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Abstract— The present work is dedicated to the numeric physical modelisation of the potential to the interface of a heterostructure in GaAsAl/GaAs. Calculs, using some projective methods, permitting the integration of Hamiltonian, with Green functions in the equation of Schrödinger, for a rigorous resolution with the equation of Poisson are elaborated. A study of convergence of globally no linear system is done and it confirmed for ten bases functions and a very determined electric wall position. The different parameter influence on performances of the GaAsAl/GaAs heterostructure is put in evidence; what will permit us subsequently to consider the dynamic of the carriers in a HEMT heterostructure by rigorous and complete manner.

Keywords- *heterojonction; quantum well; HEMT transistor; GREEN function; system of equation Poisson –Schrödinger*

I. INTRODUCTION

Quantum Systems of bass dimensionality make the object of numerous studies since about twenty years. The permanent reduction of the architecture size in micro-electronics requires to term to hold amount of quantum phenomena that considerably modifies the physical properties and drives to the new phenomena [1].

The development of semiconductor heterostructures materials gave illustrations of certain concepts of the quantum mechanical as the confinement or the quantification of energy levels[2].

In AlGaAs/GaAs heterostructures, the gas formed by electrons accumulated to the interfacing of the AlGaAs/GaAs heterojunction possesses two interesting physicals properties: a bidimentionnal caharacter and a very elevated mobility at a very bass temperature [3] .

The modelling of charge control necessity the determination of the potential profile in the heterojunction which allows calculation of energy level, the associated wave function and finally, the charge density [4].

Selft consistant solutions have been proposed, but in each case the shapes of the wave function and/or the quantum well are already supposed to be known (parabolic, or rectangular).

This work is consecrated to a numeric modelisation of a quantum well that has for aim to solve the system of equation Poisson Schrödinger where without propose any form either for the potential energy or/and for the wave function witch are characteristics parameters of a quantum well.

II. NUMERIC MODELISATION OF A QUANTUM WELL

The structure under investigation consist of an N-type AlGaAs layer , and P-type GaAs buffer layer, this structure is modelised in the effective masse approximation, at the thermodynamic equilibrium in addition in this structure nanométric:

-Quantum well have one bound state and without spacer.
-Steep: the composition of materials and doping change suddenly at the time of the passage of the interfacing plan
- Of alignment of band of energy of type I
-Very precise value of the Aluminium rate (0.25)
- Well width is taken equal to 80A°

The potential at the interface of heterojunction check simultaneously Schrödinger and Poisson equations that is why we proposed to solve with a rigorous manner the system of Schrödinger and Poisson equations given by the following formula [5]:

$$\begin{cases} Es: \dfrac{-\hbar^2}{2m_e}\Delta\Psi^i(z)+V(z)\Psi^i(z)=E^i\Psi^i(z) \\ Ep: V(z)+\dfrac{\rho(z)}{\varepsilon}=0 \end{cases} \quad (1)$$

Δ : The Laplacien operator
$m_{e:}$ effective mass of an electron
$\Psi^i(z)$: Wave function associated with energy level E^i
V (z): the potential
$\hbar$: Planck 's constant

$\rho(z)$: Density of free electron it is given by:

$$\rho(z)=\begin{cases} qN_D - q\sum n(E^i)\left|\Psi^i(z)\right|^2 \cdots in\ GaAsAl \\ -qN_A - q\sum n(E^i)\left|\Psi^i(z)\right|^2 \cdots in\ GaAs \end{cases} \quad (2)$$

q: electron charge.
qND and -qNA: fixed charge
ND: donors doping rate
NA:acceptors doping rate)

$q\sum n(E^i)\left|\Psi^i(z)\right|^2$: mobile carriers

n (Ei): carrier density (to the energy level of i number) of electrons obtained by the Dirac Fermi distribution it is given by:

$$n(E^i)=(\frac{m_e k_B T}{\pi\hbar^2})\log\left(1+\exp\frac{E_F-E^i}{k_B T}\right) \quad (3)$$

E_F: energy level of Fermi.
K_B: Boltzman constant
T: absolute temperature
i: number of state bound possible.

Our contribution relationship to the different approaches of the literatures that is we have used integral method where without propose any form either for the potential energy or/and for the wave function, this method is based on Green functions and the moments methods. Green function associated to an equation to the partial derivatives can either be defined calculated, its form depend on the physical function to study in our case the potential, and they also depend on the domain of definition and limits conditions. The mathematical interpretation to the sense of distribution of these conditions is [5]:

$$\Delta G=-\delta(z-z_0) \quad (4)$$

Application of the Galerkin method to the equation (1) yields the following equation system:

$$\sum_{n,m}^{N}\left[H_{m,n}(\alpha_1,\alpha_2,\cdots\cdots\alpha_N)\right]\alpha_n = E\sum_{m=n}^{N}\alpha_n.\delta_{mn} \quad (6)$$

In which N is the number of basis function used for expanding $\psi_i(z)$; $\alpha_n = \prec\varphi_n\psi\succ$.

The test functions used here are classical solutions obtained for a rectangular well, projected over a Galerkin basis such that

$$\varphi_n=\frac{\sin N\pi(x+w)}{2w}, H_{mn}(\alpha\succ)$$

The chosen α_n functions are eigenfunctions of the Hamiltonian of an infinite well with a width 2w, which is much greater than the dimensions of the quantum well under study. In equation (6) the unknowns to be determined are α_n and E_m .

III. NUMERIC RESULT

The resolution of a no linear system can be gotten by a choice of an appropriate numeric method. In this work the linearization of the system (system to solve) is effectuated by the method of Quasi Newton by finite difference. The most important results are the potential energy, the wave function and surfacic density. These parameters are very important seen their influence on the mobility of bidimensionnal electrons gas.

A. POTENTIAL ENERGY)

The figure (1) represents potential well profile at the interface for unique bound state[6].
The figure (2) shows the difference and the influence of different numeric physic model on the shape of the potential well. These different models proposed by authors [7, 8, 9] are based on self consist calculus that is the most often based on initial triangular potential well. On the other hand our method hasn't proposed any form to the potential and/or of wave function, it uses the resolution of the integral form of the Hamiltonian by the projective methods what showed the curvature of conduction band [6].

B. WAVE FUNCTION ASSOCIATED TO ONE BOUND STATEs

The wave function associated to one bound state is illustrated on the figure (3) where we observed that the big probability to find electrons is also located at some ten A° what implies that there is a penetration of the wave function in the potential gate[6].

C. SURFACIC DENSITY

Figure (4) shows that N_S increases slowly with doping (N_d). More doping is increasing the electron transfer GaAsAl layer (donor) to the GaAs layer (buffer layer) increases. And if AlGaAs doping increases, the surfasic density increases, the confinement of electrons in the buffer layer is effective but it will be near to a limiting value when the doping continues to increase.

So for a fixed rate of Aluminum, over doping is increasing doping workforce will increase and the transport of electron (witch located in GaAsAl layer (donor))to the layer GaAs (buffer layer) will increase witch implying an

increase of N_S .This increase will reach limited value when the doping continues to increase .

This result is in disagreement with the work of Boyer-APT Temple as it mounted on the figure(4) but is consistent with the work of A.Cappy shows that the electronic surfasic density N_S increases with the doping donor layer but it reach to a limiting value when the doping continues to increase[12] .

The figure (5) shows that for a given dopage and for a fixed rate of Aluminum that equal to 0.25, surfacic density increases when the width of the well increases but it is going to decrease when we passes a value criticizes (80A°) [12] that corresponding to a max value of NS ($0.3361 .10^{16}$ at/m^2). Beyond of this value the number of states bound is not unique what explains the reduction of Ns that in fact corresponds then to Ns[12].

By cons, the surfasic density is almost constant when varying the doping atom acceptor (N_a) which is given in figure (6), compared to the result of reference [7].

IV. CONCLUSION

Our work has as main objective the exact numerical solution of Schrödinger-Poisson system witch is globally nonlinear in order to define the potential at the interface of a heterojunction GaAsAl/GaAs. The system was solved so autocoherente, calculations, using projective method, allowing the integration of Hamiltonian using the Green function in the Schrödinger equation for autocoherente resolution with Poisson's equation are developed.

However, the resolution of this system is made by quasi Newton method [11] by finite difference. This physic – numeric modelisation that we have made can be applied to all other quantum heterojunction with inversion or accumulation layer.

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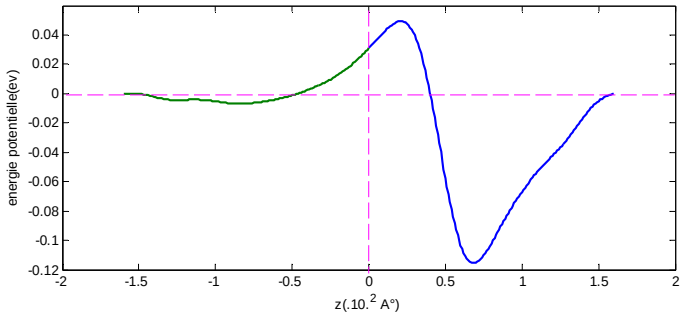

Figure 1. potential energy profile for one bound state[6]

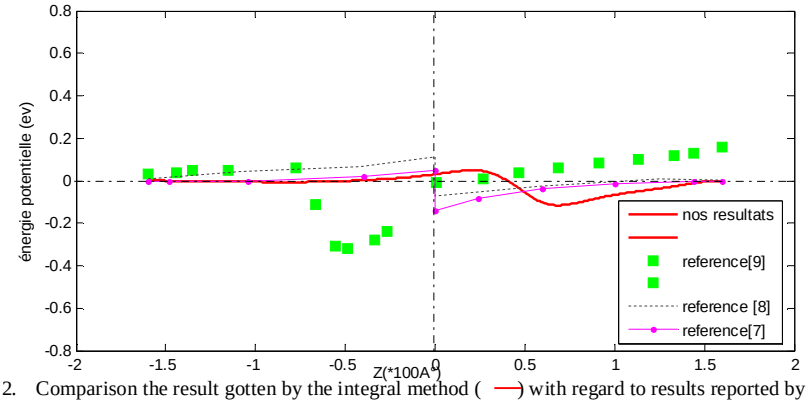

Figure 2. Comparison the result gotten by the integral method (⟶) with regard to results reported by authors[6]

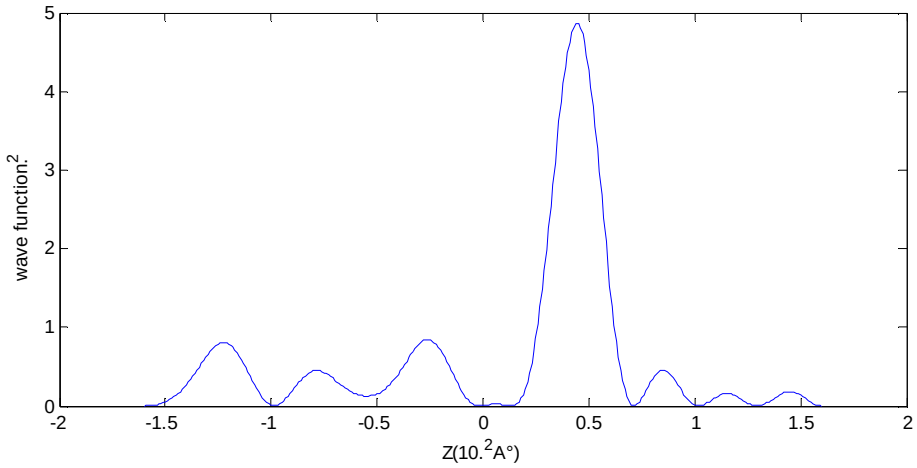

Figure 3. wave function

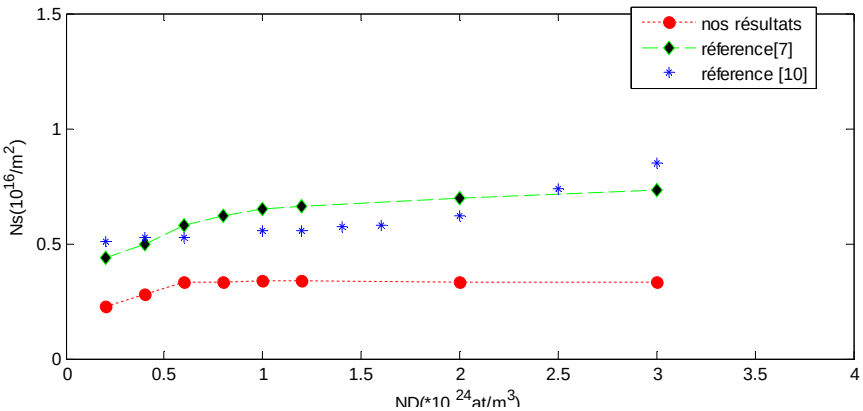

Figure 4. influence of Nd on Ns (HEMT and PHEMT structure with and without spacer) [12]

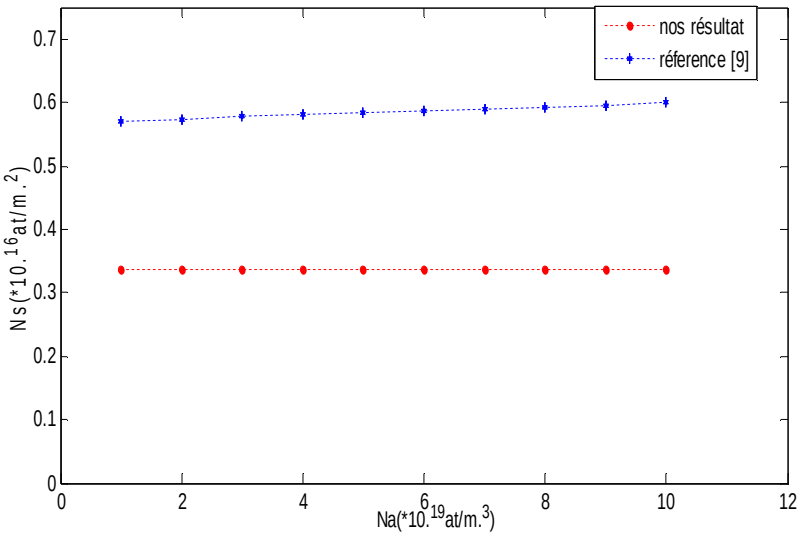

Figure 5. Influence of NA on Ns [12]

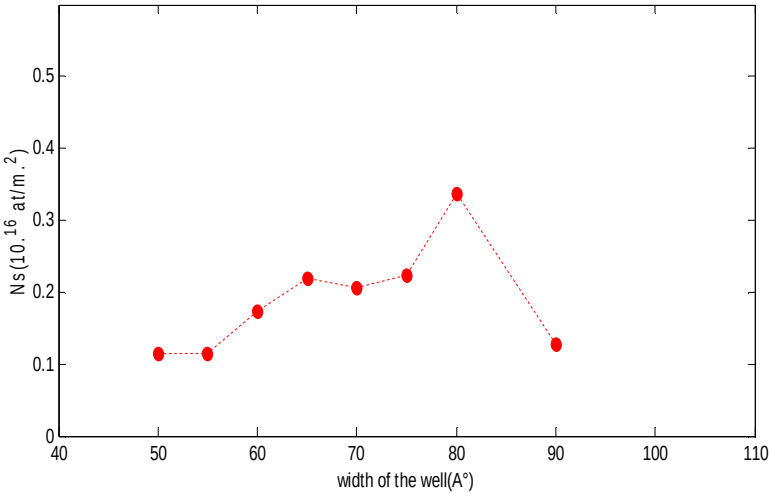

Figure 6. Variation of Ns according to the width of the well

V. AUTHORS' INFORMATION

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First I. BOUNEB obtained her BEng degree from University of Mentouri Constantine, Algeria, in June 2004, and her MSc degree in components and microsystem at the University of Mentouri, Constantine in June 2009. Her research domain is adaptation of semiconductor to the solar specter (nano PV).

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Scond M. MARIR BENABBAS he received the DES(diplome d'etude superiors) degree in physic energetic, from the university of Constantine in 1981,and the magister photovoltaic from the university of

Constantine with associated of university of Belgium, leuven 1984,his dissertation research is concerned with the breakdown phenomena in solar cells, from 1984 she joined the electronically institute of Constantine university, where she served successively as instructor, assistant master. In 1993, where she was obtained her doctorate as sciences of microelectronic from the university of Constantine with collaboration from Institute national Polytechnic (INP, ENSEEIHT) of Toulouse his dissertation is concerned with the physics and modelling quantum compound semiconductor devises such as high electron mobility transistors (HEMTS).Since 1993, she served as associate professor in the electronically department. She is now an associate research scientist in the material and electronically compound laboratory of engineering science faculty where she has been engaged in research on heterostructure quantum well devices and physics, and photovoltaic system, working on OPVC cells until a few years. She works in several scientific projects with the different institution of ministry.

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