Wavelet-Based Adaptive Computations of the Excitonic Eigenstates of Disordered Semiconductor Quantum Wires

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Abstract. A novel adaptive wavelet based method is presented that allows us to compute eigenvalues and eigenvectors of the electronic Schrödinger equation. Our method outperforms direct discretization methods with equidistant grid spacings, in particular, for problems that involve several length scales. As an application we present numerical evaluations of the energetically lowest exciton states for ordered and disordered semiconductor quantum wires.

Keywords: semiconductor quantum wires, excitons, adaptive computations, wavelets, energetic disorder.
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INTRODUCTION

Real semiconductor heterostructures, e.g., quantum wells and wires, which are fabricated using, e.g., molecular beam epitaxy, always contain a certain amount of disorder [1-6]. If the material contains more than two different atoms as in, e.g., $Al_xGa_{1-x}As$ the Al and the Ga atoms may arrange on random spatial positions which is known as compositional or alloy disorder. Another type of disorder originates from spatial variations of the interfaces between the different materials that are contained in the heterostructure. For example in quantum wells, the thickness of the well material may change by one or more atomic layers. Since these monolayer fluctuations influence the energies of the electron and hole states due to quantum confinement they have a pronounced influence on the electronic and optical properties. Similarly in quantum wires the thickness of the wire typically varies in space which leads to position dependent electronic and optical properties.

In the spectral vicinity of the band gap, the optical absorption of semiconductor heterostructures is dominated by strongly absorbing bound electron-hole complexes, i.e., excitons [1-7]. Since disorder leads to position dependent electron and hole energies, also the energy of the excitonic resonances changes in space. Besides the magnitude of the disorder-induced energy variations, also the length scale of the disorder is of relevance. If the correlation length that characterizes the disorder-induced energy variations is smaller than the size of the excitons, i.e., the exciton Bohr radius a_B, the exciton resonances are rather weakly influenced because they effectively average over the disorder variations [1,2]. In the opposite limit where the correlation length is much longer than the exciton Bohr radius the exciton energy changes smoothly in space following the disorder-induced energy variation. In any case, disorder leads to a spectral broadening of the excitonic resonances which is denoted as inhomogeneous broadening [1-6].

In the present study, we focus on thickness fluctuations of semiconductor quantum wires. The spatial variation of the electron and hole energies is included in a numerical solution of the exciton Wannier equation in real space [1-5]. To solve the Wannier equation we develop a novel adaptive method which uses wavelets as the basis functions. It is demonstrated that our method is able to efficiently compute the energetically lowest exciton states with and without disorder. To obtain the same accuracy as calculations that use equidistant grids, significantly less basis functions are needed in our adaptive approach. After projecting out the lowest state, our approach can also be used to compute energetically higher exciton states which are required in order to obtain the absorption spectrum. In the future, we plan to combine our approach with the numerical solution of dynamics equations, e.g., the semiconductor Bloch equations, and analyze nonlinear optical properties. We expect that in this case adaptive grids will greatly reduce even more the computational complexity needed for the numerical experiments.

NUMERICAL METHOD

Without disorder, e.g., in spatially homogeneous semiconductors and semiconductor heterostructures, the exciton Wannier equation describes the motion of a negatively charged conduction band electron in the presence of a positively charged valence band hole. Therefore, the Wannier equation has the same form as the Schrödinger equation of a hydrogen atom which describes the motion of a negatively charged electron and a positively charged proton and their Coulomb attraction. To describe excitons, one only needs to replace the bare electron and the proton mass, by the effective masses of the electrons and holes in the considered semiconductor material and one needs to screen the Coulomb attraction, since in a solid state system the presence of many other electrons reduces the attractive potential.

In our approach we describe a thin semiconductor quantum wire by a one-dimensional model and numerically compute the lowest eigenstate of the corresponding exciton Wannier equation. As usual, see, e.g,, [3-5], we regularize the Coulomb potential $V(x_e\text{-}x_h)$, where x_e, and x_h denote the spatial coordinates of the electron and hole, respectively, which accounts for the finite width of the quantum wire [7]. From our numerical approach we obtain the wave function of the energetically lowest exciton state $\Psi(x_e, x_h)$. Disorder is included by considering random space-dependent potentials $V_e(x_e)$ and $V_h(x_h)$ in the exciton Wannier equation. $V_e(x_e)$ is set up as a piecewise constant step function with desired number of steps, where each step height is normally distributed. As usually for the case of interface fluctuations, we use in this study correlated disorder, i.e., we assume $V(x)=V_e(x_e)=\alpha V_h(x_h)$, where α is inversely proportional to the ratio between the hole and electron effective masses.

The first step is to reformulate the eigenvalue problem in a weak sense. Our design of a new wavelet method follows a somewhat different paradigm than conventional finite difference or finite element methods in that the solution process is based directly on an infinite-dimensional representation of the problem: instead of choosing a finite subspace as a solution space, e.g., a finite element space, and performing a Galerkin discretization, we consider a suitable infinite-dimensional wavelet basis to represent the eigenvalue problem. Now we have an equivalent reformulation of the problem without any discretization error yet [9]. In this form we can apply the perturbed preconditioned inverse iteration (PPINVIT) [8] which is a highly efficient wavelet-based eigenvalue solver. The main idea of such adaptive wavelet schemes is to adaptively choose in an automated way, out of the infinite set of basis functions, only the relevant ones in order to obtain the best possible approximation of the unknown solution. For performing the involved application of the (bi-)infinite matrices up to a desired user specified accuracy, we employ an inexact adaptive operator application scheme. Essential for efficient computations is an adaptive vector approximation scheme, called coarsening. Here we use an appropriate adaptation of the APPLY scheme from [9] and the COARSE scheme from [10]. A convergence proof of the resulting scheme together with complexity estimates can be found in [11].

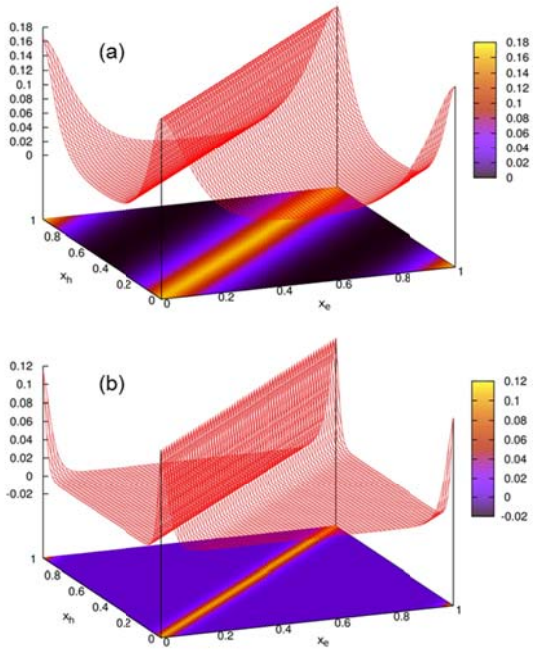

FIGURE 1. Computed $\Psi(x_e, x_h)$ of the energetically lowest exciton state for ordered quantum wires of different length L (a) L=100 nm and (b) L=400 nm.

RESULTS AND DISCUSSION

Figure 1 shows the computed wavefunctions of the lowest exciton state for ordered quantum wires of different length L. In the ordered case $\Psi(x_e, x_h)$ depends only on the distance $|x_e\text{-}x_h|$ and decays basically exponentially if one moves away from the diagonal $x_e=x_h$. The increase of Ψ towards the end of the diagonal $x_e=1\text{-}x_h$ arises from the periodic boundary conditions, i.e., $|x_e\text{-}x_h|$ needs to be evaluated as the shortest distance between equivalent points in one and adjacent unit cells.

The error in the computation of the eigenvalue of the lowest exciton state is compared in Fig. 2 for a uniform grid and our adaptive approach as function of

the considered grid points. It is clearly shown that for both approaches the error decreases basically exponentially with the number of grid points and that with the adaptive approach a better accuracy is reached than with a uniform grid for the same number of grid points.

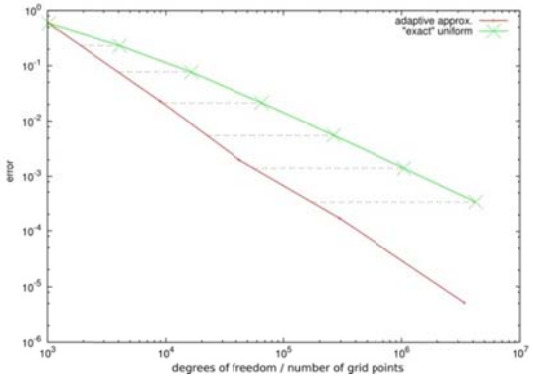

FIGURE 2. Exact eigenvalues with respect to uniform grids in comparison to the adaptive scheme for L= 800 nm.

Figure 3 shows the computed wavefunctions of the lowest exciton state for disordered quantum wires of length L=100 nm and different disorder strength. With disorder, $\Psi(x_e, x_h)$ depends not only on the distance $|x_e-x_h|$ but clearly separately on x_e and x_h. Furthermore, with increasing strength of the disorder $\Psi(x_e, x_h)$ becomes more and more localized at the spatial minimum of the disorder potential V(x).

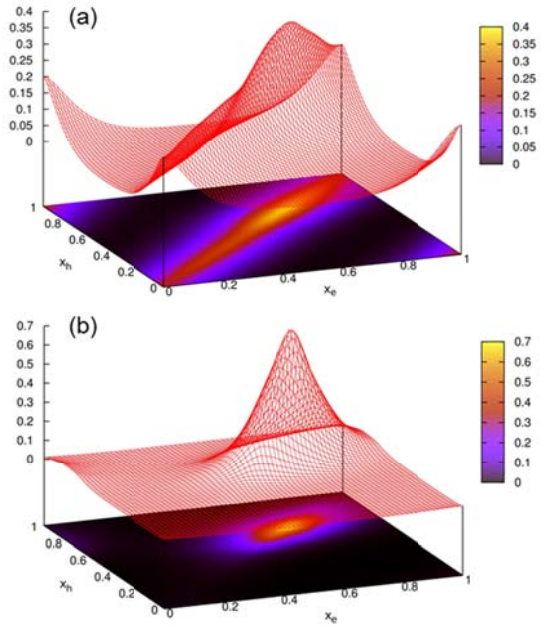

FIGURE 3. Computed $\Psi(x_e, x_h)$ of the energetically lowest exciton state for disordered quantum wires of L= 100 nm. The standard deviation of the disorder potential is (a) σ=0.013605 meV and (b) σ=0.340125 meV.

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