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Analysis and Efficient Solution of Stationary Schrödinger Equation Governing Electronic States of Quantum Dots and Rings in Magnetic Field

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Abstract. In this work the one-band effective Hamiltonian governing the electronic states of a quantum dot/ring in a homogenous magnetic field is used to derive a pair/quadruple of nonlinear eigenvalue problems corresponding to different spin orientations and in case of rotational symmetry additionally to quantum number $\pm\ell$. We show, that each of those pair/quadruple of nonlinear problems allows for the minmax characterization of its eigenvalues under certain conditions, which are satisfied for our examples and the common InAs/GaAs heterojunction. Exploiting the minmax property we devise efficient iterative projection methods simultaneously handling the pair/quadruple of nonlinear problems and thereby saving up to 40% of the computational time as compared to the nonlinear Arnoldi method applied to each of the problems separately.

AMS subject classifications: 65F15, 65F50

Key words: Quantum dot, quantum ring, nonlinear eigenvalue problem, minmax characterization, iterative projection method, electronic state, spin orbit interaction, magnetic field.

1 Introduction

The spectroscopic techniques involving magnetic field have for long been employed in experimental studies of bulk materials. However, only recently, methods like resonant spin-flip Raman scattering have been applied to quantum dots [30]. The analysis of Zeeman levels and the associated Landé factors allows the physicists for better understanding of spin effects on the optical response of low dimensional systems and is crucial for

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interpretation of the results of spectroscopic analysis, magneto-optical experiments or magneto-transport phenomena.

In this work we consider the Zeeman splitting of energy levels of quantum dots and rings in an external homogenous magnetic field. The internal Zeeman effect i.e. the splitting of electronic levels due to the interaction of the spin magnetic moment with the magnetic field acting on the electron while it is moving around the nucleus, was considered in [5]. We discuss the general three dimensional case on an example of a pyramidal quantum dot and the rotationally symmetric case on an example of an elliptical quantum ring. We assume the one-band Hamiltonian with nonparabolic effective mass approximation and the effective Landé factor for the electronic states in the conduction band. This model yields a magnetic stationary Schrödinger equation, where the eigenvalue parameter enters nonlinearly. Considering different spin orientations we obtain a pair of nonlinear eigenvalue problems, one for each spin orientation. In case of rotational symmetry additionally each of the $\pm\ell$ quantum numbers yields a separate equation resulting in a total of four different nonlinear eigenvalue problems. We derive sufficient conditions for the physically relevant eigenvalues of the corresponding variational problems to satisfy the minmax principle [39,40]. This conditions hold for the InAs/GaAs heterojunctions in our examples. Exploiting the minmax property we develop efficient iterative projection methods which simultaneously handle the pair/quadruple of the nonlinear problems considerably reducing the overall computational time.

A standard way to tackle the rational eigenproblem (cf. [15] for a quantum dot without the magnetic field) would be to multiply it by the common denominator and to linearize the resulting polynomial of degree five. Similarly, the rational problem can be linearized directly as was proposed by Su and Bai [32]. In either case one gets a linear eigenvalue problem of dimension five times as large as the original problem. This linearized problem can then be solved with standard algorithms for which off the shelf software is available. However, this approach has some significant disadvantages. Not only the dimension of the problem is increased fivefold, but also the structure of the problem (e.g. symmetry) is destroyed and moreover the desired eigenvalues are now located in the interior of the spectrum. Computation of interior eigenvalues requires shift-invert type techniques, i.e. at least a preconditioner for the linear problem with a linearization block structure, will have to be computed. Efficient non fill-in computation of such a preconditioner is an open problem.

Our paper is organized as follows. In Section 2 we introduce the magnetic one-band effective Hamiltonian which models the electronic behavior of three dimensional quantum structures. The derivation of the corresponding pair of rational eigenvalue problems and their analysis is provided in Section 3. In Section 4 we adapt the model to a nanoring in magnetic field. Further, we derive the corresponding quadruple of nonlinear eigenvalue problems and analyze it. In Section 5 we give the minmax characterization for both problems and their discretizations obtained with Galerkin methods. The resulting rational matrix eigenvalue problems are large and sparse and therefore they can be efficiently handled by iterative projection methods like e.g. Jacobi Davidson [8] or