Numerical simulation of electronic properties of quantum dots

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In semiconductor nanostructures 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.

The governing equation characterizing the relevant energy states λ and corresponding wave functions ψ is the Schrödinger equation

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

which depends nonlinearly on the eigenparameter if we assume a non-parabolic electron effective mass m.

Most simulations in the literature consider constant electron effective masses. However, numerical examples demonstrate that the electronic behavior is substantially different: for a realistic pyramidal quantum dot there are only 3 confined electron states for the linear model whereas the nonlinear model exhibits 7 confined states (i.e. energy levels which are smaller than the confinement potential).

For limited dimensions of the discretized problem (up to a few thousands) the problem can be solved by the full approximation method (FAM) where in each step a linear eigenvalue problem has to be solved. Taking advantage of variational properties of the eigenproblem (which are inherited by finite element discretizations) FAM can be enhanced substantially [5].

For higher dimension iterative projection methods of Nonlinear Arnoldi or Jacobi-Davidson type combined with safeguarded iteration prove to be very efficient [4].

The results and the methods are explicated only for quantum dots, but modifications apply also to quantum dots on wetting layers [2], and arrays of such structures. Spin orbit interaction [1] and magnetic effects can also be included [3].

References

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