Computer Physics Communications 140 (2001) 399–404

Computer Physics Communications

www.elsevier.com/locate/cpc

Electron energy level calculations for cylindrical narrow gap semiconductor quantum dot

Yiming Li [a,*], Jinn-Liang Liu [b], O. Voskoboynikov [a,c], C.P. Lee [a], S.M. Sze [a]

[a] *Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, Hsinchu 300, Taiwan*
[b] *Department of Applied Mathematics, National Chiao Tung University, Hsinchu 300, Taiwan*
[c] *Kiev Taras Shevchenko University, 64 Volodymirska st., 252030 Kiev, Ukraine*

Received 23 February 2001; accepted 4 May 2001

Abstract

Three computational techniques are presented for approximation of the ground state energy and wave function of an electron confined by a disk-shaped InAs quantum dot (QD) embedded in GaAs matrix. The problem is treated with the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, and the Ben-Daniel Duke boundary conditions. To solve the three dimensional (3D) Schrödinger equation, we employ (i) the adiabatic approximation, (ii) the adiabatic approximation with averaging, and (iii) full numerical solution. It is shown that the more efficient approximations (i) and (ii) can only be used for relatively large QD sizes. The full numerical method gives qualitative as well as quantitative trends in electronic properties with various parameters.

PACS: 73.20.Dx; 73.61.-r; 03.65.Ge; 02.60.Cb

Keywords: III-V semiconductor; Cylindrical quantum dot; Electronic structure; Electron states; Computer simulation; Calculation methods

1. Introduction

During the last decade the study of semiconductor quantum dots (QDs) has been of a great interest (see [1–3] and references therein). Unique electronic characteristics of the QDs make it possible to model atomic physics in macroscopic systems experimentally and theoretically [4]. The interest originates from an ultimate limit of size quantization in those objects. For an ideal 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 applications in micro and nano optoelectronics [2].

In this work we present and compare three computational techniques that are used to obtain the ground state energy and the corresponding wave function of an electron confined by an InAs QD embedded in GaAs matrix. The dot has a disk shape with radius ρ_0 and thickness z_0. We treat the problem with the effective one electronic

* Corresponding author.
E-mail address: ymli.ee87g@nctu.edu.tw (Y. Li).

0010-4655/01/$ – see front matter
PII: S0010-4655(01)00291-0

band Hamiltonian, the energy and position dependent electron effective mass approximation, and the Ben Daniel-Duke boundary conditions. In contrast to most of other calculations we use a hard-wall (of finite height) 3D confinement potential that is induced by real discontinuity of the conduction band at the edge of the dot. To solve the 3D Schrödinger equation we employ (i) the adiabatic approximation, (ii) the adiabatic approximation with averaged Hamiltonian along the z direction [5], and (iii) a numerical scheme for the full model by using the finite difference method, balanced and shifted QR algorithm [6,7], and inverse iteration technique [8]. We found that the approximation models (i) and (ii) lead to good results in calculating the electron ground state for relatively large sizes of QDs.

2. Model outline

We consider 3D QD structures in the one-band envelope-function formalism in which the effective Hamiltonian is given by [9]

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

where $\nabla_{\mathbf{r}}$ stands for the spatial gradient, $m(E,\mathbf{r})$ is the electron effective mass depending on both energy and position and is expressed as

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

$V(\mathbf{r})$ is the confinement potential, $E_g(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand respectively for the position dependent band gap and the spin-orbit splitting in the valence band, and P is the momentum matrix element. For systems with a sharp discontinuity of the conduction band on the interface between the quantum dot (material 1) and the crystal matrix (material 2), the hard-wall confinement potential can be presented as $V(\mathbf{r}) = 0$ for material 1, and $V(\mathbf{r}) = V_0$ for material 2, respectively. Integrating the Schrödinger equation with Hamiltonian (1) along the direction perpendicular to the interface, we obtain the Ben-Daniel Duke boundary conditions for wave function $\Psi(\mathbf{r})$

$$\begin{aligned} &\Psi_{\text{material 1}}(\mathbf{r}_s) = \Psi_{\text{material 2}}(\mathbf{r}_s), \\ &\frac{\hbar^2}{2m(E,\mathbf{r}_s)}\nabla_n\Psi(\mathbf{r}_s) = \text{const}, \end{aligned} \tag{3}$$

where $\mathbf{r}_s$ denotes position of the system interface. Eqs. (1) and (3) can be used to calculate the electron energy levels in the QD.

We consider specifically a disk-shaped QD with the radius ρ_0 and the thickness z_0 in the cylindrical coordinates (ρ,ϕ,z). The origin of the system lies at the center of the disk and the z-axis being chosen along the rotation axis. Since the system is cylindrically symmetric, the wave function can be represented as $\Psi(\mathbf{r}) = \Phi(\rho,z)\exp(\mathrm{i}l\phi)$, where $l = 0, \pm1, \pm2, \ldots$ is the orbital quantum number. To derive an equation for $\Phi(\rho,z)$, we first use the adiabatic approximation [5,10,11] in which an approximate solution can be taken of the form $\Phi(\rho,z) \simeq R(\rho)Z(z)$. The model is then reduced to a one-dimensional (1D) quantum well problem in which the electron motion is hypothetically constrained in the z-direction. The wave function of the ground state of this problem has the form

$$Z(z) = \begin{cases} A\cos(kz), & |z| < z_0/2, \\ B\exp(-\varkappa|z|), & |z| \geqslant z_0/2, \end{cases} \tag{4}$$

where A and B are related by $B = A\cos(kz_0/2)\exp(\varkappa z_0/2)$, $k(E_\rho, E_z) = \sqrt{2m_1(E)E_z}/\hbar$, and $\varkappa(E_\rho, E_z) = \sqrt{2m_2(E)(V_0 - E_z)}/\hbar$, respectively. The $m_i(E)$ is the energy dependent electron effective mass inside $(i = 1)$

and outside ($i = 2$) the dot, $E = E_\rho + E_z$ is the total electron energy that consists of the ρ and z-direction motion effective energies. From the spin independent Ben-Daniel Duke boundary conditions (3), we can obtain a transcendental equation [9]

$$\tan\left[\frac{k(E_\rho, E_z)z_0}{2}\right] = \frac{m_1(E)}{m_2(E)}\frac{\varkappa(E_\rho, E_z)}{k(E_\rho, E_z)}. \tag{5}$$

Eq. (5) gives the $E_z(E_\rho)$ dependence in an implicit form. Introducing (4) in Eq. (1), defining an effective radial Hamiltonian by taking the average $\int \mathrm{d}z\, Z^*(z)\widehat{H}Z(z) = \widehat{H}_\rho$ (after a proper normalization), and neglecting the kinetic energy contribution from the z-dependent part for $\rho \geqslant \rho_0$, we obtain the following quasi 1D Schrödinger equations in the ρ-direction [5]

$$\begin{aligned}
&-\frac{\hbar^2}{2\widetilde{m}_1(E_\rho, E_z)}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\,\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right)R_1(\rho) = E_\rho R_1(\rho), \quad \rho < \rho_0,\\
&-\frac{\hbar^2}{2m_2(E)}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\,\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right)R_2(\rho) = \big[E_\rho + E_z(E_\rho) - V_0\big]R_2(\rho), \quad \rho \geqslant \rho_0,
\end{aligned} \tag{6}$$

with the boundary conditions

$$R_1(\rho_0) = R_2(\rho_0) \quad \text{and} \quad \frac{1}{\widetilde{m}_1}\frac{\mathrm{d}R_1}{\mathrm{d}\rho}\bigg|_{\rho_0} - \frac{1}{m_2}\frac{\mathrm{d}R_2}{\mathrm{d}\rho}\bigg|_{\rho_0} = 0, \tag{7}$$

where

$$\begin{aligned}
\frac{1}{\widetilde{m}_1(E_\rho, E_z)} = C\Bigg\{&\frac{1}{m_1(E)}\left(\frac{d}{2} + \frac{m_2(E)}{\varkappa(E_\rho, E_z)m_1(E)}\sin^2\left[\frac{k(E_\rho, E_z)z_0}{2}\right]\right)\\
&+ \frac{1}{m_2(E)}\frac{\cos^2\left[\frac{k(E_\rho, E_z)z_0}{2}\right]}{\varkappa(E_\rho, E_z)}\Bigg\},
\end{aligned} \tag{8}$$

$$C(E_\rho, E_z) = \frac{2}{d + \frac{2}{\varkappa(E_\rho, E_z)}\left\{\cos^2\left[\frac{k(E_\rho, E_z)z_0}{2}\right] + \frac{m_2(E)}{m_1(E)}\sin^2\left[\frac{k(E_\rho, E_z)z_0}{2}\right]\right\}}. \tag{9}$$

Eq. (6) with the boundary conditions (7) are used to obtain the function $R(\rho)$. A formal solution of (6) is well known as follows

$$R_1(\rho) = AJ_{|l|}\big[p(E_\rho, E_z)\rho\big], \qquad R_2(\rho) = BK_{|l|}\big[\gamma(E_\rho, E_z)\rho\big],$$

where J_n and K_n are, respectively, the Bessel function and the modified Bessel function, and $p(E_\rho, E_z) = \sqrt{2\widetilde{m}_1(E)E_\rho}/\hbar$, $\gamma(E_\rho, E_z) = \sqrt{2m_2(E)(V_0 - E_\rho - E_z)}/\hbar$. Applying the boundary conditions (7), the solution leads to the following eigenvalues of energy of the problem

$$\begin{aligned}
&\frac{p(E_\rho, E_z)}{\widetilde{m}_1(E_\rho, E_z)}\left\{\frac{|l|}{p(E_\rho, E_z)\rho_0}J_{|l|}\big[p(E_\rho, E_z)\rho_0\big] - J_{|l|+1}\big[p(E_\rho, E_z)\rho_0\big]\right\}K_{|l|}\big[\gamma(E_\rho, E_z)\rho_0\big]\\
&- \frac{\gamma(E_\rho, E_z)}{m_2(E)}\left\{\frac{|l|}{\gamma(E_\rho, E_z)\rho_0}K_{|l|}\big[\gamma(E_\rho, E_z)\rho_0\big] - K_{|l|+1}\big[\gamma(E_\rho, E_z)\rho_0\big]\right\}J_{|l|}\big[p(E_\rho, E_z)\rho_0\big] = 0.
\end{aligned} \tag{10}$$

Eqs. (5) and (10) are solved to give the values of the total energy $E = E_z + E_\rho$. The energy is a complicated function of the dot parameters and the electron angular momentum. The energy system consists of discrete levels enumerated by a set of numbers $\{n, l\}$, where n denotes to the nth solution of (10) with fixed l. The energy dependence of the electron effective mass requires to solve the problem self-consistently so that more realistic values of QD characteristics can be obtained.

The approximate description of the ground state of a quantum disk based on the effective index method has both advantages and limitations [5]. More general but more expensive approaches are direct numerical solutions of the Schrödinger equation for which we consider both adiabatic and full approximations. The adiabatic approximation model for $l = 0$ is given by

$$-\frac{\hbar^2}{2m_j}\frac{1}{\rho}\left(\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}}{\mathrm{d}\rho}R\right)\right) + V_0 R = E_\rho R, \quad j = 1, 2, \tag{11}$$

$$-\frac{\hbar^2}{2m_j}\frac{\mathrm{d}^2}{\mathrm{d}z^2}Z + V_0 Z = E_z Z, \quad j = 1, 2. \tag{12}$$

The full approximation model for $l = 0$ is given by

$$-\frac{\hbar^2}{2m_j}\frac{1}{\rho}\left(\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\Phi\right)\right) - \frac{\hbar^2}{2m_j}\frac{\partial^2\Phi}{\partial z^2} + V_0\Phi = E\Phi, \quad j = 1, 2. \tag{13}$$

The models (11)–(13) are subject to proper Ben-Daniel Duke boundary conditions as discussed above.

3. Numerical methods and results

We now present three numerical algorithms for the computer simulation of the QD structures. All discretizations to Eqs. (11)–(13) are based on the finite difference method with nonuniform mesh technique. The resulting eigenvalue problems are then solved with balanced and shifted QR algorithm [6,7] as well as inverse iteration method [6,8].

Algorithm 1 (*Adiabatic Approximation Method*).
Step 1.1: Set $E_\rho = 0$, $E_Z = 0$.
Step 1.2: Set $E = E_\rho + E_Z$.
Step 1.3: Compute m_j via (2). Solve (11) for E_ρ. If E_ρ converges, then go to Step 1.4; otherwise go to Step 1.2.
Step 1.4: Set $E = E_\rho + E_Z$.
Step 1.5: Compute m_j via (2). Solve (12) for E_Z. If E_Z converges, then go to Step 1.6; otherwise go to Step 1.4.
Step 1.6: Set $E = E_\rho + E_Z$. If the total energy E converges, then stop; otherwise go to Step 1.3.

Algorithm 2 (*Adiabatic Approximation Method with Averaged Hamiltonian along z-Direction*).
Step 2.1: Set $E_\rho = 0$, $E_Z = 0$.
Step 2.2: Set $E = E_\rho + E_Z$.
Step 2.3: Compute m_j via (2). Solve (12) for E_Z. If E_Z converges, then go to Step 2.4; otherwise go to Step 2.2.
Step 2.4: Set $E = E_\rho + E_Z$.
Step 2.5: Compute m_j via (2). Take the averages of Hamiltonian along z direction, and then solve (11) for E_ρ. If E_ρ converges, then go to Step 2.6; otherwise go to Step 2.4.
Step 2.6: Set $E = E_\rho + E_Z$. If the total energy E converges, then stop; otherwise go to Step 2.3.

Algorithm 3 (*Full Approximation Method*).
Step 3.1: Set $E = 0$.
Step 3.2: Compute m_j via (2). Solve (13) for E.
Step 3.3: If E converges, then stop; otherwise update E and go to Step 3.2.

Fig. 1 illustrates ground state energies of an electron confined by an InAs quantum disk in the GaAs matrix with various disk sizes using these three algorithms. In our calculations we choose conventional semiconductor

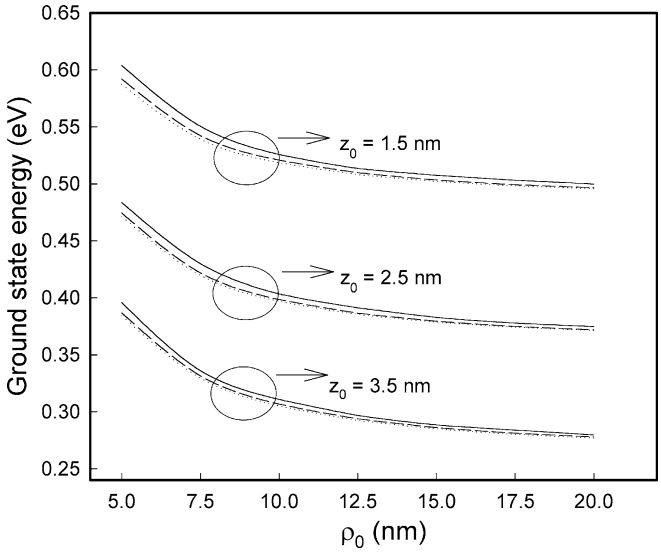

Fig. 1. The ground state energies for various disk sizes. The solid, dash, and dotted lines are the full numerical solution, adiabatic approximation, and adiabatic approximation with averaged Hamiltonian, respectively.

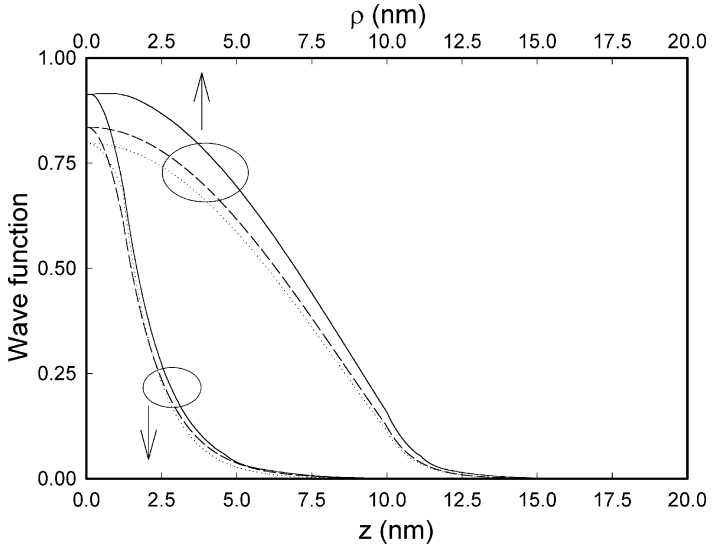

Fig. 2. The wave functions for the disk with $\rho_0 = 10.0$ nm and $z_0 = 2.5$ nm. The solid, dash, and dotted lines are the full numerical solution, adiabatic approximation, and adiabatic approximation with averaged Hamiltonian, respectively.

band structure parameters [12] for InAs: energy gap is $E_{1g} = 0.42$ eV, spin-orbit splitting is $\Delta_1 = 0.48$ eV, the value of the non-parabolicity parameter is $E_{1p} = 3m_0P_1^2/\hbar^2 = 22.2$ eV from which we recalculated P^2, m_0 is the free electron mass; and for GaAs: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, $E_{2p} = 24.2$ eV. The band offset is taken as $V_0 = 0.77$ eV.

For dots of relatively large radius ($R_0 > 20$ nm) the ground state energy can be obtained by both adiabatic algorithms in a very good agreement with the full approximation method. The results of different algorithms differ

noticeably for dots with small sizes. At the same time the electron ground state energy for dots of a small height ($z_0 \sim 1.5$ nm) demonstrate larger deviations in results even for dots with $R_0 \sim 20$ nm. This is contrary to traditional suggestions that the main adiabatic algorithms can be used when the difference between R_0 and z_0 is large [5]. This result can be understood from the following. In adiabatic algorithms we have the lowest possible estimate of the electron energy because these algorithms do not include a part of the electron kinetic energy from the matrix region [5]. At the same time, as can be seen from the ground state wave functions distributions (see Fig. 2), for dots of a small height (and of a small size in general) the electron wave function is widely spread out of the dot. In such a condition the outside part of the electron kinetic energy plays an important role and a deviation between the adiabatic algorithms and full approximation method results becomes larger. This conclusion should be taken into consideration when the adiabatic algorithms are used. We can conclude that the full numerical approximation method for three dimensional cylindrical quantum dots is necessary if one is interested in both qualitative as well as quantitative trends in electronic properties of semiconductor quantum dots.

Acknowledgements

This work was partially supported by the National Science Council of Taiwan under contract number NSC89-2215-E-009-055.

References

[1] D. Bimberg, M. Grundmann, F. Heirichdorff et al., Thin Solid Films 367 (2000) 235–249.
[2] D. Bimberg, Semicond. 33 (1999) 951–955.
[3] N.N. Ledentsov, V.M. Ustinov, V.A. Shchukin et al., Semicond. 32 (1998) 343–365.
[4] P.A. Maksym, T. Chakraborty, Phys. Rev. Lett. 65 (1990) 108–111.
[5] G. Lamouche, Y. Lépine, Phys. Rev. B 51 (1995) 1950–1955.
[6] J.H. Wilkinson, C. Reinsch, Linear Algebra II of Handbook for Automatic Computation, Springer-Verlag, 1971.
[7] D.S. Watkins, J. Comp. App. Math. (2000) 67–83.
[8] I.C.F. Ipsen, SIAM Rev. 39 (1997) 254–291.
[9] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, Les Edition de Physique, Les Ulis, 1988.
[10] F.M. Peeters, V.A. Schweigert, Phys. Rev. B 53 (1996) 1468–1474.
[11] A. Wojs, P. Hawrylak, S. Farad et al., Phys. Rev. B 54 (1996) 5604–5608.
[12] M. Levinshtein, S. Rumyantsev, Sur (Eds.), Handbook Series on Semiconductor Parameters, World Scientific, Singapore, 1999.