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An Efficient and Accurate Method to Calculate the Two-Dimensional Scattering Rates in Heterostructure Semiconductors

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Abstract

An accurate and efficient method is investigated to solve Schrödinger's equation by using variational techniques. The electronic states inside heterostructure devices are determined by a self-consistent solution of Poisson's and Schrödinger's equations. The closed forms of the wave functions are used to calculate the two-dimensional scattering rates in these structures. The computational efficiency is compared to that of conventional finite difference models.

1. Introduction

The existence of the two-dimensional electron gas (2DEG) in the vicinity of a heterointerface inside heterostructure semiconductors requires an accurate method to calculate the scattering rates and to determine the carrier transport properties in these structures. We believe that the solution of Schrödinger-Poisson system of equations will become a common simulation tool for ultra-small and heterostructure devices.

A number of authors investigated different models [1-3] which were based on the finite difference approach to solve Poisson's and Schrödinger's equations self-consistently. We have solved Schrödinger's equation by using variational methods to obtain the wave functions in terms of a number of expansion functions [4]. In the present work, this method is applied to determine the electronic states in an $AlGaAs/GaAs$ single-well heterostructure by solving Schrödinger's and Poisson's equation self-consistently. The two-dimensional scattering rates are then advantageously calculated using the obtained closed forms of the wave functions. The computational speed of this method is compared to that of conventional numerical models.

2. Model

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

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

where $V(x)$ means potential energy, E Eigenenergy, $\psi(x)$ wave function corresponds to the eigenenergy E, m^* effective mass, and $\hbar$ Planck's constant. For a semiconductor structure of width a, the eigenfunction satisfies the boundary conditions $\psi(0) = 0$, $\psi(a) = 0$. The wave functions can be expanded as

$$\psi_k = \sum_{n=1}^{N} a_{nk} \sin\left(\frac{n\,\pi\,x}{a}\right). \tag{2}$$

The accuracy of the solution depends on the number 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 obtained by means of variational integrals whose stationary values correspond to the true eigenvalues when the true eigenfunction are inserted in the integral. The variational integral for E is given by

$$E = \frac{\int_0^a \left(\frac{\hbar^2}{2\,m^*}\left(\frac{d\psi_k}{dx}\right)^2 + V(x)\,\psi_k^2\right) dx}{\int_0^a \psi_k^2\,dx} \tag{3}$$

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_k. Applying this condition, the following set of equations is obtained:

$$\sum_{n=1}^{N} a_{nk}\left(T_{ln} - \frac{2\,m^*}{\hbar^2}\,E_k\,\delta_{ln}\right) = 0 \qquad l = 1, 2, \ldots, N \tag{4}$$

$$T_{ln} = T_{nl} = \int_0^a \left(\frac{df_n}{dx}\,\frac{df_l}{dx} + \frac{2\,m^*}{\hbar^2}\,V(x)\,f_l\,f_n\right) dx \tag{5}$$

Solving these equations, the subband energies and the corresponding wave functions are determined. The electrostatic potential is then calculated by solving Poisson's equation. Knowing the electrostatic potential, the new potential energy function is calculated. For the next iteration, the effective potential energy function is expressed as a linear combination of its new and old values. The potential energy function is used to determine the wave functions which are then used to recalculate the carrier distribution. The procedure is repeated until initial and final values of $V(x)$, within the same iteration, differ by less than a specified error.

3. Two-dimensional scattering rates

The two dimensional scattering rates are calculated by defining the matrix element for scattering between the ith and the jth subbands according to

$$|M_{ij}|^2 = \int |M(Q, q)|^2\,|I_{ij}(q)|^2\,dq \tag{6}$$

where Q, $q$are the phonon wave vector components in parallel and normal to the hetero-interface, and $I_{ij}(q)$ means overlap integral

$$I_{ij}(q) = \int \psi_i(x)\,\psi_j(x)\,\exp(i\,q\,x)\,dx \tag{7}$$

$\psi(x)$ is the normalized envelope wavefunction. The closed form of the wavefunctions (2) decreases the required CPU time for calculating the 2D scattering rates compared to that of numerical integrations [1].

4. Application to an $Al_{0.7}Ga_{0.3}As/GaAs$ heterojuction

An $AlGaAs/GaAs$ heterojuction is considered with $N = 10^{21}\,cm^{-3}$ in a 0.09 μm $GaAs$ layer and $N = 10^{23}\,cm^{-3}$ in a 0.018 μm $AlGaAs$ layer. Both Rayleigh-Ritz and finite difference methods are applied to calculate the subband energies and the corresponding wavefunctions (Fig. 1). The numerical efficiency of the finite difference method is deteriorated by discretization and mesh size [3]. The wave functions are just numerically obtained so that any further application of these wave functions to calculate the scattering rates requires large CPU time because all quantities have to be calculated numerically [1]. Using Rayleigh-Ritz method, the required CPU time (Fig. 2b) to calculate the 2D scattering rates (Fig. 3) versus the number of subbands is nearly constant while it greatly changes using the finite difference method (Fig. 2a). This makes the application of the present method more practical in particular for device simulation.

5. Conclusion

An efficient variational method is applied to determine the electronic states inside heterostructure semiconductors by a self-consistent solution of Poisson's and Schrödinger's equation. Using this technique, the wave function is obtained in closed form which decreases the CPU time required for the calculation of the two-dimensional scattering rates. Moreover, the present method overcomes the limitations of the finite difference method which arise from mesh size and discretization.

Acknowledgement

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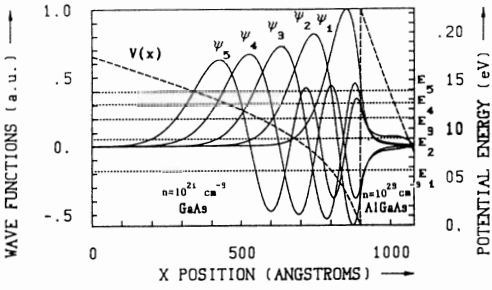

Fig.1 The self-consistent solution for the lowest five subband energies (dotted lines), the corresponding wave functions (solid lines), and the potential energy.

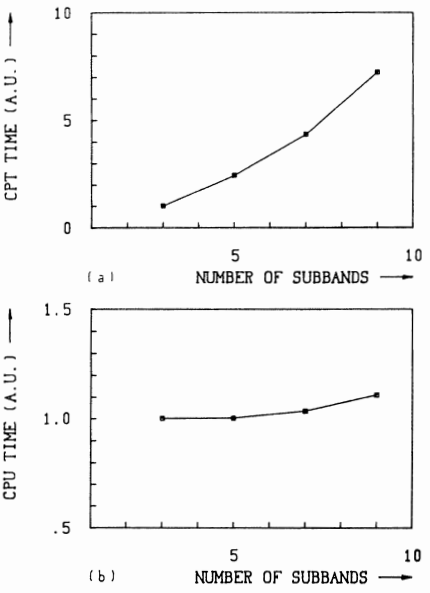

Fig.2 The required CPU time to calculate the 2D scattering rates versus the number of subbands.
a) finite difference method b) Rayleigh-Ritz method.

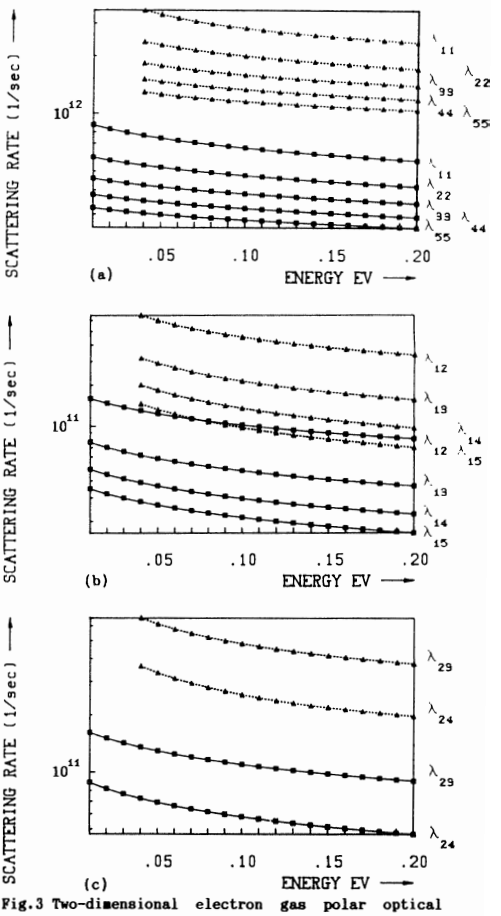

Fig.3 Two-dimensional electron gas polar optical scattering rates in the first five subbands versus electron energy. Solid lines stand for phonon absorption and dotted lines for phonon emission.
(a) intrasubband scattering.
(b) intersubband scattering for the first subband.
(c) intersubband scattering for the second subband.