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Research article

Finite element method for an eigenvalue optimization problem of the Schrödinger operator

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Abstract: In this paper, we study the optimization algorithm to compute the smallest eigenvalue of the Schrödinger operator with volume constraint. A finite element discretization of this problem is established. We provide the error estimate for the numerical solution. The optimal solution can be approximated by a fixed point iteration scheme. Then a monotonic decreasing algorithm is presented to solve the eigenvalue optimization problem. Numerical simulations demonstrate the efficiency of the method.

Keywords: eigenvalue optimization; Schrödinger operator; shape optimization; finite element method; error estimate
Mathematics Subject Classification: 35J10, 35P15, 49Q10, 65N25, 65N30

1. Introduction

The semiconductor quantum dot is a particular electronic/photonic structure in which the free carriers are confined to a small region of space by potential barriers. Due to the possibility of control over the conductive properties by adjusting its well, quantum dot structures have attracted broad attentions from mathematicians and physicists [25]. The problem of finding the optimal energy level of the structure is regarded as an important step of the research in micro- and nano-electronic/photonic devices based on the quantum dots [38], such as transistors, photodetectors, solar cells, LEDs and diode lasers. Motivated by these applications, we consider an optimization problem related to the ground state (energy) of the Schrödinger system. For simplicity, given any potential function, we solve a steady state equation which is related to the eigenvalue of the

Schrödinger operator. More precisely, given a particle with mass m and a potential function $V(x)$, the eigenvalue problem of the Schrödinger operator in Ω reads:

$$\begin{cases} -\dfrac{\hbar}{2m}\Delta u + V(x)u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \end{cases} \tag{1.1}$$

where $\hbar$ stands for the reduce Planck's constant. It is well known that for the above equation there exists a countable collection of solutions u_n (quantum states), and real numbers λ (energies). Without loss of generality, the scalar form of the Eq (1.1) will be discussed in the following sections. Let Ω be a bounded connected domain with Lipschitz boundary in $\mathbb{R}^n$ $(n = 2, 3)$. In this paper, we are interested in the eigenvalue optimization problem of the following system:

$$\begin{cases} -\Delta u + V(x)u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \end{cases} \tag{1.2}$$

where the potential function $V(x) : \Omega \to \mathbb{R}$ is a bounded function with a volume constraint, i.e., $V(x) \in \mathcal{A}_V$ where $\mathcal{A}_V$ is defined in (1.3). From [41], the system (1.2) has discrete spectrum λ_k which can be arranged in nondecreasing order as follows:

$$0 < \lambda_1 < \lambda_2 \leq \ldots \to \infty.$$

Noting that the eigenvalue λ_k depends on the choice of potential function $V(x)$, then we denote it by $\lambda_k(V)$. Let $V(x)$ vary over the admissible set

$$\mathcal{A}_V = \{V(x) \in L^\infty(\Omega) : V = \alpha\chi_D + \beta\chi_{\Omega\setminus D}, ⨍_\Omega V(x) = c\}, \tag{1.3}$$

where $D \subset \Omega$ is a measurable set, χ_D is the characteristic function of the set D, ⨍ is the average of integral function on the domain and c is a constant which satisfies: $0 \leq \alpha \leq c \leq \beta$ and it refers to the volume constraint of potential $V(x)$. Consider the following eigenvalue optimization problem:

Problem 1.

$$\min_{V(x)\in\mathcal{A}_V} \lambda_1(V).$$

Therefore a physical interpretation of the Problem 1 is: to seek the potentials that minimize the principal energy corresponding to the state Eq (1.2) relative to the constrained set $\mathcal{A}_V$. Many researchers have discussed the existence, uniqueness and other qualitative analysis of shape optimization problems for elliptic eigenvalues. It has been proved the existence and uniqueness of the minimizer in [10, 14, 31]. One can find more results in [1] and references therein. Recently, the eigenvalue optimization problems which are governed by the Schrödinger equations have been quite attractive to many mathematicians [4, 27, 30, 44]. The regularity and symmetry of the optimal solutions have been investigated in [3, 9]. In case of one dimension, the extremal eigenvalue of the Schrödinger equation is discussed in the papers [6, 11]. For the higher dimensional case, we could see that there are lots of literatures [14, 31, 39] to consider of the eigenvalue or eigenvalue function optimization problem with the potential function is allowed to vary in the ball $\|V\|_{L^P} \leq M, 1 \leq P \leq \infty$.

Extremal eigenvalue problem of the Schrödinger equations on the manifold is investigated by Harrel [13] and Freitas [34]. More results could be found in Henrot [15]. Moreover, the extremal eigenvalue has also been a hot area of research recently.

For optimization Problem 1, an important mathematical problem besides the existence is an exact description of the optimizer or optimal shape design. Therefore a great deal of papers [21, 28, 29, 39] have considered the optimality conditions and other qualitative analysis with respect to the optimal solution. This class of problems is difficult to handle because that the topology information of the optimal shape is unknown. Moreover, the classical method of shape derivative couldn't be used. So we try to study the Problem 1 in the numerical analysis. The mostly used techniques are the homogenization method [2] and the level set method [42, 43]. The homogenization method is effective but it is restricted to linear elasticity and particular functions. And it should be noticed that this method could cause numerical problems such as checkboard patterns, grey scales and artificial parameter dependance. The level set methods are popular for solving shape optimization problems. These methods have been applied to handle the eigenvalue optimization problems of inhomogeneous structure, also including the extremal eigenvalue [32] problems of the composite material, the maximum quality factor of the optical resonator [22], principal eigenvalue optimization problems in population dynamics [8]. However, the convergence of the level set method is usually slow due to the necessary reinitialization process. In addition to the above mentioned methods, there is another class of numerical optimization algorithms, in which dealing with the geometrical constraints with updating the control parameters. These algorithms rely strongly on the variational formulation of the eigenvalues and level sets or gradients of the eigenfunctions. They have been applied successfully to shape optimization problems, including eigenvalue optimization problems of elliptic operator [12, 20, 23, 24], designing the optimal shape of a stiff inclusion with given area in the membrane [16, 19, 33], optimizing principal eigenvalue of the bi-laplacian operator [7, 18], determining the optimal spatial arrangement of favorable and unfavorable regions for to survive [5, 17, 26]. Recently, this type of methods has been applied to solve a eigenvalue optimization problem [19, 30]. The algorithm we presented in this paper can be categorized into the last class. A main advantage of this approach seems to be its feasibility, stability and efficiency which could be demonstrated by the numerical experiments.

Inspired by the previous works, we exploit the optimization algorithm to compute the smallest eigenvalue of the Schrödinger operator. Our work is twofold: (1) We analysis the property of the minimizer to the continuous extremal eigenvalue problem; (2) We present an efficient numerical method to solve this problem. To be more specific, we will give an analysis on the solution of Problem 1. By means of a relaxation approach, the solution to Problem 1 is a fixed point of the Rayleigh quotient function. Then we provide a finite element method with monotonic decreasing algorithm. After a reasonable assumption to the continuous optimal solution, the error order for the smallest eigenvalue can be obtained.

The outline of this paper is as follows: in the remaining part of this section, we give some notations of function spaces. In Section 2, the property of the minimizer of the eigenvalue optimization problem is proved. In Section 3, the extremal eigenvalue problem is discretized by the finite element method and the error estimate is given. In Section 4, a monotone decreasing algorithm is introduced and some numerical examples are given to depict the efficiency of our method. We use the standard notations $W^{m,p}$ and H^m to the Sobolev space on Ω with the norm $\|\cdot\|_{W^{m,p}}$ and $\|\cdot\|_m$. The L^2 norm is simplified as $\| \cdot \|$, and $(.,.)$ is inner product in L^2 space.

2. Continuous extremal eigenvalue problem

The variational form of the Eq (1.2) is: to find $\lambda \in \mathbb{R}$ and $u \in H_0^1(\Omega)\backslash\{0\}$ such that

$$(\nabla u, \nabla w) + (Vu, w) = \lambda(u, w), \ \forall \ w \in H_0^1(\Omega). \tag{2.1}$$

We define the Rayleigh's quotients $\mathcal{R} : \mathcal{A}_V \times H_0^1(\Omega)\backslash\{0\} \to \mathbb{R}$:

$$\mathcal{R}(V, u) = \frac{\int_\Omega |\nabla u|^2 + \int_\Omega V u^2}{\int_\Omega u^2}, \tag{2.2}$$

then, for the given potential $V(x)$, by Rayleigh's principle [1],

$$\lambda_1(V) = \min_{u \in H_0^1(\Omega), u \neq 0} \mathcal{R}(V, u). \tag{2.3}$$

Therefore, Problem 1 can be equivalently reformulated by:

Problem 2.

$$\min_{V \in \mathcal{A}_V} \lambda_1(V) = \min_{V \in \mathcal{A}_V} \min_{u \in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V, u). \tag{2.4}$$

In the following, we restate some theoretical result of Problem 1. Firstly, we provide some properties of the eigenvalues and eigenfunctions associated to the Schrödinger operator which can be found in the paper [40].

Lemma 1. *Given $V \in \mathcal{A}_V$, the first eigenvalue $\lambda_1(V)$ is simple and the corresponding eigenfunction u is strictly positive in Ω (up to a nonzero constant factor), where $u \in H_0^1(\Omega)$.*

Next, we give a general existence result which can be found from Henrot [1].

Lemma 2. *There exists at least a minimizer $V^* \in \mathcal{A}_V$ to the Problem 1.*

Remark 1. *The uniqueness of the minimizer is not guaranteed. Indeed, Chanillo [39], Pedrosa [37] have indicated that if we consider a domain Ω is dumbbell, it seems that there exists at least two minimizers, each of them concentrated on the center of one disk.*

It should be noticed that the admissible set $\mathcal{A}_v$ is non-convex, by introducing its L^∞ weak star closure $\mathcal{A}$:

$$\mathcal{A} = \{V(x) \in L^\infty(\Omega) : \alpha \leq V(x) \leq \beta, ⨍_\Omega V(x) = c\}, \tag{2.5}$$

we give the following existence result from [1], which is important for $\underset{V \in \mathcal{A}}{\operatorname{argmin}}\, \lambda_1(V)$.

Lemma 3. *Let $F : \mathbb{R}^n \to \mathbb{R}$ be a continuous function. Then the Problem*

$$\min_{V \in \mathcal{A}} F(\lambda_1(V), \lambda_2(V), ..., \lambda_n(V))$$

has a solution.

Then $\forall\ V \in \mathcal{A}, u \in H_0^1(\Omega)\backslash\{0\}$, we can get the following result:

Lemma 4.

$$\min_{V\in\mathcal{A}} \min_{u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u) = \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u) = \min_{u\in H_0^1(\Omega)\backslash\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u) \tag{2.6}$$

Proof. First, we need to state that

$$\min_{V\in\mathcal{A}} \min_{u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u)$$

exists. In the following, $\forall\ V \in \mathcal{A}$, we we denote the corresponding eigenfunction as $u(V)$. Thanks to Lemma 3, it is known that the $\operatorname{argmin}_{V\in\mathcal{A}} \lambda_1(V)$ exists, which means that the solution to the left term of the Eq (2.6) could be obtained. Let $V^* \in \mathcal{A}$ be a minimizer to the Problem 1, i.e., there exists a positive real number:

$$\lambda_1^* = \min_{V\in\mathcal{A}} \lambda_1(V) = \min_{V\in\mathcal{A}} \min_{u\in H_0^1(\Omega)\backslash\{0\}} \int_\Omega |\nabla u|^2 + \int_\Omega V|u|^2, \tag{2.7}$$

where the corresponding normalized eigenfunction is u^*. For simplicity, denote this potential and corresponding eigenfunction as a pair (V^*, u^*).

Step 1. We prove the first equality relation of the Eq (2.6). Assume that it exists a minimizing sequence $\{(V_k, u_k)\}$, where $\|u_k\| = 1$, subject to

$$\lim_{k\to\infty} \int_\Omega |\nabla u_k|^2 + \int_\Omega V_k|u_k|^2 = \hat{\lambda}_1. \tag{2.8}$$

From $\|u_k\| = 1$ and (2.8), u_k is bounded in $H_0^1(\Omega)$, then there exists a subsequence (still denote as u_k), and $u_k \rightharpoonup \hat{u}$ in $H_0^1(\Omega)$. Since V_k is bounded in $L^\infty(\Omega)$, we can find a subsequence (still denote as V_k), and $V_k \overset{*}{\rightharpoonup} \hat{V}$ in $L^\infty(\Omega)$. By Sobolev embedding theorem $u_k \to \hat{u}$ in $L^2(\Omega)$, which implies that $|u_k|^2 \to |\hat{u}|^2$ in $L^1(\Omega)$. By the strong-weak convergence, we can get

$$\lim_{k\to\infty} \int_\Omega V_k|u_k|^2 = \int_\Omega \hat{V}|\hat{u}|^2. \tag{2.9}$$

From $|u_k|^2 \to |\hat{u}|^2$ in $L^1(\Omega)$, we can deduce that $\|\hat{u}\|^2 = 1$. By the weakly lower semi-continuity of the norm:

$$\int_\Omega |\nabla \hat{u}|^2 \leq \liminf \int_\Omega |\nabla u_k|^2. \tag{2.10}$$

From (2.8)–(2.10), so we can obtain that

$$\mathcal{R}(\hat{V}, \hat{u}) \leq \hat{\lambda}_1, \tag{2.11}$$

from (2.8) and (2.11), then it follows

$$\mathcal{R}(\hat{V}, \hat{u}) \leq \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \int_\Omega |\nabla u|^2 + \int_\Omega V|u|^2. \tag{2.12}$$

Notice that $\mathcal{A}$ is the L^∞ weak $*$ closure of $\mathcal{A}_V$, see Cox [40], then $\hat{V} \in \mathcal{A}$, namely

$$\mathcal{R}(\hat{V}, \hat{u}) = \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \int_\Omega |\nabla u|^2 + \int_\Omega V|u|^2. \tag{2.13}$$

Next we will prove that $\hat{\lambda}_1 = \lambda_1^*$. From (2.8) and (2.13), we can have:

$$\hat{\lambda}_1 = \mathcal{R}(\hat{V}, \hat{u}) = \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V, u). \tag{2.14}$$

Combined with (2.7), it can be obtained by

$$\hat{\lambda}_1 = \mathcal{R}(\hat{V}, \hat{u}) = \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V, u) \le \mathcal{R}(V^*, u^*) = \lambda_1^*. \tag{2.15}$$

From (2.7) and (V^*, u^*) is the corresponding potential and eigenfunction of the eigenvalue λ_1^*, we can get:

$$\lambda_1^* = \mathcal{R}(V^*, u^*) = \mathcal{R}(V^*, u(V^*)) \le \mathcal{R}(\hat{V}, u(\hat{V})). \tag{2.16}$$

Combined with (2.8), we can obtain that

$$\lambda_1^* = \mathcal{R}(V^*, u^*) = \mathcal{R}(V^*, u(V^*)) \le \mathcal{R}(\hat{V}, u(\hat{V})) \le \mathcal{R}(\hat{V}, \hat{u}) = \hat{\lambda}_1. \tag{2.17}$$

From (2.15) and (2.17), we have

$$\min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V, u) = \hat{\lambda}_1 = \lambda_1^* = \min_{V\in\mathcal{A}, u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V, u). \tag{2.18}$$

Step 2. Now we indicate that the second equality of the Eq (2.6) holds up. Similar to step 1, firstly solve the existence of

$$\min_{u\in H_0^1(\Omega)\backslash\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V, u). \tag{2.19}$$

For fixed $u \in H_0^1(\Omega)$,

$$\min_{V\in\mathcal{A}} \mathcal{R}(V, u) = \min_{V\in\mathcal{A}} \int_\Omega |\nabla u|^2 + \int_\Omega V|u|^2, \tag{2.20}$$

hence it is required to claim the existence of $\min_{V\in\mathcal{A}} \int_\Omega V|u|^2$. For $t \ge 0$, construct a auxiliary function

$$F(t) = |\{x \in \Omega : |u|^2 \ge t\}|.$$

Obviously $F(t)$ is the monotone decreasing function for the variable t. Let γ be the ratio between the area of the material with the potential α occupies and the total area $|\Omega|$. Denote

$$t^* = \inf\{t : F(t) \le \gamma|\Omega|\},$$

then we construct a potential function

$$\bar{V} = \begin{cases} \alpha, & x \in \{x : |u|^2 > t^*\}; \\ \alpha \text{ or } \beta, & x \in \{x : |u|^2 = t^*\}; \\ \beta, & x \in \{x : |u|^2 < t^*\}, \end{cases} \tag{2.21}$$

and $\bar{V} \in \mathcal{A}$. By the rearrangement inequality which can be found in Lemma 7, $\forall u \in H_0^1(\Omega)$,

$$\int_\Omega \bar{V}|u|^2 dx \le \int_\Omega V|u|^2 dx. \tag{2.22}$$

Then for given $u \in H_0^1(\Omega)$, we can find a potential function $V \in L^\infty(\Omega)$ to minimize $\mathcal{R}(V,u)$. To simplify notations, if $V \in \operatorname*{argmin}_{V\in\mathcal{A}} \mathcal{R}(V,u)$, we denote it by $V(u)$.

Then it should be proved that we can find $u \in H_0^1(\Omega)$ to minimize $\mathcal{R}(V(u),u)$. Assume that there exists a minimizing sequence $\{u_n\}$, where $\|u_n\|^2 = 1$, then we have a positive number

$$\tilde{\lambda}_1 = \lim_{n\to\infty} \min_{u_n\in H_0^1(\Omega)\setminus\{0\}} \mathcal{R}(V_n,u_n), \tag{2.23}$$

where $V_n = V(u_n) \in \operatorname*{argmin}_{V\in\mathcal{A}} \mathcal{R}(V,u_n)$. Since $\|u_n\|^2 = 1$, u_n is a bounded sequence in $H_0^1(\Omega)$, then there exists a subsequence (still denote as u_n), and $u_n \rightharpoonup \tilde{u}$ in $H_0^1(\Omega)$. Combined with V_n is a bounded sequence in $L^\infty(\Omega)$, then there exists a subsequence (still denote as V_n), and $V_n \overset{*}{\rightharpoonup} \tilde{V}$ in $L^\infty(\Omega)$. From compact embedding theorem, $u_n \to \tilde{u}$ in $L^2(\Omega)$, which means $|u_n|^2 \to |\tilde{u}|^2$ in $L^1(\Omega)$. By the strong-weak convergence, we can get

$$\lim_{n\to\infty} \int_\Omega V_n|u_n|^2 = \int_\Omega \tilde{V}|\tilde{u}|^2. \tag{2.24}$$

And from $|u_n|^2 \to |\tilde{u}|^2$ in $L^1(\Omega)$, then $\|\tilde{u}\|^2 = 1$. By the weakly lower semi-continuity of the norm:

$$\int_\Omega |\nabla\tilde{u}|^2 \le \liminf \int_\Omega |\nabla u_n|^2. \tag{2.25}$$

From (2.24) and (2.25), then

$$\mathcal{R}(\tilde{V},\tilde{u}) \le \tilde{\lambda}_1, \tag{2.26}$$

and thanks to

$$V_n \in \operatorname*{argmin}_{V\in\mathcal{A}} \mathcal{R}(V,u_n), \tag{2.27}$$

we can deduce that

$$\int_\Omega V_n|u_n|^2 \le \int_\Omega V|u_n|^2,\ \forall\ V \in H_0^1(\Omega), \tag{2.28}$$

passage to the limit the above inequality,

$$\int_\Omega \widetilde{V}|\tilde{u}|^2 \le \int_\Omega V|\tilde{u}|^2,\ \forall\ V \in H_0^1(\Omega). \tag{2.29}$$

So we can observe that $\widetilde{V} \in \operatorname*{argmin}_{V\in\mathcal{A}} \mathcal{R}(V,\widetilde{u})$, which implies that $\widetilde{V} = V(\widetilde{u})$. Then

$$\mathcal{R}(\widetilde{V},\tilde{u}) = \mathcal{R}(V(\tilde{u}),\tilde{u}), \tag{2.30}$$

Combined with (2.19) and $\mathcal{A}$ is L^∞ weak $*$ closure of $\mathcal{A}_V$, the solution to $\min_{u\in H_0^1(\Omega)\setminus\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u)$ exists. It equals that

$$\mathcal{R}(\widetilde{V},\tilde{u}) = \mathcal{R}(V(\tilde{u}),\tilde{u}) = \min_{u\in H_0^1(\Omega)\setminus\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u). \tag{2.31}$$

At last we state that the second equality of (2.6) holds up. From (2.14) and (2.30), we have

$$\min_{V\in\mathcal{A},u\in H_0^1(\Omega)\setminus\{0\}} \mathcal{R}(V,u) = \mathcal{R}(\hat{V},\hat{u}) \le \mathcal{R}(\widetilde{V},\tilde{u}) = \mathcal{R}(V(\tilde{u}),\tilde{u}). \tag{2.32}$$

Combined with (2.31) and (2.32), we can deduce that

$$\min_{V\in\mathcal{A},u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u) \leq \min_{u\in H_0^1(\Omega)\backslash\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u). \tag{2.33}$$

From (2.14), we have $(\hat{V},\hat{u}) \in \underset{V\in\mathcal{A},u\in H_0^1(\Omega)\backslash\{0\}}{\operatorname{argmin}} \mathcal{R}(V,u)$,then

$$\min_{V\in\mathcal{A},u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u) = \mathcal{R}(\hat{V},\hat{u}) = \mathcal{R}(V(\hat{u}),\hat{u}). \tag{2.34}$$

From (2.31), we can get

$$\mathcal{R}(V(\tilde{u}),\tilde{u}) \leq \mathcal{R}(V(\hat{u}),\hat{u}), \tag{2.35}$$

from (2.34), we can obtain

$$\min_{u\in H_0^1(\Omega)\backslash\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u) \leq \min_{V\in\mathcal{A},u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u). \tag{2.36}$$

Combined with (2.33) and (2.36),we have

$$\min_{u\in H_0^1(\Omega)\backslash\{0\}} \min_{V\in\mathcal{A}} \mathcal{R}(V,u) = \min_{V\in\mathcal{A},u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u), \tag{2.37}$$

which completes the proof. □

In the procedure to prove Lemma 4, a potential function $\bar{V}$ is constructed in (2.21), which can minimize $\mathcal{R}(V,u)$. This fact shows that the solution $V \in \underset{V\in\mathcal{A}}{\operatorname{argmin}} \mathcal{R}(V(u),u)$ keeps "bang-bang" property.

Remark 2. *We employ the concept "bang-bang" from the control theory, see [46]. A function $V(x) \in \mathcal{A}$ has "bang-bang" property, if $V(x) = \alpha$ or β a.e. for $x \in \Omega$.*

Therefore Problem 2 equals to the following problem

Problem 3.

$$\min_{V\in\mathcal{A}} \lambda_1(V) = \min_{V\in\mathcal{A}} \min_{u\in H_0^1(\Omega)\backslash\{0\}} \mathcal{R}(V,u). \tag{2.38}$$

3. Finite element approximation

In this section, we consider the finite element method for Problem 3 and establish the error estimate of finite element solution. Assume Ω be a polyhedral domain and let $\mathcal{T}_h$ be a quasi-uniform triangulation of Ω. We choose conformal P_1 and P_0 element spaces for the discrete solution u_h and V_h. Therefore, the discrete function space $\mathcal{V}_h$ and the discrete admissible set $\mathcal{A}_h$ are given by

$$\mathcal{V}_h = \{u_h \in C_0(\Omega), u_h|_{\Delta_h} \in P_1, \Delta_h \in \mathcal{T}_h\},$$

$$\mathcal{A}_h = \{V_h \in L^\infty(\Omega), V_h|_{\Delta_h} \in P_0, \alpha \leq V_h \leq \beta, \fint V_h = c\}.$$

Since $\mathcal{V}_h \subset H_0^1$ and $\mathcal{A}_h \subset \mathcal{A}$, Rayleigh's quotient $\mathcal{R}$ is well defined on $\mathcal{A}_h \times \mathcal{V}_h$. For any $V_h \in \mathcal{A}_h$, the discretization form of the Eq (2.1) is defined by:

$$(\nabla u_h, \nabla w_h) + (V_h u_h, w_h) = \lambda_h (u_h, w_h),\ \forall\ w_h \in \mathcal{V}_h. \tag{3.1}$$

Assume the basis function of the finite element space $\mathcal{V}_h$ be $\{\psi_i\}_{i=1}^N$, then any function $u_h \in \mathcal{V}_h$ can be represented as:

$$u_h = \sum_{i=1}^{N} c_i \psi_j. \tag{3.2}$$

We will make use of the following notation throughout this paper. Let the vector $U_h = (c_1, c_2, ..., c_N)^T$, and denote the entries of the stiffness matrix $\mathcal{K}$, the potential matrix $\mathcal{G}$, the mass matrix $\mathcal{M}$ respectively be as follows:

$$\mathcal{K}_{i,j} = (\nabla\psi_i, \nabla\psi_j),\ \mathcal{G}_{i,j} = V_h(\psi_i, \psi_j),\ \mathcal{M}_{i,j} = (\psi_i, \psi_j).$$

Then the Eq (3.1) is equivalent to a system of linear equations:

$$(\mathcal{K} + \mathcal{G})U_h = \lambda_h \mathcal{M} U_h \tag{3.3}$$

Where λ_h is generalized eigenvalue of $(\mathcal{K} + \mathcal{G})$ with $\mathcal{M}$, then the vector $U_h = (c_1, c_2, ..., c_N)^T$ is the corresponding eigenvector. Given $u_h \in \mathcal{V}_h$, $V_h \in \mathcal{A}_h$, define Rayleigh's quotient:

$$\mathcal{R}(V_h, u_h) = \frac{\int_\Omega |\nabla u_h|^2 + V_h u_h^2}{\int_\Omega u_h^2} = \frac{U_h^T(\mathcal{K} + \mathcal{G})U_h}{U_h^T \mathcal{M} U_h}, \tag{3.4}$$

Denoting by $\lambda_{1,h}(V_h)$ the smallest eigenvalue of the Eq (3.3), from the discrete Rayleigh's principle:

$$\lambda_{1,h}(V_h) = \min_{u \in \mathcal{V}_h, u \neq 0} \mathcal{R}(V_h, u_h), \tag{3.5}$$

where $u_h = \sum_{i=1}^N c_i \psi_j$, $U_h = (c_1, c_2, ..., c_N)^T$. Then the discretization of Problem 3 can be reformulated as:

Problem 4.

$$\min_{V_h \in \mathcal{A}_h} \min_{u_h \in \mathcal{V}_h \setminus \{0\}} \mathcal{R}(V_h, u_h).$$

Lemma 5. *There exists at least one optimal solution to Problem 4.*

Proof. The discrete admissible set $\mathcal{A}_h$ can be represented as:

$$\mathcal{A}_h = \{V_h : V_h = \sum_{\Delta_h} \chi_{\Delta_h} V_h|_{\Delta_h}, \alpha \le V_{\Delta_h} \le \beta, \sum_{\Delta_h} V_h|_{\Delta_h} |\Delta_h| = c \sum_{\Delta_h} \Delta_h\}.$$

where χ_{Δ_h} is the characteristic function of the element triangle Δ_h,

$$\chi_{\Delta_h}(p) = \begin{cases} 1, \text{if the point } p \text{ is in } \Delta_h; \\ 0, \text{else.} \end{cases}$$

$|\Delta_h|$ is the area of the triangle Δ_h. Notice the fact that $\lambda_{1,h}$ is a continuous function of V_h , and $V_h^k \in \mathcal{A}_h$ is a bounded set in finite dimensional space. So we can deduce that there exists a real number λ_h^* such that:

$$\lim_{k\to\infty} \mathcal{R}(V_h^k, u_h) = \lim_{k\to\infty} \frac{\int_\Omega |\nabla u_h|^2 + V_h^k u_h^2}{\int_\Omega u_h^2} = \min_{V_h\in\mathcal{A}_h} \lambda_{1,h}(V_h) = \lambda_h^*. \tag{3.6}$$

□

Let $(\lambda_1^*, V^*, u_1^*)$ is a optimal solution to Problem 3, where $\lambda_1^* = \lambda_1(V^*), u_1^* = u_1(V^*)$, From the procedure to state Lemma 4, if $V^* \in \underset{V\in\mathcal{A}}{\operatorname{argmin}} \mathcal{R}(V, u)$, then there exists $t > 0$, s.t.

$$V^*(x) = \beta \Rightarrow u^*(x) \le t,$$

$$V^*(x) = \alpha \Rightarrow u^*(x) \ge t.$$

Which means that there exists a level set $\Gamma = \{x : u^*(x) = t\}$, which could be considered as an interface between the potential values. Without loss of generality, make assumption for this level set:

Assumption 1. Γ *has finite Hausdorff measure, therefore*

$$|\Omega_{\Gamma,h}| = |\{x \in \Omega : dist(x, \Gamma) \le h\}| \le Ch.$$

Here C denotes the generic constant which doesn't depend on the choice of h. Let $\text{dist}(\Gamma, \partial\Omega) = \delta$, define

$$U_{\frac{\delta}{2}} = \{x \in \Omega : \text{dist}(x, \partial\Omega) < \frac{\delta}{2}\}.$$

Choose $h \le \frac{\delta}{2}$, then $\Omega_{\Gamma,h} \subset \Omega\backslash U_{\frac{\delta}{2}} \Subset \Omega$. From Cox [40], $\forall\ p \ge 1, u^* \in W^{2,p}_{loc}(\Omega)$, then

$$\|u^*\|_{W^{1,\infty}(\Omega_{\Gamma,h})} \le C. \tag{3.7}$$

Define the projection operator $S_h : H_0^1 \cap H^2 \mapsto \mathcal{V}_h$ and $J_h : \mathcal{A} \mapsto \mathcal{A}_h$ such that:

$$(\nabla S_h u, \nabla w_h) + (V_h S_h u, \nabla w_h) = (\nabla u, \nabla w_h) + (V_h u, \nabla w_h), \forall\ w_h \in \mathcal{V}_h, \tag{3.8}$$

$$J_h V|_{\Delta_h} = \fint_{\Delta_h} V, \forall\ \Delta_h \in \mathcal{T}_h. \tag{3.9}$$

From the error estimate of Lagrange finite element method for second-order elliptic equation [35, 36], we have:

$$\|S_h u - u\| + h\|\nabla(S_h u - u)\| \le Ch^2\|u\|_2, \tag{3.10}$$

$$J_h V^* = V_h^*, \forall\ x \notin \Omega_{\Gamma,h}. \tag{3.11}$$

By using the above assumption and the property of the solution of the finite element method, we will give the error estimate of the finite element method for the extremal eigenvalue Problem 4 to the Schrödinger equation.

Lemma 6. $\forall\ V_h \in \mathcal{A}_h$, *we have the following error estimate:*

$$\lambda_1(V_h) \le \lambda_{1,h}(V_h) \le \lambda_1(V_h) + Ch^2.$$

Proof. By $\mathcal{V}_h \subset H_0^1(\Omega)$, we have:

$$\lambda_1(V_h) = \min_{u\in H_0^1} \lambda_1(V_h) \le \min_{u\in\mathcal{V}_h} \lambda_1(V_h) = \lambda_{1,h}(V_h).$$

Next we will prove the second inequality. For simplicity, let $\lambda_1 = \lambda_1(V_h),\ u_1 = u_1(V_h)$, then:

$$\|u_1\|_2^2 \le C\|\lambda_1(V_h)u_1\|^2 \le C\lambda_1(\beta)\|u_1\|^2 \le C\frac{\lambda_1(\beta)}{\lambda_1(\beta)-\beta}\|\nabla u_1\|^2 = C\frac{\overline{\lambda}+\beta}{\overline{\lambda}},$$

where $\overline{\lambda}$ is the smallest eigenvalue of Laplace operator in the domain Ω , and for given potential function $V(x) = \beta$ of the Eq (2.3), denote the corresponding eigenvalue by $\lambda_1(\beta)$. By the definition:

$$\lambda_{1,h}(V_h) = \min_{u\in\mathcal{V}_h} \lambda_1(V_h) \le \mathcal{R}(V_h, S_h u_1) = \frac{\|\nabla S_h u_1\|^2 + \int_\Omega V_h|S_h u_1|^2}{\int_\Omega |S_h u_1|^2}.$$

By the Young inequality and the error estimate (3.10) of the finite element method, we can deduce that:

$$\int_\Omega [|u_1|^2 - |S_h u_1|^2] \le \int_\Omega [|S_h u_1 - u_1|^2 + 2|S_h u_1 - u_1||u_1|] \le Ch^2\|u_1\|_2^2.$$

From the property (3.8) of the projection operator

$$\begin{aligned}
&\|\nabla S_h u_1\|^2 + \int_\Omega V_h|S_h u_1|^2 - \|\nabla u_1\|^2 - \int_\Omega |S_h u_1|^2 \\
&= 2(\nabla S_h u_1 - \nabla u_1, \nabla u_1) - \|\nabla S_h u_1 - \nabla u_1\|^2 + 2(V_h u_1 - V_h u_1, S_h u_1) - \int_\Omega V_h|S_h u_1 - u_1|^2 \\
&\le 0.
\end{aligned}$$

Combined with the above, we can get:

$$\mathcal{R}(V_h, S_h u_1) \le \frac{\|\nabla u_1\|^2 + \int_\Omega V_h|u_1|^2}{\int_\Omega |u_1|^2 - Ch^2\|u_1\|_2^2} \le \lambda_1(V_h) + Ch^2.$$

It completes the proof. □

To simplify notations, denote $\lambda_{1,h}^* = \lambda_{1,h}^*(V_h^*), u_{1,h}^* = u_{1,h}^*(V_h^*)$. Similar to the technique in [24], we have the error estimate:

Theorem 1. *Let $(\lambda_{1,h}^*, V_h^*, u_h^*)$ be a optimal triple of the Problem 4, and Assumption 1 holds up, then we have*

$$\lambda_1^* \le \lambda_{1,h}^* \le \lambda_1^* + Ch^2.$$

Proof. Since $\mathcal{A}_h \subset \mathcal{A}$, we can get

$$\lambda_1^* = \min_{V\in\mathcal{A}} \lambda_1(V) \le \min_{V_h\in\mathcal{A}_h} \lambda_1(V) \le \min_{V_h\in\mathcal{A}_h} \lambda_{1,h}(V) = \lambda_{1,h}^*,$$

Now we turn to the second inequality. Using Lemma 6, we can deduce that:

$$\lambda_{1,h}^* \le \lambda_{1,h}(J_h V^*) \le \lambda_1(J_h V^*) + Ch^2.$$

In the following, we will provide the relation between $\lambda_1(J_hV^*)$ and λ_1^*. From

$$\lambda_1(J_hV^*) = \min_{J_hV^*\in\mathcal{A}_h} \frac{\|\nabla u_1^*\|^2 + \int_\Omega J_hV^*|u_1^*|^2}{\int_\Omega |u_1^*|^2},$$

and the regularity property (3.7) of the optimal solution u_1^*, $\forall\, x \in \Omega_{\Gamma,h}$, there exists a $\widehat{x} \in \Gamma$, if $|x-\widehat{x}| \le h$,

$$|u^*(x) - t| = |u^*(x) - u^*(\widehat{x})| \le |x - \widehat{x}|\|\nabla u^*\|_{L^\infty(\Omega_{\Gamma,h})} \le Ch.$$

Making use of (3.11) and the Assumption 1, we can get:

$$\begin{aligned} &|\int_\Omega J_hV^*|u^*|^2 - \int_\Omega V^*|u^*|^2| = |\int_{\Omega_{\Gamma,h}}(J_hV^* - V^*)(|u^*|^2 - t^2)| \\ &\le (\beta-\alpha)\int_{\Omega_{\Gamma,h}}[(u^*(x) - t)^2 + 2t|u^* - t|] \le Ch|\Omega_{\Gamma,h}| \le Ch^2, \end{aligned}$$

then we can deduce that

$$\lambda_1(J_hV^*) \le \frac{\|\nabla u_1^*\|^2 + \int_\Omega V^*|u_1^*|^2 + Ch^2}{\int_\Omega |u_1^*|^2} \le \lambda_1^* + Ch^2.$$

It completes the proof. □

4. Numerical method

In this section, we will present a monotone decreasing algorithm for the minimization problem 4. In the following of the paper, the upperscript k denotes the $k-th$ iteration.

4.1. Monotone decreasing algorithm for minimization $\lambda_{1,h}$

From the minimization problem of Problem 4

$$\min_{V_h\in\mathcal{A}_h} \lambda_{1,h} = \min_{\substack{V_h\in\mathcal{A}_h \\ (\mathcal{M}U_h,U_h)=1}} (\mathcal{K}U_h, U_h) + (\mathcal{G}U_h, U_h). \tag{4.1}$$

For each element $\{\Delta_{h,i}\}_1^N$, we suppose its basis function $\{\psi_{i,j}\}_{j=1}^3$, which are counter-clockwise arranged, the components of the corresponding eigenfunction at three nodes of $\Delta_{h,i}$ are $\{c_{i,j}\}_{j=1}^3$. Then we can get

$$U_h^T(\mathcal{K}+\mathcal{G})U_h = \sum_{i=1}^N \int_{\Delta_{h,i}} \sum_{s=1}^3\sum_{t=1}^3 \nabla\psi_{i,s}\nabla\psi_{i,t}c_{i,s}c_{i,t} + V_{h,i}\int_{\Delta_{h,i}}\sum_{s=1}^3\sum_{t=1}^3 \psi_{i,s}\psi_{i,t}c_{i,s}c_{i,t}, \tag{4.2}$$

we define $V_{h,i}$ as the value of the potential V_h in the element $\Delta_{h,i}$, where the eigenfunction U_h is normalized according to $(\mathcal{M}U_h, U_h) = 1$. Using the definition of the basis function $\{\psi_{i,j}\}_{j=1}^3$, we can deduce that:

$$\begin{aligned} \int_{\Delta_{h,i}}\sum_{s=1}^3\sum_{t=1}^3 \psi_{i,s}\psi_{i,t}c_{i,s}c_{i,t} &= \frac{|\triangle_i|}{12}\begin{pmatrix} c_{i,1} & c_{i,2} & c_{i,3}\end{pmatrix}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2\end{pmatrix}\begin{pmatrix} c_{i,1} \\ c_{i,2} \\ c_{i,3}\end{pmatrix} \\ &= \frac{|\triangle_i|}{6}(c_{i,1}^2 + c_{i,2}^2 + c_{i,3}^2 + c_{i,1}c_{i,2} + c_{i,2}c_{i,3} + c_{i,1}c_{i,3}). \end{aligned} \tag{4.3}$$

For convenience we denote by $H_i(U_h)$ the average integral term in the left side of the Eq (4.3) and have

$$(\mathcal{G}U_h, U_h) = \sum_{i=1}^{N} V_{h,i} H_i(U_h)|\Delta_{h,i}|. \tag{4.4}$$

From the above equations, we know that the course of the minimizer of the Problem 4 can now be stated as the optimization problem of the integral of the form:

$$\min_{V_h \in \mathcal{A}_h} \int_\Omega V_h(u_h)^2 dx = \min_{V_h \in \mathcal{A}_h} \sum_{i=1}^{N} V_{h,i} H_i(U_h)|\Delta_{h,i}|. \tag{4.5}$$

Above optimization problem is indeed a linear programming model. Now we have a potential value V_h^k at the iteration step k, then we can compute the eigenvalue $\lambda_{1,h}^k(V_h^k)$ and its corresponding eigenfunction $u_h^k(V_h^k)$. For simplicity, denote them as the eigenpair $(\lambda_{1,h}^k, u_h^k)$. Suppose that we give a new potential function V_h^{k+1} satisfies that:

$$\sum_{i=1}^{N} V_{h,i}^{k+1} H_i^k |\Delta_{h,i}| \leq \sum_{i=1}^{N} V_{h,i}^{k} H_i^k |\Delta_{h,i}|, \tag{4.6}$$

where H_i^k is the value of $H_i(U_h^k)$. Then a new eigenvalue $\lambda_{1,h}^{k+1}$ will be smaller since:

$$\begin{aligned} \lambda_{1,h}^{k+1} &= (\mathcal{K}U_h^{k+1}, U_h^{k+1}) + \sum_{i=1}^{N} V_{h,i}^{k+1} H_i^{k+1} |\Delta_{h,i}| \\ &\leq (\mathcal{K}U_h^{k}, U_h^{k}) + \sum_{i=1}^{N} V_{h,i}^{k+1} H_i^{k} |\Delta_{h,i}| \\ &\leq (\mathcal{K}U_h^{k}, U_h^{k}) + \sum_{i=1}^{N} V_{h,i}^{k} H_i^{k} |\Delta_{h,i}| = \lambda_{1,h}^k. \end{aligned} \tag{4.7}$$

Therefore we should find a monotonically decreasing sequence of $\sum_{i=1}^{N} V_{h,i}^k H_i^k |\Delta_{h,i}|$, where $V_h = (V_{h,1}, ..., V_{h,N}) \in \mathcal{A}_h$. It means that we should make up a suitable combination between $V_{h,i}^k$ and H_i^k, $i = 1, 2, ..., N$. We can use the following well-known rearrangement inequality in Wayne [45]:

Lemma 7. *If $a_1 \leq a_2 \leq ... \leq a_n$ and $b_1 \leq b_2 \leq ... \leq b_n$, then*

$$a_n b_1 + a_{n-1} b_2 + ... + a_1 b_n \leq a_{\tau_1} b_1 + a_{\tau_2} b_2 + ... + a_{\tau_n} b_n \leq a_1 b_1 + a_2 b_2 + ... + a_n b_n,$$

where $\{\tau_k\}_{k=1}^n$ is any permutation of indexing set $\{1, 2, ..., n\}$.

According to Lemma 7, we present a discrete monotone decreasing algorithm. See Algorithm 1.

Algorithm 1: Monotonic decreasing algorithm

1). Initial guess for $V_h^0 \in \mathcal{A}_h$, calculate $(\lambda_{1,h}^0, u_h^0)$.

2). Do while not optimal($|\lambda_h^k - \lambda_h^{k-1}| \geq \epsilon$).

2.1). $V_h^k = V_h(u_h^{k-1}) \triangleq \underset{V_h \in \mathcal{A}_h}{\operatorname{argmin}} \mathcal{R}(V_h, u_h^{k-1})$.

2.2). $u_h^k = u_h(V_h^k) \triangleq \underset{u_h \in \mathcal{V}_h \backslash \{0\}}{\operatorname{argmin}} \mathcal{R}(V_h^k, u_h)$, $\lambda_{1,h}^k = \mathcal{R}(V_h^k, u_h^k)$.

Given any initial guess $V_h^0 \in \mathcal{A}_h$, we solve the smallest eigenvalue λ_h^0 and its corresponding eigenfunction u_h^0 of Eq (3.1) for $V_h = V_h^0$, then we update V_h^1 from the eigenfunction u_h^0 such that it minimizes the Rayleigh's quotient $\mathcal{R}(V_h, u_h^0)$. Repeat this process until the stop rule is satisfied, where $\lambda_{1,h}^k = \mathcal{R}(V_h^k, u_h^k)$. In Algorithm 1, step 2.2 can be obtained by MATLAB routine *eigs*. Now we provide the details of step 2.1 to compute the minimizer V_h^k of Rayleigh's quotient $\mathcal{R}(V_h, u_h^k)$. Suppose that we have obtained the eigenpair $(\lambda_{1,h}^k, u_h^k)$ of the iteration step k. Firstly the average integration of each element $H_i^k = H_{\Delta_{h,i}}(U_h^k)$ are defined in each element $\Delta_{h,i}$, where U_h^k is the corresponding eigenvector at the k step iteration. From Lemma 7, for the minimization problem, we can sort $\{H_i^k\}_1^N$ in the ascending order as:

$$H_{\tau_1}^k \leq H_{\tau_2}^k \leq ... \leq H_{\tau_N}^k, \tag{4.8}$$

where $\{\tau_1, \tau_2, ..., \tau_N\}$ is a permutation of {1,2...,N }. Define V_h^{k+1} as follows:

$$V_{h,\tau_1}^{k+1} = ... = V_{h,\tau_{k-1}}^{k+1} = \beta, V_{h,\tau_{t+1}}^{k+1} = ... = V_{h,\tau_N}^{k+1} = \alpha, \tag{4.9}$$

where the subscript τ_t is satisfied with:

$$|\Delta_{h,\tau_1}| + ... + |\Delta_{h,\tau_{t-1}}| < \frac{c-\alpha}{\beta-\alpha}|\Omega| \leq |\Delta_{h,\tau_1}| + ... + |\Delta_{h,\tau_{t-1}}| + |\Delta_{y,\tau_t}|. \tag{4.10}$$

To fulfill the constraint, we adopt

$$\theta = V_{h,\tau_t}^{k+1} = \frac{1}{|\Delta_{h,\tau_t}|}(c|\Omega| - \beta \sum_{j=1}^{t-1} |\Delta_{h,\tau_j}| - \alpha \sum_{j=t+1}^{N} |\Delta_{h,\tau_j}|). \tag{4.11}$$

Notice that step (2.1) in Algorithm 1 is implemented by the Eqs (4.8)–(4.11). In fact, we have the following conclusion from the step (2.1) in Algorithm 1:

Proposition 1. *If we define the potential value V_h^* by step 2.1 in Algorithm 1, then it is a minimizer of the Rayleigh's quotient $\mathcal{R}(V_h, u_h)$ over $\mathcal{A}_h$.*

Proof. For any given $V_h \in \mathcal{A}_h$, recall that from the Eq (4.3)

$$H_i(U_h) = \frac{1}{6}(c_{i,1}^2 + c_{i,2}^2 + c_{i,3}^2 + c_{i,1}c_{i,2} + c_{i,2}c_{i,3} + c_{i,1}c_{i,3}).$$

Where U_h is the corresponding eigenvector. Then it is sufficient to check that

$$\sum_{i=1}^{N} V_{h,i}^* H_i |\Delta_{h,i}| \leq \sum_{i=1}^{N} V_{h,i} H_i |\Delta_{h,i}|,$$

where $V_h^* = \{V_{h,i}^*\}_{i=1}^N$. Define $e_i = V_{h,i} - V_{h,i}^*$, $\mathcal{I}_\beta = \{\tau_1, ..., \tau_{t-1}\}$, $\mathcal{I}_\alpha = \{\tau_{t+1}, ..., \tau_N\}$, $\mathcal{I}_\theta = \{\tau_t\}$. Then we have

$$\sum_{i=1}^N V_{h,i}H_i|\Delta_{h,i}| - \sum_{i=1}^N V_{h,i}^*H_i|\Delta_{h,i}| = \sum_{i\in\mathcal{I}_\alpha} e_iH_i|\Delta_{h,i}| + \sum_{i\in\mathcal{I}_\beta} e_iH_i|\Delta_{h,i}| + e_{\tau_t}H_{\tau_t}|\Delta_{h,\tau_t}|.$$

Since $\sum_{i=1}^N V_{h,i}|\Delta_{h,i}| = \sum_{i=1}^N V_{h,i}^*|\Delta_{h,i}|$, which means that $\sum_{i=1}^N e_i|\Delta_{h,i}| = 0$, then

$$e_{\tau_t}|\Delta_{h,\tau_t}| = -(\sum_{i\in\mathcal{I}_\alpha\cup\mathcal{I}_\alpha} e_i|\Delta_{h,i}|).$$

It could deduce that

$$\sum_{i=1}^N V_{h,i}H_i|\Delta_{h,i}| - \sum_{i=1}^N V_{h,i}^*H_i|\Delta_{h,i}| = \sum_{i\in\mathcal{I}_\alpha} e_i|\Delta_{h,i}|(H_i - H_{\tau_t}) + \sum_{i\in\mathcal{I}_\beta} e_i|\Delta_{h,i}|(H_i - H_{\tau_t}).$$

From the rearrangement inequality (4.8), we can observe that:

$$\begin{cases} H_{\tau_t} \le H_i, & \forall\ i \text{ in } \mathcal{I}_\alpha, \\ H_i \le H_{\tau_t}, & \forall\ i \text{ in } \mathcal{I}_\beta. \end{cases}$$

And from the fact that $\alpha \le V_h \le \beta$, it implies that

$$\begin{cases} e_i|\Delta_{h,i}|(H_i - H_{\tau_t}) = |\Delta_{h,i}|(V_{h,i} - \alpha)(H_i - H_{\tau_t}) \ge 0, & \forall\ i \text{ in } \mathcal{I}_\alpha, \\ e_i|\Delta_{h,i}|(H_i - H_{\tau_t}) = |\Delta_{h,i}|(V_{h,i} - \beta)(H_i - H_{\tau_t}) \ge 0, & \forall\ i \text{ in } \mathcal{I}_\beta. \end{cases}$$

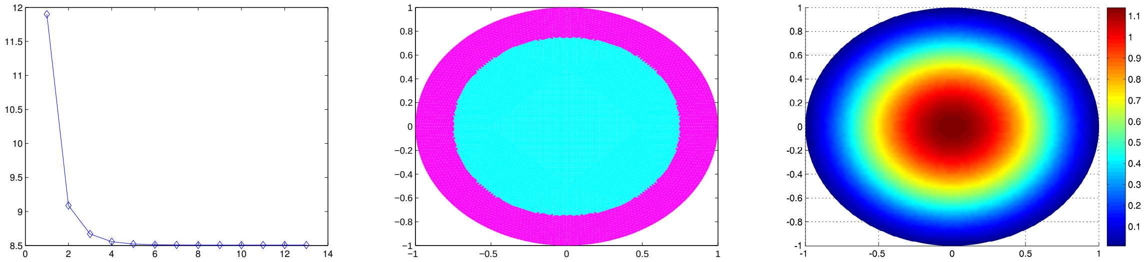
Combining with above we can obtain the desired result. □

4.2. Numerical experiment

In this section, we provide some numerical experiments for the extremal problem on planar regions to verify the effect of Algorithm 1. The color of the area shows the distribution of the potential, where the color magenta represents the potential value of the area is β, the color cyan represents the potential value of the area is α.

Example 1. *Consider a disk* $\Omega = \{0 \le x^2 + y^2 \le 1.0\}$. *Choose* $\alpha = 2.0, \beta = 18.0$*, and* $c = 9.0$.

Eigenvalue optimization problems in disk have been considered in [1]. In our numerical example, we initially divide the domain into 4 triangles, then refine the mesh by subdividing each triangle into 4 triangles. The numerical results are done on the 7-th refinement which gives 4^8 triangles. The stopping criterion we adopt is the L^2 norm of the difference between current and previous configuration of the potential is less than 10^{-10}. At the left of Figure 1 is the iterative process of the eigenvalue $\lambda_{1,h}$,in the middle of of Figure 1 is the approximate optimal potential distribution, at the right of Figure 1 is the corresponding eigenfunction. At 12-th iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 8.504640. In Table 1, we present the corresponding smallest eigenvalues $\lambda_{1,h}^*$ for 5 successive mesh refinements. The first two lines of Table 1 show that the smallest eigenvalue decreases while the mesh is refined. The third line is the difference between two successive smallest eigenvalues. From the fourth line, we note that our convergence order is close to 2, which is predicted in Theorem 1.



(a) Iterative process of $\lambda_{1,h}$ **(b)** The potential distribution **(c)** The eigenfunction

Figure 1. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* = 8.504640$ to the circular case.

Table 1. Grid refinement analysis for the extremal eigenvalue of the disk case.

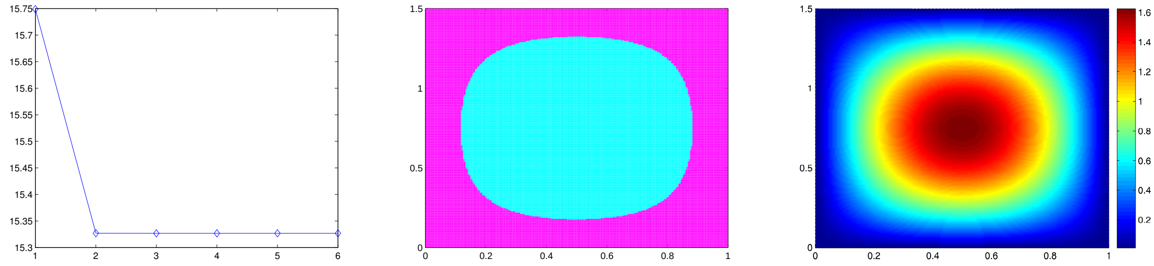
N	4^3	4^4	4^5	4^6	4^7	4^8
λ_1^N	8.698680	8.550880	8.516318	8.507116	8.505131	8.504640
e_N	0.147800	0.034562	0.009202	0.001985	0.000491	
order	2.09639	1.90913	2.21263	2.01689		

Example 2. *Consider a rectangular* $\Omega = [0, 1] \times [0, 1.5]$. *Choose* $\alpha = 2.0, \beta = 2.0$*, and* $c = 1.5$.

The numerical results are done on the 7-th refinement which gives 131072 triangles. The stopping criterion adopted is the same as Example 1. At the left of Figure 2 is the iterative process of the eigenvalue $\lambda_{1,h}$,in the middle of Figure 2 is the approximate optimal potential distribution, at the right of Figure 2 is the corresponding eigenfunction. At 5-th iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 15.325775. In Table 2, we present the corresponding smallest eigenvalues $\lambda_{1,h}^*$ for 5 successive mesh refinements. The first two lines of Table 2 show that the smallest eigenvalue decreases while the mesh is refined. The third line is the difference between two successive smallest eigenvalues. From the fourth line, we note that our convergence order is also close to 2.

Table 2. Grid refinement analysis for the extremal eigenvalue of the rectangular case

N	128	512	2048	8192	32678	131072
λ_1^N	15.709809	15.420859	15.349355	15.331401	15.326897	15.325775
e_N	0.288950	0.071503	0.017954	0.004505	0.001122	
order	2.01474	1.99369	1.99485	2.00555		

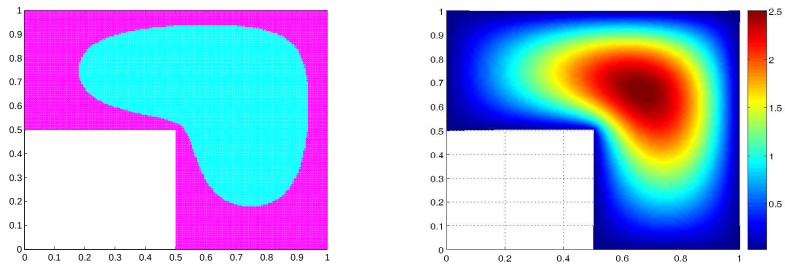


(**a**) Iterative process of $\lambda_{1,h}$ (**b**) The potential distribution (**c**) The eigenfunction

Figure 2. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* = 15.325775$ to the rectangular case.

Example 3. *Consider a L-Shape domain* $\Omega = [0, 1.0] \times [0, 1.0] \backslash [0, 0.5) \times [0, 0.5)$. *Choose* $\alpha = 2.0, \beta = 2.0$, *and* $c = 1.5$.

In numerical example, we divide the domain into 6×4^6 triangles. The stopping criterion adopted is the same as Example 1. At the left of Figure 3 is the approximate optimal potential distribution, at the right of Figure 3 is the corresponding eigenfunction. At 8-th iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 39.657491.



(**a**) The potential distribution (**b**) The eigenfunction

Figure 3. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* = 39.657491$ to the L-Shape.

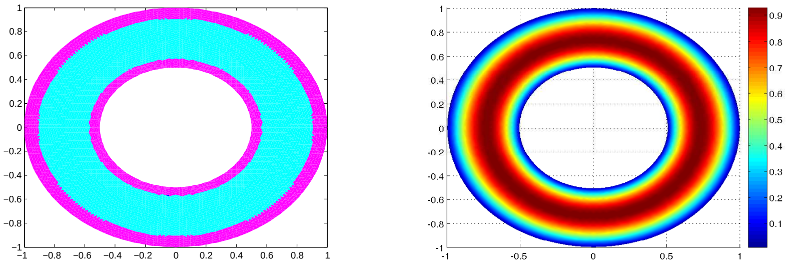
Example 4. *Consider an annular shape domain* $\Omega = \{(x, y)|0.25 \le x^2 + y^2 \le 1.0\}$. *Choose* $\alpha = 2.0, \beta = 18.0$. *For the volume constraint c, we study two cases: one is* $c = 5.5$, *and another is* $c = 7.5$.

The numerical results are done on the mesh which gives 12×4^5 triangles. The stopping criterion we adopt is the difference between eigenvalues in two consecutive iterations is less than 10^{-6}.

(1). If $c = 5.5$, at the left of Figure 4 is the approximate optimal potential distribution, at the right of Figure 4 is the corresponding eigenfunction. At 3rd iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 41.914713.

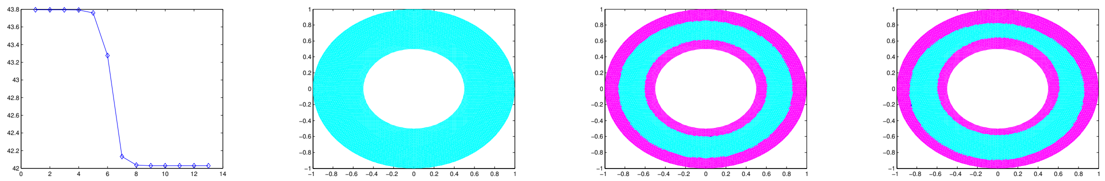
(2). If $c = 7.5$, Figure 5 (a) shows the iterative process of the eigenvalue $\lambda_{1,h}$. Figure 5(b)–(d) show the evolution process of the potential distribution. At 13-th iteration, we find the extremal eigenvalue

$\lambda_{1,h}^*$ is 42.028784. At the left of Figure 6 is the approximate optimal potential distribution, at the right of Figure 6 is the corresponding eigenfunction.



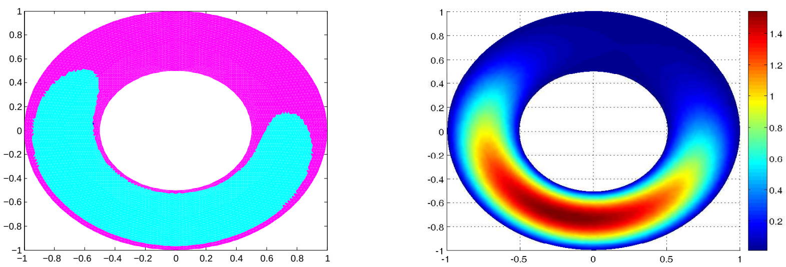
(a) The potential distribution **(b)** The eigenfunction

Figure 4. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* = 41.914713$ to the annular case, where $c = 5.5$.



(a) $\lambda_{1,h}$ **(b)** $k = 0$ **(c)** $k = 5$ **(d)** $k = 6$

Figure 5. Iterative process of the eigenvalue $\lambda_{1,h}$ and the potential V.



(a) The potential distribution **(b)** The eigenfunction

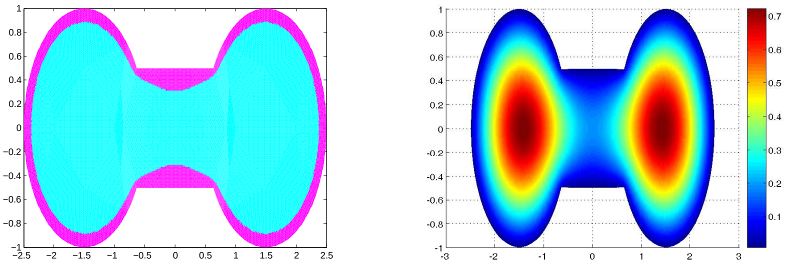
Figure 6. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* = 42.028784$ to the annular case, where $c = 7.5$.

Example 5. *Consider a dumbbell shape domain* $\Omega_h = B_1(-1.5, 0) \cup ((-1.5, 1.5) \times \times (-h, h)) \cup B_1(1.5, 0)$, *and* $B_r(p) = \{x \in \mathbb{R}^2 : |x - p| < r\}$. *Choose* $\alpha = 1.0, \beta = 2.0$, *and* $c = 1.2$. *For* $h \in (0, 1)$, *define the dumbbell with the handle width* $2h$.*The parameter* h *will be chosen as:* $h = 0.5$ *and* $h = 0.3$.

The numerical results are done on the mesh which gives 58×4^5 triangles. The stopping criterion we adopt is the same as Example 4.

(1) If $h = 0.5$, at the left of Figure 7 is the approximate optimal potential distribution, at the right of Figure 7 is the corresponding eigenfunction. At 14-th iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 6.360768.

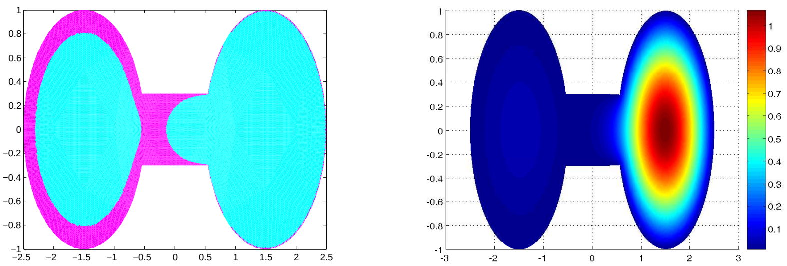
(2) If $h = 0.3$, at the left of Figure 8 is the approximate optimal potential distribution, at the right of Figure 8 is the corresponding eigenfunction. At 15-th iteration, we find the extremal eigenvalue $\lambda_{1,h}^*$ is 6.669552.



(a) The potential distribution

(b) The eigenfunction

Figure 7. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* =$ 6.360768 to the dumbbell case, where $h = 0.5$.



(a) The potential distribution

(b) The corresponding eigenfunction

Figure 8. The potential distribution V_h^* and the corresponding eigenfunction u_h^* with $\lambda_{1,h}^* =$ 6.669552 to the dumbbell case, where $h = 0.3$.

One interesting phenomena called *symmetry − breaking* is found in the second case of Example 4, Example 5, which has been studied in many papers, see [37, 39]. Chanillo and others have pointed out that if the annulus and the handle becomes "thinner", then symmetry breaking occurs, which is verified by our method. As we all know that, the symmetry breaking phenomena implies non-uniqueness of the solution: such as Example 5, the pair (V_h', U_h') obtained from the pair (V_h, U_h) for the extremal eigenvalue $\lambda_{1,h}^*$ by reflection in the y−axis will be a solution, which also verify that the solution to the minimization problem doesn't hold uniqueness.

5. Conclusions

In this paper, finite element method with a monotonic decreasing algorithm is applied to solve the smallest eigenvalue optimization problem of the Schrödinger operator. We have performed an analysis which shows that the optimizer of this problem is a fixed point of the variational formulation of the eigenvalue optimization problem. From the numerical examples, we can see that our algorithm is feasible and efficient. In the future, the study on the nonlinear eigenvalue problems of the Schrödinger operator will be considered.

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Conflict of interest

The authors declare that they have no conflict of interest.

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