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# Numerical computation of pyramidal quantum dots with band non-parabolicity

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ABSTRACT

This paper presents an effective and feasible eigen-energy scanning method to solve polynomial matrix eigenvalues introduced by 3D quantum dots problem with band non-parabolicity. The pyramid-shaped quantum dot is placed in a computational box with uniform mesh in Cartesian coordinates. Its corresponding Schrödinger equation is discretized by the finite difference method. The interface conditions are incorporated into the discretization scheme without explicitly enforcing them. By comparing the eigenvalues from isolated quantum dots and a vertically aligned regular array of them, we investigate the coupling effect for variable distances between the quantum dots and different size.



## 1. Introduction

Nanoscale semiconductor quantum dots (QDs) have been investigated extensively in science [1–3] and for applications [4–6]. Besides theoretical and experimental methods, numerical simulation can offer insights into the electronic and optical properties of quantum dots [7,8]. There is a wide range of numerical methods: expressing the wave function as a series of orthogonal functions [9], Fourier expansion [10], plane wave expansion [11], $\mathbf{k}\cdot\mathbf{p}$ perturbation theory [12], finite element method [13], finite differences [14] and so on. When moving to higher dimensions, the methods based on Fourier-type expansions and direct diagonalization become expensive in terms of both memory and CPU time. The finite difference method, simple, flexible and portable, has found widespread application in scientific and technical computation. When dealing with 3D quantum structures, especially if

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taking the spin-orbit split-off effect into account, the CPU time and memory resources soon get exhausted because there are too many mesh nodes. In order to solve a large and complex 3D system, one has to resort to a different, less demanding computational technique.

In this paper we present a novel energy scanning method. Although based on the finite difference method, the characteristics of the wave functions are estimated which allows to control and dynamically adjust the relevant parameters.

Pyramid-shaped quantum dots are a standard product of modern semiconductor manufacturing. For that reason we aim at computing the relevant energy states (eigenvalues) and the corresponding wave functions (eigenvectors) of an regular three-dimensional array of such quantum dots. We explain and test our computational scheme for electrons in a non-parabolic conduction band. Thereby the coupling between neighboring quantum dots can be analyzed as well.

## 2. Theoretical model

We consider a pyramidal InAs quantum dot embedded in the center of a cuboid GaAs matrix. The baselines of both should be parallel. Fig. 1 illustrates this. $h$ is the height of the quantum dot pyramid and $a$ its base length.

The governing equation for this problem is the Schrödinger equation

$$-\nabla \cdot \left\{ \frac{\hbar^2}{2m(\boldsymbol{r},\lambda)} \nabla\psi \right\} + V(\boldsymbol{r})\psi = \lambda\psi, \tag{1}$$

where $\hbar$ is Planck's constant, $\lambda$ the unknown energy eigenvalue and $\psi = \psi(\boldsymbol{r})$ the corresponding eigenfunction for the electron under discussion. The effective electron mass $m = m(\boldsymbol{r},\lambda)$ and the confinement potential $V = V(\boldsymbol{r})$ are discontinuous across the heterojunction.

The dependence of $m(\boldsymbol{r},\lambda)$ on $\lambda$ can be calculated from eight-band $\mathbf{k}\cdot\mathbf{p}$ analysis and effective mass theory [15]. With properly chosen base functions, the effective Hamiltonian $H_{\text{eff}}$ defined in (1) can be block-diagonalized and gives the effective mass $m(\boldsymbol{r},\lambda)$.

Let us denote by $m_1(\lambda)$ the effective mass within the quantum dot and by $m_2(\lambda)$ the effective mass of the matrix. Likewise, $V_1(\lambda)$ is the effective potential of the quantum dot and $V_2$ of the matrix. Kane's matrix element [16] $P_k$ is given by

$$P_k^2 = \frac{3\hbar^2}{2} \frac{1/m_k(\lambda) - 1/m_0}{2/(\lambda + g_k - V_k) + 1/(\lambda + g_k - V_k + \delta_k)}. \tag{2}$$

Here, $m_0, g_k$ and $\delta_k$ are the bulk effective mass, the conduction and spin-orbit split-off band gaps for the quantum dot $(i = 1)$ and for the matrix $(i = 2)$. Because the effective masses $m_k$ are much smaller that the bulk effective electron mass $m_0$ one may approximate by

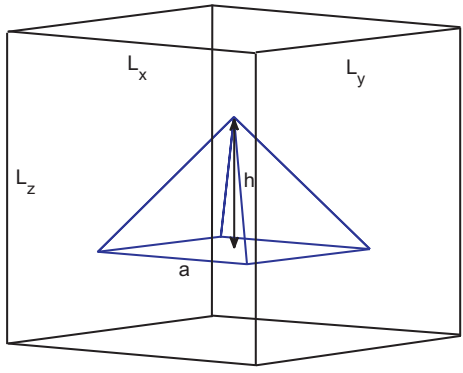


**Fig. 1.** Scheme of a single pyramid quantum dot with height $h$ and base length $a$ embedded in the center of a cuboid GaAs matrix cell of dimensions $L_x, L_y$ and $L_z$, respectively.