

## VERIFIED EIGENVALUE EVALUATION FOR THE LAPLACIAN OVER POLYGONAL DOMAINS OF ARBITRARY SHAPE\*

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**Abstract.** The finite element method (FEM) is applied to bound leading eigenvalues of the Laplace operator over polygonal domains. Compared with classical numerical methods, most of which can only give concrete eigenvalue bounds over special domains of symmetry, our proposed algorithm can provide concrete eigenvalue bounds for domains of arbitrary shape, even when the eigenfunction has a singularity. The problem of eigenvalue estimation is solved in two steps. First, we construct a computable a priori error estimation for the FEM solution of Poisson's problem, which holds even for nonconvex domains with reentrant corners. Second, new computable lower bounds are developed for the eigenvalues. Because the interval arithmetic is implemented throughout the computation, the desired eigenvalue bounds are expected to be mathematically correct. We illustrate several computation examples, such as the cases of an L-shaped domain and a crack domain, to demonstrate the efficiency and flexibility of the proposed method.

**Key words.** eigenvalue problem, elliptic operator, finite element method, min-max principle, verified computation, Prager–Synge's theorem

**AMS subject classifications.** 34L15, 80M10

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**1. Introduction.** The eigenvalue problem for the Laplacian,  $-\Delta u = \lambda u$ , has been well investigated in history, mainly in the study of acoustic theory and problems of vibrating elastic membranes and electromagnetic waveguides. There is considerable literature on approximating the eigenvalues by numerical methods; see, e.g., the review papers of Boffi [5] and Kuttler and Sigillito [19] and the lecture book of Weinberger [41].

In this paper, we aim to provide concrete lower and upper bounds for eigenvalues of the Laplacian over a polygonal domain. The need for such bounds arises in many practical problems, for example, the estimation of the Poincaré constant in the embedding theorem of Sobolev spaces (see, e.g., [16]) and the investigation of the spectral distribution of the differential operator when exploring the existence of solutions of nonlinear differential equations (see, e.g., [30, 27]). All these problems are closely related to the elliptic eigenvalue problem. Moreover, to apply the computational results to a mathematical proof, strictly correct eigenvalue bounds are desired.

It is well known that the upper bound for eigenvalues can be easily computed using the Rayleigh–Ritz method, while the lower bound cannot be determined easily. Many theories propose a qualitative analysis of eigenvalue approximation using various numerical methods, but a concrete lower bound is usually unavailable because of the appearance of unknown constants in the estimation formula. In the following, we present a short review of methods that can provide explicit bounds:

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- (i) The finite difference method [14, 40] can provide bounds on eigenvalues in domains of regular shape. For a general domain, it is difficult to process the boundary strip using this method, especially for domains with a reentrant corner.
- (ii) The intermediate method, also known as the Weinstein–Aronszajn method (see, e.g., [42]), can give lower bounds for eigenvalues. However, it requires complex manipulation of constraint conditions and a base problem with an explicit spectrum is necessary.
- (iii) The point-matching method or collocation method (see, e.g., [11, 25, 35]) can give precise bounds for eigenvalues by calculating the existence interval. As only the existence of the eigenvalue is guaranteed, such a method cannot verify the eigenvalue indexes. Based on these high-precision computed results, a discussion on the eigenmodes of planar regions can be found in [38].
- (iv) The finite element method (FEM), which has a solid foundation of mathematical theories, can effectively approximate eigenvalues (see, e.g., [37]) with a comprehensive analysis on error estimation. In particular, some non-conforming FEM can give lower bounds of eigenvalues directly when the mesh size is sufficiently small; see [44] for a survey. However, since most of the theories on nonconforming FEMs are limited to asymptotic analysis, it is difficult to check when the mesh size is small enough. In this paper, we reconsider the theories, especially the ones for conforming FEMs, to construct explicit eigenvalue bounds by evaluating the constants appearing in the error estimation formulation.
- (v) Katou’s bound and the Lehmann–Goerisch method [23, 12, 3] can provide precise lower bounds for up to the  $n$ th eigenvalue if the lower bound  $\nu$  for the  $(n+1)$ th eigenvalue is available. However, finding a proper a priori estimation  $\nu$  is not an easy task. Numerical computation for an L-shaped domain has been performed to show the efficiency of this method [45], where a pseudo lower bound  $\nu$  is used.

To apply the eigenvalue estimation result to a mathematical proof, one needs to have the eigenvalue bounds and indexes strictly guaranteed. In addition to the function approximation error in evaluating the eigenvalue, the rounding error in floating-point number computation also needs to be considered. IEEE Standard 754 makes it possible to estimate the rounding error by applying interval arithmetic (see, e.g., [26]). Once both the approximation error and the rounding error are effectively estimated, one can enclose the exact result by a narrow interval through numerical computation, which we call *verified computation*. The available verified evaluation of eigenvalues is summarized as follows:

- (i) In [28], Nakao, Yamamoto, and Nagatou developed a method to verify the nonexistence of eigenvalues in small intervals. By excluding the nonexistence small intervals that start from zero, a lower bound for the eigenvalue is available.
- (ii) In [29], Plum developed the *homotopy method* based on the operator comparison theorem to bound eigenvalues. This method provides a rough lower bound of the  $k$ th eigenvalue for certain  $k$ , which can act as the a priori estimation needed by the Lehmann–Goerisch method. The dependency of the homotopy method on the base problem, i.e., the one with an explicit spectrum, restricts its application in solving problems of general domains. For a domain of irregular shape, a transformation of the domain to a regular shape, e.g., a square, is needed.

In Theorem 4.3, we propose an explicit bound for Laplacian eigenvalues based on the FEM

$$(1.1) \quad \lambda_k^h / (1 + M_h^2 \lambda_k^h) \leq \lambda_k \leq \lambda_k^h,$$

where  $\lambda_k$  is the  $k$ th eigenvalue to be estimated,  $\lambda_k^h$  is an approximation to  $\lambda_k$ , and  $M_h$  is a computable quantity related to the FEM error estimation. By inheriting the advantages of FEM, such a method can deal with a polygonal domain of arbitrary shape in a natural way. Because interval arithmetic is implemented in the computation, the obtained result is expected to be mathematically correct.

The main contributions of this paper can be summarized as follows:

- (i) A computable a priori estimation is developed for the projection  $P_h$  that projects the solution of Poisson's equation into the FEM function space. Such an estimation holds even for nonconvex domains, where singularities appear around reentrant corners. The *hypercircle equation* from the Prager–Synge theorem [31] and the mixed Raviart–Thomas FEM play an important role in estimating  $P_h$  when the solution has a singularity.
- (ii) An improvement is achieved for the classical qualitative error estimation for FEM eigenvalue approximation [37, 33, 20], and an explicit lower bound based on the error estimation for the projection  $P_h$  is proposed. Such a bound can work as a good candidate for the a priori estimation needed by the Lehmann–Goerisch method to sharpen the bounds.

The remainder of this paper is organized as follows. In section 2, we provide some preliminary background. In section 3, an explicit a priori error estimate is deduced for the FEM solution of Poisson's problem, where much effort is focused on the case of domains of singularity. In section 4, the a priori error estimate from section 3 is applied to construct an explicit lower bound for eigenvalues. In section 5, the computation results are presented. Finally, in section 6, we state our conclusions and discuss the scope for future work.

**2. Preliminaries.** We shape our discussion within the framework of Sobolev spaces [1]. Let  $\Omega$  be a connected bounded polygonal domain with arbitrary shape and let the boundary of  $\Omega$  be divided into two disjoint parts,  $\partial\Omega = \Gamma_D \cup \Gamma_N$ . The function space  $L_2(\Omega)$  is constructed by all the real square integrable functions over  $\Omega$ , and  $H^n(\Omega)$  ( $n = 1, 2, \dots$ ) are the  $n$ th order Sobolev function spaces that the function has up to the  $n$ th derivative to be in  $L_2(\Omega)$ . We further introduce subspace  $V \subset H^1(\Omega)$  associated with homogeneous boundary conditions such that, for  $\Gamma_D \neq \emptyset$ ,

$$(2.1a) \quad V = \{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_D\}.$$

If  $\Gamma_D$  is the empty set, we define  $V$  by

$$(2.1b) \quad V = \left\{ v \in H^1(\Omega) \mid \int_{\Omega} v dx = 0 \right\}.$$

Denote by  $\|v\|_{L_2}$  the  $L_2$  norm of  $v \in L_2(\Omega)$  and denote by  $|v|_{H^k(\Omega)}$  and  $\|v\|_{H^k(\Omega)}$  the seminorm and norm of  $H^k(\Omega)$ , respectively. Integration  $(\cdot, \cdot)$  is the inner product in  $L_2(\Omega)$  or  $(L_2(\Omega))^2$ . Using such notation, the variational form of the Laplacian eigenvalue problem  $-\Delta u = \lambda u$  reads as

$$(2.2) \quad \text{Find } \lambda \in \mathbb{R} \text{ and } u \in V \text{ s.t. } (\nabla u, \nabla v) = \lambda(u, v) \quad \forall v \in V.$$

Here,  $\nabla$  is the gradient operator. As the inverse of the Laplacian is a compact self-adjoint operator, the spectral theorem shows that problem (2.2) has a spectrum of infinitely many eigenvalues (see, e.g., [10]),  $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \dots$ .

The associated eigenfunctions  $u_1, u_2, \dots$  can be normalized to form an orthogonal set in  $L_2(\Omega)$ , that is,  $(u_i, u_j) = \delta_{ij}$ , where  $\delta_{ij}$  is Kronecker's delta. In the sense of distributions, we have  $-\Delta u_i = \lambda_i u_i$ .

Let  $\mathcal{T}^h$  be a triangulation of domain  $\Omega$ . The piecewise-continuous linear finite element space  $V^h(\subset V)$ , which has the hat function as its basis function, is adopted here as the approximation space. Suppose that  $\dim(V^h) = n$ . The Ritz-Galerkin method solves the variation problem (2.2) in  $V^h$ ,

$$(2.3) \quad \text{find } \lambda^h \in \mathbb{R} \text{ and } u_h \in V^h \text{ s.t. } (\nabla u_h, \nabla v_h) = \lambda^h (u_h, v_h) \quad \forall v_h \in V^h .$$

The eigenvalue problem (2.3) has finitely many eigenpairs, which we denote by  $\{\lambda_i^h, u_i^h\}_{i=1}^n$ , and we assume that  $\lambda_1^h \leq \lambda_2^h \leq \dots \leq \lambda_n^h$  and  $(u_i^h, u_j^h) = \delta_{i,j}$ . Take the basis function of  $V^h$  as  $\{\phi_i\}_{i=1}^n$ ; then, problem (2.3) is to solve the generalized eigenvalue problem of  $n \times n$  matrices  $A^h$  and  $B^h$ ,

$$(2.4) \quad A^h x = \lambda^h B^h x, \text{ where } A_{i,j}^h = (\nabla \phi_i, \nabla \phi_j), B_{i,j}^h = (\phi_i, \phi_j) .$$

Let us introduce the Rayleigh quotient over space  $V$ ,

$$(2.5) \quad R(v) := (\nabla v, \nabla v)/(v, v) \quad \text{for } v \in V .$$

The Poincaré min-max principle asserts that

$$(2.6) \quad \lambda_k = \min_{H_k \subset V} \max_{v \in H_k} R(v), \quad \lambda_k^h = \min_{H_k \subset V^h} \max_{v_h \in H_k} R(v_h),$$

where  $H_k$  denotes any  $k$ -dimensional subspace of  $V$  or  $V^h$ . Thus, the discrete eigenvalue  $\lambda_k^h$  provides an upper bound for  $\lambda_k$ , which is also called the *Rayleigh-Ritz bound*. From numerical analysis, we find that  $\lambda_k^h$  acts as an accurate upper bound for  $\lambda_k$  (see, e.g., [37]). However, it is difficult to obtain a concrete lower bound for the eigenvalues, which is the primary objective of this paper. Note that the eigenfunction approximation error will not be discussed here.

**Interpolation function and error estimation.** We introduce two interpolation operators,  $\pi_{0,h}$  and  $\pi_{1,h}$ , which will enable explicit a priori error estimation for the FEM. For each  $u \in L_2(\Omega)$ ,  $\pi_{0,h}u$  is a piecewise constant function over  $\mathcal{T}^h$  such that on each element  $K$ ,

$$(2.7) \quad (\pi_{0,h}u)|_K \equiv \text{average of } u \text{ on } K = \int_K u(x) dx / (\text{area of } K) .$$

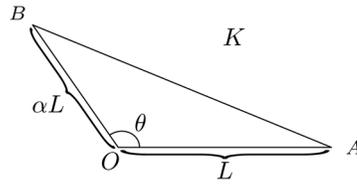
For  $u \in H^2(\Omega)$ ,  $\pi_{1,h}u \in V^h$  is the Lagrange interpolation of  $u$ , that is,

$$(2.8) \quad (\pi_{1,h}u)(p_i) = u(p_i) \text{ for each node } p_i \text{ of triangulation } \mathcal{T}^h .$$

The computable interpolation error estimation for  $\pi_{0,h}$  and  $\pi_{1,h}$  has been investigated extensively; for example, see [8, 39, 16, 24, 18], according to which

$$(2.9) \quad \|u - \pi_{0,h}u\|_{L_2} \leq C_0 h |u|_{H^1} \text{ for } u \in H^1(\Omega),$$

$$(2.10) \quad |u - \pi_{1,h}u|_{H^1} \leq C_1 h |u|_{H^2} \text{ for } u \in H^2(\Omega),$$

FIG. 2.1. Configuration of triangle element  $K$  by  $(\alpha, \theta, L)$ .

where  $h$  is the mesh size to be specified; constants  $C_0$  and  $C_1$  are defined as

$$(2.11) \quad C_i := \max_{K \in \mathcal{T}^h} C_i(K)/h \quad (i = 0, 1).$$

Here,  $C_i(K)$  ( $i = 0, 1$ ) are constants defined on triangle element  $K$  of  $\mathcal{T}^h$ :

$$C_0(K) := \sup_{v \in H^1(K)} \frac{|v|_{H^1(K)}}{\|v\|_{L_2(K)}}, \quad C_1(K) := \sup_{v \in H^2(K), v(O)=v(A)=v(B)=0} \frac{|v|_{H^2(K)}}{|v|_{H^1(K)}}.$$

For each  $K$  (see Figure 2.1), let  $L$  be the median edge length, i.e.,  $|OB| \leq L = |OA| \leq |AB|$ , let  $\theta$  be the maximum angle, and let  $\alpha L$  ( $0 < \alpha \leq 1$ ) be the smallest edge length; thus, Liu and Kikuchi [24] obtained the following result:

$$C_0(K) \leq \frac{L}{\pi} \sqrt{1 + |\cos \theta|}, \quad C_1(K) \leq 0.493L \frac{1 + \alpha^2 + \sqrt{1 + 2\alpha^2 \cos 2\theta + \alpha^4}}{\sqrt{2(1 + \alpha^2 - \sqrt{1 + 2\alpha^2 \cos 2\theta + \alpha^4})}}.$$

Another estimate for  $C_0$  is given by Laugesen and Siudeja [21]:  $C_0(K) \leq |AB|/j_{1,1}$ , where  $j_{1,1} \approx 3.8317$  denotes the first positive root of the Bessel function  $J_1$ . In the case of  $\mathcal{T}^h$  being a uniform mesh with isosceles right triangle elements, we can take

$$h = \text{leg length of right triangle element}, \quad C_0 = 1/\pi, \quad C_1 = 0.493.$$

**3. Explicit a priori error estimation for the FEM solution of Poisson's problem.** In this section, we construct an explicit error estimation for the FEM solution of Poisson's equation, which is the key part of the algorithm to bound the Laplacian eigenvalues. We consider Poisson's equation associated with the mixed boundary condition: for  $f \in L_2(\Omega)$ , find  $u$  such that

$$(3.1) \quad -\Delta u = f \quad \text{in } \Omega, \quad u = 0 \text{ on } \Gamma_D, \quad \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma_N.$$

A weak formulation of the above problem is to find  $u$  in  $V$  such that

$$(3.2) \quad (\nabla u, \nabla v) = (f, v) \quad \forall v \in V.$$

The FEM solution  $u_h \in V^h$  is given by solving the above weak formulation in  $V^h$ :

$$(3.3) \quad (\nabla u_h, \nabla v_h) = (f, v_h) \quad \forall v_h \in V^h.$$

The selection of  $V$  and  $V^h$  in section 2, along with the Lax–Milgram theorem, ensures the existence and uniqueness of solutions  $u$  and  $u_h$  (see, e.g., [37]).

Let us introduce the projection  $P_h : V \rightarrow V^h$  such that for  $v \in V$ ,

$$(\nabla(v - P_h v), \nabla v_h) = 0 \quad \forall v_h \in V^h.$$

Therefore,  $u_h = P_h u$ . The classical error estimation theory gives the a priori estimation for projection  $P_h$  in a qualitative way,

$$\|u - P_h u\|_{H^1} \leq Ch^\gamma \|f\|_{L_2},$$

where the constant  $C$ , independent of  $f$ , is bounded but usually unknown; the exponent  $\gamma$  is the convergence order in terms of the mesh size  $h$ . In the case of homogeneous Dirichlet or Neumann boundary conditions over convex domains, we know that the solution  $u$  of (3.2) belongs to  $H^2(\Omega)$ , which we call  $H^2$ -regularity (see, e.g., [13]), and the order  $\gamma$  can be one. However, such a regularity cannot be expected for a non-convex domain or the mixed boundary condition, which makes FEM error estimation difficult.

In sections 3.1 and 3.2, we introduce a computable quantity  $M_h$  such that

$$\sup_{f \in L_2} \inf_{v_h \in V^h} \frac{|u_f - v_h|_{H^1}}{\|f\|_{L_2}} \leq M_h,$$

where  $u_f$  denotes the solution of Poisson's equation with data  $f$ . Such a quantity leads to the a priori error estimation for the FEM solution,

$$(3.4) \quad |u - P_h u|_{H^1} \leq M_h \|f\|_{L_2}, \quad \|u - P_h u\|_{L_2} \leq M_h^2 \|f\|_{L_2}.$$

The discussion will be divided into two cases, one in which the solution  $u$  of problem (3.1) has  $H^2$ -regularity, and the other in which  $u$  is singular, i.e.,  $u \notin H^2(\Omega)$ .

**3.1. A priori estimation for solution of  $H^2$ -regularity.** For all  $u \in H^2(\Omega)$  that are solutions of problem (3.1), we know that  $|u|_{H^2} = \|\Delta u\|_{L_2} = \|f\|_{L_2(\Omega)}$ ; see, e.g., Theorem 4.3.1.4 of [13]. Thus, the explicit a priori estimation can be easily obtained by applying Céa's lemma and the Aubin–Nitsche duality technique,

**THEOREM 3.1** (a priori error estimation). *Let  $u \in V$  and  $u_h \in V^h$  be the solutions of (3.2) and (3.3), respectively. In the case that  $u \in H^2(\Omega)$ , it holds that*

$$|u - u_h|_{H^1} \leq C_1 h |u|_{H^2} = C_1 h \|f\|_{L_2},$$

where the constant  $C_1$  is the one defined in (2.11). Let  $\phi \in V$  be the solution of the dual problem  $(\nabla \phi, \nabla v) = (u - u_h, v) \forall v \in V$ . If  $\phi \in H^2(\Omega)$ , then

$$\|u - u_h\|_{L_2} \leq C_1 h |u - u_h|_{H^1} \leq C_1^2 h^2 \|f\|_{L_2}.$$

Thus, we can take  $M_h := C_1 h$  in the estimation (3.4).

**3.2. A priori error estimate for solution without  $H^2$ -regularity.** In this subsection, we will apply the hypercircle method in order to facilitate a priori error estimation. Such an analysis uses only the first-order derivative of solution  $u$ . Thus, it can deal with elliptic problems, even if  $H^2$ -regularity is not available. The hypercircle method has also been used in a posteriori error estimation; cf., Kikuchi and Saito [17], Braess [6], etc.

First, let us review several classical finite element spaces:

- (i) Piecewise constant function space  $X^h$ :

$$X^h := \{v \in L_2(\Omega) \mid v \text{ is constant on each element of } \mathcal{T}^h\}$$

In the case of  $\Gamma_N = \partial\Omega$ , the function  $f_h$  in  $X^h$  is required to satisfy  $\int_\Omega f_h dx = 0$ .

(ii) Lowest-order Raviart–Thomas mixed FEM space  $W^h$ :

$$W^h := \{\mathbf{p}_h \in H(\operatorname{div}, \Omega) \mid \mathbf{p}_h = (a_K + c_K x, b_K + c_K y) \text{ in } K \in \mathcal{T}^h, \mathbf{p}_h \cdot \vec{n} = 0 \text{ on } \Gamma_N\},$$

where  $a_K, b_K, c_K$  are constants on element  $K$ , and  $H(\operatorname{div}, \Omega)$  is defined by

$$H(\operatorname{div}, \Omega) = \{\mathbf{q} \in (L_2(\Omega))^2 \mid \operatorname{div} \mathbf{q} \in L_2(\Omega)\}.$$

(iii) Subset  $W_{f_h}^h$  of  $W^h$  corresponding to  $f_h \in X^h$ :

$$W_{f_h}^h := \{\mathbf{p}_h \in W^h \mid \operatorname{div} \mathbf{p}_h + f_h = 0 \text{ on each } K \in \mathcal{T}^h\}.$$

The classical analysis shows that  $\operatorname{div}(W^h) = X^h$  (cf. Chapter IV.1 of [7]). From the definition of  $\pi_{0,h}$  in (2.7), we see that  $\pi_{0,h}$  is also the projection of  $L_2(\Omega)$  onto  $X^h$  under the  $L_2$  norm: for  $v \in L_2(\Omega)$ ,  $\pi_{0,h}v \in X^h$  satisfies

$$(3.5) \quad (v - \pi_{0,h}v, v_h) = 0 \quad \forall v_h \in X^h.$$

We introduce a computable quantity  $\kappa_h$  for the purpose of developing the a priori estimation. The computation of  $\kappa_h$  will be discussed in section 3.3.

$$(3.6) \quad \kappa_h := \max_{f_h \in X^h \setminus \{0\}} \min_{v_h \in V^h} \min_{\mathbf{p}_h \in W_{f_h}^h} \|\mathbf{p}_h - \nabla v_h\|_{L_2} / \|f_h\|_{L_2}.$$

**THEOREM 3.2.** *Given  $f_h \in X^h$ , let  $\tilde{u} \in V$  and  $\tilde{u}_h \in V^h$  be the solutions of the variational problems*

$$(3.7) \quad (\nabla \tilde{u}, \nabla v) = (f_h, v) \quad \forall v \in V; \quad (\nabla \tilde{u}_h, \nabla v_h) = (f_h, v_h) \quad \forall v_h \in V^h,$$

respectively. Then, we have the following computable error estimate:

$$(3.8) \quad |\tilde{u} - \tilde{u}_h|_{H^1} \leq \kappa_h \|f_h\|_{L_2}.$$

*Proof.* First, we present the *hypercircle equation* from the Prager–Synge theorem [31]: for  $\tilde{u}$  in (3.7) and any  $v_h \in V^h$ ,  $\mathbf{p}_h \in W_{f_h}^h$ ,

$$(3.9) \quad \|\nabla \tilde{u} - \nabla v_h\|_{L_2}^2 + \|\nabla \tilde{u} - \mathbf{p}_h\|_{L_2}^2 = \|\mathbf{p}_h - \nabla v_h\|_{L_2}^2.$$

To see why the above equality holds, we consider the cross term

$$(3.10) \quad (\nabla \tilde{u} - \nabla v_h, \nabla \tilde{u} - \mathbf{p}_h) = \sum_{K \in \mathcal{T}^h} \int_{\partial T} (\tilde{u} - v_h) [(\nabla \tilde{u} - \mathbf{p}_h) \cdot \tilde{\mathbf{n}}] ds + (\tilde{u} - v_h, f_h + \operatorname{div} \mathbf{p}_h),$$

where  $\tilde{\mathbf{n}}$  is the unit normal vector on the boundary. To see that the first term on the right-hand side of (3.10) vanishes, we note that it is zero on inner element edges owing to the continuity of  $\mathbf{p}_h \cdot \tilde{\mathbf{n}}$  and  $v_h$ , and it vanishes on  $\partial\Omega$  owing to the boundary condition associated with  $V^h$  and  $W^h$ . The second term on the right-hand side of (3.10) vanishes because of  $f_h + \operatorname{div} \mathbf{p}_h = 0$ . Thus, the cross term is zero.

From the hypercircle equation (3.9), we see that

$$\|\nabla \tilde{u} - \nabla v_h\|_{L_2} \leq \|\nabla v_h - \mathbf{p}_h\|_{L_2} \quad \forall v_h \in V^h, \forall \mathbf{p}_h \in W_{f_h}^h.$$

Since  $\tilde{u}_h = P_h \tilde{u}$ , the error estimate for  $\tilde{u} - \tilde{u}_h$  is given as

$$\|\nabla \tilde{u} - \nabla \tilde{u}_h\|_{L_2} = \min_{v_h \in V^h} \|\nabla \tilde{u} - \nabla v_h\|_{L_2} \leq \min_{v_h \in V^h} \min_{\mathbf{p}_h \in W_{f_h}^h} \|\mathbf{p}_h - \nabla v_h\|_{L_2}.$$

From the definition of  $\kappa_h$ , we obtain the error estimation (3.8).  $\square$

Next, we state the main theorem on computable a priori estimation.

**THEOREM 3.3** (a priori error estimation). *For any  $f \in L_2(\Omega)$ ,  $\int_{\Omega} f dx = 0$  when  $\Gamma_N = \partial\Omega$ , let  $u \in V$  and  $u_h \in V^h$  be the solutions of variational problems (3.2) and (3.3), respectively. Let  $M_h := \sqrt{C_0^2 h^2 + \kappa_h^2}$ , where  $C_0$  is the constant defined in (2.11). Then, we have*

$$(3.11) \quad |u - u_h|_{H^1} \leq M_h \|f\|_{L_2}, \quad \|u - u_h\|_{L_2} \leq M_h^2 \|f\|_{L_2}.$$

*Proof.* We introduce two auxiliary functions  $\tilde{u}$  and  $\tilde{u}_h$ , which are solutions of the following problems, respectively:

$$(3.12) \quad (\nabla \tilde{u}, \nabla v) = (\pi_{0,h} f, v) \quad \forall v \in V; \quad (\nabla \tilde{u}_h, \nabla v_h) = (\pi_{0,h} f, v_h) \quad \forall v_h \in V^h.$$

The minimization principle gives  $|u - u_h|_{H^1} \leq |u - \tilde{u}_h|_{H^1}$ . Decomposing  $u - \tilde{u}_h$  by  $(u - \tilde{u}) + (\tilde{u} - \tilde{u}_h)$ , we have

$$(3.13) \quad |u - u_h|_{H^1} \leq |u - \tilde{u}_h|_{H^1} \leq |u - \tilde{u}|_{H^1} + |\tilde{u} - \tilde{u}_h|_{H^1}.$$

From the definitions of  $u$  and  $\tilde{u}$ , for any  $v \in V$ ,

$$(\nabla(u - \tilde{u}), \nabla v) = (f - \pi_{0,h} f, v) = ((I - \pi_{0,h})f, (I - \pi_{0,h})v),$$

where  $I$  is the identity operator. Taking  $v = u - \tilde{u}$  and applying the error estimation for interpolation  $\pi_{0,h}$ , we get

$$|u - \tilde{u}|_{H^1}^2 \leq \|(I - \pi_{0,h})f\|_{L_2} \|(I - \pi_{0,h})(u - \tilde{u})\|_{L_2} \leq \|(I - \pi_{0,h})f\|_{L_2} C_0 h |u - \tilde{u}|_{H^1}.$$

Hence,

$$(3.14) \quad |u - \tilde{u}|_{H^1} \leq C_0 h \|(I - \pi_{0,h})f\|_{L_2}.$$

When  $\Gamma_N = \partial\Omega$ ,  $\int_{\Omega} \pi_{0,h} f dx = \int_{\Omega} f dx = 0$ ; thus, the a priori estimate in (3.8) still holds for  $f_h = \pi_{0,h} f$ . Substituting (3.8) and (3.14) into (3.13), we have

$$|u - u_h|_{H^1} \leq C_0 h \|(I - \pi_{0,h})f\|_{L_2} + \kappa_h \|\pi_{0,h} f\|_{L_2} \leq \sqrt{C_0^2 h^2 + \kappa_h^2} \|f\|_{L_2}.$$

The estimate for  $\|u - u_h\|_{L_2}$  can be obtained using the Aubin–Nitsche method.

*Remark 3.1.* The concept of introducing an auxiliary problem in (3.12) is inspired by the approach of Kikuchi and Saito et al. [17], who discussed a posteriori error estimation based on the Prager–Synge theorem.

*Remark 3.2.* The a priori estimation considered here is limited to the case that  $f \in L_2(\Omega)$ . For the function  $f \in H^1(\Omega)$ , for example, the right-hand side used for eigenvalue problem (2.2), smaller error constants, and a higher convergence order are expected; however, this is not discussed here.

*Remark 3.3.* We present a concise discussion on the convergence order of  $\kappa_h$  and  $M_h$  in terms of the mesh size  $h$ . For each  $f_h \in X^h$ , let  $\tilde{u}$  be the exact solution of Poisson’s equation (3.1) with  $f = f_h$ . Define  $\mathbf{p}_h \in W_{f_h}^h$  by the one minimizing  $\|\nabla \tilde{u} - \mathbf{p}_h\|_{L_2}$  and  $u_h := P_h \tilde{u}$ . From the hypercircle equation (3.9), we have

$$(3.15) \quad \kappa_h^2 = \max_{\|f_h\|_{L_2}=1} \|\nabla \tilde{u} - \mathbf{p}_h\|^2 + \|\nabla \tilde{u} - \nabla u_h\|^2.$$

For a regular mesh, i.e., when the minimum inner angles of triangle elements are not very small, the classical error estimation for  $u_h$  and  $\mathbf{p}_h$  reads (see, e.g., [37, 32])

$$(3.16) \quad \|\nabla \tilde{u} - \mathbf{p}_h\|_{L_2} \leq Ch^\gamma \|f_h\|_{L_2}, \quad \|\nabla \tilde{u} - \nabla u_h\|_{L_2} \leq Ch^\gamma \|f_h\|_{L_2},$$

where  $C$  is a bounded constant independent of  $f_h$ ;  $\gamma$  is the convergence order. In the case of a regular problem, that is,  $|\tilde{u}|_{H^2} \leq C' \|f_h\|_{L_2}$  for a certain constant  $C'$ , we have  $\gamma = 1$ . Otherwise, the convergence order  $\gamma$  will be less than one. As a consequence of (3.15) and (3.16),  $\kappa_h$  converges to zero with the same order  $\gamma$ . Since  $M_h = \sqrt{\kappa_h^2 + (C_0 h)^2}$ , the quantity  $M_h$  has the same convergence order as  $\kappa_h$ . In section 5, we will verify the convergence order numerically.

We also point out that the convergence order of  $M_h$  cannot be greater than 1, even if a high-order degree FEM space is adopted. This is because for general  $f \in L_2(\Omega)$ , the solution of Poisson's equation cannot be expected to be as smooth as  $H^2$ -regularity. Thus, the convergence order  $\gamma$  in (3.15) and (3.16) is at most 1 (see, e.g., Theorems 3.2.2 and 3.2.5 of [9]).

*Remark 3.4.* In [43], Yamamoto and Nakao developed another type of computable a priori error estimate for an L-shaped domain. The vector space  $\hat{V}_h \times \hat{V}_h$ ,  $\hat{V}_h$  being the piecewise continuous linear FEM space without the boundary constraint, is used to approximate  $\nabla u$ ; the extension of the domain from the nonconvex  $\Omega$  to a bigger convex one  $\Omega_*$  ( $\Omega \subset \Omega_*$ ) is also necessary. The evaluation of various constants is too complex to handle in a domain of general shape. In section 5, numerical comparisons show that our estimation in Theorem 3.3 gives a much better result.

**3.3. Computation of  $\kappa_h$  by solving matrix eigenvalue problem.** The quantity  $\kappa_h$  is evaluated in two steps. First, for fixed  $f_h$ , we deduce explicit forms of  $u_h \in V^h$  and  $\mathbf{p}_h \in W_{f_h}$  that optimize  $\|\mathbf{p}_h - \nabla u_h\|_{L_2}$ . Second, we find  $f_h$  that maximizes the value of  $\|\mathbf{p}_h - \nabla u_h\|_{L_2} / \|f_h\|_{L_2}$  by solving an eigenvalue problem.

For fixed  $f_h \in X^h$ , we consider the optimization problem

$$(3.17) \quad \min_{v_h \in V^h} \min_{\mathbf{p}_h \in W_{f_h}} \|\mathbf{p}_h - \nabla u_h\|_{L_2}^2.$$

From the hypercircle equation (3.9), the problem above is equivalent to

$$\min_{v_h \in V^h} \min_{\mathbf{p}_h \in W_{f_h}} \|\nabla \tilde{u} - \nabla v_h\|_{L_2}^2 + \|\nabla \tilde{u} - \mathbf{p}_h\|_{L_2}^2,$$

where  $\tilde{u}$  is the exact solution corresponding to  $f_h$ . Since  $v_h$  and  $\mathbf{p}_h$  can be taken independently, the value of (3.17) can be obtained by optimizing the following two parts separately:

$$(3.18) \quad \min_{v_h \in V^h} \|\nabla \tilde{u} - \nabla v_h\|_{L_2}, \quad \min_{\mathbf{p}_h \in W_{f_h}} \|\nabla \tilde{u} - \mathbf{p}_h\|_{L_2}.$$

The theory on the conforming FEM and the Raviart–Thomas FEM [7] states that the minimizers of (3.18) are given by the solutions of the following two problems:

(a) Find  $\mathbf{p}_h \in W^h$  and  $\rho_h \in X^h$  such that

$$\begin{cases} (\mathbf{p}_h, \tilde{\mathbf{p}}_h) + (\rho_h, \operatorname{div} \tilde{\mathbf{p}}_h) = 0 & \forall \tilde{\mathbf{p}}_h \in W^h, \\ (\operatorname{div} \mathbf{p}_h, \tilde{q}_h) + (f_h, \tilde{q}_h) = 0 & \forall \tilde{q}_h \in X^h. \end{cases}$$

(b) Find  $u_h \in V^h$  such that

$$(\nabla u_h, \nabla v_h) = (f_h, v_h) \quad \forall v_h \in V^h.$$

Let  $R_h : X^h \rightarrow X^h$ ,  $S_h : X^h \rightarrow W^h$ , and  $T_h : X^h \rightarrow V^h$  denote the solution operators coming from (a) and (b), i.e.,  $R_h f_h = \rho_h$ ,  $S_h f_h = \mathbf{p}_h$ , and  $T_h f_h = u_h$ , where  $\{\mathbf{p}_h, \rho_h\}$  and  $u_h$  solve equations (a) and (b), respectively. We observe that the operators  $T_h$  and  $R_h$  are symmetric: for any  $f_h, g_h \in X_h$ ,

$$\begin{aligned} (T_h f_h, g_h) &= (\nabla T_h f_h, \nabla T_h g_h) = (f_h, T_h g_h), \\ (R_h f_h, g_h) &= -(R_h f_h, \operatorname{div} S_h g_h) = (S_h f_h, S_h g_h). \end{aligned}$$

Since  $(\nabla T_h f_h, S_h g_h) = -(T_h f_h, \operatorname{div} S_h g_h) = (T_h f_h, g_h)$ , we have

$$\begin{aligned} &(\nabla T_h f_h - S_h f_h, \nabla T_h g_h - S_h g_h) \\ &= (\nabla T_h f_h, \nabla T_h g_h) - (S_h f_h, \nabla T_h g_h) - (\nabla T_h f_h, S_h g_h) + (S_h f_h, S_h g_h) \\ &= (T_h f_h, g_h) - 2(T_h f_h, g_h) - (R_h f_h, \operatorname{div} S_h g_h) \\ (3.19) \quad &= -(T_h f_h, g_h) + (R_h f_h, g_h) = -(f_h, T_h g_h) + (f_h, R_h g_h). \end{aligned}$$

Thus, the error  $\|\nabla u_h - \mathbf{p}_h\|_{L_2}$  becomes

$$(3.20) \quad \|\nabla u_h - \mathbf{p}_h\|_{L_2}^2 = -(f_h, T_h f_h) + (f_h, R_h f_h).$$

Let the basis functions of the FEM spaces be

$$W^h = \operatorname{span}\{\psi_i\}_{i=1}^p, \quad V^h = \operatorname{span}\{\phi_i\}_{i=1}^n, \quad X^h = \operatorname{span}\{q_i\}_{i=1}^m.$$

Define matrices  $P_{p \times p}, G_{n \times p}, S_{n \times n}, B_{n \times m}, M_{m \times m}, N_{m \times p}$  with their elements as

$$\begin{aligned} P_{i,j} &= (\psi_i, \psi_j), & S_{i,j} &= (\nabla \phi_i, \nabla \phi_j), \\ B_{i,j} &= (\phi_i, q_j), & M_{i,j} &= (q_i, q_j), & N_{i,j} &= (q_i, \operatorname{div} \psi_j). \end{aligned}$$

Let us represent the function  $f_h \in X^h$  by a column vector  $f \in \mathbb{R}^m$ , that is,  $f_h = (q_1, \dots, q_m) \cdot f$ . With such a notation, problems (a) and (b) become

$$(3.21) \quad \begin{cases} Px + N^T z = 0, \\ Nx + Mf = 0, \end{cases} \quad Sy = Bf.$$

Define a matrix  $A$  by

$$A := \begin{pmatrix} P & N^T \\ N & 0 \end{pmatrix}.$$

Thus, the solution of (a) can be expressed by

$$z = -A^{-1}(p + 1 : p + m, p + 1 : p + m)Mf = -HMf,$$

where  $H := A^{-1}(p + 1 : p + m, p + 1 : p + m)$  denotes the last  $m$  rows and last  $m$  columns of  $A^{-1}$ . The solutions of (a) and (b) are summarized as follows:

$$z = -HMf, \quad y = S^{-1}Bf.$$

From (3.20), we have

$$\|\nabla u_h - \mathbf{p}_h\|_{L_2}^2 = -f^T B^T S^{-1} B f - f^T M^T H M f.$$

Let  $Q := -B^T S^{-1} B - M^T H M$ . Thus, the evaluation of  $\kappa_h$  becomes

$$\kappa_h = \max_{f_h \in X^h} \frac{\|\nabla u_h - \mathbf{p}_h\|_{L_2}}{\|f_h\|_{L_2}} = \max_{f \in R^m} \left( \frac{f^T Q f}{f^T M f} \right)^{1/2}.$$

Equation (3.19) implies that  $Q$  is symmetric. Therefore, the quantity  $\kappa_h$  is the square root of the maximum eigenvalue of the eigenvalue problem

$$(3.22) \quad Qf = \lambda Mf.$$

We point out that the above matrix  $M$  is a diagonal matrix, whereas  $Q$  is a full matrix. In practical computation, to obtain the approximate value of  $\kappa_h$ , the explicit forms of  $S^{-1}$ ,  $H$ , and  $Q$  are not required if we adopt the iterative method to solve the matrix eigenvalue problem (3.22): the iteration  $M^{-1}Qf^{(n)} \rightarrow f^{(n+1)}$  for solving (3.22) can be computed by solving problems (a) and (b), and the eigenvalue of the largest magnitude can be easily computed by applying, e.g., Lanczos's method. Thus, the heavy computation of  $Q$  can be avoided. The number of iterations for practical computation is reported in section 5.

However, to obtain a verified upper bound on the eigenvalue (3.22), the currently available method, e.g., [2], involves verifying that  $\hat{\lambda}M - Q$  is positive definite for a proper upper bound  $\hat{\lambda}$ , where the explicit form of full matrix  $Q$  is needed. Thus, verified estimation of  $\kappa_h$  will require considerable computing resources.

*Remark 3.5.* To speed up the solution calculation of (a) and (b), we carry out LDL-decomposition of sparse matrices  $A$  and  $S$  with element reordering, i.e.,  $P_A A P_A^T = L_A D_A L_A^T$ ,  $P_S S P_S^T = L_S D_S L_S^T$ , where  $P_A$  and  $P_S$  are permutation matrices. Such decomposition is performed only one time, and the sparsity of the matrices  $A$  and  $S$  can be effectively conserved. In the computation example for an L-shaped domain, the sparsity of obtained triangle matrices is only around five times that of  $A$  and  $S$ . Thus, the iteration  $f^{(n+1)} = M^{-1}Qf^{(n)}$  is efficiently computed by solving linear equations with the sparse matrices  $P_A$ ,  $L_A$ ,  $D_A$ ,  $P_S$ ,  $L_S$ ,  $D_S$ .

**4. Lower and upper bounds of eigenvalues.** In this section, we will show how to apply the a priori error estimate for the projection  $P_h$  to deduce explicit eigenvalue bounds.

**4.1. Result of Birkhoff et al.** Birkhoff, et al. [4] considered an eigenvalue problem in the form of the Rayleigh quotient  $R(u) := N(u, u)/D(u, u)$ , where  $N(u, v)$  and  $D(u, v)$  are symmetric bilinear forms of  $u, v \in V$  and  $D(u, u) > 0$  for  $u \neq 0$ . Let  $\{\lambda_k, u_k\}_{k=1}^n$  be the first  $n$  stationary values and the critical points of  $R(u)$  on the space  $V$  with increasing order on  $\lambda_k$ . Let  $\tilde{P}$  be any linear approximation scheme defined on  $V$  and  $T_n$  the subspace of  $V$  spanned by  $\{\tilde{P}u_k\}_{k=1, \dots, n}$ . Define  $\mu_k$  by

$$\mu_k := \min_{H_k \subset T_n} \max_{v \in H_k} R(v),$$

where  $H_k$  denotes any  $k$ -dimensional subspace of  $T_n$ . In case that  $N(u, u)$  is nonnegative for any  $u \in V$ , the result in [4] is summarized as follows.

**THEOREM 4.1.** *Let  $e_i = \tilde{P}u_i - u_i$ ,  $i = 1, \dots, k$ . If  $\sum_{i=1}^k D(e_i, e_i) < 1$ , then*

$$(4.1) \quad \lambda_k \leq \mu_k \leq \lambda_k + \left( \sum_{i=1}^k N(e_i, e_i) \right) / \left( 1 - \left( \sum_{i=1}^k D(e_i, e_i) \right)^{1/2} \right)^2.$$

*Remark 4.1.* By selecting the linear map  $\tilde{P}$  in Theorem 4.1 as the spline interpolation operator, Birkhoff et al. [4] gave concrete eigenvalue bounds for the one-dimensional Sturm–Liouville problem. However, their technique cannot be easily applied to a two-dimensional (2D) eigenvalue problem, especially for a domain with a reentrant corner.

We apply the theorem of Birkhoff et al. to the Laplacian eigenvalue problem over the 2D domain, while the operator  $\tilde{P}$  is taken as the projection  $P_h : V \rightarrow V_h$ . Let  $N(u, v) := (\nabla u, \nabla v)$  and  $D(u, v) := (u, v)$ . As the normalized eigenfunction  $u_i$  is also the weak solution of Poisson’s equation (3.2) with  $f = \lambda_i u_i$ , from the error estimate of (3.4), we have

$$|u_i - P_h u_i|_{H^1} \leq M_h \lambda_i \|u_i\|_{L_2} = M_h \lambda_i, \quad \|u_i - P_h u_i\|_{L_2} \leq M_h^2 \lambda_i.$$

Noting that  $\lambda_i \leq \lambda_i^h$ , we obtain an a priori estimate for  $\lambda_k^h$ .

**THEOREM 4.2.** *Let  $\lambda_k$  and  $\lambda_k^h$  be the ones defined in section 2. If the mesh size  $h$  is sufficiently small such that  $\sum_{i=1}^k (\lambda_i^h)^2 < M_h^{-4}$ , a lower bound on  $\lambda_k$  is given by*

$$(4.2) \quad \lambda_k^h - M_h^2 \sum_{i=1}^k (\lambda_i^h)^2 \left/ \left( 1 - M_h^2 \left( \sum_{i=1}^k (\lambda_i^h)^2 \right)^{1/2} \right)^2 \right. \leq \lambda_k.$$

**4.2. Our proposal.** The bounds based on Theorems 4.1 and 4.2 are not very sharp, as is shown by the computational example in section 5. An improved theoretical result has been reported by, e.g., Strang and Fix [37] (see also Raviart and Thomas [33] and Larsson and Thomée [20]):

$$(4.3) \quad \lambda_k^h \leq \lambda_k (1 + C \sup_{v \in E_k, \|v\|_{L_2}=1} |v - P_h v|_{H^1}^2),$$

where  $E_k$  is the space spanned by the eigenfunctions  $\{u_i\}_{i=1}^k$ . The qualitative estimation of (4.3) enables us to deduce concrete eigenvalue bounds. By adopting the explicit a priori estimation for projection  $P_h$  and dropping one overestimation in the classical proof for (4.3) (see Remark 4.3), the result is further improved.

**THEOREM 4.3** (explicit eigenvalue bounds). *Assume that  $\lambda_k M_h^2 < 1$  for  $k \leq \dim(V^h)$ . Then, a lower bound for  $\lambda_k$  can be given by*

$$(4.4) \quad \lambda_k \geq \lambda_k^h / (1 + M_h^2 \lambda_k^h).$$

*Remark 4.2.* In practical computation, the mesh size of the triangulation is chosen to be sufficiently small such that  $\lambda_k^h M_h^2 < 1$ . Thus, as  $\lambda_k \leq \lambda_k^h$ , the assumption  $\lambda_k M_h^2 < 1$  in this theorem will hold.

*Proof.* Let  $E_k$  be the space spanned by the orthonormal eigenfunctions  $\{u_i\}_{i=1}^k$ . For any  $v = \sum_{i=1}^k c_i u_i \in E_k$ ,  $\|v\|_{L_2} = 1$ , we have

$$(\nabla v, \nabla w) = \left( \sum_{i=1}^k \lambda_i c_i u_i, w \right) \quad \forall w \in V,$$

which means that  $v$  solves the weak formulation of Poisson’s equation with data  $f = \sum_{i=1}^k \lambda_i c_i u_i$ . For such  $f$ , it is easy to see that  $\|f\|_{L_2} \leq \lambda_k$ . Therefore,

$$(4.5) \quad |P_h v - v|_{H^1} \leq M_h \|f\|_{L_2} \leq M_h \lambda_k, \quad \|P_h v - v\|_{L_2} \leq M_h^2 \lambda_k.$$

From the assumption  $\lambda_k M_h^2 < 1$ , we have

$$\|P_h v\|_{L_2} \geq 1 - \|v - P_h v\|_{L_2} \geq 1 - M_h^2 \lambda_k > 0.$$

As  $E_k$  is a  $k$ -dimensional space,  $P_h E_k$  is also a  $k$ -dimensional space.

Now, from the min-max principle,

$$\begin{aligned} \lambda_k^h &\leq \max_{v_h \in P_h E_k} \frac{|v_h|_{H^1}^2}{\|v_h\|_{L_2}^2} = \max_{v \in E_k} \frac{|P_h v|_{H^1}^2}{\|P_h v\|_{L_2}^2} \\ (4.6) \quad &= \max_{v \in E_k} \frac{|v|_{H^1}^2 - |v - P_h v|_{H^1}^2}{\|v\|_{L_2}^2 + 2(v, P_h v - v) + \|P_h v - v\|_{L_2}^2}. \end{aligned}$$

Since  $\|v - P_h v\|_{L_2} \leq M_h |v - P_h v|_{H^1}$  and  $|v|_{H^1}^2 / \|v\|_{L_2}^2 \leq \lambda_k$  for  $v \in E_k (\subset V)$ ,

$$\begin{aligned} \lambda_k^h &\leq \max_{v \in E_k, \|v\|=1} \frac{\lambda_k - |v - P_h v|_{H^1}^2}{1 - 2\|P_h v - v\|_{L_2} + \|P_h v - v\|_{L_2}^2} \\ &\leq \max_{v \in E_k, \|v\|=1} \frac{\lambda_k - |v - P_h v|_{H^1}^2}{(1 - M_h |P_h v - v|_{H^1})^2}. \end{aligned}$$

Let  $g(t) := (\lambda_k - t^2)/(1 - M_h t)^2$ . It is easy to verify that  $g(t)$  is monotonically increasing if  $t$  satisfies  $t \leq M_h \lambda_k$  and  $t < 1/M_h$ . From (4.5) and the assumption  $\lambda_k M_h^2 < 1$ , we have  $|P_h v - v|_{H^1} \leq M_h \lambda_k < 1/M_h$ . Hence,

$$(4.7) \quad \lambda_k^h \leq \max_{v \in E_k, \|v\|=1} g(|P_h v - v|_{H^1}) \leq \max_{v \in E_k, \|v\|=1} g(M_h \lambda_k) = \lambda_k / (1 - M_h^2 \lambda_k).$$

Now, it is trivial to deduce the conclusion in (4.4).  $\square$

*Remark 4.3.* In [37, 33, 20], the classical method estimates the term  $|P_h v|_{H^1}$  in (4.6) by  $|P_h v|_{H^1} \leq |v|_{H^1}$ . Because of the missing term  $|v - P_h v|_{H^1}$ , the final estimation will be  $\lambda_k^h \leq \lambda_k / (1 - M_h^2 \lambda_k)^2$ , which is slightly rougher than (4.7).

*Remark 4.4.* To obtain sharper eigenvalue bounds, it is natural to consider mesh refinement, which, however, will lead to large-scale matrices. The Lehmann–Goerisch method is a useful approach for obtaining greatly sharpened bounds. Suppose that an a priori estimation for a certain eigenvalue  $\lambda_N$  is available, that is,  $\lambda_N < \nu \leq \lambda_{N+1}$ . Then, the Lehmann–Goerisch method can give high-precision bounds for eigenvalues  $\lambda_1, \dots, \lambda_N$ . The homotopy method developed by Plum provides such a priori estimation, which is slightly complex to deal with in a domain of general shape, especially for problems with the Neumann boundary condition. In fact, our proposed method based on FEM robustly enables such a priori estimation. A combination of the Lehmann–Goerisch method and our algorithm will be reported in subsequent papers.

**5. Computation results and applications.** This section demonstrates the efficiency and flexibility of our proposed algorithm by solving several eigenvalue problems over different domains.

**5.1. Preparation.** In previous sections, we developed a framework to provide computable bounds for eigenvalues of the Laplacian as follows:

- (1) Set up the finite element space  $V^h$  over triangulation of domain  $\Omega$ .
- (2) Solve  $A^h x = \lambda^h B^h x$  to get the upper bounds for the eigenvalues.

- (3) Evaluate  $M_h$  and calculate the eigenvalue bounds using Theorem 4.3. If the condition  $\lambda_k^h M_h^2 < 1$  for the desired  $k$  is not satisfied, refine the mesh and compute again.

Interval arithmetic is implemented in the numerical computation, where the rounding error in floating-point computation is estimated. Thus, the desired results can be expected to be mathematically accurate. Note that having a verified result is not as trivial as replacing each floating-point manipulation by interval manipulation. The algorithm for obtaining an approximate numerical result and that for obtaining the desired verified solution may differ significantly.

In our computation, the Boost interval library (<http://www.boost.org>) and the INTLAB toolbox for MATLAB (developed by Rump [34]) are used for interval computation; the method of Behnke [2] is adopted to bound eigenvalues of the generalized matrix eigenvalue problem. All the eigenvalue bounds to be shown in the following examples are obtained through verified computation. Detailed discussions on the techniques for implementing verified computation will be given in subsequent papers.

**Computation time and precision.** The verified evaluation of upper bounds for eigenvalues takes around 1.1 times the computing time required by approximate computation, which is independent from the regularity of the eigenfunctions. The computing time for lower bounds differs greatly upon the regularity of the eigenfunctions. For the problem with  $H^2$ -regularity, the lower bound is up to several constants  $C_0$  and  $C_1$ , which can be evaluated easily. However, for the eigenvalue problem without  $H^2$ -regularity, even the approximate evaluation of  $\kappa_h$  is time-consuming, and the verified evaluation requires much more time. As for the precision of computational results, it is observed that the rounding error accumulation in floating-point computation is usually not significant, especially when compared with the function approximation error. Detailed discussions on precision and computation time are provided in the appendix.

**5.2. Triangle domain.** We consider the eigenvalue problem over a unit isosceles right triangle. By  $\{\lambda_{D,i}, u_{D,i}\}$  and  $\{\lambda_{N,i}, u_{N,i}\}$ , we denote the Laplacian eigenpairs in the cases of homogeneous Dirichlet and Neumann boundaries, respectively. By applying the reflection technique to extend the triangle domain to a unit square (see, for instance, [15]), the explicit eigenpairs are easily obtained:

$$\begin{aligned} \{\lambda_D = (m^2 + n^2)\pi^2, u_D = \sin m\pi x \sin n\pi y - \sin n\pi x \sin m\pi y\}_{m>n\geq 1}, \\ \{\lambda_N = (m^2 + n^2)\pi^2, u_N = \cos m\pi x \cos n\pi y + \cos n\pi x \cos m\pi y\}_{m\geq n\geq 0}. \end{aligned}$$

As the domain in consideration is convex, we have two candidates for  $M_h$ :  $M_h = C_1 h$  and  $M_h = \sqrt{\kappa_h^2 + C_0^2 h^2}$ . The latter involves complicated computation, and, as we can see in Table 5.1, it does not give a smaller value of  $M_h$ . Thus, we take  $M_h = C_1 h$  for a convex domain. The values listed in Table 5.1 indicate that the convergence order of  $\kappa_h$ , denoted by  $\kappa_h$ -order, is close to 1.

The numerical results for the eigenvalue bounds under the Dirichlet boundary conditions are listed in Table 5.2. Note that both the conditions on  $M_h$  in Theorems 4.2 and 4.3 can be easily satisfied, even with a rough mesh ( $h = 1/8$ ), if only the first five eigenvalues are considered. The relative error for the lower bound  $\lambda_{low}$  and the upper bound  $\lambda_{upper}$  is estimated by  $\text{ReErr} := 2(\lambda_{upper} - \lambda_{low}) / (\lambda_{upper} + \lambda_{low})$ . A comparison between the results of Birkhoff et al. (4.2) and our results (4.4) is given in Figure 5.1, which definitively shows that our method gives a better lower bound for eigenvalues.

TABLE 5.1  
Quantities for bounding eigenvalues (Dirichlet b.d.c.).

$h$	$\kappa_h$	$C_0h$	$\sqrt{\kappa_h^2 + C_0^2h^2}$	$C_1h$	$\kappa_h$ -order
1/4	0.0949	0.0796	0.124	0.108	-
1/8	0.0534	0.0398	0.067	0.054	0.83
1/16	0.0288	0.0199	0.035	0.031	0.89
1/32	0.0150	0.0100	0.018	0.016	0.94

TABLE 5.2  
Bounding eigenvalues on triangle domain by using (4.4) (Dirichlet b.d.c.).

$\lambda_{D,i}$	Exact value	$h = 1/32$			$h = 1/64$		
		Lower	Upper	ReErr	Lower	Upper	ReErr
1	$5\pi^2 \approx 49.348$	48.976	49.553	1.2E-2	49.254	49.400	2.9E-3
2	$10\pi^2 \approx 98.696$	97.331	99.633	2.3E-2	98.352	98.931	5.9E-3
3	$13\pi^2 \approx 128.305$	125.85	129.73	3.0E-2	127.68	128.67	7.6E-3
4	$17\pi^2 \approx 167.783$	163.69	170.32	4.0E-2	166.74	168.42	9.9E-3
5	$20\pi^2 \approx 197.392$	192.37	201.58	4.7E-2	196.12	198.44	1.2E-2

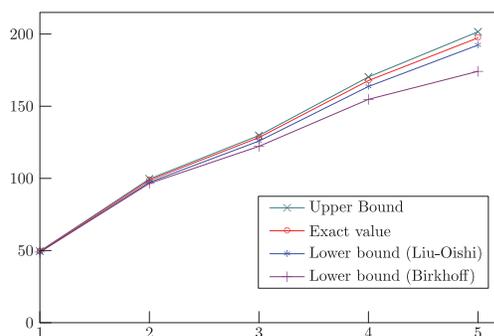


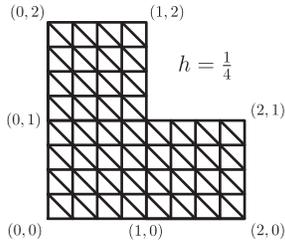
FIG. 5.1. Upper and lower bounds for the leading five eigenvalues ( $h = 1/32$ ).

**5.3. Domain with reentrant corner: L-shaped one.** Let us consider an eigenvalue problem with the homogeneous Dirichlet boundary condition over domain  $\Omega = (0, 2) \times (0, 2) \setminus [1, 2] \times [1, 2]$ . As a model problem, we know that an eigenfunction may have singularities around the reentrant corner. In fact, the first eigenfunction has the leading term of the singularity as  $r^{2/3}$  and the singularity of the second one is  $r^{4/3}$ . However, the third eigenfunction is analytic; the explicit form is  $u_3 = \sin(\pi x) \sin(\pi y)$ . To obtain the optimal convergence rate for the eigenfunction even with lower regularity, we choose a geometrically graded mesh: for the element  $K$  with distance to the singular point being  $r$ , the diameter of  $K$ , denoted by  $h(r)$ , is set to  $h(r) = O(r^{1/3})$  for small  $r$ . The reason for choosing such a mesh is that the interpolation error for the leading singular part  $\psi := r^{2/3}$  of  $u_1$  is around  $|\pi_{1,h}\psi - \psi|_{H^1(K)} \leq C_1(K)h(r)|\psi|_{H^2(K)} = h(r)|K|O(r^{-4/3})$ .

The quantities for error estimation of the projection  $P_h$ , such as,  $\kappa_h$ ,  $C_0h$ , and  $M_h$ , are listed in Tables 5.3 and 5.4: the former is based on a uniform mesh and the

TABLE 5.3

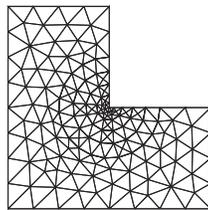
Uniform mesh of L-shaped domain and the quantities in computation.



h	N	$n_{itr}$	$C_0h$	$\kappa_h$	$M_h$	$\gamma(\kappa_h)$
1/4	96	2	0.080	0.147	0.167	-
1/8	384	2	0.040	0.0882	0.0968	0.73
1/16	1536	2	0.020	0.0538	0.0574	0.71
1/32	6144	1	0.010	0.0332	0.0348	0.70

TABLE 5.4

Nonuniform mesh of L-shaped domain and the quantities in computation.



N	$n_{itr}$	$C_0h$	$\kappa_h$	$M_h$	$\gamma(\kappa_h)$
278	7	0.0959	0.0777	0.1234	-
982	8	0.0536	0.0440	0.0694	0.90
3748	14	0.0297	0.0233	0.0377	0.95
14666	12	0.0151	0.0119	0.0192	0.98

latter on a nonuniform one. The Lanczos method is adopted to solve the eigenvalue problem  $Qx = \lambda Mx$  for calculating the value of  $\kappa_h$ . In the case that the number of Lanczos vectors is 15, the iteration numbers, denoted by  $n_{itr}$ , are listed in Tables 5.3 and 5.4.

Let us examine the convergence rate over the mesh with adaptivity. By  $\gamma(\kappa_h)$ , we denote the convergence order of  $\kappa_h$  with respect to the square root of the number of elements. As is implied in Table 5.4, the graded mesh recovers the optimal convergence order of  $\kappa_h$ . However, since the quantity  $M_h$  involves the global mesh parameter  $h$ , the precision of the lower bound of eigenvalues cannot be improved significantly, as compared with the result using a uniform mesh.

The eigenvalue problem over an L-shaped domain has been well investigated by many researchers, e.g., Fox, Henrici, and Moler [11] and Yuan and He [45]. In Table 5.5, we list the first six approximate eigenvalues given by [11] and the lower and upper bounds given by our proposed method using a uniform mesh. It is important to note that our method also gives the eigenvalue indexes strictly, whereas most classical methods, e.g., [11], can only guarantee the existence of eigenvalues in a narrow interval.

We also compare our estimation of  $M_h$  with the result of Yamamoto and Nakao [43]. For a uniform mesh with mesh size  $h = 0.05$ , they showed that  $M_h \leq 0.082$ , which is around two times the estimation by our method,  $M_h \leq 0.041$ .

Yuan and He [45] adopted the Lehmann–Goerisch method to produce high-precision eigenvalue bounds for an L-shaped domain, for example,  $9.6397238404 \leq \lambda_1 \leq 9.6397238444$ . However, the a priori estimation  $\lambda_{11} < \nu = 71 < \lambda_{12}$  used in [45] is based on the eigenvalue bound from [36], which is not a verified result and is available only for special domains of symmetry. This implies that the combination of the Lehmann–Goerisch method and our algorithm can give high-precision eigenvalue bounds, even for a domain of general shape.

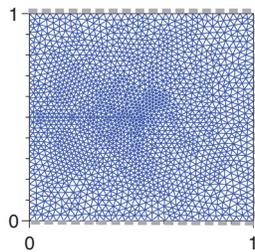
TABLE 5.5

Eigenvalue evaluation for L-shaped domain (uniform mesh with  $h = 1/32$ ). The third eigenpair is known:  $\{\lambda_3 = 2\pi^2, u_3 = \sin \pi x \sin \pi y\}$ .

$\lambda_i$	Lower bound	Approx. [11]	Upper bound	ReErr
1	9.5585	9.63972	9.6699	0.012
2	14.950	15.1973	15.225	0.018
3	19.326	19.7392	19.787	0.024
4	28.605	29.5215	29.626	0.035
5	30.866	31.9126	32.058	0.038
6	39.687	41.4745	41.680	0.049

TABLE 5.6

Sample nonuniform triangulation (left) and eigenvalue estimation result (right).



$\lambda_i$	Lower	Upper	ReErr
1	12.233	12.343	0.009
2	16.087	16.276	0.012
3	31.392	32.119	0.022
4	51.049	52.998	0.037
5	68.241	71.768	0.050

**5.4. Domain with crack.** Let  $\Omega$  be a unit square domain with a crack  $\{(x, 0.5) | 0 < x < 0.5\}$ . Divide the boundary into two parts:

$$\Gamma_D = \partial\Omega \cap \{(x, y) | y = 1 \text{ or } y = 0 \text{ or } x = 1\}, \quad \Gamma_N = \partial\Omega \setminus \Gamma_D.$$

We solve the eigenvalue problem associated with the mixed boundary condition:

$$-\Delta u = \lambda u \text{ in } \Omega, \quad u = 0 \text{ on } \Gamma_D, \quad \partial u / \partial n = 0 \text{ on } \Gamma_N.$$

Around the center of the domain, the eigenfunctions of the above problem may have the worst singularity as  $r^{1/2}$ . In the computation, we adopted nonuniform triangulation, which has a denser mesh around the central point  $(0.5, 0.5)$ . The graph alongside Table 5.6 shows a sample triangulation. The basic data for the computation results listed in Table 5.6 are

$$\text{Number of elements} = 5312; \quad M_h = 0.027.$$

Some of the eigenfunctions have explicit forms, for example,  $\cos(n - \frac{1}{2})\pi x \sin m\pi y$  ( $n, m \in N^+$ ). Thus, we have the following values as exact eigenvalues:

$$\left\{ \frac{5}{4}\pi^2, \frac{13}{4}\pi^2, \frac{29}{4}\pi^2 \right\} \approx \{12.337, 32.076, 71.555\}.$$

The eigenvalue bounds are listed in Table 5.6. The contour lines of eigenfunctions corresponding to the least four eigenvalues are plotted in Figure 5.2.

**5.5. Applications.** We show applications of verified eigenvalue evaluation in estimating the error constants that appear in numerical analysis.

- (i) According to the Poincaré inequality in the embedding theorem of Sobolev spaces, for a bounded domain  $\Omega$ , there exists a constant  $C'$  such that

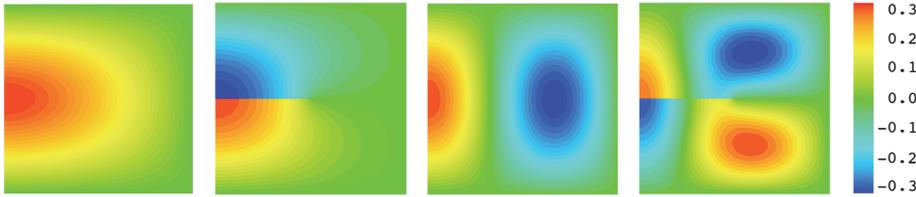


FIG. 5.2. Contour lines of eigenfunctions corresponding to the leading four eigenvalues.

$$\|u\|_{L_2} \leq C'|u|_{H^1(\Omega)} \text{ for any } u \in H^1(\Omega) \text{ and } u = 0 \text{ on } \partial\Omega .$$

- (ii) The average interpolation  $\pi_0 u$  for  $u \in H^1(\Omega)$  is defined by  $\pi_0 u := \int_{\Omega} u dx / \int_{\Omega} dx$ , which has an error estimate

$$\|u - \pi_0 u\|_{L_2} \leq C''|u|_{H^1(\Omega)} .$$

The evaluation of the constants  $C'$  and  $C''$  leads to solving the eigenvalue problem of the Laplacian associated with the Dirichlet boundary condition and the Neumann boundary condition, respectively. Our computation result implies that for  $\Omega$  being a unit isosceles right triangle,

$$C' \leq 1/\sqrt{49.254} \leq 0.1425, \quad C'' \leq 1/\sqrt{9.8542} \leq 0.3186 .$$

Denote by  $|\Omega|$  and  $\text{Diam}(\Omega)$  the area and diameter of the triangle, respectively. According to the theoretical analysis, for the current domain  $\Omega$  (see, e.g., [22, 21]),

$$C' \leq |\Omega|^{1/2} \sqrt{2}/4 = 0.25, \quad C'' \leq \text{Diam}(\Omega)/3.8317 \approx 0.3691 .$$

Thus, our proposed method gives better estimates than the theoretical method.

**6. Conclusion and further work.** For classical eigenvalue problems of the Laplacian over the 2D domain, we proposed a novel and robust method to give accurate lower and upper bounds for the eigenvalues. This method can deal with both convex and nonconvex domains. Thus, it can solve a wide variety of eigenvalue problems. The method developed in this paper can also be extended to a general self-adjoint elliptic operator,  $L := -\text{div}A(x)\nabla u + c(x)u$ , for which new a hypercircle such as (3.9) is required; in such a case, the cross term will not vanish as in the case of (3.10), owing to the discontinuity along the element interface and the nonzero residue error  $-\text{div}A(x)p_h + c(x)u_h - f_h$ . Thus, we need to pay efforts to estimating these terms while being careful not to use the second derivative information of solution  $u$ . The eigenvalue problem with a nonhomogeneous boundary is also of great interest, especially when we consider the estimation of various interpolation constants in numerical analysis; see, e.g., [24].

**Appendix A. Approximate computation versus verified computation.**

Here, by examining the eigenvalue bounds obtained through (4.3) on an L-shaped domain, we give a comparison of the two computation modes: approximate computation and verified computation. As it is time-consuming to execute loops in MATLAB, we build sparse matrices by using the Boost interval C++ library, and then we load them into MATLAB. The matrix eigenvalue problem is solved using the INTLAB toolbox for MATLAB.

First, we discuss the computation time. Denote by  $t_{matrix}$ ,  $t_{upper}$ , and  $t_{low}$  the time required for matrix initialization, lower bound estimation, and upper bound

TABLE A.1

Computation time for calculating eigenvalue bounds (unit: second). The dash implies that the computation failed because of large memory requirements.

$h$ (#element)	Approx.			Verified		
	$t_{matrix}$	$t_{upper}$	$t_{low}$	$t_{matrix}$	$t_{upper}$	$t_{low}$
1/8 (384)	0.071	0.018	0.026	0.17	0.019	2.21
1/16 (1536)	0.29	0.028	0.082	0.57	0.030	129.1
1/32 (6144)	1.42	0.08	0.41	2.7	0.082	10997.7
1/64 (24576)	8.90	0.51	4.22	13.5	0.53	-
1/128 (98304)	74.1	2.93	23.3	112.3	3.1	-

TABLE A.2

Computation precision comparison of the two computation modes.

Error estimation	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$
$\lambda_{upper} - \lambda_{low}$	8.4E-1	3.0E-1	1.1E-1	4.2E-2
$\lambda_{upper}^v - \lambda_{upper}$	3.7E-14	7.6E-14	1.7E-13	1.1E-12
$\lambda_{low} - \lambda_{low}^v$	9.4E-12	9.5E-11	4.5E-10	-

estimation, respectively. The results are listed in Table A.1. Owing to the extra computation, e.g., rounding mode switch, in interval arithmetic, the verified computation of matrices usually takes longer than approximate computation with the fixed rounding mode. However, in many cases, the verified result is obtained via a posteriori error estimation of the approximate solution, and it may not be very time-consuming. To obtain verified eigenvalues bounds, it suffices to perform interval computation of the Rayleigh quotient with approximated eigenvectors. As we can see, it takes only around 10% longer to obtain the exact upper bound, as compared to the approximate bound. However, to obtain the lower eigenvalue bound, the algorithm for approximate computation and that for verified computation differ significantly: the former does not need the explicit form of the full matrix  $Q$ , whereas the latter does. For a triangulation with the mesh size  $h = 1/128$ , around 80 GB of memory is required to store the matrix  $Q$ .

Next, we discuss the computation precision in eigenvalue bound estimation. As approximate computation with fixed rounding-to-nearest mode will often give satisfactory approximation of the desired exact value, we measure the difference between the approximate and verified results and take it as the rounding error.

Let  $\lambda_{upper}$  and  $\lambda_{low}$  be the upper and lower bounds for the first eigenvalue, which are numerically evaluated using (2.4) and (4.4), respectively. Denote by  $\lambda_{upper}^v$  and  $\lambda_{low}^v$  the verified computation results of  $\lambda_{upper}$  and  $\lambda_{low}$ , respectively. Thus, the rounding error can be measured by two terms:  $\lambda_{low} - \lambda_{low}^v$  and  $\lambda_{upper}^v - \lambda_{upper}$ . The value  $\lambda_{upper} - \lambda_{low}$  can be regarded as the function approximation error, which is dependent on mesh size.

The results in Table A.2 indicate that the rounding error for eigenvalue bounds accumulates as the amount of calculation increases; however, compared with the function approximation error, the rounding error is not very significant.

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