

# Electron energy level calculations for semiconductor nanostructures

Marta M. Betcke<sup>1</sup> and Heinrich Voss<sup>2\*</sup>

<sup>1</sup> The University of Manchester, School of Mathematics, Oxford Road, M13 9PL, Manchester, United Kingdom

<sup>2</sup> Hamburg University of Technology, Institute of Numerical Simulation, D-21071 Hamburg, Germany

Although self-assembled quantum dots are grown on wetting layers, most simulations exclude the wetting layer. The neglected effects on the electronic structure of a pyramidal InAs quantum dot embedded in a GaAs matrix are investigated based on the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, and a finite height hard-wall 3D confinement potential.

Copyright line will be provided by the publisher

## 1 The governing Schrödinger equation

Semiconductor nanostructures have attracted tremendous attention in the past few years because of their unique physical properties and their potential for applications in micro- and optoelectronic devices. In such nanostructures, the free carriers are confined to a small region of space by potential barriers, and if the size of this region is less than the electron wavelength, the electronic states become quantized at discrete energy levels. The ultimate limit of low dimensional structures is the quantum dot, in which the carriers are confined in all three directions.

Quantum dots can be produced today by the Stranski–Krastanov process which uses the relief of the elastic energy when two materials with a large lattice mismatch form an epitaxial structure. The deposited layer initially grows as a thin two dimensional (2D) wetting layer. As the deposited layer exceeds a critical thickness, the growth mode switches from 2D to 3D leading to the formation of a self-assembled quantum dot on top of the wetting layer.

Most simulations neglect the effect of wetting layers on the electronic structure of self-assembled quantum dots (cf. [2, 4] and the literature given therein). In this paper we report on numerical simulations investigating the effect of a wetting layer on the electronic structure of a pyramidal InAs quantum dot embedded in a GaAs matrix. We consider the one-band envelope-function formalism assuming non-parabolicity for the electron's dispersion relation and an electron effective mass depending on the position and the energy level.

Let  $\Omega_q \subset \mathbb{R}^3$  be a domain occupied by the quantum dot with the possible inclusion of the wetting layer, which is embedded in a bounded matrix  $\Omega_m$  of different material. A typical example is an InAs pyramidal quantum dot grown on a wetting layer, which is embedded in a cuboid GaAs matrix. The governing equation is the Schrödinger equation

$$-\nabla \cdot \left( \frac{\hbar^2}{2m(x, \lambda)} \nabla \psi \right) + V(x)\psi = \lambda\psi, \quad x \in \Omega_q \cup \Omega_m, \quad (1)$$

where  $\hbar$  is the reduced Planck constant,  $m$  is the effective mass of electrons in the conduction band, which is a function of the energy level  $\lambda$ ,  $V$  denotes the position dependent confinement potential, and  $\psi$  is the wave function.

Assuming non-parabolicity for the electron's dispersion relation, the electron effective mass  $m(\lambda, x)$  is constant on  $\Omega_q$  and on the matrix  $\Omega_m$  for every fixed energy level  $\lambda$ , and is given by [2]

$$\frac{1}{m_j(\lambda)} := \frac{1}{m(\lambda, x)} \Big|_{x \in \Omega_j} = \frac{P_j^2}{\hbar^2} \left( \frac{2}{\lambda + E_{g,j} - V_j} + \frac{1}{\lambda + E_{g,j} - V_j + \Delta_j} \right), \quad (2)$$

for  $j \in \{m, q\}$ , where the confinement potential  $V_j := V|_{\Omega_j}$  is piecewise constant, and  $P_j$ ,  $E_{g,j}$  and  $\Delta_j$  denote the momentum matrix element, the band gap, and the spin-orbit splitting in the valence band for the quantum dot material ( $j = q$ ) and the matrix ( $j = m$ ), respectively.

Since the wave function decays outside of the quantum dot (and possibly the wetting layer) very rapidly, it is reasonable to assume homogeneous Dirichlet conditions  $\psi = 0$  on the horizontal part  $\partial\Omega_h$  of the outer boundary of  $\Omega_m$ . On the vertical part the outer boundary of  $\Omega_m$  we impose Neumann boundary conditions  $\frac{\partial\psi}{\partial n} = 0$ , since far away from the quantum dot wave functions must approach asymptotically ordinary quantum well envelope functions (where the wetting layer is the quantum well). On the interface between the quantum dot material and the matrix the Ben Daniel–Duke condition holds

$$\frac{1}{m_q} \frac{\partial\psi}{\partial n_q} \Big|_{\partial\Omega_q} = \frac{1}{m_m} \frac{\partial\psi}{\partial n_m} \Big|_{\partial\Omega_m}, \quad x \in \partial\Omega_q \cap \partial\Omega_m. \quad (3)$$

Here  $n_q$  and  $n_m$  denote the outward unit normal on the boundary of  $\Omega_q$  and  $\Omega_m$ , respectively.

\* Corresponding author: e-mail: voss@tu-harburg.de, Phone: +49 40 42878 3279, Fax: +49 40 42878 2696

**Table 1** Electronic eigenstates

	pure QD	QD/WL 0.3 nm	QD/WL 0.6 nm	pure WL 0.6 nm
dimension	46291	65505	48778	10555
CPU	92.1	155.3	381.0	16.1
$\lambda_1$	0.3679	0.3504	0.3340	0.6962
$\lambda_{2/3}$	0.5338	0.5092	0.4858	0.7055
$\lambda_4$	0.6464	0.6173	0.5887	0.7147
$\lambda_5$	0.6541	0.6243	0.5954	0.7328
$\lambda_6$	0.7154	0.6827	0.6498	0.7328
$\lambda_7$	0.7473	0.7171	0.6839	0.7417

Let  $\Omega := \bar{\Omega}_q \cup \Omega_m$  and  $H := \{\psi \in H^1(\Omega) : \psi = 0 \text{ on } \partial\Omega_h\}$ . Multiplying equation (1) by  $\phi \in H$  and integrating by parts, one gets the variational form of the Schrödinger equation, and similar to [4] the nonlinear minmax theory [5] yields, that there exists a countable set of positive eigenvalues  $0 < \lambda_1 \leq \lambda_2 \leq \dots \rightarrow \infty$  of finite multiplicity.

Discretizing by finite elements results in a rational matrix eigenvalue problem

$$T(\lambda)x = \lambda Mx - \frac{1}{m_1(\lambda)} A_1 x - \frac{1}{m_2(\lambda)} A_2 x - Bx = 0 \quad (4)$$

with symmetric  $T(\lambda) \in \mathbb{R}^{n \times n}$  which has also real eigenvalues.

Typically  $T(\lambda)$  is large and sparse, and its eigenvalues can be determined by iterative projection methods like the nonlinear Arnoldi or the Jacobi–Davidson method where the projected eigenvalue problems can be solved by safeguarded iteration [1, 3].

## 2 Numerical results

We consider a pyramidal quantum dot with width 12.4 nm and height 6.2 nm embedded in a cuboid matrix of size 24.8 nm × 24.8 nm × 18.6 nm. We computed the electronic levels of the pure dot without a wetting layer, for the combined quantum dot and wetting layer structures for two wetting layers of thickness 0.3 nm and 0.6 nm, respectively, and of the corresponding pure wetting layers. In our numerical simulations we used the following semiconductor band structure parameters:  $P_q = 0.8503$ ,  $E_{g,q} = 0.42$ ,  $\delta_q = 0.48$ , and  $V_q = 0$  for InAs;  $P_m = 0.8878$ ,  $E_{g,m} = 1.52$ ,  $\delta_m = 0.34$ , and  $V_m = 0.77$  for GaAs.

We discretized the Schrödinger equation by the finite element method with quadratic Lagrangian elements on a tetrahedral grid. Since the envelope functions are mainly confined to the quantum dot (which occupies less than 3% of  $\Omega$ ) and the wetting layer, and since they decay very rapidly outside the quantum dot/wetting layer structure, we chose a non-uniform grid such that roughly half of the degrees of freedom correspond to the InAs structure and the remaining ones to the GaAs matrix.

The arising rational eigenvalue problems were solved under MATLAB 2006b on an Intel Xeon processor with 8 GByte RAM and 3.4 GHz by the nonlinear Arnoldi method. We started the method with a constant vector on  $\bar{\Omega}_q \cup \Omega_m$  which is far away from an eigenvector, and we terminated the iteration for an eigenvalue, if the residual norm was less than  $10^{-8}$ . Due to the symmetry of the problem there exist multiple eigenvalues (for instance the second eigenvalue in all cases). The Arnoldi method had no problems to detect these multiple eigenvalues with the right multiplicity.

We first consider the pure quantum dot problem which has seven energy eigenvalues smaller than the confinement potential  $V_m = 0.77$  displayed in the second column of Tab. 1. The discretized problem has 46291 degrees of freedom, and it takes 92.1 seconds to solve it. The envelope functions  $\psi_j$  corresponding to these states are essentially confined to the quantum dot.

Next we added to the quantum dot a wetting layer of thickness 0.3 nm and 0.6 nm, respectively. In this case there are 10 and 17 eigenvalues smaller than  $V_m$ , respectively, most of them being approximate quantum well eigenstates corresponding to the pure wetting layer. The smallest 7 eigenvalues are shown in columns 3 and 4 in Tab. 1. They are substantially smaller than the corresponding ones of the pure quantum dot demonstrating that the wetting layer can not be neglected when simulating the electronic behavior of semiconductor nanostructures.

## References

- [1] M.M. Betcke. *Iterative Projection Methods for Symmetric Nonlinear Eigenvalue Problems with Applications*. PhD thesis, Institute of Numerical Simulation, Hamburg University of Technology, 2007.
- [2] Y. Li. Numerical calculation of electronic structure for three-dimensional nanoscale semiconductor quantum dots and rings. *J. Comput. Electronics*, 2:49 – 57, 2003.
- [3] H. Voss. An Arnoldi method for nonlinear eigenvalue problems. *BIT Numerical Mathematics*, 44:387 – 401, 2004.
- [4] H. Voss. A rational eigenvalue problem governing relevant energy states of a quantum dots. *J. Comput. Phys.*, 217:824 – 833, 2006.
- [5] H. Voss and B. Werner. A minimax principle for nonlinear eigenvalue problems with applications to nonoverdamped systems. *Math. Meth. Appl. Sci.*, 4:415–424, 1982.