A minimization problem for an elliptic eigenvalue problem with nonlinear dependence on the eigenparameter

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Abstract

In this paper we examine an eigenvalue optimization problem. Given two nonlinear functions $\alpha(\lambda)$ and $\beta(\lambda)$, find a subset D of the unit ball of measure A for which the first Dirichlet eigenvalue of the operator $-\text{div}((\alpha(\lambda)\chi_D + \beta(\lambda)\chi_{D^c})\,\nabla u) = \lambda u$ is as small as possible. This sort of nonlinear eigenvalue problems arises in the study of some quantum dots taking into account an electron effective mass. We establish the existence of a solution, and we propose a numerical algorithm to obtain an approximate description of the optimizer.

Keywords: Nonlinear eigenvalue problem, Shape optimization, Eigenvalue optimization, Quantum Dots
2000 MSC: 35Q93, 49R05, 35P15, 49Q10

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1. Introduction

Let Ω be a bounded, connected, open set in $\mathbb{R}^N$ with smooth boundary. Assume that A is a given positive number, $0 < A < |\Omega|$, where $|.|$ denotes the Lebesgue measure. Given a measurable set $D \subset \Omega$ with $|D| = A$ and continuous positive functions $\alpha(\lambda)$ and $\beta(\lambda)$ for $\lambda \geq 0$, consider the following nonlinear eigenvalue problem

$$-\text{div}(G(\lambda, x)\nabla u) = \lambda u \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

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where $G(\lambda, x) = \alpha(\lambda)\chi_D + \beta(\lambda)\chi_{D^c}$, $\alpha(\lambda) \geq \beta(\lambda)$. In this paper, λ is the principal eigenvalue (ground state energy) or the smallest positive eigenvalue of (1.1) and $u = u(x)$ is a corresponding eigenfunction.

We are interested in the cases where $\alpha(\lambda)$ and $\beta(\lambda)$ are nonlinear functions of the parameter λ. Indeed, equation (1.1) can be regarded as a nonlinear elliptic eigenvalue problem such that the nonlinearity originates from the nonlinear dependence on the eigenparameter.

Such nonlinear eigenvalue problems appear as the Hamiltonian equation governing some quantum dot nanostructures, where $\alpha(\lambda)$ and $\beta(\lambda)$ correspond to the effective mass of the carrier (electron or hole) and the surrounding matrix, respectively, and λ is the ground state energy [1, 2, 3, 4]. A real physical phenomenon modeled by equation (1.1) is the heterostructures of different semiconductors where the electron effective mass depends on both the energy and position [1, 2].

It is known that the ground state energy of (1.1) depends on the set D, the region with effective mass α, and we use the notation $\lambda(D)$ as we want to emphasize this dependence. To determine the system's profile which gives the minimum ground state energy, we study the following optimization problem

$$\inf_{\substack{D\subset\Omega \\ |D|=A}} \lambda(D). \tag{1.2}$$

Solutions of minimization problem (1.2) correspond to the physical systems where have lowest ground state energies and so are most stable structures from a physical point of view. Regarding the importance of stable structures in designing electronic and photonic devices based on quantum dots, it would be interesting to find them.

Problem (1.1) is in fact a generalization of the linear case $G(\lambda, x) = \alpha\chi_D(x) + \beta\chi_{D^c}(x)$ where α and β are two positive constants, $\alpha > \beta$. In the linear case, the optimization problem (1.2) is the problem of optimal design where two material phases are to be distributed inside a fixed region Ω. This problem is known to often have no solution other than microstructural designs [5]. However, the original problem (1.2) may still have a solution for specific Ω for instance when Ω is a ball. Existences of a radially symmetric optimal set for the linear case has been established in [6] when $\Omega = \mathcal{B}(0, R)$ is a ball with radius R centered at the origin. Conca *et al.* have revived interest in this problem by giving a new simpler proof of the existence result only using rearrangement techniques [7]. For the one-dimensional case, Krein has shown in [8] that the unique minimizer is a ball $\mathcal{B}(0, R^*)$. This suggests for higher dimensions that $\mathcal{B}(0, R^*)$ is a natural candidate to be the optimal domain. This conjecture has been supported by numerical tests in [9]. In addition, it has been shown in [10] employing second order shape derivative calculus that $\mathcal{B}(0, R^*)$ is a local minimum for the optimization problem when A is small enough. In spite of the above evidences, it has been established in [11] that the conjecture is not true at least in two- or three- dimensional spaces when α and β are close to each other (low contrast regime) and A is sufficiently large. This makes clear that the optimal domain can not be a ball. The theoretical base for the result is an asymptotic expansion of the eigenvalue with respect to $\alpha - \beta$ as $\alpha \to \beta$, which allows one to approximate the optimization problem by a simple minimization problem. Based upon the properties of Bessel functions, it has been proved in [12] that the conjecture is not true not only for two- or three-dimensional spaces, but also for all dimensions $n \geq 2$. Recently, Laurian has proved that the optimal domain in low contrast regime is either a centered ball or the union of a centered ball and a centered ring touching the boundary, depending on the prescribed volume ratio between the two materials [13].

In this paper we want to generalize those investigations to the case where $\alpha(\lambda)$ and $\beta(\lambda)$ are nonlinear functions of the parameter λ. First, we will show the existence of a solution for the case where Ω is a ball centered at the origin. Thereafter we will address the question of the configuration of the optimal domain. It will be demonstrated that the optimal set in the one-dimensional problem is a symmetric interval centered at the origin. Despite the conclusion in $\mathbb{R}^1$, a ball is not an optimal shape thanks to findings of the linear cases in two- or three-dimensional space. At last, we need an algorithm that allows us to compute numerical approximations of the optimal solution of the problem (1.2). An efficient and convergent numerical algorithm will be derived based upon the level sets of the gradient of the eigenfunction and the safeguarded iteration.

Let us recall here that nonlinear eigenvalue problems and optimization problems have many applications in engineering and applied sciences and these problems have been intensively attractive to mathematicians in the past decades [14]. However, it should be mentioned that the majority of the investigated nonlinear models are nonlinear in their differential operator part [15, 16, 17]. We note that the equation (1.1) has nonlinear dependence on the parameter λ and such systems have been under less attention in this field of study [18, 19].

Throughout this paper $\langle \cdot, \cdot \rangle$ denotes the inner product in $H_0^1(\Omega)$, and we use the abbreviation a.e. when we desire to say that a property holds almost everywhere.

The remainder of this paper is organized as follows. In section 2, we prove the existence of a solution for problem (1.2). In section 3, we introduce and analyze an algorithm which generates a decreasing sequence of principal eigenvalues. In section 4, we apply our algorithm to some minimization problems and present the numerical results to show the efficiency of our algorithm and its drawbacks.

2. Existence result for optimization problem (1.2)

This section is devoted to prove the existence of a solution for problem (1.2). We take advantage of a variational characterization of the ground state energy which follows immediately from a generalization of the minmax characterization of the eigenvalues of Poincaré to eigenvalue problems depending nonlinearly on the eigenparameter given in [20, 21, 22].

A variational formula is derived for a more general function $G(\lambda, x)$ than a step function. We assume that in (1.1)

$$G(\lambda, \cdot) \text{ is bounded for every } \lambda \geq 0, \tag{2.1}$$

$$G(\cdot, x) \text{ is a continuous function.} \tag{2.2}$$

Multiplying (1.1) by $\varphi \in H_0^1(\Omega)$ and integrating by parts, one gets the following variational formulation of (1.1): Find $\lambda \in \mathbb{R}$ and $u \in H_0^1(\Omega)$, $u \neq 0$ such that

$$\int_\Omega G(\lambda, x)\nabla u \cdot \nabla\varphi dx = \lambda \int_\Omega u\varphi dx, \tag{2.3}$$

for all φ in $H_0^1(\Omega)$.

Both integrals in (2.3) can be viewed as bounded linear functionals on $H_0^1(\Omega)$, and thanks to the Riesz representation theorem, (2.3) is equivalent to the nonlinear eigenvalue problem

$$\langle \mathcal{F}(\lambda)u, \varphi\rangle = \lambda \int_\Omega u\varphi dx - \int_\Omega G(\lambda, x)\nabla u \cdot \nabla\varphi dx = 0,$$

for all φ in $H_0^1(\Omega)$, or

$$\mathcal{F}(\lambda)u = 0, \tag{2.4}$$

where $\mathcal{F}(\lambda) : H_0^1(\Omega) \to H_0^1(\Omega)$, is a family of self-adjoint and bounded operators for $\lambda \geq 0$.

We take advantage of the following minmax characterization for nonlinear eigenvalue problems which is a special case of the more general result in [20, 22]:

Theorem 2.1. *Let $\mathcal{H}$ be a Hilbert space with scalar product $\langle\cdot,\cdot\rangle$. Consider the nonlinear eigenvalue problem*

$$\mathcal{F}(\lambda)u = 0, \tag{2.5}$$

where $\mathcal{F}(\lambda) : \mathcal{H} \to \mathcal{H}$ is a family of self-adjoint and bounded operators on $\mathcal{H}$ depending continuously on a parameter $\lambda \in J$, and J is an open real interval.

Assume that

(A_1) for every fixed $u \in \mathcal{H}$, $u \neq 0$ the real equation

$$f(\lambda; u) := \langle\mathcal{F}(\lambda)u, u\rangle = 0 \tag{2.6}$$

has exactly one solution $\lambda := \mathcal{P}(u) \in J$.

(A_2) for every $u \neq 0$ and every $\lambda \in J$ with $\lambda \neq \mathcal{P}(u)$ it holds that

$$(\lambda - \mathcal{P}(u))f(\lambda, u) > 0, \tag{2.7}$$

(A_3) for every $\lambda \in J$ the supremum of the essential spectrum of $\mathcal{F}(\lambda)$ is negative.

Then problem (2.5) has a countable set of eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots$, and it holds that

$$\lambda_j = \min_{\dim V = j} \max_{0 \neq u \in V \subset \mathcal{H}} \mathcal{P}(u). \tag{2.8}$$

Remark 2.1. The requirements (A_1), (A_2) and (A_3) are generalizations for the ones for linear eigenvalue problems. Equation $f(\lambda; u) = 0$ defines a functional $\mathcal{P}$ on $\mathcal{H} \setminus \{0\}$, which generalizes the Rayleigh quotient for linear eigenvalue problems with $\mathcal{F}(\lambda) = \lambda I - A$, and therefore it is called Rayleigh functional of (2.5), and (A_2) generalizes the definiteness requirement for linear pencils $\mathcal{F}(\lambda) = \lambda B - A$.

Theorem 2.1 applies to G if we further assume

$$G(0, \cdot) > 0, \quad \text{a.e. in } \Omega. \tag{2.9}$$

and that $G(\lambda, x)$ is a non-increasing function with respect to λ for every $x \in \Omega$, i.e.

$$G(\lambda_1, \cdot) \geq G(\lambda_2, \cdot) \text{ a.e. in } \Omega \text{ for } \lambda_1, \lambda_2 \geq 0 \text{ with } \lambda_1 < \lambda_2. \tag{2.10}$$

Then, in view of (2.9) and (2.10) we see

$$f(\lambda, u) := \langle\mathcal{F}(\lambda)u, u\rangle = \lambda\|u\|^2_{L^2(\Omega)} - \int_\Omega G(\lambda, x)|\nabla u|^2 dx, \tag{2.11}$$

for $u \neq 0$ is strictly monotonically non-decreasing and $f(0, u) < 0$. Hence, the conditions of Theorem 2.1 are satisfied, and we obtain

Theorem 2.2. *Suppose that conditions* (2.1)*,* (2.2)*,* (2.9) *and* (2.10) *hold. Then the principal eigenvalue of* (1.1) *allows for a variational formulation*

$$\lambda = \min_{\substack{v \in H_0^1(\Omega) \\ \|v\|_{L^2(\Omega)}=1}} \mathcal{P}(v) = \int_\Omega G(\lambda, x)|\nabla u|^2 dx, \tag{2.12}$$

where u is the associated eigenfunction.

We gain some insight into the eigenfunction of problem (1.1) associated with the principal eigenvalue from the following lemma.

Lemma 2.3. *Let u be an eigenfunction corresponding to the first eigenvalue of* (1.1) *then*

(i) $u \in H_0^1(\Omega) \cap C^{0,\delta}(\overline{\Omega})$ *for some* $\delta \in (0, 1)$ *when* $N \leq 3$*,*

(ii) $u > 0$ *in* Ω*,*

(iii) u is unique up to a constant factor,

(iv) level sets of the function $|\nabla u|$ have measure zero.

Proof. (i) follows from standard regularity results for elliptic partial differential equations, see [23].

(ii) In view of (2.12), we can regard $|u|$ as an eigenfunction. Applying Harnack's inequality [23], leads us to the fact that eigenfunctions associated to λ have a constant sign.

(iii) Let $\widetilde{u}$ be an eigenfunction of (1.1) corresponding to λ. According to part (ii), we have $\int_\Omega \widetilde{u} dx > 0$ and so there exists a real constant τ such that $\int_\Omega u - \tau\widetilde{u} dx = 0$. But since $u - \tau\widetilde{u}$ is also a solution of (1.1) associated to the principal eigenvalue λ and $\int_\Omega u - \tau\widetilde{u} dx = 0$, one arrives at $u \equiv \tau\widetilde{u}$.

(iv) All level sets $\{x : |\nabla u| = s\}$ have measure zero because of Lemma 7.7 in [23] and part (ii).

□

Having the variational formulation (2.12) for the first eigenvalue, we devote the rest of this section to demonstrate that the optimization problem (1.2) has a solution if $\Omega = B(0, R)$. Note that $G(\lambda, x) = \alpha(\lambda)\chi_D + \beta(\lambda)\chi_{D^c}$ satisfies conditions (2.1), (2.2), (2.9) and (2.10) if the continuous functions $\alpha(\cdot)$ and $\beta(\cdot)$ are positive and non-increasing, and $\alpha(\lambda) \geq \beta(\lambda)$ for every $\lambda \geq 0$.

Theorem 2.4. *Let $\Omega = \mathcal{B}(0, R)$, and assume that the conditions* (2.1)*,* (2.2)*,* (2.9) *and* (2.10) *satisfied. Then, the minimization problem* (1.2) *is solvable, i.e. there exists $\widetilde{D} \subset \Omega$ with $|\widetilde{D}| = A$, such that*

$$\widehat{\lambda} = \lambda(\widetilde{D}) = \inf_{\substack{D\subset\Omega\\|D|=A}} \lambda(D).$$

Proof. For fixed $\lambda \in J = (0, +\infty)$ we consider the following linear eigenvalue problem

$$-\mathrm{div}(G(\lambda, x)\nabla u) = \mu(\lambda, D)u \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega,$$

where $\mu(\lambda, D)$ is the principal eigenvalue that depends upon both λ and D.

Applying results of Alvino and Conca [6, 7], the minimization problem

$$\zeta(\lambda) = \inf_{\substack{D\subset\Omega\\|D|=A}} \mu(\lambda, D),$$

admits a radially symmetric solution D for every $\lambda \geq 0$. Hence, the function $\zeta : J \to \mathbb{R}$ is well defined and

$$\zeta(\lambda) = \inf_{\substack{D\subset\Omega;\ |D|=A\\ u\in H_0^1(\Omega);\ \|u\|_{L^2(\Omega)}=1}} \int_\Omega G(\lambda, x)|\nabla u|^2 dx. \tag{2.13}$$

In the following we show that this function has a fixed point, $\zeta(\widetilde{\lambda}) = \widetilde{\lambda}$.

Step 1. Consider a function $u \in H_0^1(\Omega)$ with $\|u\|_{L^2(\Omega)} = 1$ and $D \subset \Omega$ with $|D| = A$. According to (2.10), we have

$$\int_\Omega (\alpha(\lambda_1)\chi_D + \beta(\lambda_1)\chi_{D^c})\, |\nabla u|^2 dx \geq \int_\Omega (\alpha(\lambda_2)\chi_D + \beta(\lambda_2)\chi_{D^c})\, |\nabla u|^2 dx,$$

whenever $\lambda_1 < \lambda_2$, and therefore it follows from (2.13) that ζ is non-increasing.

Step 2. Assume that $\{\lambda_n\}$ is a non-decreasing sequence of positive numbers tending to $\widehat{\lambda}$. Employing (2.13) and the monotonicity of ζ derived in step 1, we have

$$\begin{aligned} 0 \leq \zeta(\lambda_n) - \zeta(\widehat{\lambda}) &= \int_\Omega (\alpha(\lambda_n)\chi_{D_n} + \beta(\lambda_n)\chi_{D_n^c})|\nabla u_n|^2 dx - \int_\Omega (\alpha(\widehat{\lambda})\chi_{\widehat{D}} + \beta(\widehat{\lambda})\chi_{\widehat{D}^c})|\nabla \widehat{u}|^2 dx \\ &\leq \int_\Omega (\alpha(\lambda_n)\chi_{\widehat{D}} + \beta(\lambda_n)\chi_{\widehat{D}^c})|\nabla \widehat{u}|^2 dx - \int_\Omega (\alpha(\widehat{\lambda})\chi_{\widehat{D}} + \beta(\widehat{\lambda})\chi_{\widehat{D}^c})|\nabla \widehat{u}|^2 dx \\ &= \int_\Omega \Big((\alpha(\lambda_n) - \alpha(\widehat{\lambda}))\chi_{\widehat{D}} + (\beta(\lambda_n) - \beta(\widehat{\lambda}))\chi_{\widehat{D}^c}\Big)\, |\nabla \widehat{u}|^2 dx, \end{aligned}$$

and hence $\zeta(\lambda_n)$ converges to $\zeta(\widehat{\lambda})$ as λ_n tends to $\widehat{\lambda}$, i.e. ζ is left continuous.

Step 3. Let $\{\lambda_n\}$ be a non-increasing sequence of positive numbers tending to $\widehat{\lambda}$. Applying (2.13) and the monotonicity of ζ, one can infer

$$
\begin{aligned}
0 \le \zeta(\widehat{\lambda}) - \zeta(\lambda_n) &\le \int_\Omega (\alpha(\widehat{\lambda})\chi_{D_n} + \beta(\widehat{\lambda})\chi_{D_n^c})|\nabla u_n|^2 dx - \int_\Omega (\alpha(\lambda_n)\chi_{D_n} + \beta(\lambda_n)\chi_{D_n^c})|\nabla u_n|^2 dx \\
&= \int_\Omega \left[\left(\alpha(\widehat{\lambda}) - \alpha(\lambda_n)\right)\chi_{D_n} + \left(\beta(\widehat{\lambda}) - \beta(\lambda_n)\right)\chi_{D_n^c}\right] |\nabla u_n|^2 dx \\
&\le \| \left(\alpha(\widehat{\lambda}) - \alpha(\lambda_n)\right)\chi_{D_n} + \left(\beta(\widehat{\lambda}) - \beta(\lambda_n)\right)\chi_{D_n^c}\|_{L^\infty(\Omega)} \|u_n\|^2_{H_0^1(\Omega)}.
\end{aligned}
$$

The righthand side of the last inequality converges to zero if the sequence $\|u_n\|_{H_0^1(\Omega)}$ is bounded from above. Invoking (2.13) and the monotonicity of ζ, we observe

$$
\beta(\lambda_n)\|u_n\|^2_{H_0^1(\Omega)} \le \zeta(\lambda_n) \le \alpha(\lambda_n)\|\psi\|^2_{H_0^1(\Omega)},
$$

where ψ is the normalized eigenfunction corresponding to the principal eigenvalue of Laplacian with Dirichlet's boundary condition. Recall that $\alpha(.)$ is a non-increasing continuous function. Hence, the sequence $\|u_n\|_{H_0^1(\Omega)}$ cannot be unbounded, and ζ is also a right continuous function.

In summary, ζ is a non-increasing continuous function with positive values which yields that ζ has a positive fixed point $\widetilde{\lambda}$ where

$$
\widetilde{\lambda} = \zeta(\widetilde{\lambda}) = \inf_{\substack{D\subset\Omega \\ |D|=A}} \mu(\widetilde{\lambda}, D) = \inf_{\substack{D\subset\Omega;\ |D|=A \\ u\in H_0^1(\Omega);\ \|u\|_{L^2(\Omega)}=1}} \int_\Omega G(\widetilde{\lambda}, x)|\nabla u|^2 dx \tag{2.14}
$$

Step 4. The infimum in the last equality is attained by a radially symmetric set $\widetilde{D}$. Moreover,

$$
-\text{div}((\alpha(\widetilde{\lambda})\chi_{\widetilde{D}} + \beta(\widetilde{\lambda})\chi_{\widetilde{D}^c})\nabla\widetilde{u}) = \widetilde{\lambda}\widetilde{u} \quad \text{in } \Omega, \qquad \widetilde{u} = 0 \quad \text{on } \partial\Omega,
$$

in the weak sense using (2.13).

Now, we claim that $\widetilde{D}$ is a minimizer of problem (1.2). Consider an eigenvalue of (1.1), $\overline{\lambda}(\overline{D})$, where $\overline{\lambda}(\overline{D}) < \widetilde{\lambda}(\widetilde{D})$, then one can observe using (2.10) and (2.14) that

$$
\begin{aligned}
\overline{\lambda}(\overline{D}) &= \int_\Omega (\alpha(\overline{\lambda})\chi_{\overline{D}} + \beta(\overline{\lambda})\chi_{\overline{D}^c})|\nabla\overline{u}|^2 dx \ge \int_\Omega (\alpha(\widetilde{\lambda})\chi_{\overline{D}} + \beta(\widetilde{\lambda})\chi_{\overline{D}^c})|\nabla\overline{u}|^2 dx \\
&\ge \int_\Omega (\alpha(\widetilde{\lambda})\chi_{\widetilde{D}} + \beta(\widetilde{\lambda})\chi_{\widetilde{D}^c})|\nabla\widetilde{u}|^2 dx = \widetilde{\lambda}(\widetilde{D}),
\end{aligned}
$$

which is a contradiction. Therefor, $\widetilde{\lambda}$ is the minimum value of the optimization problem (1.2) associated to the radially symmetric set $\widetilde{D}$. □

Remark 2.2. From the physics point of view it is important to know the configuration of the optimal set $\widetilde{D}$. However, from the above proof we only get that the optimal set is radially symmetric, and for instance it could be a wild set including infinitely many annuli centered at the origin.

We would like to clarify what kind of radially symmetric shape is a minimizer. In the one dimensional case, Krein has proved for the linear case, [8], that the unique minimizer is obtained by putting the material with the highest phase in one piece in the center of the domain. Switching to the nonlinear case, one can discover that the infimum is attained in formula (2.14) by a ball centered at the origin and in fact the minimizer set $\widetilde{D}$ is a ball centered at the origin when $N = 1$. For higher dimensions, the exact shape of the optimizer is an open problem even for the linear case. This motivates a numerical approach to approximate an optimal set.

3. A descent approach

In this section we describe an algorithm which starts from a given initial set D_0 and determines a new set D_1 such that the principal eigenvalue is diminished, i.e.

$$\lambda(D_1) \leq \lambda(D_0).$$

The algorithm relies strongly on the Rayleigh functional $\mathcal{P}$. It includes the ideas which have been applied successfully to minimize an eigenvalue in [11, 24, 25, 26, 27]. It relies on the variational formulation of the eigenvalues and uses level sets of the eigenfunctions or gradients of them. In contrast to the method proposed in [11], for our problem we do not have an explicit expression of the Rayleigh functional and this raises some technical problems. Employing the level sets of the eigenfunction or its gradient, we need some modification of the bathtub principle with an eye on our problem.

Lemma 3.1. *Let $f \in L^1(\Omega)$ be a nonnegative function and*

$$\mathcal{M} = \{\eta \in L^\infty(\Omega) \, : \, \beta \leq \eta(x) \leq \alpha \text{ a.e. in } \Omega, \int_\Omega \eta(x)dx = \alpha A + \beta(|\Omega| - A)\}.$$

Then the minimization problem

$$\inf_{\eta \in \mathcal{M}} \int_\Omega f(x)\eta(x)dx, \tag{3.1}$$

is solvable by some $\widehat{\eta}(x) = \alpha\chi_{\widehat{D}}(x) + \beta\chi_{\widehat{D}^c}(x)$.

With

$$t = \inf\{s \in \mathbb{R} : |\{x : \ f(x) \le s\}| \ge A\} \tag{3.2}$$

it holds that

$$|\widehat{D}| = A \text{ and } \{x : \ f(x) < t\} \subseteq \widehat{D} \subseteq \{x : \ f(x) \le t\}. \tag{3.3}$$

Proof. We recall that $\mathcal{M}$ is a convex subset of $L^\infty(\Omega)$, that is compact for the weak-* convergence and its extremal points are exactly of the type $\alpha\chi_D + \beta\chi_{D^c}$ for some measurable subset D of Ω [28, 29]. For this extremal points, we have $|D| = A$ regarding the integral constraint in the definition of $\mathcal{M}$. Due to the continuity of integration in (3.1) and the compactness of the set $\mathcal{M}$, the minimization problem (3.1) has a minimum among the extremal points of the convex set $\mathcal{M}$. Hence, we have a solution of the form $\alpha\chi_{\widehat{D}} + \beta\chi_{\widehat{D}^c}$ for a measurable subset $\widehat{D} \subset \Omega$, $|\widehat{D}| = A$.

In view of (3.1), $\widehat{D} \subset \{x : \ f(x) \le s\}$ for some $s > 0$, and we choose

$$t = \inf\{s \in \mathbb{R} : |\{x : \ f(x) \le s\}| \ge A\}.$$

To gain more insight into the optimal set $\widehat{D}$ we consider two different cases. Firstly, assume that $|\{x : \ f(x) \le t\}| = A'$ for some $A' > A$. Invoking (3.2), we have for any $\epsilon > 0$

$$|\{x : \ f(x) \le t - \epsilon\}| < A < A'.$$

Setting $\delta = A' - A$, we observe that

$$\begin{aligned} 0 < \delta < A' - |\{x : \ f(x) \ \le \ t - \epsilon\}| &= A' - |\{x : \ f(x) \le t\}| + |\{x : \ t - \epsilon < f(x) \le t\}| \\ &= |\{x : \ t - \epsilon < f(x) \le t\}|, \end{aligned}$$

which, passing to the limit $\epsilon \to 0$, leads us to

$$|\{x : \ f(x) = t\}| \ge \delta > 0.$$

Then, $|\{x : \ f(x) < t\}| = A' - |\{x : \ f(x) = t\}| \le A' - \delta = A$. Since $|\widehat{D}| = A$, we have

$$\{x : \ f(x) < t\} \subseteq \widehat{D} \subseteq \{x : \ f(x) \le t\},$$

and $\widehat{D}$ contains a subset of $\{x : \ f(x) = t\}$. In particular, the minimizer $\widehat{D}$ is not unique since there is no unique subset of $\{x : \ f(x) = t\}$ as a part of $\widehat{D}$.

Secondly, suppose that $|\{x : \ f(x) \le t\}| = A$. Since $\widehat{D} \subset \{x : \ f(x) \le t\}$ and $|\widehat{D}| = A$, then $\widehat{D}$ can be determined uniquely by

$$\widehat{D} = \{x : \ f(x) \le t\}.$$

□

Lemma 3.1 is the basis for constructing a sequence of domains D_n such that $|D_n| = A$ for every n and

$$\lambda(D_{n+1}) \leq \lambda(D_n). \tag{3.4}$$

Denote by u_n a normalized eigenfunction of problem (1.1) with $D = D_n$, let $f(x) := |\nabla u_n(x)|^2$ and fix $\lambda > 0$. By Lemma 3.1 there exists $D_{n+1} \subset \Omega$ with $|D_{n+1}| = A$ such that

$$\int_\Omega (\alpha(\lambda)\chi_{D_n} + \beta(\lambda)\chi_{D_n{}^c})|\nabla u_n|^2 dx \geq \int_\Omega (\alpha(\lambda)\chi_{D_{n+1}} + \beta(\lambda)\chi_{D_{n+1}{}^c})|\nabla u_n|^2 dx. \tag{3.5}$$

According to (2.2) and (2.10) both sides of the above inequality are non-increasing continuous functions of λ, and due to

$$\lambda_n = \int_\Omega (\alpha(\lambda_n)\chi_{D_n} + \beta(\lambda_n)\chi_{D_n{}^c})|\nabla u_n|^2 dx,$$

$\lambda_n = \lambda(D_n)$ is a fixed point of the left hand side of (3.5).

In accordance with (2.12) a fixed point of the right hand side of (3.5) is $\mathcal{P}_{D_{n+1}}(u_n)$, where $\mathcal{P}_{D_{n+1}}$ denotes the Rayleigh functional of (1.1) corresponding to $D = D_{n+1}$. Recall that both sides of (3.5) are non-increasing continuous functions of λ. Then it is obvious that the fixed point of the left hand side of (3.5) is greater than or equal to the fixed point of its right hand side. Hence,

$$\lambda(D_n) \geq \int_\Omega (\alpha(\lambda_n)\chi_{D_{n+1}} + \beta(\lambda_n)\chi_{D_{n+1}{}^c})|\nabla u_n|^2 dx \geq \mathcal{P}_{D_{n+1}}(u_n) \geq \lambda(D_{n+1}).$$

Remark 3.1. Employing part (iv) of Lemma 2.3, level sets of the function $f(x) = |\nabla u_n(x)|$ have measure zero. Therefore, the set D_{n+1} is determined uniquely as $D_{n+1} = \{x : |\nabla u_n(x)| \leq t\}$ where t is calculated by (3.2).

Thanks to (3.3)-(3.5), we have

$$\int_{D_n} |\nabla u_n|^2 dx \geq \int_{D_{n+1}} |\nabla u_n|^2 dx, \tag{3.6}$$

and equality holds in (3.6) if and only if $D_n = D_{n+1}$. On the other hand, equality holds in (3.6) if and only if equality holds in (3.4). In summary, we can say that $\lambda(D_n)$ is equal to $\lambda(D_{n+1})$ if and only if $D_{n+1} = D_n$. One can be sure that λ evolves into a lower value when $D_{n+1} \neq D_n$.

4. Implementation of the descent method

This section provides the details of an implementation for the descent approach introduced in section 3 and some examples chosen to illustrate its efficiency.

At iteration step n, there is a guess for an optimal configuration which is denoted by D_n. We use the finite element method with the piecewise linear basis functions to discretize equation (1.1) with $D = D_n$.

We determine the eigenfunction u_n and eigenvalue $\lambda_n = \lambda(D_n)$ of the generated discrete system, which is a nonlinear matrix eigenvalue problem:

$$\mathcal{F}(\lambda)v = 0, \tag{4.1}$$

where $\mathcal{F}(\lambda)$ is a family of symmetric matrices depending nonlinearly on the parameter λ.

$\mathcal{F}(\cdot)$ satisfies the conditions of Theorem 2.1, and therefore its principle eigenvalue can be characterized as the minimum value of the Rayleigh functional corresponding to problem (4.1).

There is a close relation between the nonlinear problem (4.1) and the symmetric linear eigenproblem

$$\mathcal{F}(\lambda)v = \mu v. \tag{4.2}$$

In particular, $\widehat{\lambda} > 0$ is the principle eigenvalue of (4.1) if and only if $\mu = 0$ is the maximal eigenvalue of problem (4.2) with $\lambda = \widehat{\lambda}$. The so called safeguarded iteration in algorithm 1 converges globally to the first eigenvalue of (4.1) and the convergence is quadratic, [20, 30, 31]. The tolerance TOL which is used in algorithm 1 is in the order of the machine precision.

Combining the finite element method and the safeguarded iteration, we derive $\lambda_n = \lambda(D_n)$ and a corresponding eigenfunction u_n. Employing (3.3) and (3.2) based on the level sets of $f(x) = |\nabla u_n|^2$, we construct a new set D_{n+1} with $|D_{n+1}| = A$ and

$$\lambda(D_{n+1}) \leq \lambda(D_n).$$

We repeat the above procedure until no furthermore improvement of the eigenvalue can be obtained. The algorithm stops when $|\lambda(D_{n+1}) - \lambda(D_n)|$ is less than a prescribed tolerance TOL.

The resulting algorithm 2, is shown in table 2.

Let us explain more precisely the implementation of step 3 in algorithm 2. As stated in [11], a difficulty when one solves the discrete problem is the volume constraint $|D_{n+1}| = A$. Indeed, from a numerical point of view it is not possible to

Table 1

Algorithm 1. Safeguarded iteration
Data: Nonlinear eigenproblem (4.1) and λ' an approximation of its first eigenvalue
Result: λ, the first eigenvalue of (4.1) and u an associated eigenvector
1. Determine an eigenvector v corresponding to μ, the largest eigenvalue of the matrix $\mathcal{F}(\lambda')$;
2. If $\lvert\mu\rvert < TOL$ then
Set $u = v$ and $\lambda = \lambda'$;
Stop;
else
Evaluate new λ' by solving $v^T\mathcal{F}(\lambda')v = 0$ for λ';
Go to step 1;

satisfy the volume constraint exactly because of the discretization. We describe here how this difficulty can be overcome.

Let us for simplicity now assume $\Omega = \mathcal{B}(0,1)$ in $\mathbb{R}^2$ or $\mathbb{R}^3$. Thus, one can employ polar coordinates in $\mathbb{R}^2$ or spherical coordinates in $\mathbb{R}^3$ and then (1.1) reduces to the following differential equation

$$-\frac{d}{dr}(r^{N-1}G(\lambda,r)u'(r)) = \lambda r^{N-1}u(r) \quad 0 \le r < 1, \ \ N = 2,3.$$

We suppose that the proportion $d = A/|\Omega|$ is a rational number. A specific mesh in each iteration is used: Node points x_j, $0 \le ... < x_j < x_{j+1} < ... \le 1$, $j = 0..l$, are chosen such that

$$\pi(x_{j+1}^2 - x_j^2) = \pi q,$$

for the two-dimensional problem and

$$(4\pi/3)(x_{j+1}^3 - x_j^3) = (4\pi/3)q,$$

for the three-dimensional problem. The number q is a rational number less than one where $d/q = k$ and k is an integer. Recall from Remark 3.1 and Lemma 3.1 that

$$D_{n+1} = \{x : \ |\nabla u_n(x)| \le t\}, \quad |D_{n+1}| = A.$$

We do not have to calculate the parameter t, but since we are using piecewise linear basis functions in the finite element method, $|\nabla u_n|$ has a constant value in

Table 2

Algorithm 2. Eigenvalue minimization

Data: An initial set D_0
Result: A sequence of decreasing eigenvalues $\lambda(D_n)$
1. Set $n = 0$;
2. Compute u_n and $\lambda(D_n)$ applying the finite element method and safeguarded iteration;
3. Compute D_{n+1} applying relations (3.2) and (3.3);
4. Compute u_{n+1} and $\lambda(D_{n+1})$ applying the finite element method and safeguarded iteration;
5. If $\|\lambda(D_{n+1}) - \lambda(D_n)\| < TOL$ then stop;
    else
            Set $n = n + 1$;
            Go to step 3;

each element. The value of $|\nabla u_n(x)|$ in an element $T_j = [x_{j-1}, x_j]$ is denoted by ξ_j, $j = 1, .., l$. We renumber the elements T_j (still denoted by T_j) such that the quantities ξ_j, $j = 1, .., l$ are in ascending order

$$\xi_1 \leq \xi_2 \leq ... \leq \xi_l.$$

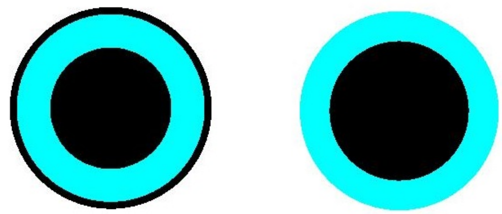
Recalling $kq\pi = A$, a subset D_{n+1} with measure A of $\mathcal{B}(0, 1)$ in $\mathbb{R}^2$ is constructed as follows. Consider elements $T_j = [x_{j-1}, x_j]$, $j = 1, .., l$ in their new order. Starting with $D_{n+1} = \emptyset$, for $j = 1, 2, \ldots, k$, we add the annulus with outer radius x_j and inner radius x_{j-1} one by one to the set D_{n+1}. Each of the annuli have same measure $q\pi$ and so we exactly add k annuli to each other regarding the constraint $|D_{n+1}| = A$. In other words, we do not need to add a part of an annulus as a subset of D_{n+1} or to refine the mesh. Hence, the concluded set satisfies the size condition with the smallest error.

The derivation of D_{n+1} in $\mathbb{R}^3$ is the same as that of the two-dimensional case and is omitted.

Let us close this section with some numerical examples. We consider simulations in two and three dimensions for $\Omega = \mathcal{B}(0, 1)$, unit circle or unit sphere. In these examples, we derive the optimal set by starting algorithm 2 from three different initial sets

$$D_0^1 = \mathcal{B}(0, R_1),\ D_0^2 = \mathcal{B}(0, R_2) \backslash \mathcal{B}(0, R_3),\ D_0^3 = \mathcal{B}(0, 1) \backslash \mathcal{B}(0, R_4),$$

where these initializers have the same measure A and $0 < R_i < 1$, $i = 1..4$.



(a) $\lambda_{\min} = 1.95, \theta = 0.01$ (b) $\lambda_{\min} = 0.71, \theta = 10$

Figure 1: The black region corresponds to the minimizer set

Invoking these sets, our numerical tests typically converge to the global optimal set of the respective problem, although this has not been established theoretically.

In the following examples, the grid is made of $l = 10^3$ points and in Algorithm 2 we set $TOL = 5 \times 10^{-3}$. Algorithm 2 converges in less than 5 iterations for all examples. Using a tolerance in the order of the machine precision, the safeguarded method in the second step of Algorithm 2, with a suitable initial approximation λ', does not exceed 50 iterations.

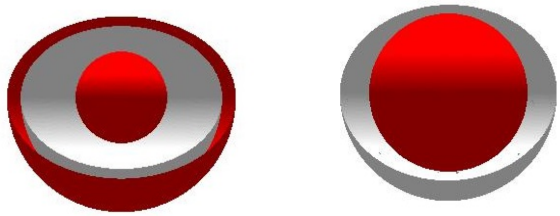
Example 4.1. In this example, we verify our problem in the unit circle. Functions $\alpha(\lambda)$ and $\beta(\lambda)$ are assumed to be rational functions

$$\alpha(\lambda) = 1/(1 + \lambda), \quad \beta(\lambda) = 1/(1 + \theta + \lambda), \quad \theta > 0.$$

Thus, equation (1.1) can be considered as the Schrödinger equation governing a quantum dot with effective mass where we have mostly set relevant physical constants to unity [3, 4]. For $A/|\Omega| = 0.5$ the minimizing set and the ground state energy corresponding to two different values of θ are shown in figure 1.

Example 4.2. In the second example, we check algorithm 2 where Ω is the unit sphere and we use the same rational functions $\alpha(\lambda)$ and $\beta(\lambda)$ as in example 4.1. Again equation (1.1) can be interpreted as the Schrödinger equation governing the electronic behavior of a quantum dot with effective mass. With $A/|\Omega| = 0.4$ the minimizing sets and the minimum value of the principal eigenvalue corresponding to two different values of θ are shown in figure 2 .

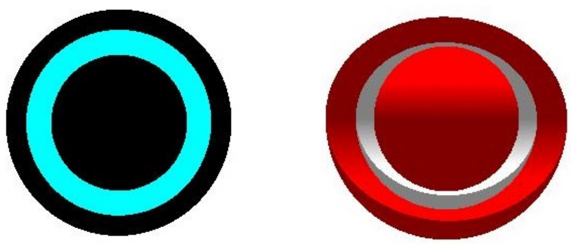
Utilizing the terminology from [9, 11], the minimizer sets in figures 1a and 2a of the above examples are in low contrast regime and the minimizer sets in figure 1b and 2b are in high contrast regime. These numerical examples show that the optimal set of the nonlinear problem inherit a disconnectivity from the linear



(a) $\lambda_{\min} = 2.67, \theta = 0.01$ (b) $\lambda_{\min} = 1.16, \theta = 10$

Figure 2: The red region corresponds to the optimal set

problem in low contrast regime. Indeed, the optimal set contains a ball centered at the origin and a neighborhood of the boundary of Ω.



(a) $\lambda_{\min} = 1.20$ (b) $\lambda_{\min} = 1.22$

Figure 3: The dark region corresponds to the minimizer set

Example 4.3. The functions $\alpha(\lambda)$ and $\beta(\lambda)$ are not restricted to rational functions. In this example we consider

$$\alpha(\lambda) = \mathrm{e}^{-\lambda}, \quad \beta(\lambda) = \frac{3\cos(\lambda) - 1}{\cos(\lambda)},$$

which have a more complicated nonlinearity. Figure 3a shows the optimal set for the two dimensional with the parameter $A/|\Omega| = 0.7$, and figure 3b displays the minimizer in the three dimensional case with the parameter $A/|\Omega| = 0.8$.

Acknowledgments. This work was initiated when the first author visited Hamburg University of Technology. He would like to thank Professor H. Voss for his great hospitality. The authors would like to express their deep gratitude to anonymous referees for helpful comments and useful suggestions.

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