Determination of Electronic States in Low Dimensional Heterostructure and Quantum Wire Devices

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Abstract

An efficient variational technique is applied to solve Schrödinger's equation in two dimensions. This model is then self-consistently used with a two-dimensional Poisson's equation solver to determine the electronic states inside low dimensional heterostructure and quantum wire devices. Finally, the advantages and limitations of the present model are discussed.

1. Introduction

The existance of a one-dimensional electron gas in low dimensional and quantum wire heterostructure devices requires an accurate and efficient model to determine the electronic states and the carrier transport properties in these devices. The self-consistent solution of Poisson's and Schrödinger's equations is belived to be one of the most accurate methods which can be used to characterize the operation and to optimize the structure of these devices.

A number of authors investigated different models which are based on the finite difference method to solve Poisson's and Schrödinger's equations self-consistently in two dimensions [1-3]. The accuracy and the computational efficiency of these models strongly depend on mesh size and discretization techniques. An alternative efficient method to solve Schrödinger's equation in one dimension by using a variational technique has been suggested [4-6]. In the present work, this method is extended to two dimensions to determine the electronic states in low dimensional and quantum wire heterostructure devices. Finally, the advantages and limitations of this method are discussed.

2. Model

The effective mass, two-dimensional Schrödinger equation is given by

$$-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right]+V(x,y)\psi=E\psi \qquad (1)$$

where V(x,y) means potential energy, E eigenenergy, ψ wave function corresponding to the eigenenergy E, m^* effective mass, and $\hbar$ Planck's constant. For a semiconductor structure of length a and width b, the wave equation can be expanded as

$$\psi = \sum_{n=1}^{N} \sum_{m=1}^{M} a_{nm} \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b}. \tag{2}$$

The accuracy of this solution depends on the number of the expansion functions N and M. If N and M are infinite, the obtained wave functions are identical to the true ones. However, finite N and M still lead to very good accuracy.

The coefficients a_{nm} are obtained by means of variational integrals whose stationary values correspond to the true eigenvalues when the true eigenfunctions are inserted in the integral. The variational integral for E is given by

$$E = \frac{\frac{\hbar^2}{2m^*} \int_0^a \int_0^b [(\frac{\partial \psi}{\partial x})^2 + (\frac{\partial \psi}{\partial y})^2] dxdy + \int_0^a \int_0^b V(x,y)\psi^2 dxdy}{\int_0^a \int_0^b \psi^2(x,y) dxdy}. \tag{3}$$

The condition that (3) should be stationary is satisfied if the first-order variation in E vanishes for an arbitrary first-order variation $\delta\psi$ in ψ. Applying this condition, a matrix equation $[R]\mathbf{A} = E\mathbf{A}$ is obtained where $\mathbf{A}$ is a column vector with the elements a_{nm} and $R_{nm,n'm'} = \mathbf{I}_1 + \mathbf{I}_2$ where $\mathbf{I}_1$ and $\mathbf{I}_2$ are given by

$$\mathbf{I}_1 = \frac{\hbar^2}{2m^*} \int_0^a \int_0^b [(\frac{\partial \psi}{\partial x})^2 + (\frac{\partial \psi}{\partial y})^2] dxdy = \frac{\hbar^2}{2m^*} [(\frac{n\pi}{a})^2 + (\frac{m\pi}{b})^2] \delta_{nn'} \delta_{mm'}, \tag{4}$$

$$\mathbf{I}_2 = \int_0^a \int_0^b V(x,y)\psi^2 dxdy = \frac{4}{ab} \int_0^a \int_0^b V(x,y) \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{n'\pi x}{a} \sin \frac{m'\pi y}{b} dxdy. \tag{5}$$

Solving these equations, the subband energies and the corresponding wave functions are determined and then used to calculate the carrier distribution. Knowing the carrier distribution, the electrostatic potential is then calculated by solving Poisson's equation in two dimensions. Knowing the electrostatic potential, the new potential energy function V(x,y) is calculated and the effective V(x,y) is expressed as a linear combination of its new and old values given by

$$V_{new}(x,y) = \omega V_{old}(x,y) + (1-\omega) V_{old}(x,y) \tag{6}$$

where ω means relaxation constant which is introduced to obtain the solution safely. Schrödinger's equation is again solved to determine the new eigenenergies and the corresponding wave functions which are then used to recalculate the carrier distribution. The procedure is repeated until the initial and final values of V(x,y), within the same iteration, differ by less than a specified error.

3. Numerical results and computational performance

Schrödinger's and Poisson's equation are solved self-consistently to determine the electronic states of the structure shown in fig. 1. The electronic states and hence the device operation are strongly affected by the terminal voltages. The applied potential V_{g3} can be varied to control the barrier height and the distance between the quantum wires. The potential energy and the carrier distribution for different bias are displayed in figures 2 and 3, respectively.

From these results one can see that the present model is able to accurately determine the electronic states in two-dimensional structures. The method is able to take into account the variations in the effective mass and the boundary conditions in a more flexible way than previous models. Moreover, the accuracy does not depend on mesh size and discretization and is only affected by the number of expansion functions N and M. Using 20 expansion functions in each direction, 20-30 iterations are required to get the solution with a maximum error of 0.5 meV in V(x,y). The required CPU time for each iteration is about 80 seconds on a HP700 work station.

4. Conclusions

An efficient variational technique is investigated to solve Schrödinger's equation in 2D and is applied with a 2D Poisson solver to determine the electronic states inside low-dimensional heterostructure devices. This method overcomes the limitations of previous finite-difference methods which are arising from mesh size and discretization. Moreover, the closed form of the wave functions makes the model more tractable to determine scattering rates and transport properties inside these devices.

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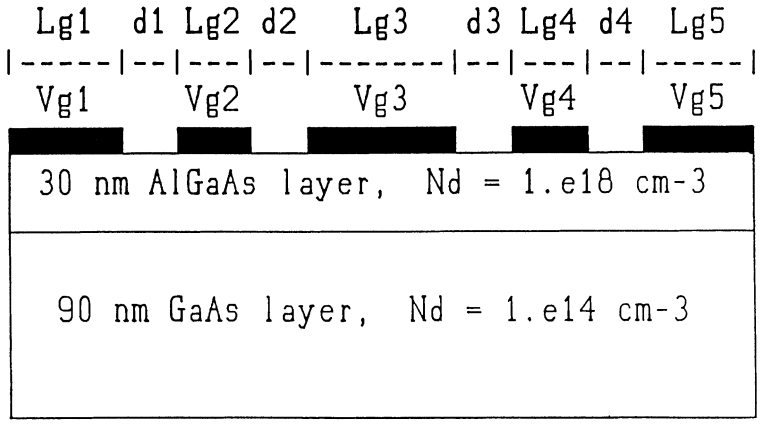
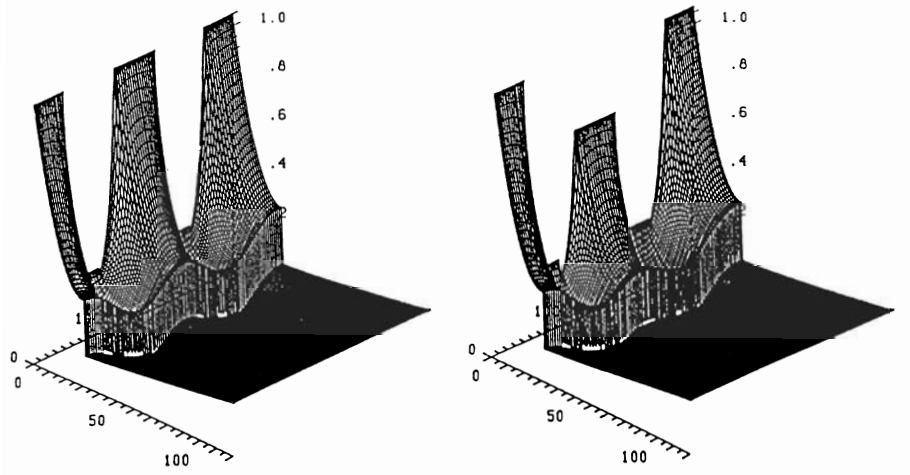
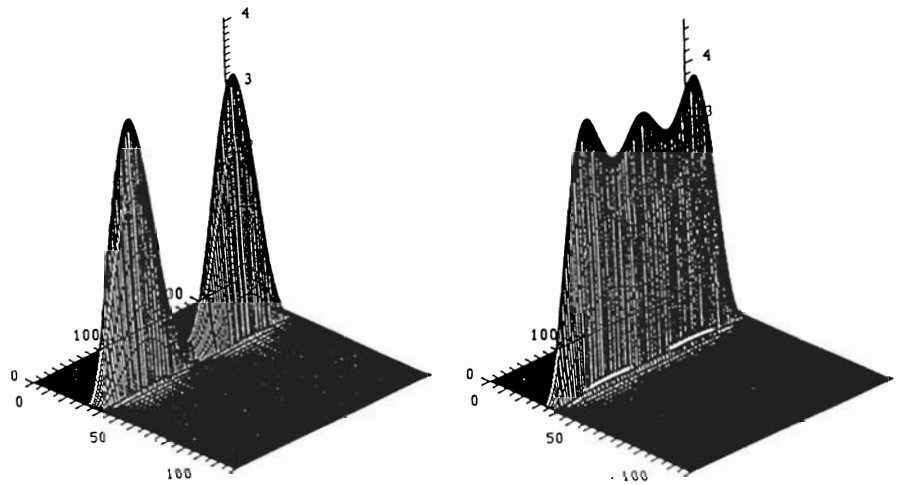


Fig. 1 The simulated AlGaAs/GaAs heterostructure.
$L_{g1}=L_{g5}=36$ nm, $L_{g2}=L_{g4}=24$ nm, $L_{g3}=48$ nm, $d_1=d_2=d_3=d_4=18$ nm



(a) (b)

Fig. 2 The potential energy distribution [eV]
(a) $V_{g1}=V_{g5}=V_{g3}=0.0$ V, $V_{g2}=V_{g4}=0.8$ V
(b) $V_{g1}=V_{g5}=0.0$ V, $V_{g3}=0.3$ V, $V_{g2}=V_{g4}=0.8$ V



(a) (b)

Fig. 3 The carrier concentration [$10^{17} cm^{-3}$]
(a) $V_{g1}=V_{g5}=V_{g3}=0.0$ V, $V_{g2}=V_{g4}=0.8$ V
(b) $V_{g1}=V_{g5}=0.0$ V, $V_{g3}=0.3$ V, $V_{g2}=V_{g4}=0.8$ V