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A comparison between different numerical methods used to solve Poisson's and Schroedinger's equations in semiconductor heterostructures

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A comparison between different numerical methods which are used to solve Poisson's and Schroedinger's equations in semiconductor heterostructures is presented. Considering Schroedinger's equation, both the Rayleigh–Ritz method and the finite difference method are examined. The accuracy and the computational speed are investigated as a function of both the mesh size and the number of Rayleigh–Ritz functions and the numerical results are compared with analytical solutions for special cases. To solve Poisson's equation, direct and iterative methods are implemented and the advantages and limitations of each method are discussed. The previous methods are used to solve Poisson's and Schroedinger's equations self-consistently in typical heterostructures to obtain the wave functions, the carrier distribution, and the subband energies.

I. INTRODUCTION

Based on technological advances, ultrasmall and highly doped heterostructure devices (with scales down to nanometer range and doping levels up to 10^{19} cm^{-3}) have been fabricated and have exhibited very good performance.[1–3] The physical phenomena which are taking place in such small devices require accurate physical models to characterize device operation and to optimize the structures. We believe that a coupled solution of Poisson's and Schroedinger's equation will become a common simulation tool for heterostructure and quantum devices.

A number of authors investigated different models[4–7] which were based on the finite-difference approach to solve Poisson's and Schroedinger's equations self-consistently. A new method has been introduced to solve Schroedinger's equation by using the Rayleigh–Ritz technique.[8] The closed form of the wave functions, which are obtained by this method, makes the calculations of the scattering rates and the determination of the carrier transport properties easier.

In the present work, some different methods for solving Poisson's and Schroedinger's equations are examined. The accuracy and the computational speed of these methods are compared. In Sec. II, Schroedinger's equation and its solution methods are introduced. To check the validity of these methods, the obtained results are compared with analytical solutions which are known for special cases. The direct and iterative methods which are used to solve Poisson's equation are discussed in Sec. III. In Sec. IV, Poisson's and Schroedinger's equations are solved self-consistently in a typical heterostructure to obtain the wave functions, the eigenenergies, and the carrier distribution. Conclusions and remarks are given in Sec. V.

II. SCHROEDINGER'S EQUATION

A. Description of the models

The effective mass, one-dimensional Schroedinger equation is given by

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi_i(x)}{\partial x^2}+V(x)\psi_i(x)=E_i\psi_i(x), \tag{1}$$

$$V(x)=-e\phi(x)+V_h(x)+V_{ex}(x), \tag{1a}$$

where $\phi(x)$ means electrostatic potential, $V_h(x)$ potential step function at the heterointerface, $V_{ex}(x)$ local exchange potential, E_i eigenenergy, $\psi_i(x)$ wave function corresponding to the eigenenergy E_i, e magnitude of electronic charge, m^* effective mass, and $\hbar$ Planck's constant.

The finite difference method is probably the easiest and most popular method to solve Eq. (1). However, the accuracy of this method is strongly affected by the mesh size and the discretization method.[4] In the present work, the three-point finite difference method with uniform meshes is used to solve Eq. (1). This method offers a relatively easy and effective way to determine the effects of the mesh size on accuracy and computational speed.

The discretized form of Eq. (1) is given by

$$-\frac{\hbar^2}{2m_j^*}\frac{\psi_{i,j+1}-2\psi_{i,j}+\psi_{i,j-1}}{(\Delta x)^2}+V_j\psi_{i,j}=E_i\psi_{i,j}. \tag{2}$$

Subscript j denotes the one-dimensional grid mesh point. Equation (2) constitutes a set of linear homogeneous equations with symmetric triangular form that simplifies the calculation of the eigenvalues and the wave functions.

We have investigated another method to solve Eq. (1) by using the Rayleigh–Ritz method which is usually applied to solve the electromagnetic wave equation and field problems.[9] The formal similarity between Schroedinger's equation and the wave equation suggests the extension of that method to the solution of wave propagation in crystals. For a semiconductor structure of width a, if the eigenfunction satisfies the boundary conditions $\psi(0)=0$, $\psi(a)=0$, the wave functions can then be expanded as

$$\psi_k=\sum_{n=1}^{N} a_{nk}f_n, \tag{3}$$

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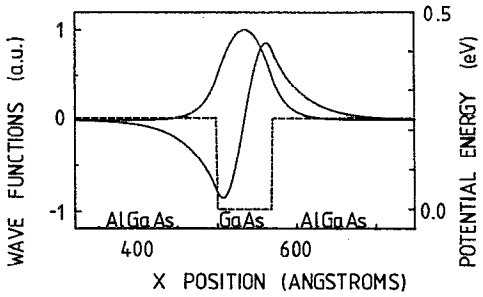

FIG. 1. An AlGaAs/GaAs/AlGaAs rectangular potential well and the first two wave functions. (The well height is 0.23 eV.)

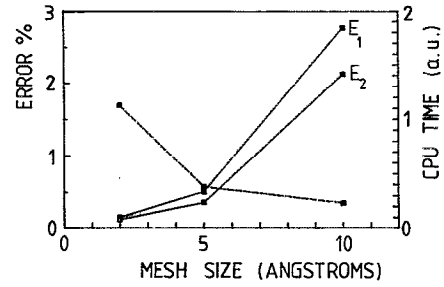

FIG. 3. The percentage error in the first two eigenenergies (compared with with the analytical solution) and the total CPU time vs the mesh size used in the finite-difference method.

$$f_n=\left(\frac{2}{a}\right)^{1/2}\sin\left(\frac{n\pi x}{a}\right). \tag{3a}$$

The accuracy of the solution depends on the number N of Rayleigh–Ritz functions N. If N is infinite, the obtained wave functions are identical to the true ones. However, a finite N still leads to very good accuracy. The coefficients a_{nk} are determined from the set of homogeneous equations

$$\sum_{n=1}^{N} a_{nk}\left[T_{ln}-\frac{2m^*}{\hbar^2}E_k\delta_{ln}\right]=0 \quad l=1,2,...,N, \tag{4}$$

$$T_{ln}=T_{nl}=\int_o^a\left(\frac{df_n}{dx}\frac{df_l}{dx}+\frac{2m^*}{\hbar^2}V(x)f_lf_n\right)dx. \tag{4a}$$

The wave functions can be calculated if the potential-energy function $V(x)$ is known. In semiconductor devices, the potential-energy function $V(x)$ is analytically obtained by making some approximations or numerically by solving Poisson's equation. The closed form of the wave functions makes the calculation of the scattering rates and the carrier transport properties much easier.

B. Applications

The solution of Schroedinger's equation for both a rectangular and a triangular potential well is analytically known. These expressions will be used to check the validity and the accuracy of our solution methods.

The eigenenergies of a rectangular potential well, shown in Fig. 1, are calculated by both finite-difference and the Rayleigh–Ritz methods. In our case, the width of the well is set equal to 70 Å. This insures the applicability for multilayer heterostructures because the potential well width may be of that order. The percentage error with respect to the analytical solutions for the eigenenergies of the the lowest two subbands and the total CPU time as a function of the mesh size (in the case of the finite-difference method and as a function of the number of the Rayleigh–Ritz functions) is displayed in Figs. 2 and 3, respectively.

Another illustration uses a triangular potential well (Fig. 4) as an extreme case in which the wave functions extend over a wide distance inside the device. The analytical solution for the eigenenergies, which is obtained by using Airy functions, is given by

$$E_i=\left[\frac{3\pi\hbar e}{2}E_F\left(i+\frac{3}{4}\right)\right]^{2/3}\left(\frac{1}{2m^*}\right)^{1/3}, \tag{5}$$

where E_F means electric field. The percentage error and the CPU time are displayed once more in Figs. 5 and 6, respectively.

For a certain accuracy, the CPU time of the finite-difference method is poorer than that of the Rayleigh–Ritz method. The advantage of the Rayleigh–Ritz method is that both CPU time and accuracy do not depend on a numerical parameter (the mesh sizes) and that the wave functions are obtained in closed form.

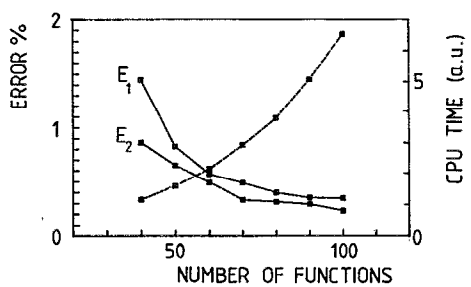

FIG. 2. The percentage error in the first two eigenenergies (compared with the analytical solution) and the total CPU time vs the number of Rayleigh–Ritz functions.

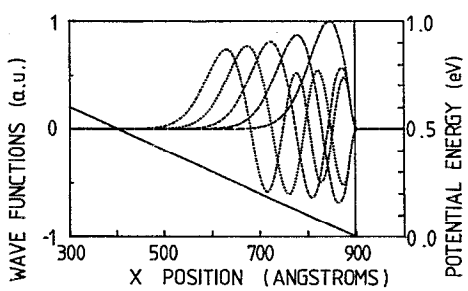

FIG. 4. An AlGaAs/GaAs triangular potential well and the first five wave functions.

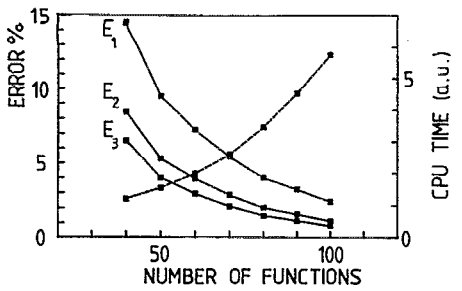

FIG. 5. The percentage error in the first three eigenenergies (compared with the analytical solution) and the total CPU time vs the number of Rayleigh–Ritz functions N.

III. POISSON'S EQUATION

The one-dimensional Poisson equation is given by

$$\frac{d}{dx}\epsilon_0\epsilon_r(x)\frac{d}{dx}\phi(x)=-e[N_d^+(x)-n(x)], \tag{6}$$

where $\epsilon_r(x)$ means relative dielectric constant. $N_d^+(x)$ is the ionized donor concentration which is given by[10]

$$N_d^+(x)=\frac{N_d}{1+\Sigma_r g_r \exp[(E_f-E_{dr})/kT]} \quad r=\Gamma,L,X, \tag{6a}$$

while the electron concentration $n(x)$ is given by

$$n(x)=n_{\text{subband}}(x)+n_{\text{bulk}}(x), \tag{6b}$$

where

$$n_{\text{subband}}(x)=\sum_i \frac{m^*kT}{\pi\hbar^2}\ln\{1+\exp[(E_f-E_i)/kT]\}|\psi_i(x)|^2, \tag{6c}$$

$$n_{\text{bulk}}(x)=\sum_r \frac{N_{cr}}{0.25+[\exp(E_{cr}-E_f)/kT]} \quad r=\Gamma,L,X, \tag{6d}$$

$$N_{cr}=2\left(\frac{2\pi m_r^*kT}{h}\right)^{3/2}. \tag{6e}$$

N_d means the donor density, g_r degeneracy factor, E_{dr} donor level, k Boltzmann's constant, T absolute temperature, E_f energy of the Fermi level, E_i and ψ_i energy and corresponding wave function of subband i, and E_{cr} energy of the bottom of the r band.

In previous works, Poisson's equation (6) is integrated to obtain a relationship between the electric field and the electrostatic potential for all x. A second integration yields $\phi(x)$. This method is relatively time-consuming and requires special treatments to achieve an accurate solution at the heterointerface.[4,5] In the present model, Poisson's equation is discretized and the obtained system of linear equations is then solved by using both direct and iterative methods.

The direct methods are faster but require larger memory size. For a large number of equations, the round-off error deteriorates the accuracy. Iterative methods, on the other hand, are simpler than direct methods and require smaller memory size. Their computational errors are automatically eliminated so that accuracy and hence CPU time both depend on the limit after which the iterations will be stopped. Both direct and iterative methods are used here to solve Poisson's equation self-consistently with Schroedinger's equation.

IV. SELF-CONSISTENT SOLUTION OF POISSON'S AND SCHROEDINGER'S EQUATIONS

A. Self-consistent procedure

Equations (1) and (6) are solved iteratively until a self-consistent solution is obtained. For the first iteration, the potential energy function $V(x)$ and the corresponding wave functions are calculated by using the triangular wave approximation. The electrostatic potential $\phi(x)$ is then calculated by solving Eq. (6). The boundary conditions imposed on the structure are that the differences between the Fermi level and the bottom of the conduction band at both ends are constant and equal to the bulk values. These values are calculated by knowing the occupancy of the deep centers and the electron concentration.[12] Poisson's equation is solved and the new potential energy function is then calculated using Eq. (1a). For the next iteration, the effective potential energy function is recalculated from a linear combination of new and old values of $V(x)$:

$$V_{\text{new}}(x)=\omega V_{\text{new}}(x)+(1-\omega)V_{\text{old}}(x), \tag{7}$$

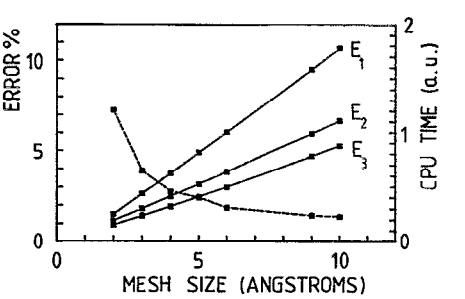

FIG. 6. The percentage error in the first three eigenenergies (compared with the analytical solution) and the total CPU time vs the mesh size used in the finite-difference method.

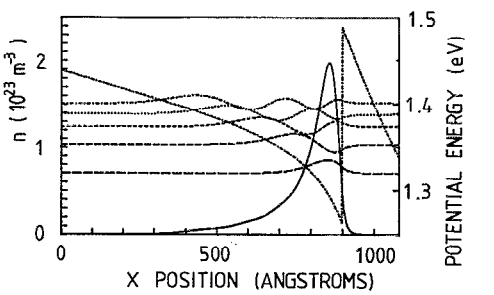

FIG. 7. The self-consistent solution for the lowest five wave functions, the potential energy (dashed lines), and the carrier concentration (solid line) of a $GaAs/Al_{0.3}Ga_{0.7}As$ heterojunction. (The potential energy is measured from the top of the valence band of GaAs.)

TABLE I. A comparison between different combinations of the solution methods.

Solution method of Schroedinger's eq.	Solution method of Poisson's eq.	Number of iterations	CPU time (a.u.)	Relaxation parameter
Rayleigh–Ritz	direct method	17	12.6	0.3
finite-difference	direct method	17	1.67	0.3
finite-difference	simple iterations	12	43.2	0.4
finite-difference	SOR iterations	16	2.68	0.3

where ω is a relaxation constant which is introduced to obtain the solution safely.[6] From Eqs. (4) and (4a), the potential-energy function $V(x)$ is used to determine the wave functions which are then used to recalculate the carrier distribution according to Eq. (6c). The procedure is repeated until initial and final values of $V(x)$, within the same iteration, differ by less than a specified error.

B. Applications

1. AlGaAs/GaAs heterojunction

A GaAs/AlGaAs heterojunction is considered with $N_{d1}=10^{21}$ cm^{-3} in a 0.09 μm GaAs layer and $N_{d2}=10^{23}$ cm^{-3} in a 0.018 μm $Al_{0.3}Ga_{0.7}As$ layer. Schroedinger's and Poisson's equations are solved self-consistently. The iterations are stopped when the difference between the initial and the final values of $V(x)$, within the same iteration, is less than 0.1 meV.

The self-consistent solutions of the potential energy, the lowest five wave functions, and the carrier concentration are displayed in Fig. 7. Different combinations of the solution method are given in Table I together with the number of iterations and the required CPU time for each of them. The relaxation parameter ω is adjusted to obtain fast convergence. The number of Rayleigh–Ritz functions which are used to solve Schroedinger's equation are 60, while the mesh size is set equal to 2 Å for the finite difference method. The relaxation parameter which is used to solve Poisson's equation is 1.98.

Considering Schroedinger's equation, the finite-difference method is faster than the Rayleigh–Ritz method. On the other hand, the accuracy of the Rayleigh–Ritz method is not affected by the mesh size. This offers an advantage in semiconductor-device simulation because the mesh size should be as wide as possible to save the computational time.

To solve Poisson's equation, direct methods generally are faster than iterative methods. However, the computational speed is dramatically improved by using the successive overrelaxation (SOR) method.[11] On the other hand, the memory size is smaller and the computational algorithm is simpler in the case of iterative methods. This offers an advantage in two-dimensional and three-dimensional device simulation where the number of equations and unknowns are too large to be solved by direct methods.

V. CONCLUSIONS

A comparison between the different methods which are used to solve Poisson's and Schroedinger's equations is presented. Considering Schroedinger's equation, the finite-difference method generally is faster than the Rayleigh–Ritz method. The accuracy of the finite-difference method is affected by the mesh size while the number of functions used in the expression of the wave functions is the main parameter in the case of the Rayleigh–Ritz method. For Poisson's equation, direct methods are more efficient than iterative methods in one-dimensional simulations. However, the computational speed of iterative methods is greatly improved by using the SOR technique. In two-dimensional and three-dimensional simulations, the iterative methods are expected to be more accurate and more efficient than the direct methods. The choice of an efficient combination of the solution methods depends on the required accuracy, on the device structure and dimensions, and on further applications of the solution.

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