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Electron energy level calculation for a three dimensional quantum dot

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Abstract: In this paper we consider the rational eigenvalue problem governing the relevant energy levels and wave functions of a three dimensional quantum dot. We present iterative projection methods of Arnoldi and of Jacobi–Davidson type for computing a few eigenpairs of this system. Solving the projected nonlinear eigenvalue problems we take advantage of a minmax characterization of the eigenvalues.

Keywords: Quantum dot, effective mass, Rayleigh functional, Arnoldi method, Jacobi–Davidson method

Mathematics Subject Classification: 65F15

1 The governing equation

We consider the problem to compute relevant energy states and corresponding wave functions of a three dimensional semiconductor quantum dot. Let $\Omega_q \subset \mathbb{R}^3$ be a domain occupied by the quantum dot, which is embedded in a bounded matrix Ω_m of different material. A typical example is an InAs pyramidal quantum dot embedded in a cuboid GaAs matrix.

The governing equation is the Schrödinger equation

$$-\nabla \cdot \left(\frac{\hbar^2}{2m(x,\lambda)} \nabla u \right) + V(x)u = \lambda u, \ x \in \Omega_q \cup \Omega_m, \tag{1}$$

where $\hbar$ is the reduced Planck constant, m is the effective electron mass depending on both, energy level λ and position x, V is the confinement potential depending on x, and u is the wave function. Since the wave function decays outside the quantum dot very rapidly it is reasonable to assume homogeneous Dirichlet conditions $u = 0$ on the outer boundary of Ω_m, and on the interface between the quantum dot and the matrix the Ben Daniel–Duke condition holds

$$\frac{1}{m_q} \frac{\partial u}{\partial n_q}\bigg|_{\partial\Omega_q} = \frac{1}{m_m} \frac{\partial u}{\partial n_m}\bigg|_{\partial\Omega_m}, \ x \in \partial\Omega_q \cap \partial\Omega_m. \tag{2}$$

Here n_q and n_m denote the outward unit normal on the boundary of Ω_q and Ω_m, respectively.

Assuming non-parabolicity for the electron's dispersion relation the effective mass is given as [3]

$$\frac{1}{m_j(\lambda)} = \frac{P_j^2}{\hbar^2} \left(\frac{2}{\lambda + g_j - V_j} + \frac{1}{\lambda + g_j - V_j + \delta_j} \right) \tag{3}$$

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where the confinement potential $V_j := V|_{\Omega_j}$ is piecewise constant, and P_j, g_j and δ_j are the momentum matrix element, the conduction and the spin-orbit split-off band gap for the quantum dot ($j = q$) and the matrix ($j = m$), respectively.

Multiplying (1) by $v \in H_0^1(\Omega)$, $\Omega := \bar{\Omega}_q \cup \Omega_m$, and integrating by parts one gets the variational form of the Schrödinger equation

$$\begin{aligned} a(u,v;\lambda) &:= \frac{\hbar^2}{2m_q(\lambda)} \int\limits_{\Omega_q} \nabla u \cdot \nabla v \, dx + \frac{\hbar^2}{2m_m(\lambda)} \int\limits_{\Omega_m} \nabla u \cdot \nabla v \, dx + V_q \int\limits_{\Omega_q} uv \, dx + V_m \int\limits_{\Omega_m} uv \, dx \\ &= \lambda \int\limits_{\Omega} uv \, dx =: \lambda b(u,v) \quad \text{for every } v \in H_0^1(\Omega). \end{aligned} \tag{4}$$

It is easily seen that for fixed $u \in H_0^1(\Omega)$, $u \neq 0$ the real equation

$$f(\lambda; u) := \lambda b(u,u) - a(u,u;\lambda) = 0 \tag{5}$$

has a unique solution $\lambda =: p(u)$. It therefore defines a functional $p : H_0^1(\Omega) \setminus \{0\} \to \mathbb{R}^+$ which is called the Rayleigh functional of the rational eigenvalue problem (4). With this functional the following variational characterization of eigenvalues of problem (4) which generalizes the well known minmax characterization of Poincaré for linear eigenproblems (cf. [7]).

THEOREM 1

(i) The Schrödinger equation (4) *with effective mass given in* (3)*, which models the energy states and wave functions of a quantum dot, has a countable set of eigenvalues* $0 < \lambda_1 \leq \lambda_2 \leq \ldots$. *Each of the eigenvalues has finite multiplicity, and the only cluster point is* ∞.

(ii) The j-th smallest eigenvalue λ_j *can be characterized as*

$$\lambda_j = \min_{\dim V = j} \max_{u \in V, u \neq 0} p(u). \tag{6}$$

Discretizing problem (4) by finite elements results in a rational matrix eigenvalue problem

$$T(\lambda)x = \lambda M x - \frac{1}{m_1(\lambda)} A_1 x - \frac{1}{m_2(\lambda)} A_2 x - Bx = 0 \tag{7}$$

where $T(\lambda) \in \mathbb{R}^{n \times n}$ is symmetric, and also satisfies the conditions the of minmax characterization [7] for $\lambda > 0$. Hence, it has n eigenvalues $0 < \tilde{\lambda}_1 \leq \ldots \tilde{\lambda}_n$, and it follows from the characterization (6) that $\lambda_j \leq \tilde{\lambda}_j$ for $j = 1, \ldots, n$.

2 Iterative projection methods

Typically $T(\lambda)$ is large and sparse, and its eigenvalues can be determined by iterative projection methods [4]. Here the underlying eigenproblem is projected to a sequence of subspaces of $\mathbb{R}^n$ which are expanded in the course of the algorithm by vectors with high approximation potential for the eigenvector wanted next.

Typical examples are the nonlinear Jacobi–Davidson method [1], and the nonlinear Arnoldi method [5], a template of which is listed below:

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1: Start with an initial shift σ and initial orthonormal basis V
2: determine preconditioner M ≈ T(σ)^{-1}
3: while m ≤ number of wanted eigenvalues do
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compute the m-th smallest eigenvalue μ of projected problem $V^TT(\lambda)Vy = 0$
determine Ritz vector $u = Vy$, $\|u\| = 1$, and residual $r = T(\mu)u$
if $\|r\| < \varepsilon$ **then**
accept eigenpair $\lambda_m = \mu$, $x_m = u$
choose new shift σ and update preconditioner M if indicated
restart if necessary
m=m+1
end if
$v = Mr$; $v = v - VV^Tv$; $v = v/\|v\|$; $V = [V, v]$;
reorthogonalize if necessary
end while

There are many details that have to be considered when implementing the nonlinear Arnoldi method concerning the choice of the initial basis, when and how to update the preconditioner, and how to restart the method. A detailed discussion is given in [5].

A crucial point in iterative methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method to converge to the same eigenvalue repeatedly. For linear eigenvalue problems this is easy to do by using Schur forms or generalized Schur forms for the projected problem and then locking or purging certain eigenvalues. For nonlinear problems, however, such Schur forms do not exist and this presents one of the most difficult tasks in achieving good convergence.

For symmetric nonlinear eigenproblems satisfying a minmax characterization (6) however, its eigenvalues can be computed safely one after the other. The proof of Theorem 1 shows that the minimum in (6) is attained by the invariant subspace of $T(\lambda_j)$ corresponding to the j largest eigenvalues, and the maximum by every eigenvector corresponding to the eigenvalue 0. This suggests the safeguarded iteration for computing the j-th smallest eigenvalue:

Start with an approximation μ_1 to the j-th eigenvalue of $T(\lambda)x = 0$
for $k = 1, 2, \ldots$ until convergence do
determine eigenvector u corresponding to the j-largest eigenvalue of $T(\mu_k)$
evaluate $\mu_{k+1} = p(u)$
end for

The safeguarded iteration has the following convergence properties [6]: It converges globally to the smallest eigenvalue λ_1. The (local) convergence to simple eigenvalues is quadratic. If $T'(\lambda)$ is positive definite, and u in Step 3 of the last algorithm is replaced by an eigenvector of $T(\sigma_k)x = \mu T'(\sigma_k)x$ corresponding to the j-th largest eigenvalue, then the convergence is even cubic. Moreover, a variant exists which is globally convergent also for higher eigenvalues.

3 Numerical results

We consider a pyramidal quantum dot with width 12.4 nm and height 6.2 nm embedded in a cubic matrix of size 24.8 nm×24.8 nm×18.6 nm with the following parameters $P_q = 0.8503$, $g_q = 0.42$, $\delta_q = 0.48$, $V_q = 0$, $P_m = 0.8878$, $g_m = 1.52$, $\delta_m = 0.34$, and $V_m = 0.7$. This model was already treated by Hwang, Lin, Wang, and Wang in [2].

The authors of [2] presented a discretization of problem (4) by the finite volume method based on a uniform grid. The corresponding finite dimensional problem (7) was multiplied by the denominators, and the resulting polynomial eigenvalue problem of degree 5 was solved by the Jacobi–Davidson method.

We solved the rational eigenproblem (7) directly by the nonlinear Arnoldi method [5] (not taking advantage of the fact that the stencils are identical for all discretization points in the matrix and in the quantum dot, respectively) under MATLAB 7.0.4 on an AMD Opteron processor with 4

GByte RAM and 2.2 GHz. The following Table contains the approximations to the smallest 5 eigenvalues and the CPU times.

dim	λ_1	$\lambda_{2/3}$	λ_4	λ_5	CPU time
$2'475$	0.41195	0.58350	0.67945	0.70478	0.68 s
$22'103$	0.40166	0.57668	0.68418	0.69922	8 s
$186'543$	0.39878	0.57477	0.68516	0.69767	151 s
$1'532'255$	0.39804	0.57427	0.68539	0.69727	4018 s
$12'419'775$	0.39785	0.57415			overnight

The uniform grid does not seem to be appropriate for discretizing (4) since the wave functions corresponding to small energy levels are mainly concentrated on the quantum dot and decay rapidly outside, whereas the volume occupied by the quantum dot is only less than 3 % of Ω. We discretized (4) by cubic Lagrangian elements on a tetrahedal grid with 96'640 degrees of freedom such that 43'615 DoFs where located in the quantum dot, 43'897 DoFs in the matrix, and 9'128 DoFs on the interface. We solved the rational eigenproblem by the nonlinear Arnoldi method and the Jacobi–Davidson method. The following table contains the approximations to the smallest 5 eigenvalues, the number of iterations to obtain the approximations, and the CPU times. Notice, that in this case by Theorem 1 one gets upper bounds of the corresponding eigenvalues of problem (4). Hence, the approximations to λ_j, $j = 1, 2, 3$ are definitely better than the ones obtained by the finite volume method with more than 12 million DoFs.

dim	λ_1	λ_2	λ_3	λ_4	λ_5	CPU time
$96'640$	0.39779	0.57411	0.57411	0.68547	0.69714	
Arnoldi	44 it.	29 it.	29 it.	24 it.	21 it.	189 s
JD	9 it.	7 it.	9 it.	5 it.	6 it.	205 s

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