A Nonlinear Iterative Method for InAs/GaAs Semiconductor Quantum Dots Simulation

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Abstract

A computational efficient nonlinear iterative method for computing the ground and excited state energies of an electron confined by an InAs quantum dot embedded in GaAs matrix is proposed. We treat the problem with the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, and the Ben Daniel-Duke boundary conditions. Computational results show that the parabolic band approximation is valid only for the dots with large volume. For excited states the nonparabolic effect has also been found to be stronger than for ground states.

1 Introduction

During the last decade the experimental development and theoretical study of semiconductor quantum dots (QDs) have been of great interests. For a well-fabricated QD the electron spectrum consists of a set of discrete levels and the density of levels becomes a set of δ-functions. This makes the semiconductor QDs very attractive for various applications in micro and nano optoelectronics [1-2].

In the modelling and simulation of semiconductor quantum dots, one needs a physical assumption about the electronic confinement potential in the QD system. Among those applied confinement potential models (the parabolic lateral potential and the infinite wall potential) (see [3] and references therein), a finite hard wall boundary potential model is the most realistic approach. In this case the problem cannot be solved analytically and it requires a computer modelling for the numerical simulation of such problems. In this paper, a computational efficient nonlinear iterative method for computing the ground and excited state energies and the corresponding wave functions of an electron confined by an InAs QD embedded in GaAs semiconductor matrix is presented for the first time. The model is formulated with the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation (so-called nonparabolic band approximation), and the Ben Daniel-Duke boundary conditions. In contrast to most of other calculations, our model includes a hard-wall (of finite height) 3D confinement potential that is induced by real discontinuity of the conduction band at

the edge of the InAs/GaAs QD. Based on a nonlinear iterative, the balanced and shifted QR, and inverse iteration methods, a novel solution algorithm for InAs/GaAs QD simulation is developed and successfully implemented. With the developed QD simulator, the effects of parabolic and nonparabilic band approximation in energy levels are studied for different shapes of QD. Our results show that the parabolic band approximation (effective mass is independent on energy) is applicable only for the dots with large volume. For excited electron states the nonparabolic effect has also been found to be stronger than for ground states. In Sec. 2, the QD model and computational method are stated. Results and discussions are presented in Sec. 3. Conclusions are given in Sec. 4.

2 A Quantum Dot Model and Computational Algorithm

We consider electrons confined in QD and use one-band effective Hamiltonian H [4].

$$H = -\frac{\hbar^2}{2}\nabla_r\left(\frac{1}{m(E,r)}\right)\nabla_r + V(r), \tag{1}$$

where $m(E, r)$ is the electron effective mass that depends on both energy and position

$$\frac{1}{m(E,r)} = \frac{P^2}{\hbar^2}\left[\frac{2}{E + E_g(r) - E_c(r)} + \frac{1}{E + E_g(r) + \Delta(r) - E_c(r)}\right], \tag{2}$$

and $V(r) = E_c(r)$ is the QD confinement potential. The $E_c(r)$, $E_g(r)$, $\Delta(r)$, and P are the position dependent electron band edge, band gap, spin-orbit splitting in the valance band, and momentum matrix element, respectively [9]. When the QD has a disk, ellipsoid, or conical shape of radius R_0 and of height z_0 we can solve the problem with cylindrical coordinate (R, ϕ, z). The QD system is cylindrical symmetry, so the wave function can be written as: $\Phi(r) = \Phi(R, z)\exp(il\phi)$, where $l = 0,\pm1,\pm2,...$ is the electron orbital quantum number and the model is reduced to

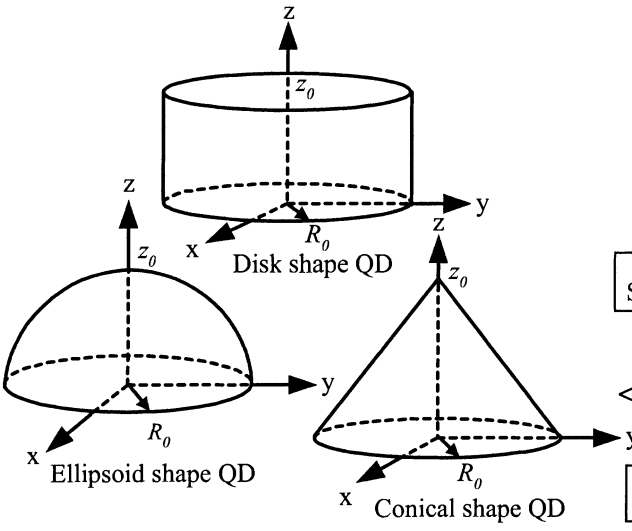
$$-\frac{\hbar^2}{2m_i(E)}\left(\frac{\partial^2}{\partial R^2} + \frac{\partial}{R\partial R} + \frac{\partial^2}{\partial z^2} - \frac{l^2}{R^2}\right)\Phi_i(R,z) + V_i(R,z)\Phi_i(R,z) = E\Phi_i(R,z) \tag{3}$$

where $V_{i=1}(R, z) = 0$ is inside the dot and $V_{i=2}(R, z) = V_0$ is outside the dot. The boundary conditions are

$$\Phi_1 = \Phi_2 \text{ and } \frac{1}{m_1(E)}\left\{\frac{\partial\Phi_1}{\partial R} + \frac{df_s}{dR}\frac{\partial\Phi_1}{\partial z}\right\} = \frac{1}{m_2(E)}\left\{\frac{\partial\Phi_2}{\partial R} + \frac{df_s}{dR}\frac{\partial\Phi_2}{\partial z}\right\}, \tag{4}$$

where $z = f_s(R, z)$ (s is disk, ellipsoid, or conical shape QD, see Fig. 1) presents a contour generator of the QD structure in (R, z) plane. To obtain a "self-consistent" solution of the model, we propose here a nonlinear iterative algorithm as shown in

Fig. 2. The feedback nonlinear iteration scheme is: (a) Set an initial energy E_0, (b) Compute effective mass m, (c) Solve Schrödinger equation with boundary conditions for energy E, (d) Back to (b). The iteration loop will be terminated when a specified stopping criterion on energy is reached. To solve the Schrödinger equation in step (c) a finite difference method with nonuniform mesh, balanced and shifted QR algorithm, and inverse iteration technique are applied in this work. The dominant method for solving matrix eigenvalue problem is still the QR algorithm, in the year 2000 [5].



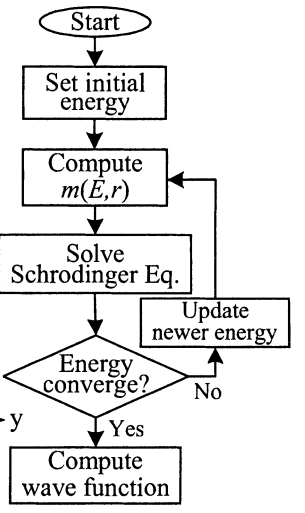


Fig. 1. Schematic diagram for various QDs. **Fig. 2.** A solution procedure for QD simulation.

3 Results and Discussions

The proposed nonlinear iterative method converges for various QD structures. It takes about 8-10 iteration loops to reach a stopping criterion in maximum energy error less than 10^{-7}. The global convergence mechanism is due to the effective mass is a monotone function in energy E. Fig. 3 shows the computed ground state ($l=0$) energies with parabolic and nonparabolic band effective mass approximations for R_0 = 10.0 nm (a) disk, (b) ellipsoid, and (c) conical shape QD, respectively. Similarly, Fig. 4 gives the excited state ($l=1$) energies for various QD shapes.

4 Conclusions

A novel computational technique for QD simulation has been proposed. With the developed QD simulator, we have found that the widely used the parabolic band approximation lead to a large discrepancy in calculation results for electron energy states in various small QDs. This parabolic approximation can be used only for large size QDs in the calculation of ground and excited state energies. The modelling, numerical method, and study presented here not only provide a novel way to calculate the energy levels of QD but also are useful to clarify principal

dependencies of QD energy states on material band parameter and QDs size for various QD shapes.

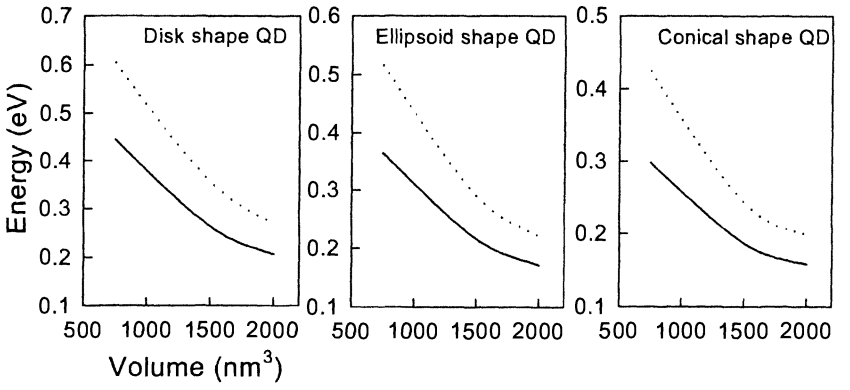


Fig. 3. Ground state (*l=0*) energy with nonparabolic (solid line) and parabolic (dot line) band effective mass approximations for (a) disk, (b) ellipsoid, and (c) conical shape InAs/GaAs QD.

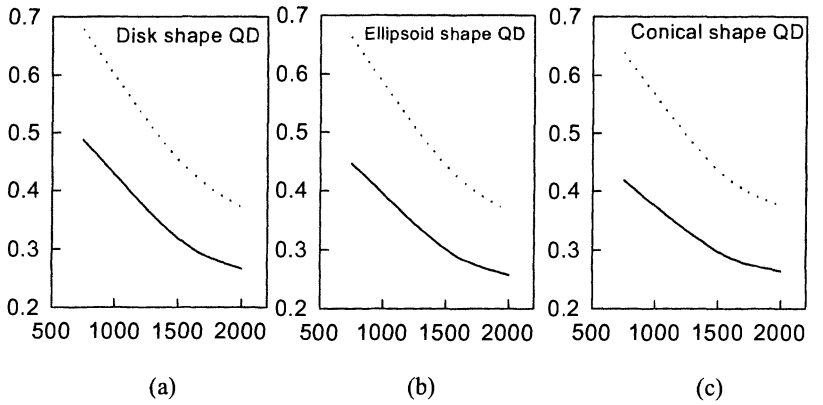


Fig. 4. Simulated results of the excited state (*l=1*) energy for various InAs/GaAs QDs.

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