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An efficient finite-difference scheme for computation of electron states in free-standing and core–shell quantum wires

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ABSTRACT

The electron states in axially symmetric quantum wires are computed by means of the effective-mass Schrödinger equation, which is written in cylindrical coordinates φ, ρ, and z. We show that a direct discretization of the Schrödinger equation by central finite differences leads to a non-symmetric Hamiltonian matrix. Because diagonalization of such matrices is more complex it is advantageous to transform it in a symmetric form. This can be done by the Liouville-like transformation proposed by Rizea et al. (2008), which replaces the wave function $\psi(\rho)$ with the function $F(\rho) = \psi(\rho)\sqrt{\rho}$ and transforms the Hamiltonian accordingly. Even though a symmetric Hamiltonian matrix is produced by this procedure, the computed wave functions are found to be inaccurate near the origin, and the accuracy of the energy levels is not very high. In order to improve on this, we devised a finite-difference scheme which discretizes the Schrödinger equation in the first step, and then applies the Liouville-like transformation to the difference equation. Such a procedure gives a symmetric Hamiltonian matrix, resulting in an accuracy comparable to the one obtained with the finite element method. The superior efficiency of the new finite-difference scheme (*FDM*) is demonstrated for a few ρ-dependent one-dimensional potentials which are usually employed to model the electron states in free-standing and core–shell quantum wires. The new scheme is compared with the other *FDM* schemes for solving the effective-mass Schrödinger equation, and is found to deliver energy levels with much smaller numerical error for all the analyzed potentials. It also gives more accurate results than the scheme of Rizea et al., except for the ground state of an infinite rectangular potential in freestanding quantum wires. Moreover, the $\mathcal{PT}$ symmetry is invoked to explain similarities and differences between the considered *FDM* schemes.

1. Introduction

Recent advances in nanowire (quantum wire) fabrication technology have led to an increased interest in the *vapor–liquid–solid* (VLS) method [1]. It is a bottom-up process, which has been used to produce freestanding quantum wires [2], core–shell quantum wires [3,4], nanowire superlattices [5], branched nanowires [6], etc. They have been made out of various semiconductors, including III–V compounds [3], silicon [7], germanium [8], and their alloys. The huge progress in the field has been driven by actual and potential applications of nanowires in electronics and photonics. For example, transistors [9], photovoltaic devices [10], light-emitting diodes [11], lithium batteries [12], and chemical and biological sensors [13] have all been realized using nanowires.

In addition to advances in production tools, the models of electronic structure of quantum wires has substantially progressed during time, both in increasing complexity and higher precision [14]. For example, *ab initio* methods are currently able to predict experimental results with sub-meV accuracy [14], but are over-complex to use for large wires. For the latter, however, use of the effective methods, such as the effective-mass and $\mathbf{k}\cdot\mathbf{p}$ theories, may be suitable [15–18]. We note that modeling of electronic structure is essentially important to understand transport and optical properties of nanostructures and nanodevices. Moreover, the electronic structure models of quantum wires provide a reliable and an inexpensive way to design quantum wire systems with specific properties.

A convenient model for the electron states in quantum wires which are wider than about 2 nm is the effective-mass theory. It has the form of the Schrödinger equation written for the case of position dependent effective mass, and is able to capture the essential physics of the electron states. In practice it usually

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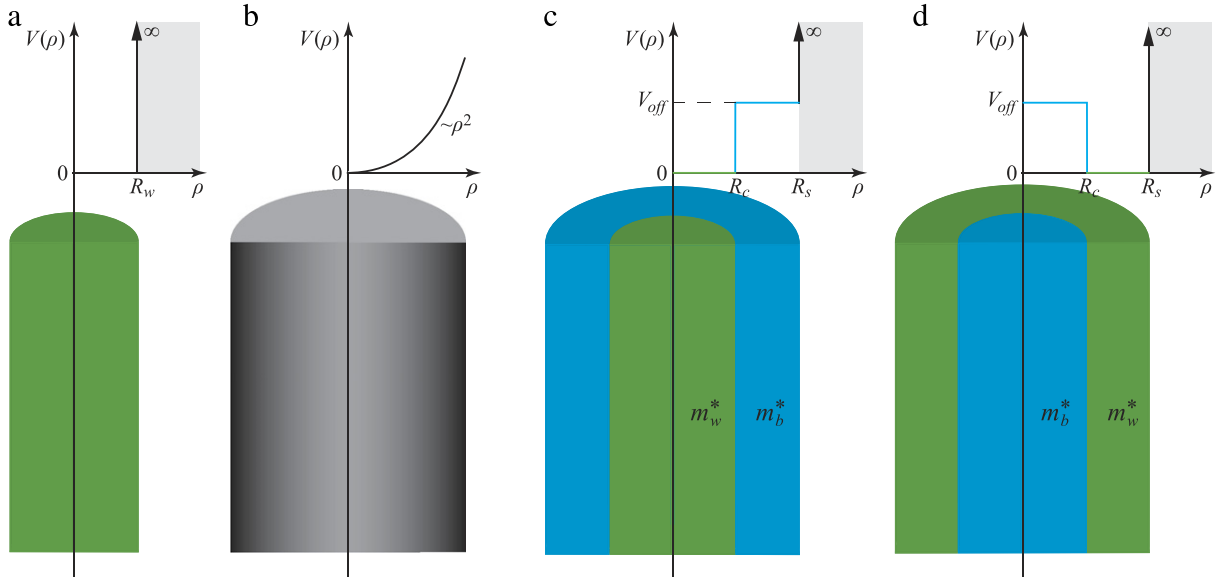

Fig. 1. The considered potentials in the analyzed cylindrical quantum wires: (a) the infinite rectangular potential well in a free-standing quantum wire, (b) the potential of a linear harmonic oscillator, (c) the confining potential inside the core of a core–shell quantum wire, and (d) the confining potential inside the shell of a core–shell quantum wire.

assumes that the confinement potential arises from a band offset between different semiconductors, yet the eigenproblem is usually only numerically solvable. For example, the wave function can be expanded in a basis of analytical functions [19]. But such an approach is known to produce dense Hamiltonian matrices, and could have low accuracy of the wave functions around numerical boundaries [20]. An attractive alternative is the finite-difference method (*FDM*) [21], which employs a discretization of the wave function and its derivatives on a grid [22,23]. Finite difference approximations are usually of low order [23], therefore the *FDM* delivers sparse matrices which could be diagonalized extremely fast. As a matter of fact, the *FDM* has been adopted to numerically solve various equations in physics [24–26]. For example, the Poisson equation and the Schrödinger equation are solved together in the Hartree calculation of exciton states by using the same *FDM* discretization [27]. The robustness of the *FDM* has been an essential criterion for its frequent use to model systems where the electrons are confined in more than one dimension, quantum wires and quantum dots [27], for example.

When applying the *FDM* to solve the Schrödinger equation, a grid should be constructed with special care about the regions close to the interfaces. It is not a difficult task when quantum wires have axial symmetry, which allows reducing the eigenproblem to the computation of matrix elements that depend on only the ρ coordinate of the cylindrical system. However, the effective-mass Schrödinger equation contains a term proportional to the first derivative of the wave function with respect to the radius. Because of this term the finite-difference approximation makes the Hamiltonian matrix nonsymmetric.

In this paper, we study how the *FDM* is used to solve the effective-mass Schrödinger equation for axially symmetric potentials that appear in freestanding and core–shell quantum wires. In the case of freestanding quantum wires, an infinite rectangular potential and the potential of a 2D linear harmonic oscillator are analyzed, shown schematically in Figs. 1(a) and (b). Core–shell quantum wires are considered for: (1) the type-Ic potential [17], where the electron is confined inside the core, and (2) the type-Is potential [17], which confines the electron in the shell. Both analyzed potentials in core–shell quantum wires are assumed to have stepwise variation with ρ, which is displayed in Figs. 1(c) and (d). A few discretization *FDM* schemes are constructed to solve the eigenproblem. *First*, the original Schrödinger equation is discretized by central differences, and it is demonstrated that the Hamiltonian matrix is asymmetric. Furthermore, for computing the states of zero orbital momentum two types of boundary conditions are tested and compared. *Second*, the Schrödinger equation is transformed into another equation [28] by the Liouville-like (*LL*) transformation, which removes the problematic term from the Hamiltonian. When the *LL*-transformed Schrödinger equation is discretized by the *FDM*, the Hamiltonian matrix becomes symmetric. However, the boundary condition at the inner boundary is such that the wavefunctions are inaccurately computed close to the origin. The *third* method is an approach developed by us, which employs the finite-difference discretization of the original Schrödinger equation, and subsequently applies the Liouville-like transformation to the obtained difference equation. This approach is novel to the best of our knowledge and is able to solve the problem of insufficient accuracy of the solution of the *LL*-transformed Schrödinger equation, and in the same time delivers a symmetric Hamiltonian matrix. The accuracies of the three discretization schemes are mutually compared for the analyzed model potentials, and we compare the results with those from the finite element method (*FEM*).

The paper is organized as follows. In Section 2 the discretization schemes to solve the effective-mass Schrödinger equation for quantum wires are presented. Section 3 contains the error analysis on the example of a constant effective mass in the structure. Section 4 presents the results of our computations. We conclude in Section 5.

2. The model of the electron states and the FDM schemes

2.1. The model

We compute the electron states by using the effective-mass Schrödinger equation

$$H_{3D}\Psi_{3D}(\mathbf{r}) = E\Psi_{3D}(\mathbf{r}). \tag{1}$$

Here, H_{3D} denotes the single-band effective-mass Hamiltonian,

$$H_{3D} = \frac{1}{2}\mathbf{p}\frac{1}{m^*(\mathbf{r})}\mathbf{p} + V(\mathbf{r}), \tag{2}$$

where $m^*(\mathbf{r})$ is the position dependent electron effective mass, $\mathbf{p} = -i\hbar\nabla$ is the canonical momentum operator, and $V(\mathbf{r})$ is

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