obtained, as usual, from the Poisson equation. Analytical solutions are found when a linear uniform distribution of charge along the wire direction is considered. We shall call this potential $\phi_{dop}(x,y)$, in allusion to the doping concentration fixed by the growing conditions. That term is given by the following expression:

$$\phi_{dop}(x,y) = -\frac{\lambda}{2\pi\varepsilon} \int_{-a}^{+a} dX \int_{-b}^{+b} dY \ln\left(\sqrt{(x-X)^2 + (y-Y)^2}\right) \tag{1}$$

where a and b are the lateral dimensions of our quantum wire, λ is the linear charge density, and ε is the dielectric constant. Integration of Eq. 1 can be done analytically, but this is out of our scope here. The solution of the Schrödinger equation for this potential provides the quantum energy levels and states accessible to electrons.

Each particular electronic level can receive as many electrons as it is allowed: 4 (spin degeneracy multiplied by the bi-directional possibility of movement) times the integral over the one-dimensional density of states. For $T = 0K$, electrons start to fill the first excited state only after the ground state is completely occupied. This process continues up to the total energy, which is given by the summation of each electron energy, and reaches the Fermi level, which is taken as a constant parameter and is given by conditions of growing.

Electrons filling eigenstates of energy will behave exactly as quantum wires of negative charge whose space distributions are dependent on the (square) wave-function geometries. Consequently, they will also contribute to the electrostatic potential, but with a repulsive term given by the following expression:

$$\phi_{acu}(x,y) = -\frac{1}{2\pi\varepsilon} \int_{-\infty}^{+\infty} dX \int_{-\infty}^{+\infty} dY\, n(x,y) \ln\left(\sqrt{(x-X)^2 + (y-Y)^2}\right) \qquad (2)$$

where $n(x,y)$ is the one-dimensional electron density. The potential energy to be considered in the Hamiltonian at this point is the sum of both the "doping" and the "accumulation" terms, in which e represents the charge of the electron:

$$V(x,y) = -|e|\left(\phi_{dop}(x,y) + \phi_{acu}(x,y)\right). \qquad (3)$$

The electronic density is dependent on the Fermi distribution function $f(E)$, the one-dimensional density of states $D^1(E)$, and the "shape" of the electrons, which is written as a summation over all occupied wave functions $\psi(x,y)$:

$$n(x,y) = -|e| \sum_{i=1}^{\infty} \int_{E_i}^{\infty} |\psi_i(x,y)|^2 \; D_i^1(E)\; f(E)\, dE. \qquad (4)$$

The temperature is a parameter to be fixed initially. For $T = 0\,K$, the expression above can be considerably simplified without lack of generality. In that case, the summation above shall be limited to a fixed value ief. To determine ief, we take into account the neutrality of charges and assume the electronic effective mass approximation m^* to write

$$\sum_{i=1}^{ief} \frac{g_s\,|e|\,\sqrt{2m^*(E_F - E_i)}}{\pi\hbar} = \lambda \qquad (5)$$

where g_s is the spin degeneracy, E_i is the i-th eigenvalue, $\hbar$ is Planck's constant, and a factor 2 has been considered to describe the degeneracy of the movement along the $\hat{z}$ direction.

Our first self-consistent system of equations is hereafter evidenced since the potential energy expressed in Eq. 3 is explicitly dependent, through Eqs. 2 and 4, on the form of the wave functions and energy eigenvalues. These eigenstates are themselves directly dependent on the potential to be considered because of the Schrödinger equation to be solved.

In order to solve the bi-dimensional Schrödinger equation involved in the self-consistent system described in this paper, we have made use of a variational method already tested in many other situations. The analytical procedure is quite simple and consists of changing a differential equation into a matrix eigenvalue problem. We have made use of cubic β-spline functions as a basis set, with the variational parameters being the amplitudes of specific polynomials. Such a method was presented by Porto and Sanchez-Dehesa [8]; it has been extensively tested in many different cases, and it works very well.

We have studied quantum wires with surface areas varying typically from 10 Å × 40 Å up to 40 Å × 100 Å. The doping concentration is considered as an input parameter, and we take values between $0.8 \times 10^8 \mathrm{m}^{-1}$ and $4.0 \times 10^8 \mathrm{m}^{-1}$. The electronic effective mass of GaAs, $m^\star = 0.0667$, was used. Finally, all results in this paper are presented for $T = 0\,K$. Temperature effects and the effective mass variation will be discussed in a later communication.

We choose to exhibit numerical results for a quantum wire whose dimensions are 40 Å × 100 Å. However, we applied our method without major problems for a wide range of surface area varying from 10 Å × 10 Å up to 150 Å × 150 Å. The self-consistent calculation must be pursued very carefully to avoid numerical problems and misunderstanding of results. Many details have to be considered: *e.g.*, looking for the ideal size of the integration cell, choosing the best number of β-splines functions, *etc.*

Ending the first part of this study, we mention that absolutely no effect of bi-stability was observed. If this result is intuitive when considering square quantum wires, it's less obvious for rectangular forms where asymmetric wave functions are obtained. However, hysteresis effects do not appear in the calculation of any variable applied to this system.

Due to the current controversy about hysteresis effects

in quantum wire systems, as for example bi-stability in the carrier concentrations, we pursued this work by including a new energy term in the total potential energy. This new energy is due to a local-field approximation for many-body interactions of electrons. It's usually called the exchange-correlation energy and has been neglect up to this point.

In spite the fact that many different formulations exist to express the exchange-correlation energy, we considered the same expression as proposed by Takagaki and Ploog [5] in order to be consistent with previous results already presented in the literature. Therefore, we included in Eq. 3 the following term:

$$V_{xc}(x,y) = -\frac{0.0784e^2 \sqrt[3]{n(x,y)}}{\varepsilon}\left(1 + 0.0338\frac{\ln\left(1 + 18.38a_0\sqrt[3]{n(x,y)}\right)}{a_0\sqrt[3]{n(x,y)}}\right) \qquad (6)$$

where the cited authors defined $a_0 = 4\pi\varepsilon\hbar^2/m^*e^2$ as the effective Bohr radius. This term is obviously self-consistent.

The final self-consistent form of the new potential energy presents some differences from previous calculation. When V_{xc} is included into the Schrödinger equation, self-consistency is obtained faster. In Fig. 1, we show V_{xc}, considering the same wire as before. Since neutrality of electric charges is imposed, the electrical field far from the wire must be zero or very small; consequently, the self-consistent potential is constant.

In Fig. 2, we show that hysteresis effects are effectively present. These effects are observed only when the doping concentrations correspond to the limit in which a particular energy level is very close to the Fermi energy, *i.e.*, when the doping concentration is being increased (decreased) and the system is near the limit that one more energy level must be added (retired) to maintain the total electrical-charge neutrality. Numerically, this is done

by the following procedure: we start with the smallest (largest) value of λ (doping concentration) presented in Fig. 2 and solve the self-consistent Schrödinger-Poisson system of equations taking into account V_{dop}. After this calculation is over, we increase (decrease) the value of λ and re-start the calculation, but we take into account the former self-consistent potential obtained as the initial input.

It's clear from our results that bi-stability effects are present only when the potential energy of the exchange-
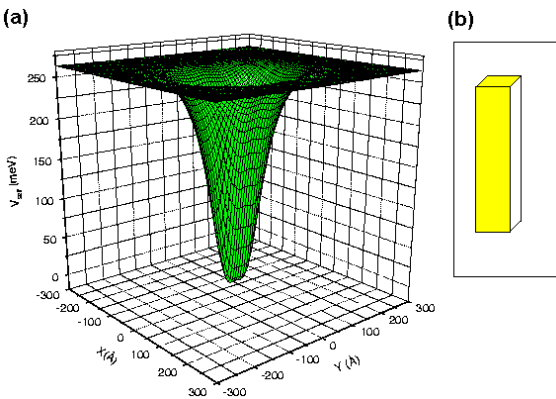

Fig. 1. (a) Potential energy term due to many body effects expressed as an exchange-correlation factor calculated by mean-field approximation theory was included in the Hamiltonian. The details of the calculation were presented in the references cited in the text. Inclusion of this term improves the convergence of self-consistent calculations. (b) In the insert we see a schematic representation of rectangular carriers.
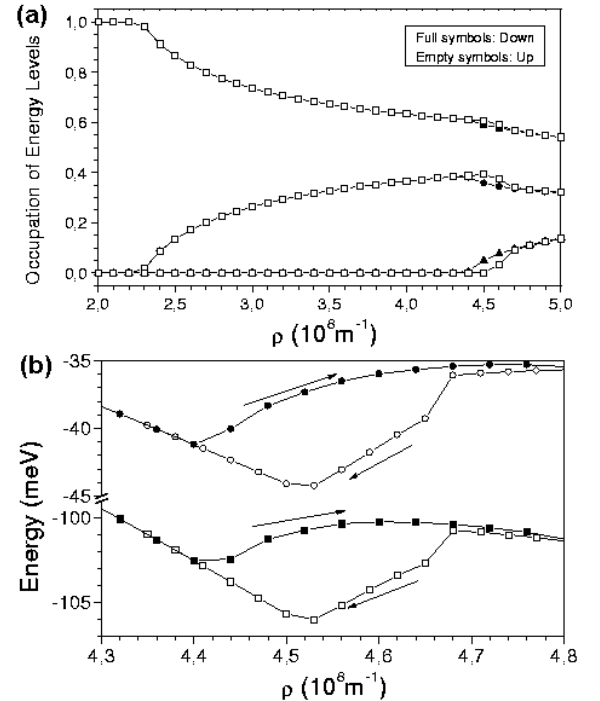

Fig. 2. Hysteresis or bi-stability effect on (a) electronic occupation and (b) energies levels as functions of the doping carrier concentrations. These effects only occur when the potential energy due to the exchange correlation is taken into account. We conclude that bi-stability is not an effect of symmetry, but is due to electron-electron interactions.

correlation term is taken into account. On the contrary, when the Schrödinger-Poisson equations are coupled only by Eq. 3, no hysteresis effect is noted, even for rectangular quantum wires for which very asymmetric wavefunctions are obtained and for which hysteresis could be *a priori* expected. In fact, it seems absolutely correct that such an effect of bistability appears when exchange correlation is taken into account. It is normally accepted that exchange correlation, as the name implies, is a direct measure of how much the system is correlated. For the situation considered in this paper, it represents the correlation among all the electrons composing the system.

To visualize the effect of exchange correlation, we can imagine a flexible line joining all the electrons involved in our description. Therefore, we can talk about some form of **state of correlation**. This line is responsible for trying, as much as possible, to keep the system in the same **state of correlation** it was in before any kind of variation. When the number of occupied levels is expected to change due to the variation of the Fermi level (or equivalently in our formulation to the variation of λ), the **state of correlation** obviously change too, since electrons will be forced to re-organize themselves in another spatial configuration. Thus, hysteresis is a direct consequence of the presence of such a "line." Near the crossing of the electronic energy eigenstate with the Fermi level, electrons try to remain in the state of lower energy when λ (the quantum wire charge density) increases while in the absence of correlation they would already be in a higher level for the same variation. On the contrary, when λ is decreasing, the electrons change their configuration to remain in the higher level. This rearrangement will not occur in the absence of exchange correlation because all electrons are independent of each other. The intensity, or relevance, of bistability is related to the coefficients entering the formulation of the local-field-approximation described in Eq. 6. We associate the word "intensity" in this context with the area inside the hysteresis region.

We presented here a complete self-consistent calculation of the electronic levels for two-dimensional systems. Particularly, we applied our method to rectangularly shaped quantum wires. The electrostatic potential for the rectangular charge distribution was presented and was used as the seed to start the convergence process for the self-consistent eigenvalues of the system. The central conclusion of this work is related to the origin of hysteresis effects on electrical quantities of quantum wires, such as the occupation number of levels. Exchange-correlation was considered in the usual form presented in the literature, and it was responsible for every hysteresis effect observed. Even for rectangular systems, for which wave functions are not symmetric, hysteresis effects are not present in the absence of an exchange correlation contribution. On the other hand, even for square quantum-wires, which present very symmetric eigenstates, hysteresis effects emerge when we include exchange correlation.

REFERENCES

[1] M. Tadić and Z. Ikonić, Phys. Rev. B **50**, 7680 (1994).
[2] D. Agosti, F. Pederiva, E. Lipparini and K. Takayanagi. Phys. Rev. B **57**, 14869 (1998).
[3] V. Türck, O. Stier, F. Heinrichsdorff, M. Grundmann and D. Bimberg. Phys. Rev. B **55**, 7733 (1997).
[4] N. Mutluay and B. Tanatar. Phys. Rev. B **55**, 6697 (1997).
[5] Y. Takagaki and K. Ploog. J. Phys.: Condens. Matter **7**, 731 (1995).
[6] Cathy Guasch, PhD Dissertation, Institut National des Sciences Appliqueés (INSA, Toulouse France, 1994), p. 38.
[7] C. Guasch, F. Voillot, M. Goiran, J. P. Peyrade, E. Bedel, C. Fontaine, H. Atmani and A. Rocher. Solid-State Electronics **37**, 567 (1994).
[8] J. A. Porto and José Sanchez-Dehesa. Phys. Rev. B **51**, 4352 (1995).