

Excitonic Eigenstates of Disordered Semiconductor Quantum Wires: Adaptive Wavelet Computation of Eigenvalues for the Electron-Hole Schrödinger Equation

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Received 8 October 2011; Accepted (in revised version) 26 July 2012

Communicated by Chi-Wang Shu

Available online 18 October 2012

Abstract. A novel adaptive approach to compute the eigenenergies and eigenfunctions of the two-particle (electron-hole) Schrödinger equation including Coulomb attraction is presented. As an example, we analyze the energetically lowest exciton state of a thin one-dimensional semiconductor quantum wire in the presence of disorder which arises from the non-smooth interface between the wire and surrounding material. The eigenvalues of the corresponding Schrödinger equation, i.e., the one-dimensional exciton Wannier equation with disorder, correspond to the energies of excitons in the quantum wire. The wavefunctions, in turn, provide information on the optical properties of the wire.

We reformulate the problem of two interacting particles that both can move in one dimension as a stationary eigenvalue problem with two spacial dimensions in an appropriate weak form whose bilinear form is arranged to be symmetric, continuous, and coercive. The disorder of the wire is modelled by adding a potential in the Hamiltonian which is generated by normally distributed random numbers. The numerical solution of this problem is based on adaptive wavelets. Our scheme allows for a convergence proof of the resulting scheme together with complexity estimates. Numerical examples demonstrate the behavior of the smallest eigenvalue, the ground state energies of the exciton, together with the eigenstates depending on the strength and spatial correlation of disorder.

AMS subject classifications: 81Q05, 65N25, 65N50, 65Zxx

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Key words: Semiconductor quantum wire, disorder, Schrödinger equation, eigenvalue problem, weak formulation, bounded and coercive bilinear form, adaptive wavelet method, convergence, complexity, ground state energies, exciton.

1 Introduction

Semiconductors and semiconductor nanostructures, e.g., wells, wires, and dots, play a prominent role in modern technology: computer chips are based on their electronic properties; the optical and optoelectronic properties of semiconductors are exploited in solar cells, light emitting diodes, and lasers, and, furthermore, future applications in the area of quantum communications and computing are expected to be within reach of current technology [3, 15, 20, 27]. In this paper, we consider thin semiconductor quantum wires which are essentially one-dimensional systems, see Fig. 1. This approximation is appropriate if the diameter is much smaller than the intrinsic electronic length scale of the problem which is the exciton Bohr radius since we study the optical absorption close to the fundamental band gap. By optical excitation, one generates an electron-hole pair whose states are described by a two-particle time-dependent Schrödinger equation. Due to the unavoidable imperfections during the growth of such structures, the interface between the wire and the surrounding material cannot be considered to be perfectly smooth. We call this a *disordered* quantum wire and model it by an additional disorder potential in the Hamiltonian describing the spatial variation of the electron and hole energies. Thus, we analyze a model with diagonal disorder [2, 39], which has recently been used to study linear and nonlinear optical properties of semiconductor nanostructures together with a tight-binding model, see, e.g., [17, 25, 27, 30]. From this, we formulate a stationary eigenvalue problem in two spatial dimensions describing the two interacting one-dimensional particles.

For the numerical solution, we seek for a highly efficient method, i.e., employing degrees of freedom for the computation and representation of eigenenergies and eigenstates only where actually needed. This paradigm has, from a numerical point of view, triggered much more substantial advancements in highly accurate simulations than increased computer power and larger storage systems. Thus, for us, it is indispensable to utilize a) an *adaptive* method which introduces during the computation and depending on the residuals of the operator equation and singularities of the problem additional degrees of freedom according to a user-specified accuracy. In view of extensions to quantum films and a resulting partial differential operator in four space dimensions to be considered at a later stage, we want to ensure that our method could b) systematically be adapted to higher spatial dimensions. In addition, it is important to us to c) be able to prove *convergence* of the numerical method. This means that an addition of degrees of freedom provably reduces the numerical error. Lastly, we want to assure that d) our method provides *optimal computational complexity*. This means that the algorithm has an