Electron energy level calculations for semiconductor nanostructures

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Semiconductor nanostructures have attracted tremendous interest in the past few years because of their special 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, thus reducing the degrees of freedom to zero. A quantum dot can therefore be thought of as an artificial atom, and it makes it possible to model atomic physics in macroscopic systems experimentally and theoretically.

We consider the problem to compute relevant energy states and corresponding wave functions of a three dimensional semiconductor quantum dot embedded in a bounded matrix of different material assuming an effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, and a finite height hard-wall 3D confinement potential.

The governing equation characterizing the energy states E and corresponding wave functions ϕ is the Schrödinger equation

$$-\nabla\cdot\left(\frac{\hbar^2}{2m(E)}\nabla\phi\right)+V\phi=E\phi, \tag{1}$$

where the confinement potential V and the electron effective mass m are discontinous across the interface between the dot and the matrix. Assuming non-parabolicity for the electron effective mass, m depends nonlinearly on the energy state E, and (1) becomes a rational eigenvalue problem. Discretizing by FE or FV methods it results in a nonlinear sparse matrix eigenvalue problem.

For sparse linear eigenvalue problems iterative projection methods (Lanczos, Arnoldi, and Jacobi–Davidson method, e.g.) are known to be very efficient, where approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem of small dimension which are expanded in the course of the algorithm. We take advantage of generalizations to nonlinear problems of Arnoldi [2] or Jacobi-Davidson type [3]. These are particularly efficient since the eigenvalues of (1) satisfy a minmax property which is inherited by finite element discretizations [1, 4].

References

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