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STATIONARY SCHRÖDINGER EQUATIONS GOVERNING ELECTRONIC STATES OF QUANTUM DOTS IN THE PRESENCE OF SPIN-ORBIT SPLITTING

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Abstract. In this work we derive a pair of nonlinear eigenvalue problems corresponding to the one-band effective Hamiltonian accounting for the spin-orbit interaction governing the electronic states of a quantum dot. We show that the pair of nonlinear problems allows for the minmax characterization of its eigenvalues under certain conditions which are satisfied for our example of a cylindrical quantum dot and the common InAs/GaAs heterojunction. Exploiting the minmax property we devise an efficient iterative projection method simultaneously handling the pair of nonlinear problems and thereby saving about 25 % of the computation time as compared to the Nonlinear Arnoldi method applied to each of the problems separately.

Keywords: quantum dot, nonlinear eigenvalue problem, minmax characterization, iterative projection method, electronic state, spin orbit interaction

MSC 2000: 65F15, 65F50

1. Introduction

The recent technological progress made the spin of the electron more than only a theoretical property. The new type of electronic devices utilizes the spin of an electron along with its charge. This development makes it necessary to incorporate the spin effects into the mathematical models, and in fact spin-orbit interaction has been found to significantly affect the electronic states of various quantum structures and semiconductor nanostructures. The latter have been an object of intensive research in the past few years because of their unique physical properties and their potential for applications in micro-, optoelectronic and only recently also spintronics devices. In semiconductor 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 free carriers are confined in all three directions of space. Such an energy quantization is an intrinsic property of an atom, which makes the quantum dot an interesting model for investigating the properties of systems at the atomic level.

Modeling quantum dots by the one-band Hamiltonian with nonparabolic effective mass approximation including the spin-orbit interaction one arrives at a stationary Schrödinger equation which is nonlinear with respect to the eigenvalue parameter. It can be further transformed into a form where the spin dependence only dwells in the boundary conditions [6], [14] resulting in two Schrödinger equations which differ only on the interface conditions between the quantum dot and the surrounding bulk material. Numerical experiments demonstrating the influence of the spin-orbit splitting on the relevant energy levels for rotationally symmetric quantum dots are contained in [9], [10], [15], [16], [17], where the Schrödinger equations are discretized by finite differences, and the resulting nonlinear eigenproblem is solved by the full approximation method.

In this paper we propose to include the interface contribution corresponding to the spin dependent interface condition directly into the nonlinear eigenvalue problem in variational formulation. This leads to a pair of nonlinear eigenvalue problems. We derive a sufficient condition for the physically relevant eigenvalues of both the problems to satisfy the minmax principle [21]. This condition holds for the InAs/GaAs heterojunction in our example. Exploiting the minmax property we develop an efficient iterative method which simultaneously handles the pair of the nonlinear problems considerably reducing the overall computational time.

Our paper is organized as follows. In Section 2 we introduce the one band effective Hamiltonian with spin-orbit interaction which models the electronic behavior of quantum dots. The derivation of the corresponding pair of rational eigenvalue problems and their analysis is provided in Section 3. Discretization by a Galerkin method yields in both cases a sparse rational matrix eigenvalue problem. Section 4 briefly describes the iterative projection method introduced already in [20] and asserts its scope of application. Further, the solution of the projected rational eigenproblems by safeguarded iteration is expounded in detail. Section 5 demonstrates the efficiency of our method on a numerical example, and it describes how the iterative projection methods can be modified to simultaneously handle the pair of nonlinear eigenvalue problems. The conclusions and some ideas for future research are summarized in the last section.

2. One-band effective Hamiltonian with spin-orbit interaction

We consider the one-band effective Hamiltonian for electrons in the conduction band [8], [11]

$$H = H_0 + H_{\mathrm{so}}. \tag{2.1}$$

In equation (2.1) H_0 denotes the Hamiltonian without the spin-orbit interaction,

$$H_0 = -\frac{\hbar^2}{2}\nabla \cdot \Big(\frac{1}{m(\lambda, x)}\nabla\Big) + V(x), \tag{2.2}$$

where $\hbar$ is the reduced Planck constant, $m(\lambda, x)$ is the position and energy dependent electron effective mass, V is the confinement potential, and ∇ denotes the spatial gradient. Assuming nonparabolicity for the electron's dispersion relation, the electron effective mass $m(\lambda, x)$ is constant on the dot Ω_q and on the surrounding bulk material Ω_b for every fixed energy level λ, and is taken as [2], [5]

$$\frac{1}{m_j(\lambda)} := \frac{1}{m(\lambda, x)}\Big|_{x\in\Omega_j} = \frac{P_j^2}{\hbar^2}\Big(\frac{2}{\lambda + E_{g,j} - V_j} + \frac{1}{\lambda + E_{g,j} - V_j + \Delta_j}\Big) \tag{2.3}$$

for $j \in \{b, q\}$. Here the confinement potential $V_j := V|_{\Omega_j}$ is piecewise constant, and P_j, $E_{g,j}$ and Δ_j are the momentum matrix element, the band gap, and the spin-orbit splitting in the valence band for the quantum dot ($j = q$) and the bulk material ($j = b$) called a matrix, respectively.

The spin-orbit interaction in equation (2.1) is described by [6], [14]

$$H_{\mathrm{so}} = \mathrm{i}\nabla\alpha(\lambda, x) \cdot [\sigma \times \nabla], \tag{2.4}$$

where σ is the vector of Pauli matrices and $\alpha(\lambda, x)$ is the spin-coupling parameter

$$\begin{aligned} \alpha_j(\lambda) &:= \alpha(\lambda, x)|_{x\in\Omega_j} \\ &= \frac{P_j^2}{2}\Big(\frac{1}{\lambda + E_{g,j} - V_j} - \frac{1}{\lambda + E_{g,j} + \Delta_j - V_j}\Big), \quad j \in \{b, q\} \end{aligned} \tag{2.5}$$

with the materials parameters defined above. Analogously to the effective mass, for a fixed energy level λ, $\alpha(\lambda, x)$ is a piecewise constant function.

From now on for the sake of simplicity we focus on a cylindrical quantum dot, but the ideas presented herein are applicable to dots of arbitrary shapes. We consider a cylindrical quantum dot of radius R_q and height Z_q centrally embedded into a cylindrical matrix of radius R_b and height Z_b (see Fig. 2.1). To determine the

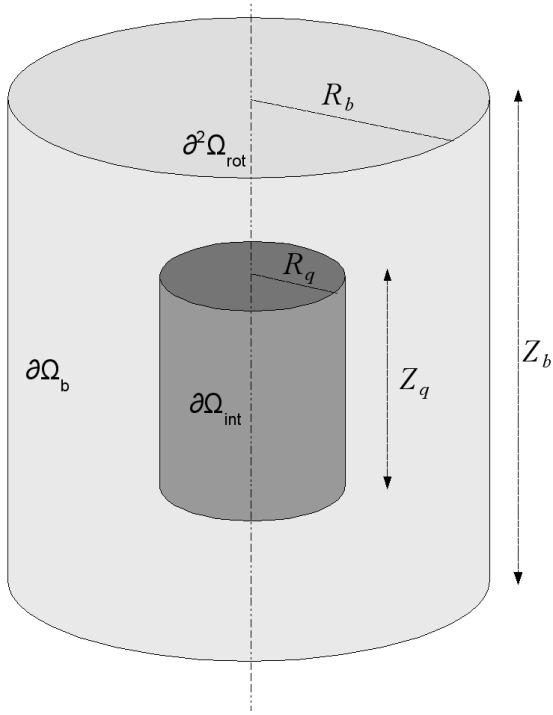

Figure 2.1. Cylindrical quantum dot centrally embedded into a cylindrical matrix.

relevant energy states and the corresponding wave functions Φ we have to solve the governing stationary Schrödinger equation in cylindrical coordinates (r, θ, z):

$$\frac{-\hbar^2}{2m_j(\lambda)}\Big[\frac{1}{r}\frac{\partial}{\partial r}\Big(r\frac{\partial\Phi}{\partial r}\Big) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial z^2}\Big] + V_j\Phi = \lambda\Phi, \quad j \in \{b, q\}. \tag{2.6}$$

In the modeling of quantum dots the knowledge of the positive eigenvalues smaller than the confinement potential is the key issue. These are also called the confined states since the corresponding wave functions mainly live on the quantum dot and rapidly decay outside of the dot. Thus it is reasonable to assume homogeneous Dirichlet conditions $\Phi = 0$ on the outer boundary of the matrix.

On the interface $\partial\Omega_{\text{int}}$ between the dot and the matrix the electron wave function Φ is continuous, and the spin-dependent Ben Daniel-Duke boundary condition

$$\Big\{\frac{\hbar^2}{2m(\lambda, x)} - \mathrm{i}\alpha(\lambda, x)[\sigma \times \nabla]\Big\}_{\bar{n}}\Phi(x) = \text{const}, \quad x \in \partial\Omega_{\text{int}} \tag{2.7}$$

is satisfied [10].

Due to the rotational symmetry of the problem we make the following ansatz for the solution:

$$\Phi(r,\theta,z) = \varphi(r,z)\psi(\theta), \tag{2.8}$$

and separating the variables we obtain two independent equations

$$\frac{\hbar^2}{2m_j(\lambda)}\Big[\frac{\partial}{\partial r}\Big(-r\frac{\partial\varphi(r,z)}{\partial r}\Big) - r\frac{\partial^2\varphi(r,z)}{\partial z^2} + \frac{l^2}{r}\varphi(r,z)\Big] + r(V_j-\lambda)\varphi(r,z) = 0, \tag{2.9}$$

$$\frac{\partial^2\psi(\theta)}{\partial\theta^2} + l^2\psi(\theta) = 0. \tag{2.10}$$

The solution of the latter equation (2.10) is well known to be a plane wave

$$\psi_l(\theta) = \mathrm{e}^{\mathrm{i}l\theta}, \quad l = 0, \pm1, \pm2, \ldots \tag{2.11}$$

while the first equation is a nonlinear eigenvalue problem in the plane defined by r and z.

On the outer boundary of the matrix $\partial\Omega_b$ homogeneous Dirichlet conditions are inherited from the three dimensional problem. On the rotational axis $\partial\Omega^2_{\mathrm{rot}}$ we assume for continuity reasons homogeneous Neumann conditions $\partial\varphi/\partial r = 0$ for $l = 0$ and homogeneous Dirichlet conditions $\varphi = 0$ for $l \neq 0$. On the interface $\partial\Omega_{\mathrm{int}}$ we obtain from (2.7)

$$\begin{gathered}\frac{1}{m_b}\frac{\partial\varphi(r,z)}{\partial z}\Big|_{z=\pm Z_q/2} - \frac{1}{m_q}\frac{\partial\varphi(r,z)}{\partial z}\Big|_{z=\pm Z_q/2} = 0, \quad r \leqslant R_q, \\ \frac{1}{m_b}\frac{\partial\varphi(r,z)}{\partial r}\Big|_{r=R_q} - \frac{1}{m_q}\frac{\partial\varphi(r,z)}{\partial r}\Big|_{r=R_q} + \frac{2\sigma_z(\alpha_b-\alpha_q)}{\hbar^2}\frac{l}{R_q}\varphi(R_q,z) = 0, \quad |z| \leqslant Z_q\end{gathered} \tag{2.12}$$

where $\sigma_z = \pm1$ is the third component of the vector of Pauli matrices σ in cylindrical coordinates. Since the latter equation depends exclusively on $l\sigma_z$ we end up with two distinguished cases, $\pm|l\sigma_z|$.

The eigenvalues of the three dimensional problem (2.6) are the ordered eigenvalues of the series of the two dimensional problems (2.9) for $\sigma_z|l| = 0, \pm1, \pm2, \ldots$ and the eigenfunctions are

$$\Phi(r,\theta,z) = \varphi_l(r,z)\mathrm{e}^{\mathrm{i}l\theta},$$

where $\varphi_l(r,z)$ is the corresponding eigenfunction of the plane problem. The spin dependent boundary conditions (2.12) result in a pair of Schrödinger equations to solve for each $|l| \neq 0$ which differ only in the interface condition.

3. Variational characterization of eigenvalues

We already pointed out that the eigenvalues of physical relevance are the ones not exceeding the confinement potential. We gage the potential to $V_q = 0$ and characterize the eigenvalues of the Schrödinger equation in the interval $J = (0, V_b)$ as minmax values of Rayleigh functionals. To this end we rewrite it in variational form.

Let $\Omega := (0, R_b) \times (-Z_b/2, Z_b/2)$, $\Omega_q := (0, R_q) \times (-Z_q/2, Z_q/2)$, $\Omega_b := \Omega \setminus \overline{\Omega}_q$. For $l = 0$ where the interface conditions (2.12) do not depend on the spin-orbit splitting it is appropriate to describe the problem in the weighted spaces

$$H := \{\varphi\colon\ r|\nabla\varphi|^2 \in L^1(\Omega),\ \varphi(r, \pm Z_b/2) = 0,\ 0 \leqslant r \leqslant R_b,\\ \varphi(R_b, z) = 0,\ -Z_b/2 \leqslant z \leqslant Z_b/2\}$$

with a scalar product $\langle \varphi, \psi \rangle_H := \int_\Omega r\nabla\varphi \cdot \nabla\psi \,\mathrm{d}(r, z)$, and $W := \{\varphi\colon\ r\varphi^2 \in L^1(\Omega)\}$ with $\langle \varphi, \psi \rangle_W := \int_\Omega r\varphi\psi \,\mathrm{d}(r, z)$. Then H is compactly embedded in W (cf. [13, Thm. 7.13]).

Multiplying equation (2.9) by $\psi \in H$ and integrating by parts, we obtain the variational form of the Schrödinger equation for $l = 0$:

Find $\varphi \in H$, $\varphi \neq 0$ and $\lambda \in J$ such that

$$\begin{aligned} a_0(\varphi, \psi; \lambda) := {} & \frac{\hbar^2}{2m_q(\lambda)} \int_{\Omega_q} r\nabla\varphi \cdot \nabla\psi \,\mathrm{d}(r, z) \\ & + \frac{\hbar^2}{2m_b(\lambda)} \int_{\Omega_b} r\nabla\varphi \cdot \nabla\psi \,\mathrm{d}(r, z) + V_b \int_{\Omega_b} r\varphi\psi \,\mathrm{d}(r, z) \\ = {} & \lambda \int_\Omega r\varphi\psi \,\mathrm{d}(r, z) =: \lambda b(\varphi, \psi) \quad \text{for every } \psi \in H. \end{aligned} \tag{3.1}$$

We assume that $E_{g,j} - V_j > 0$ for $j \in \{b, q\}$. Then the functions $\lambda \mapsto 1/m_j(\lambda)$ are defined for $\lambda \geqslant 0$, and are positive and monotonically decreasing.

The quadratic form $b(\cdot, \cdot)$ obviously is bilinear, positive, and bounded on W, and $a_0(\cdot, \cdot; \lambda)$ is symmetric and bounded (cf. Thm. 1.14 in [13]) on H for every fixed $\lambda \in J$, and from

$$a_0(\varphi, \varphi; \lambda) \geqslant \min\Big(\frac{\hbar^2}{2m_q(V_b)}, \frac{\hbar^2}{2m_b(V_b)}\Big) \int_\Omega r|\nabla\varphi|^2 \,\mathrm{d}(r, z)$$

it follows that $a_0(\cdot, \cdot)$ is H-elliptic. Hence, if we fix λ on the left-hand side of (3.1) then the linear eigenproblem

$$\text{Find } \mu \text{ and } \varphi \in H,\ \varphi \neq 0 \text{ with } a_0(\varphi, \psi; \lambda) = \mu b(\varphi, \psi) \quad \text{for every } \psi \in H$$

has a countable set of eigenvalues $0 < \mu_1^0 \leqslant \mu_2^0 \leqslant \dots$ which can be characterized as minmax values of its Rayleigh quotient (cf. [1]):

$$\mu_j^0 = \min_{\dim V = j} \max_{\varphi \in H,\, \varphi \neq 0} \frac{a_0(\varphi, \varphi; \lambda)}{b(\varphi, \varphi)}.$$

For $l \neq 0$ the following setting is appropriate. Let H be the weighted Sobolev space

$$H = H_0^1(\Omega, r, 1/r) := \{\varphi\colon\ r|\nabla\varphi|^2 \in L^1(\Omega),\ \frac{1}{r}\varphi^2 \in L^1(\Omega),\ \varphi = 0 \text{ on } \partial\Omega\}$$

with a scalar product

$$\langle \varphi, \psi \rangle := \int_\Omega \Big(r\nabla\varphi \cdot \nabla\psi + \frac{1}{r}\varphi\psi \Big) \,\mathrm{d}(r, z)$$

and set W as before. Then by [13, Thm. 18.12 and Exmpl. 18.15], H is compactly embedded in W. The variational form of (2.9), (2.12) reads

Find $\varphi \in H$, $\varphi \neq 0$ and $\lambda \in J$ such that

$$\begin{aligned} a_\pm(\varphi, \psi; \lambda) := {} & \frac{\hbar^2}{2m_q(\lambda)} \int_{\Omega_q} \Big(r\nabla\varphi \cdot \nabla\psi + \frac{l^2}{r}\varphi\psi \Big) \,\mathrm{d}(r, z) \\ & + \frac{\hbar^2}{2m_b(\lambda)} \int_{\Omega_b} \Big(r\nabla\varphi \cdot \nabla\psi + \frac{l^2}{r}\varphi\psi \Big) \,\mathrm{d}(r, z) \\ & + V_b \int_{\Omega_b} r\varphi\psi \,\mathrm{d}(r, z) \pm |l|\beta(\lambda) \int_{-Z_q/2}^{Z_q/2} \varphi(R_q, z)\psi(R_q, z) \,\mathrm{d}z \\ = {} & \lambda \int_\Omega r\varphi\psi \,\mathrm{d}(r, z) =: \lambda b(\varphi, \psi) \quad \text{for every } \psi \in H, \end{aligned} \tag{3.2}$$

where $\beta(\lambda) = \alpha_q(\lambda) - \alpha_b(\lambda)$.

The following lemma contains a sufficient condition for $a_\pm(\cdot, \cdot; \lambda)$ to be H-elliptic such that the linear eigenvalue problem

$$\text{Find } \mu \text{ and } \varphi \in H,\ \varphi \neq 0 \text{ with } a_\pm(\varphi, \psi; \lambda) = \mu b(\varphi, \psi) \quad \text{for every } \psi \in H \tag{3.3}$$

has a countable set of eigenvalues which can be characterized by the minmax principle of Poincaré.

Lemma 3.1. *Let $\kappa_{\min}$ be the minimal eigenvalue of the Steklov type eigenvalue problem*

$$c(\varphi,\psi) := \int_\Omega (r\nabla\varphi\cdot\nabla\psi + \frac{l^2}{r}\varphi\psi)\,\mathrm{d}(r,z) = \kappa\int_{-Z_q/2}^{Z_q/2}\varphi(R_q,z)\psi(R_q,z)\,\mathrm{d}z \quad \text{for every } \psi\in H. \tag{3.4}$$

If

$$\min\Big\{\frac{\hbar^2}{2m_q(\lambda)},\frac{\hbar^2}{2m_b(\lambda)}\Big\} > \frac{|l\beta(\lambda)|}{\kappa_{\min}} \quad \text{for every } \lambda\in J, \tag{3.5}$$

then $a_\pm(\cdot,\cdot;\lambda)$ is H-elliptic for every fixed $\lambda\in J$.

P r o o f. For $\varphi\in H$ we have

$$\begin{aligned} a_\pm(\varphi,\varphi;\lambda) &\geqslant \min\Big\{\frac{\hbar^2}{2m_q(\lambda)},\frac{\hbar^2}{2m_b(\lambda)}\Big\}c(\varphi,\varphi) - |l\beta(\lambda)|\int_{-Z_q/2}^{Z_q/2}\varphi(R_q,z)^2\,\mathrm{d}z \\ &\geqslant \Big(\min\Big\{\frac{\hbar^2}{2m_q(\lambda)},\frac{\hbar^2}{2m_b(\lambda)}\Big\} - \frac{|l\beta(\lambda)|}{\kappa_{\min}}\Big)c(\varphi,\varphi) \\ &\geqslant \frac{1}{l^2}\Big(\min\Big\{\frac{\hbar^2}{2m_q(\lambda)},\frac{\hbar^2}{2m_b(\lambda)}\Big\} - \frac{|l\beta(\lambda)|}{\kappa_{\min}}\Big)\|\varphi\|^2. \end{aligned}$$

□

The variational characterizations for a linear eigenproblem $a(\varphi,\psi)=\lambda b(\varphi,\psi)$ employ the Rayleigh quotient $R(\varphi) := a(\varphi,\varphi)/b(\varphi,\varphi)$ which is the unique solution of the real equation $F(\lambda;\varphi)=\lambda b(\varphi,\varphi)-a(\varphi,\varphi)$. More generally, a variational characterization of real eigenvalues of a nonlinear eigenvalue problem like (3.1) or (3.2) requires the existence of a Rayleigh functional, which is a solution of the corresponding equation

$$f_\diamond(\lambda;\varphi) := \lambda b(\varphi,\varphi) - a_\diamond(\varphi,\varphi;\lambda) = 0, \quad \diamond\in\{0,+,-\}. \tag{3.6}$$

We observe that $f_0(\cdot,\varphi)$ is monotonically increasing, and $f_0(0,\varphi) = -a_0(\varphi,\varphi;0) < 0$ for every $\varphi\neq 0$. Hence, $f_0(\cdot,\varphi)=0$ has at most one solution, and therefore defines a Rayleigh functional p_0 on a subset D_0 of H.

The following lemma contains a sufficient condition for the existence of Rayleigh functionals for the cases $\diamond\in\{+,-\}$.

Lemma 3.2. *Assume that the conditions of Lemma* 3.1 *hold, and*

$$-\frac{\hbar^2}{2}\max\Big(\Big(\frac{1}{m_q(\lambda)}\Big)',\Big(\frac{1}{m_b(\lambda)}\Big)'\Big)\geqslant\frac{|l\beta'(\lambda)|}{\kappa_{\min}}\quad\text{for every }\lambda\in J \tag{3.7}$$

where $\kappa_{\min}$ *denotes the minimal eigenvalue of the Steklov type eigenvalue problem* (3.4).

Then for every $\varphi\in H$, $\varphi\neq 0$ *each of the real equations*

$$f_\pm(\lambda;\varphi):=\lambda b(\varphi,\varphi)-a_\pm(\varphi,\varphi;\lambda)=0$$

has at most one solution $p_\pm(\varphi)\in J$.

P r o o f. We prove that $f_\pm(0,\varphi)<0$ and $\frac{\partial}{\partial\lambda}f_\pm(\lambda,\varphi)>0$ for every $\varphi\in H$, $\varphi\neq 0$ and every $\lambda\in J$.

First, $f_\pm(0,\varphi)=-a_\pm(\varphi,\varphi;0)<0$ follows immediately from the ellipticity of $a_\pm(\cdot,\cdot;0)$. Second,

$$\begin{aligned}\frac{\partial}{\partial\lambda}f_\pm(\lambda;\varphi)&=\int_\Omega r\varphi^2\,\mathrm{d}(r,z)-\Big(\frac{\hbar^2}{2m_q(\lambda)}\Big)'\int_{\Omega_q}\Big(r|\nabla\varphi|^2+\frac{l^2}{r}\varphi^2\Big)\,\mathrm{d}(r,z)\\&\quad-\Big(\frac{\hbar^2}{2m_b(\lambda)}\Big)'\int_{\Omega_b}\Big(r|\nabla\varphi|^2+\frac{l^2}{r}\varphi^2\Big)\,\mathrm{d}(r,z)\\&\quad\pm|l\beta'(\lambda)|\int_{-Z_q/2}^{Z_q/2}\varphi(R_q,z)^2\,\mathrm{d}z\\&>\min\Big\{-\Big(\frac{\hbar^2}{2m_q(\lambda)}\Big)',-\Big(\frac{\hbar^2}{2m_b(\lambda)}\Big)'\Big\}c(\varphi,\varphi)\\&\quad-|l\beta'(\lambda)|\int_{-Z_q/2}^{Z_q/2}\varphi(R_q,z)^2\,\mathrm{d}z\\&\geqslant\Big(\min\Big\{-\Big(\frac{\hbar^2}{2m_q(\lambda)}\Big)',-\Big(\frac{\hbar^2}{2m_b(\lambda)}\Big)'\Big\}-\frac{|l\beta'(\lambda)|}{\kappa_{\min}}\Big)c(\varphi,\varphi)\geqslant 0.\end{aligned}$$

□

Under the conditions of Lemma 3.2, for each of the eigenvalue problems in (3.1) and (3.2) a Rayleigh functional

$$p_\diamond\colon\ H\supset D_\diamond\to J$$

is defined. The general conditions of the minmax theory for nonlinear eigenvalue problems in [21] are satisfied, and Theorems 2.1 and 2.9 of [21] imply the following characterization of eigenvalues of (3.1) and (3.2) in the interval J.

Theorem 3.3. *Assume that the conditions of Lemma 3.2 are satisfied. Then each of the three Schrödinger equations in (3.1) and (3.2) has a finite number of eigenvalues in J, and*

(i) *the kth smallest eigenvalue can be characterized by*

$$\lambda_k^\diamond = \min_{\dim V = k,\, V \cap D_\diamond \neq \emptyset} \; \max_{\varphi \in V \cap D_\diamond} p_\diamond(\varphi); \tag{3.8}$$

(ii) *the minimum in (3.8) is attained for the subspace which is spanned by the eigenelements corresponding to the k smallest eigenvalues of the linear eigenproblem*

$$a_\diamond(\varphi, \psi, \lambda_k^\diamond) = \mu b(\varphi, \psi) \quad \text{for every } \psi \in H.$$

Discretizing the Schrödinger equations by a Galerkin method (finite elements, e.g.) one gets rational matrix eigenvalue problems

$$S_\diamond(\lambda)x := \lambda M x - \frac{\hbar^2}{2m_q(\lambda)} K_q x - \frac{\hbar^2}{2m_b(\lambda)} K_b x - M_b x \pm |l| \beta(\lambda) D x = 0, \tag{3.9}$$

where for $j \in \{b, q\}$

$$K_j = \left(\int_{\Omega_j} r \nabla \varphi_k \cdot \nabla \varphi_n + \frac{l^2}{r} \varphi_k \varphi_n \, \mathrm{d}(r, z) \right)_{k,n},$$

$$D = \left(\int_{-Z_q/2}^{Z_q/2} \varphi_k(R_q, z) \varphi_n(R_q, z) \, \mathrm{d}z \right)_{k,n},$$

$$M = \left(\int_{\Omega} r \varphi_k \varphi_n \, \mathrm{d}(r, z) \right)_{k,n},$$

and

$$M_b = V_b \left(\int_{\Omega_b} r \varphi_k \varphi_n \, \mathrm{d}(r, z) \right)_{k,n},$$

and φ_i denotes a basis of the ansatz space.

It is obvious that for the discretized problem (3.9) discrete versions of the conditions of Lemma 3.2 are sufficient for the existence of Rayleigh functionals $q_\diamond$ corresponding to $S_\diamond$ on the interval J, and that the eigenvalues of $S_\diamond$ in J are minmax values of $q_\diamond$. Moreover, it follows from the minmax characterization that the kth smallest eigenvalue of $S_\diamond$ is an upper bound of the corresponding eigenvalue of (3.1) and (3.2).

4. Solving the discretized problem

In this section we consider the problem to compute a few eigenvalues and the corresponding eigenvectors at the lower end of the spectrum of the discretization (3.9) of the Schrödinger equation. Since the methods apply to all three problems $S_\diamond(\lambda)x = 0$ we omit the subscript in this section.

For linear sparse eigenproblems $S(\lambda) = \lambda B - A$ very efficient methods are the iterative projection methods like the Lanczos, the Arnoldi, and the Jacobi-Davidson method, e.g., where approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem to subspaces of small dimension which are expanded in the course of the algorithm.

Let $V \in \mathbb{R}^{n\times k}$ be an (orthonormal) basis of the current search space $\mathcal{V} \subset \mathbb{R}^n$, assume that (θ, y), $y \in \mathbb{R}^k$ is an eigenpair of the projected eigenvalue problem

$$V^T S(\lambda) V y = 0, \tag{4.1}$$

and denote by $x := Vy$ the corresponding Ritz vector. To obtain an improved approximation it is reasonable to expand $\mathcal{V}$ by a direction with a high approximation potential for the eigenvector wanted next.

There are two approaches in literature for expanding the search space, both approximating the inverse iteration: a Jacobi-Davidson type method [4] and the Arnoldi method [19] based on the residual inverse iteration. Here we restrict ourselves to the latter.

Residual inverse iteration (introduced by Neumaier [12]) suggests the expansion

$$v = S(\sigma)^{-1} S(\theta) x \tag{4.2}$$

of the search space $\mathcal{V}$, where σ is a fixed parameter close to the wanted eigenvalues.

For a linear eigenproblem $S(\lambda) = A - \lambda B$ this is exactly the Cayley transformation with pole σ and zero θ, and since $(A-\sigma B)^{-1}(A-\theta B) = I + (\sigma-\theta)(A-\sigma B)^{-1}B$ and the Krylov spaces are shift-invariant the resulting projection method expanding $\mathcal{V}$ by v is nothing else but the shift-and-invert Arnoldi method.

If the linear system $S(\sigma)v = S(\theta)x$ is too expensive to solve for v we may choose as a new direction $v = K^{-1}S(\theta)x$ with $K \approx S(\sigma)$, and for the linear problem we obtain an inexact Cayley transformation or a preconditioned Arnoldi method. The resulting iterative projection method given in Algorithm 1 is therefore called the nonlinear Arnoldi method, although no Krylov space is constructed and no Arnoldi recursion holds.

Algorithm 1. Nonlinear Arnoldi Method

```
start with an initial pole σ and an initial orthonormal basis V, V^T V = I
determine preconditioner K ≈ S(σ), σ close to the smallest eigenvalue
k = 1
while k ⩽ number of wanted eigenvalues do
  compute the kth smallest eigenvalue μ and the corresponding normalized
  eigenvector y of the projected problem V^T S(μ) V y = 0
  determine Ritz vector u = V y and residual r = S(μ) u
  if ‖r‖ < ε then
    accept eigenvalue λ_k = μ, and eigenvector x_k = u,
    choose new pole σ and update preconditioner K ≈ S(σ) if indicated
    restart if necessary
    k = k + 1
  end if
  solve K v = r for v
  v = v − V V^T v, ṽ = v/‖v‖, V = [V, ṽ]
  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 [19].

A crucial point in iterative projection methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method from converging 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 eigenvectors. For nonlinear problems, however, such normal 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, however, its eigenvalues can be computed safely one after the other. The minimum in (3.8) is attained by the invariant subspace of $S(\lambda_k)$ corresponding to the k largest eigenvalues, and the maximum by every eigenvector corresponding to the eigenvalue 0. This suggests the safeguarded iteration for computing the kth smallest eigenvalue which is presented in Algorithm 2 for the projected eigenproblem $P(\lambda)y := V^T S(\lambda) V y = 0$:

Algorithm 2. Safeguarded iteration

1: Start with an approximation μ_1 to the kth smallest eigenvalue of $P(\lambda)y = 0$
2: **for** $l = 1, 2, \ldots$ until convergence **do**
3: determine an eigenvector u corresponding to the kth largest eigenvalue of the matrix $P(\mu_l)$
4: evaluate $\mu_{l+1} = p(u)$, i.e. solve $u^T P(\mu_{l+1})u = 0$ for μ_{l+1}
5: **end for**

The safeguarded iteration has the following convergence properties [18]: It converges globally to the smallest eigenvalue λ_1. The (local) convergence to simple eigenvalues is quadratic. If $P'(\lambda)$ is positive definite, and u in Step 3 of Algorithm 2 is replaced by an eigenvector of $P(\mu_l)u = \mu P'(\mu_l)u$ corresponding to the kth largest eigenvalue, then the convergence is even cubic. Moreover, a variant exists which is globally convergent also for higher eigenvalues.

5. Numerical experiments

We consider a cylindrical InAs quantum dot of radius 5 nm and height 9 nm centrally embedded into a GaAs cylindrical matrix of radius 10 nm and height 13.5 nm and we assume the one-band effective Hamiltonian with spin-orbit interaction (2.1). Following [10] we use the semiconductor band structure parameters $P_q = 0.7509$, $E_{g,q} = 0.42$, $\Delta_q = 0.48$, and $V_q = 0$ for InAs, and $P_b = 0.7848$, $E_{g,b} = 1.52$, $\Delta_b = 0.34$, and $V_b = 0.77$ for GaAs.

Problems of this type have been computationally treated by Li, Voskoboynikov, Lee, Liu, Sze and Tretyak in [9], [10], [17] using the so called Full Approximation Method, where each eigenvalue is targeted separately and where each iteration step requires the solution of a linear eigenproblem. Hence, for reasonably fine discretizations $S_\diamond(\lambda)x = 0$ this method is much too expensive.

Using FEMLAB [7] we discretized the Schrödinger equations by the finite element method with quadratic Lagrangian elements on a triangular grid. The matrix D in (3.9) corresponding to the interface integrals was directly computed from the mesh data, which can be extracted from the FEMLAB model. The physically interesting energy levels are the ones which are confined to the dot. Since the envelope functions are mainly concentrated on the quantum dot and since they decay very rapidly outside the dot, we chose a non-uniform grid which is the finest on the dot-matrix interface, fine on the dot and quite coarse on the matrix.

All the computations were performed under MATLAB 7.1.0 on an Intel Pentium D processor with 4 GByte RAM and 3.2 GHz. As a preconditioner for the iterative

projection methods we used the incomplete LU decomposition with threshold 0.01 of $S_\pm(0.1)$ but without the splitting term. We initialized the methods with a constant vector on $\overline{\Omega}_q \cup \Omega_b$ which is far away from an eigenvector, and we terminated the iteration for an eigenvalue provided the residual norm was less than 10^{-6}.

To guarantee the nonlinear Arnoldi method to work we need to fulfil conditions (3.5) and (3.7) for the discrete problem $S_\pm$, where $\kappa_{\min}$ is the smallest eigenvalue of the corresponding discretized Steklov type problem

$$Kx = \kappa Dx, \tag{5.1}$$

where K depends on l.

The minimal eigenvalues of the Steklov type problem (5.1) are displayed in Tab. 5.1 for $|l| = 1, 2, 3$. For $|l| \geqslant 4$ no confined states of the one-band Hamiltonian (2.1) exist. Condition (3.5) is equivalent to

$$\kappa_{\min} > \frac{|l\beta(\lambda)|}{\min\left\{\frac{\hbar^2}{2m_q(\lambda)}, \frac{\hbar^2}{2m_b(\lambda)}\right\}} \quad \text{for every } \lambda \in J,$$

and since $\lambda \to 1/m_j(\lambda)$, $j \in \{b, q\}$ are monotonically decreasing functions and $|\beta(\lambda)|$ is monotonic,

$$\kappa_{\min} > \frac{|l| \max\{|\beta(0)|, |\beta(V_b)|\}}{\min\left\{\frac{\hbar^2}{2m_q(V_b)}, \frac{\hbar^2}{2m_b(V_b)}\right\}}, \tag{5.2}$$

is sufficient for (3.5). Tab. 5.1 demonstrates that (5.2) is satisfied for all relevant l.

$\lvert l\rvert$	1	2	3
$\kappa_{\min}$	3.5189	4.976	6.6932
RHS	0.40411	0.80821	1.2123

Table 5.1. Minimal eigenvalues of (5.1) for $|l| = 1, 2, 3$.

Fig. 5.1 shows that (3.7) is also satisfied for $|l| = 1, 2, 3$ in the interval of interest $J = (0, V_b)$.

Tab. 5.2 displays all confined states of the problems $S_\diamond$ where we used a discretization with about 70000 degrees of freedom. The high dimension of the problem is necessary in order to guarantee correct capturing of the spin-orbit effect which is of the order of meV. Column 4 shows the CPU times needed for solving S_0, and S_+, S_- for $|l| = 1, 2, 3$ by the nonlinear Arnoldi method. The CPU times are given for every individual eigenvalue, though the eigenvalues of each plane problem $S_\diamond$ for fixed l are computed in one run.

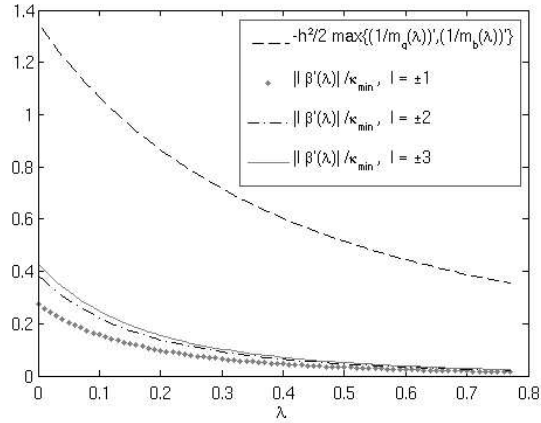

Figure 5.1. Condition (3.7) for $|l| = 1, 2, 3$ in the interval $J = (0, V_b)$.

$\pm\|l\|$	local order	λ	time [s]	time [s] (simultaneous)
0	1	0.2341	29.5	
−1	1	0.4000	33.7	16.5
0	2	0.4029	37.1	
1	1	0.4031	34.5	33.2
−1	2	0.5382	37.9	16.8
1	2	0.5402	37.7	29.9
−2	1	0.5725	33.7	13.0
2	1	0.5784	34.0	33.4
0	3	0.6195	30.3	
0	4	0.6255	29.1	
−2	2	0.6885	33.4	19.4
2	2	0.6927	32.0	32.8
−1	3	0.7285	27.3	11.0
1	3	0.7296	27.3	25.3
0	5	0.7345	26.1	
−3	1	0.7453	36.6	9.6
3	1	0.7531	36.5	36.2

Table 5.2. Confined states of a cylindrical quantum dot of radius 5 nm and height 9 nm and the CPU times for their simultaneous and separate computation for a given eigenvalue.

The physical background of the pair of the nonlinear eigenvalue problems $S_\pm$ is the energy level splitting in the internal magnetic field, which suggests that they are strongly correlated. This is reflected by the mathematical model, since the pair differs only by an interface contribution, which for a discrete problem corresponds to a low rank matrix. Because of the local nature of this contribution it is justified to expect the eigensubspaces of both the problems to be close to each other. Indeed,

if X_-^l and X_+^l denote the subspaces spanned by the eigenvectors corresponding to the three smallest eigenvalues of S_- and S_+ for $l = 1, 2, 3$, respectively, then the singular values of the matrix $[X_-^l, X_+^l]$ for $l = 1, 2, 3$ show a clear gap between the largest three singular values and the remaining ones (cf. Tab. 5.3), which indicates an overlap of the eigenspaces spanned by X_-^l and X_+^l.

$\|l\|$	σ_1	σ_2	σ_3	σ_4	σ_5	σ_6
1	1.6975	1.4142	1.0575	0.0063532	0.0063432	0.0027425
2	1.6125	1.4142	1.1831	0.0091780	0.0089219	0.0038084
3	1.5575	1.4142	1.2547	0.0095062	0.0087885	0.0042112

Table 5.3. Singular values of $[X_-^l, X_+^l]$, for $l = 1, 2, 3$.

This experiment suggests that the solution of one problem can benefit from the solution of the other one, and leads us to the following approach. We apply an iterative projection method, such as described in the last section, to the pair of problems $S_\pm(\lambda)x = 0$ simultaneously in such a way that they both use the same search subspace $\mathcal{V}$.

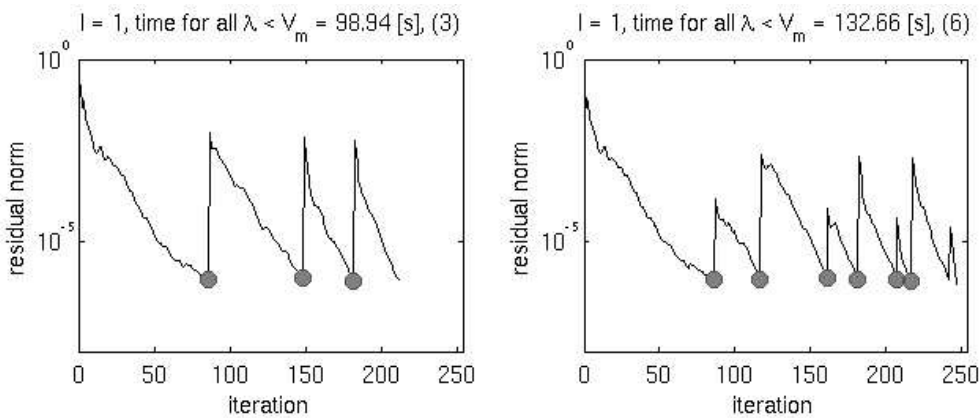

Figure 5.2. Convergence of the nonlinear Arnoldi method for S_-, $l = 1$ (left), and of the simultaneous computation for problems $S_\pm$, $l = 1$ (right).

The left subplot in Fig. 5.2 shows the convergence history of the nonlinear Arnoldi method for S_- and $l = 1$ (where we computed one more eigenvalue than required since we do not know a priori the number of confined states). For S_+ the picture looks very similar. We solved the problems S_+ and S_- for fixed $l = 1, 2, 3$ simultaneously, i.e. after having found λ_k^+ the Arnoldi method aimed at λ_k^-, and thereafter at λ_{k+1}^+, etc. The convergence history for $l = 1$ is shown in the right subplot of Fig. 5.2. It demonstrates that the computation of λ_k^- requires less iterations than the computation of λ_k^+. The last column of Tab. 5.2 shows that the total computing

time is reduced by approximately 25% by this simultaneous computation of confined states.

The same approach can also be used with the Jacobi Davidson subspace expansion. In [3] we compared the robustness of the Jacobi Davidson and nonlinear Arnoldi subspace expansion subject to the quality of the preconditioner. We found that the Jacobi Davidson subspace expansion is favorable if the size of the problem does not allow for a good quality preconditioner. Otherwise the residual inverse type expansion as in nonlinear Arnoldi is more efficient. In this work we focused on the latter since for two dimensional problems a good quality preconditioner can be obtained inexpensively.

6. Conclusions

We directly included the spin-orbit interaction into the one-band Hamiltonian with nonparabolic effective mass in weak form, which results in a pair of rational eigenproblems. We derived a minmax characterization of its eigenvalues allowing to compute the confined states efficiently by an iterative projection method like the nonlinear Arnoldi or the Jacobi-Davidson method. Handling a pair of problems with opposite spin simultaneously the CPU time can be further reduced by approximately 25%. We plan to extend the ideas presented in this work to problems where the energy level splitting originates from the external magnetic field.

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