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Computable Error Estimates for Ground State Solution of Bose–Einstein Condensates

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Abstract
In this paper, we propose a computable error estimate of the Gross–Pitaevskii equation for the ground state solution of the Bose–Einstein condensate by the general conforming finite element method on general meshes. Based on this error estimate, the asymptotically lower and upper bound for the smallest eigenvalue and ground state energy can be calculated. Several numerical examples are presented to validate the theoretical results in this paper.

Keywords Bose–Einstein condensate · Gross–Pitaevskii equation · Finite element method · Computable error estimates · Lower bound

Mathematics Subject Classification 65N30 · 65N25 · 65L15

1 Introduction

Bose–Einstein condensation (BEC) predicted by A. Einstein is a new state of matter at the beginning of the last century. When a dilute gas of trapped bosons (of the same species) is cooled down to ultra-low temperatures (close to absolute zero), BEC could be formed [6,18]. Since 1995, the first experimental achievement of BEC in dilute ^{87}Rb gases [6], which is one of the most important scientific discoveries in the last century, a nonlinear Schrödinger equation known as the Gross–Pitaevskii equation (GPE) [21,30] has been used extensively to describe the single particle properties of BEC. It has been found that the results obtained

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by solving the GPE are in excellent agreement with most of the experiments (cf. [5,17,19]). A lot of numerical methods for the computation of the time-independent GPE for the ground state and the time-dependent GPE for finding the dynamics of the BEC has been developed, please refer to [2,9,10,23,36,37] and references cited therein.

In this paper, we focus on ground state of BEC, which can be obtained by minimizing the following energy functional (cf. [24])

$$E(\phi) = \int_\Omega \left(|\nabla \phi|^2 + W|\phi|^2 + \frac{\zeta}{2}|\phi|^4 \right) \mathrm{d}\Omega \tag{1.1}$$

with respect to wavefunctions ϕ under the following constraint

$$\int_\Omega |\phi|^2 \mathrm{d}\Omega = 1,$$

where $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ denotes the computing domain which has the cone property [1], $\zeta > 0$ is a constant, $\inf_{|x|>r} W(x) \to \infty$ as $r \to \infty$ and $W(x) \in L^\infty(\Omega)$. From [13], (1.1) has exactly two minimizers u and $-u$. We denote by λ the corresponding Lagrange multiplier. The Euler–Lagrange equation corresponding to this minimization problem is the so-called GPE: Find $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ such that

$$\begin{cases} -\Delta u + Wu + \zeta |u|^2 u = \lambda u, & \text{in } \Omega. \\ \int_\Omega |u|^2 d\Omega = 1. \end{cases} \tag{1.2}$$

The eigenfunction u is a solution to the nonlinear eigenvalue problem (1.2) corresponding to the smallest eigenvalue λ of (1.2) which is non-degenerate [13]. In this paper, we denote by u the unique positive solution of (1.1) and (1.2), and u is one of the ground state solutions of BEC. We call (λ, u) as the principal eigenpair (i.e. the eigenpair corresponding to the ground state solution u) of (1.2) and the corresponding ground state energy can be given as $E(u)$.

The lower bounds of the principal eigenvalue of (1.2) and the ground state energy (1.1) are very useful since they can give important guidance for the physical experiments and reveal very useful physical information (see e.g., [24]). Owing to using the conforming finite element method, we can obtain the upper bounds of the principal eigenvalue and the ground state energy. Hence, the main aim of this paper is to consider the lower bounds of the principal eigenvalue and the ground state energy.

So far, there have been developed some methods to get lower bound of eigenvalue, primarily including the nonconforming finite element methods (see e.g., [7,25,26,29,40]), interpolation constant based methods (see e.g., [27,28,39]) and computational error estimate methods (see e.g., [15,32,38]) for the linear eigenvalue problem. But there are no results about lower bounds of the semilinear eigenvalue problems. This paper is the first attempt in this direction.

In order to deduce the lower bounds of the principal eigenvalue and the ground state energy, we begin with the computable error estimates for the ground state of GPE by the finite element method. For this aim, we first propose a computable method to obtain an asymptotically upper bound of the error estimate for the ground state eigenfunction approximation by the general conforming finite element methods on general meshes. The approach is based on complementary energy method from [22,31,33,34]. Of course, the computable error estimates can also provide a type of the a posteriori error estimate for the partial differential equations by the finite element method, please refer to [3,4,8,11,35] and references cited therein. In addition, [14] is based on planewaves and combines the adaptive procedure directly into an iterative algorithm for the ground state of the GPE.

An outline of the paper goes as follows. In Sect. 2, we introduce the finite element method for the GPE. An asymptotically upper bound for the error estimate of the principal eigenfunction approximation is given in Sect. 3. In Sect. 4, asymptotically lower bounds of the principal eigenvalue and ground state energy are also obtained based on the results in Sect. 3. Some numerical examples are presented in Sect. 5 to validate the theoretical results in this paper. Some concluding remarks are given in the last section.

2 Finite Element Method for GPE

In this section, we introduce some notation and finite element method for GPE (1.2). We will use standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms $\|\cdot\|_{s,p,\Omega}$ and seminorms $|\cdot|_{s,p,\Omega}$ (see, e.g., [1]). For $p=2$, we denote $H^s(\Omega)=W^{s,2}(\Omega)$ and $H_0^1(\Omega)=\{v\in H^1(\Omega):\ v|_{\partial\Omega}=0\}$, where $v|_{\partial\Omega}=0$ is in the sense of trace, $\|\cdot\|_{s,\Omega}=\|\cdot\|_{s,2,\Omega}$. In this paper, we set $V:=H_0^1(\Omega)$ and use $\|\cdot\|_{s,p}$ to denote $\|\cdot\|_{s,p,\Omega}$ for simplicity.

For the aim of finite element discretization, we define the corresponding variational form for (1.2) as follows: Find $(\lambda,u)\in\mathbb{R}\times V$ such that $b(u,u)=1$ and

$$\hat{a}(u,v)=\lambda b(u,v),\quad \forall v\in V, \tag{2.1}$$

where

$$\hat{a}(u,v):=a(u,v)+\int_\Omega\big((W-1)uv+\zeta|u|^2uv\big)\,\mathrm{d}\Omega,$$
$$a(u,v):=\int_\Omega(\nabla u\nabla v+uv)\,d\Omega,\quad b(u,v)\ :=\ \int_\Omega uv d\Omega.$$

It is obvious that $a(v,v)\ge 0$ for all $v\in V$. Then we define $\|v\|_a=\sqrt{a(v,v)}$ for all $v\in V$ in this paper.

The following Rayleigh quotient expression holds for the principal eigenpair (λ,u)

$$\lambda=\frac{\hat{a}(u,u)}{b(u,u)}. \tag{2.2}$$

Now, let us demonstrate the finite element method [11,16] for the semilinear eigenvalue problem (2.1). First we generate a shape-regular decomposition for the computational domain $\Omega\subset\mathbb{R}^d$ $(d=2,3)$ into triangles or rectangles for $d=2$ (tetrahedrons or hexahedrons for $d=3$) and the diameter of a cell $K\in\mathcal{T}_h$ is denoted by h_K. The mesh diameter h describes the maximum diameter of all cells $K\in\mathcal{T}_h$. Based on the mesh $\mathcal{T}_h$, we construct the conforming finite element space denoted by $V_h\subset V$. The family of finite-dimensional spaces V_h is assumed to satisfy the following assumption:

$$\lim_{h\to 0}\inf_{v_h\in V_h}\|w-v_h\|_a=0,\quad \forall w\in V. \tag{2.3}$$

Define $X_h=\{\phi_h\in V_h:\int_\Omega|\phi_h|^2\mathrm{d}\Omega=1\}$. We shall introduce the following minimization problem

$$u_h=\arg\inf_{\phi_h\in X_h}E(\phi_h). \tag{2.4}$$

The existence of a minimizer of (2.4) can be obtained. However, the uniqueness is unknown [13]. It is easy to know that the minimizer u_h of (2.4) and $(u_h,u)>0$ solves the following eigenvalue problem

$$\hat{a}(u_h,v_h)=\lambda_h b(u_h,v_h),\quad \forall v_h\in V_h, \tag{2.5}$$

with the Lagrange multiplier λ_h. Define the set of finite dimensional ground state eigenpairs

$$\Theta_h = \{(\lambda_h, u_h) \in \mathbb{R} \times X_h : (\lambda_h, u_h) \text{ solves (2.5) and } (u_h, u) > 0\}.$$

Then, the discrete ground state energy of BEC is given by

$$E(u_h) = \int_\Omega \left(|\nabla u_h|^2 + W|u_h|^2 + \frac{\zeta}{2}|u_h|^4 \right) d\Omega, \tag{2.6}$$

where $(\lambda_h, u_h) \in \Theta_h$.

From (2.5), the following Rayleigh quotient for λ_h holds

$$\lambda_h = \frac{\hat{a}(u_h, u_h)}{b(u_h, u_h)}. \tag{2.7}$$

In order to give the error estimates for the finite element method, we define the following notation

$$\delta_h(u) := \inf_{v_h \in V_h} \|u - v_h\|_a. \tag{2.8}$$

Lemma 2.1 [13, Theorem 1] *There exists $h_0 > 0$ such that for all $0 < h < h_0$, the principal eigenpair $(\lambda, u) \in \mathbb{R} \times V$ and its approximation $(\lambda_h, u_h) \in \Theta_h$ satisfy following error estimates*

$$\|u - u_h\|_a \le C_u \delta_h(u), \tag{2.9}$$

$$\|u - u_h\|_0 \le C_u \eta_a(h) \|u - u_h\|_a \le C_u^2 \eta_a(h) \delta_h(u), \tag{2.10}$$

$$\begin{aligned} |\lambda - \lambda_h| &\le C_u \|u - u_h\|_a^2 + C_u \|u - u_h\|_0 \\ &\le C_u^2 (\delta_h(u) + \eta_a(h)) \|u - u_h\|_a, \end{aligned} \tag{2.11}$$

where $\eta_a(h)$ is defined as follows:

$$\eta_a(h) = \sup_{f \in L^2(\Omega), \|f\|_0 = 1} \inf_{v_h \in V_h} \|Tf - v_h\|_a \tag{2.12}$$

with the operator T being defined as follows: Find $Tf \in u^\perp$ such that

$$\langle (E''(u) - \lambda) Tf, v \rangle = (f, v), \quad \forall v \in u^\perp, \tag{2.13}$$

where

$$\langle (E''(u) - \lambda) w, v \rangle = (\nabla w, \nabla v) + ((W - \lambda) \nabla w, \nabla v) + 3(\zeta |u|^2 w, v),$$

and $u^\perp = \left\{ v \in V : | \int_\Omega uv d\Omega = 0 \right\}$. Here and hereafter C_u (with or without subscripts) is some constant depending on the eigenpair (λ, u) but independent of the mesh size h.

Remark 2.1 In Lemma 2.1, the error estimates are a bit more complicated than that of linear elliptic eigenvalue problems. The definition of $\eta_a(h)$ and the operator T come from the error analysis for the semilinear eigenvalue problems in [13]. Since we are concerned with the principal eigenvalue, the operator T is bounded and elliptic. For more information, please refer to [13].

3 Computable Error Estimates

First, we define $H(\text{div};\Omega) := \{\mathbf{p} \in (L^2(\Omega))^d : \text{div}\mathbf{p} \in L^2(\Omega)\}$ $(d = 2, 3)$ and let $\mathbf{W} := H(\text{div};\Omega)$ for simplicity.

Theorem 3.1 *There exists $h_0 > 0$ such that for all $0 < h < h_0$, the principal eigenpair (λ, u) of (2.1) and its approximation $(\lambda_h, u_h) \in \Theta_h$ satisfy the following error estimate:*

$$\|u - u_h\|_a \leq \frac{1}{\theta_1} \min_{\mathbf{p}\in\mathbf{W}} \eta(\lambda_h, u_h, \mathbf{p}), \tag{3.1}$$

where θ_1, $\eta(\lambda_h, u_h, \mathbf{p})$ and α are defined as follows

$$\theta_1 = 1 - \alpha(\delta_h(u) + \eta_a(h)), \tag{3.2}$$

$$\eta(\lambda_h, u_h, \mathbf{p}) = \left(\|\lambda_h u_h - W u_h - \zeta u_h^3 + \text{div}\mathbf{p}\|_0^2 + \|\mathbf{p} - \nabla u_h\|_0^2\right)^{1/2}, \tag{3.3}$$

$$\alpha = \max\left\{C_u^2, C_u(C_u + \|W\|_{0,\infty} + 1 + |\lambda_h|)\right\}. \tag{3.4}$$

Here $\eta_a(h)$ is given by (2.12) and the constant C_u is independent of the mesh size h, vector function $\mathbf{p}$ and the eigenfunction approximation u_h. Furthermore, the following asymptotic property holds

$$\lim_{h\to 0} \theta_1 = 1. \tag{3.5}$$

Proof Let us define $w = u - u_h$ in this proof. Combining (2.1), (2.5) and the following Green's formula

$$\int_\Omega \text{div}\mathbf{p} v \text{d}\Omega + \int_\Omega \mathbf{p}\cdot\nabla v \text{d}\Omega = 0, \quad \forall \mathbf{p} \in \mathbf{W} \text{ and } \forall v \in V,$$

we have

$$\begin{aligned}
a(u - u_h, w) &\leq a(u - u_h, w) + (\zeta(u^3 - u_h^3), w) \\
&= \int_\Omega \lambda u w \text{d}\Omega - \int_\Omega ((W-1)uw)\,\text{d}\Omega \\
&\quad - \int_\Omega (\nabla u_h \cdot \nabla w + u_h w + \zeta u_h^3 w)\text{d}\Omega + \int_\Omega \text{div}\mathbf{p} v \text{d}\Omega + \int_\Omega \mathbf{p}\cdot\nabla v d\Omega \\
&= \underbrace{\int_\Omega \left((\lambda_h u_h - W u_h - \zeta u_h^3 + \text{div}\mathbf{p})w + (\mathbf{p} - \nabla u_h)\cdot\nabla w\right)\text{d}\Omega}_{A_1} \\
&\quad + \underbrace{\int_\Omega ((\lambda u - \lambda_h u_h) - (W-1)(u - u_h))\, w \text{d}\Omega}_{A_2} \\
&=: A_1 + A_2.
\end{aligned} \tag{3.6}$$

For A_1, by using Cauchy–Schwarz inequality, the following inequalities hold

$$\begin{aligned}
A_1 &\leq \|\lambda_h u_h - W u_h - \zeta|u_h|^2 u_h + \text{div}\mathbf{p}\|_0 \|w\|_0 + \|\mathbf{p} - \nabla u_h\|_0 \|\nabla w\|_0 \\
&\leq \left(\|\lambda_h u_h - W u_h - \zeta u_h^3 + \text{div}\mathbf{p}\|_0^2 + \|\mathbf{p} - \nabla u_h\|_0^2\right)^{1/2} \|w\|_a \\
&=: \eta(\lambda_h, u_h, \mathbf{p})\|w\|_a.
\end{aligned} \tag{3.7}$$

The second term A_2 has the following estimate

$$A_2 \le \underbrace{\int_\Omega (\lambda - \lambda_h) u w \mathrm{d}\Omega}_{B_1} + \underbrace{\int_\Omega (\lambda_h - W + 1)(u - u_h) w \mathrm{d}\Omega}_{B_2} =: B_1 + B_2.$$

For B_1, B_2 and $\|u\|_0 = \|u_h\|_0 = 1$, using Lemma 2.1, we have following inequalities

$$B_1 \le |\lambda - \lambda_h| \|u\|_0 \|w\|_a \le C_u^2(\delta_h(u) + \eta_a(h)) \|u - u_h\|_a \|w\|_a, \tag{3.8}$$

$$\begin{aligned} B_2 &\le (\|W\|_{0,\infty} + 1 + |\lambda_h|) \|u - u_h\|_0 \|w\|_a \\ &\le C_u(\|W\|_{0,\infty} + 1 + |\lambda_h|) \eta_a(h) \|u - u_h\|_a \|w\|_a. \end{aligned} \tag{3.9}$$

Summing B_1 and B_2 leads to

$$\begin{aligned} A_2 &\le \left(C_u^2 \delta_h(u) + C_u(C_u + \|W\|_{0,\infty} + 1 + |\lambda_h|)\eta_a(h)\right) \|u - u_h\|_a \|w\|_a \\ &=: \alpha(\delta_h(u) + \eta_a(h)) \|u - u_h\|_a \|w\|_a, \end{aligned} \tag{3.10}$$

where $\alpha = \max\left\{C_u^2, C_u(C_u + \|W\|_{0,\infty} + 1 + |\lambda_h|)\right\}$.

Therefore, from (3.6), (3.7) and (3.10), we can draw the following conclusion

$$\|u - u_h\|_a \le \eta(\lambda_h, u_h, \mathbf{p}) + \alpha(\delta_h(u) + \eta_a(h)) \|u - u_h\|_a, \quad \forall \mathbf{p} \in \mathbf{W}.$$

Then the desired result (3.1) can be obtained by the arbitrariness of $\mathbf{p} \in \mathbf{W}$. The property (3.5) can be deduced from $\lim_{h\to 0} \delta_h(u) = \lim_{h \to 0} \eta_a(h) = 0$ and the proof is complete. □

From (3.1), in order to produce asymptotically upper bound error estimate for the eigenfunction approximation, it is a natural way to find a function $\mathbf{p}^* \in \mathbf{W}$ to satisfy the following optimization problem

$$\eta(\lambda_h, u_h, \mathbf{p}^*) = \min_{\mathbf{p} \in \mathbf{W}} \eta(\lambda_h, u_h, \mathbf{p}). \tag{3.11}$$

Lemma 3.1 [33] *The optimization problem (3.11) is equivalent to the following partial differential equation: Find* $\mathbf{p}^* \in \mathbf{W}$ *such that*

$$a^*(\mathbf{p}^*, \mathbf{q}) = \mathcal{F}^*(\mathbf{q}), \quad \forall \mathbf{q} \in \mathbf{W}, \tag{3.12}$$

where

$$a^*(\mathbf{p}^*, \mathbf{q}) = \int_\Omega \left(\mathrm{div}\mathbf{p}^* \mathrm{div}\mathbf{q} + \mathbf{p}^* \cdot \mathbf{q}\right) \mathrm{d}\Omega,$$

$$\mathcal{F}^*(\mathbf{q}) = -\int_\Omega \left(\lambda_h u_h - \zeta u_h^3 - (W - 1)u_h\right) \mathrm{div}\mathbf{q} \mathrm{d}\Omega.$$

Moreover, $a^*(\cdot, \cdot)$ *defines an inner product for the space* $\mathbf{W}$. *The corresponding norm is* $|||\mathbf{p}|||_*^2 = a^*(\mathbf{p}, \mathbf{p})$, *and the auxiliary problem (3.12) has a unique solution.*

Now, we state some properties of the estimator $\eta(\lambda_h, u_h, \mathbf{p})$.

Lemma 3.2 [33] *Assume* $\mathbf{p}^*$ *be the solution of the (3.12) and let* $\lambda_h \in \mathcal{R}$, $u_h \in V$ *and* $\mathbf{p} \in \mathbf{W}$ *be arbitrary. Then the following equality holds*

$$\eta^2(\lambda_h, u_h, \mathbf{p}) = \eta^2(\lambda_h, u_h, \mathbf{p}^*) + |||\mathbf{p}^* - \mathbf{p}|||_*^2. \tag{3.13}$$

It is easy to state the following upper bound property by combining Theorems 3.1 and (3.13).

Corollary 3.1 *Under the conditions of Theorem 3.1, the following upper bound holds*

$$\|u - u_h\|_a \leq \frac{1}{\theta_1}\eta(\lambda_h, u_h, \mathbf{p}^*). \tag{3.14}$$

4 Asymptotically Lower Bounds of the Principal Eigenvalue and Ground State Energy

In this section, based on the upper bound of the error estimate for the principal eigenfunction approximation in Theorem 3.1, we give an asymptotically lower bounds of the principal eigenvalue and ground state energy. Actually, the process is direct since we have the following Rayleigh quotient expansion.

Lemma 4.1 *Assume $(\lambda, u) \in \mathbb{R} \times V$ is the principal eigenpair of the original problem (2.1), $(\lambda_h, u_h) \in \mathbb{R} \times V_h$ is the eigenpair of the discrete problem (2.5). We have the following expansion:*

$$\begin{aligned}\lambda_h - \lambda = \|u_h - u\|_a^2 - \lambda\|u_h - u\|_0^2 + \int_\Omega (W-1)(u_h - u)^2 \mathrm{d}\Omega \\ + \int_\Omega \zeta(|u|^2u - |u_h|^2u_h - |u_h|^2u - |u|^2u_h)(u_h - u)\mathrm{d}\Omega.\end{aligned} \tag{4.1}$$

Proof From (2.1), (2.2), (2.5), (2.7), and direct calculation, we have

$$\begin{aligned}\lambda_h - \lambda &= \hat{a}(u_h, u_h) - \lambda b(u_h, u_h) \\ &= a(u_h, u_h) + \int_\Omega \big((W-1)u_hu_h + \zeta|u_h|^2u_hu_h\big)\,\mathrm{d}\Omega - \lambda b(u_h, u_h) \\ &= a(u_h - u, u_h - u) + 2a(u, u_h) - a(u, u) \\ &\quad + \int_\Omega \big((W-1)u_hu_h + \zeta|u_h|^2u_hu_h\big)\,\mathrm{d}\Omega - \lambda b(u_h, u_h) \\ &= \|u_h - u\|_a^2 + 2\lambda b(u, u_h) - 2\int_\Omega \big((W-1)uu_h + \zeta|u|^2uu_h\big)\,\mathrm{d}\Omega \\ &\quad - \lambda b(u, u) + \int_\Omega \big((W-1)uu + \zeta|u|^2uu\big)\,\mathrm{d}\Omega \\ &\quad + \int_\Omega \big((W-1)u_hu_h + \zeta|u_h|^2u_hu_h\big)\,\mathrm{d}\Omega - \lambda b(u_h, u_h) \\ &= \|u_h - u\|_a^2 - \lambda\|u_h - u\|_0^2 + \int_\Omega (W-1)(u - u_h)^2\mathrm{d}\Omega \\ &\quad + \int_\Omega \zeta(|u|^2u - |u_h|^2u_h - |u_h|^2u - |u|^2u_h)(u - u_h)\mathrm{d}\Omega.\end{aligned}$$

This is the desired result (4.1) and the proof is complete. □

Theorem 4.1 *Under conditions of Theorem 3.1, we have the following error estimate:*

$$|\lambda_h - \lambda| \leq \frac{C_3\,(\delta_h(u) + \eta_a(h))}{1 - \alpha\,(\delta_h(u) + \eta_a(h))}\eta(\lambda_h, u_h, \mathbf{p}), \quad \forall \mathbf{p} \in \mathbf{W}, \tag{4.2}$$

where

$$C_3 = \max\left\{C_u, C_u^3\left(\|W\|_{0,\infty}+1+|\lambda|\right)\delta_h(u)\eta_a(h) + \zeta C_u C_\Omega^3\left(\|u\|_a^3+\|u_h\|_a^3+\|u_h\|_a^2\|u\|_a+\|u\|_a^2\|u_h\|_a\right)\right\}.$$

Moreover, if h is such small that

$$\frac{C_3\left(\delta_h(u)+\eta_a(h)\right)}{1-\alpha\left(\delta_h(u)+\eta_a(h)\right)} \le 1,$$

the following explicit and asymptotically result holds

$$\lambda_h^L := \lambda_h - \eta(\lambda_h, u_h, \mathbf{p}) \le \lambda, \quad \forall \mathbf{p} \in \mathbf{W}, \tag{4.3}$$

where λ_h^L denotes an asymptotically lower bound of the principal eigenvalue λ.

Proof From (4.1) and $b(u_h, u_h) = 1$, we have following estimates

$$\begin{aligned}
|\lambda_h - \lambda| \le\ & \|u_h - u\|_a^2 + \left(\lambda\|u_h-u\|_0^2 + (\|W\|_{0,\infty}+1)\|u_h-u\|_0^2\right) \\
&+ \int_\Omega |\zeta|(|u|^2|u| + |u_h|^2|u_h| + |u_h|^2|u| + |u|^2|u_h|)|u_h - u|\mathrm{d}\Omega \\
\le\ & \underbrace{\|u_h-u\|_a^2}_{A_1} + \underbrace{(\|W\|_{0,\infty}+1+|\lambda|)\|u_h-u\|_0^2}_{A_2} \\
&+ \underbrace{|\zeta|\int_\Omega |u|^2|u||u_h-u|\mathrm{d}\Omega}_{A_3} + \underbrace{|\zeta|\int_\Omega |u_h|^2|u_h||u_h-u|\mathrm{d}\Omega}_{A_4} \\
&+ \underbrace{|\zeta|\int_\Omega |u_h|^2|u||u_h-u|\mathrm{d}\Omega}_{A_5} + \underbrace{|\zeta|\int_\Omega |u|^2|u_h||u_h-u|\mathrm{d}\Omega}_{A_6} \\
=:\ & \sum_{i=1}^{6} A_i.
\end{aligned}$$

Using Lemma 2.1, the following estimates for A_1 and A_2 hold

$$\begin{aligned}
A_1 &\le C_u\delta_h(u)\|u-u_h\|_a, \\
A_2 &\le (\|W\|_{0,\infty}+1+|\lambda|)C_u^2\eta_a^2(h)\|u-u_h\|_a^2 \\
&\le (\|W\|_{0,\infty}+1+|\lambda|)C_u^3\eta_a^2(h)\delta_h(u)\|u_h-u\|_a.
\end{aligned}$$

From Sobolev imbedding theorem (cf. [1])

$$W^{s,p}(\Omega) \hookrightarrow L^q(\Omega), \text{ for } p \le q \le p^* = dp/(d-sp), \ \Omega \subset \mathbb{R}^d,$$

we have

$$\|v\|_{0,12} \le C_\Omega\|v\|_a, \quad \|v\|_{0,6} \le C_\Omega\|v\|_a, \ \forall v \in V, \ \text{for } d = 2, \tag{4.4}$$

where C_Ω is a constant depending only on Ω.

For A_2, combing Lemma 2.1, (4.4) and the Hölder inequality, we have

$$A_3 \le \zeta\left(\int_\Omega (|u|^2)^3\mathrm{d}\Omega\right)^{1/3}\left(\int_\Omega |u|^6\mathrm{d}\Omega\right)^{1/6}\left(\int_\Omega |u_h-u|^2\mathrm{d}\Omega\right)^{1/2}$$

$$\leq \zeta \|u\|_{0,6}^2 \|u\|_{0,6} \|u-u_h\|_0 \leq \zeta C_u C_\Omega^3 \|u\|_a^3 \eta_a(h) \|u-u_h\|_a.$$

Similarly, A_3, A_4 and A_5 have following estimates

$$A_4 \leq \zeta C_u C_\Omega^3 \|u_h\|_a^3 \ \eta_a(h) \|u-u_h\|_a,$$
$$A_5 \leq \zeta C_u C_\Omega^3 \|u_h\|_a^2 \|u\|_a(h) \eta_a(h) \|u-u_h\|_a,$$

and

$$A_6 \leq \zeta C_u C_\Omega^3 \|u\|_a^2 \|u_h\|_a \ \eta_a(h) \|u-u_h\|_a.$$

Combining (3.1) and the above estimates, we have

$$\begin{aligned} |\lambda_h - \lambda| &\leq \left(C_u + (\|W\|_{0,\infty} + 1 + |\lambda|) C_u^3 \eta_a^2(h)\right) \delta_h(u) \|u_h - u\|_a \\ &\quad + \left(\zeta C_u C_\Omega^3 \left(\|u\|_a^3 + \|u_h\|_a^3 + \|u_h\|_a^2 \|u\|_a + \|u\|_a^2 \|u_h\|_a\right) \eta_a(h) \|u-u_h\|_a \\ &\leq C_3 \left(\delta_h(u) + \eta_a(h)\right) \|u-u_h\|_a \\ &\leq \frac{C_3(\delta_h(u) + \eta_a(h))}{1-\alpha(\delta_h(u)+\eta_a(h))} \eta(\lambda_h, u_h, \mathbf{p}), \quad \forall \mathbf{p} \in \mathbf{W}, \end{aligned}$$

where

$$\begin{aligned} C_3 = \max \Big\{ C_u + \left(\|W\|_{0,\infty} + 1 + |\lambda|\right) C_u^3 \eta_a^2(h), \zeta C_u C_\Omega^3 \Big(\|u\|_a^3 \\ + \ \|u_h\|_a^3 + \|u_h\|_a^2 \|u\|_a + \|u\|_a^2 \|u_h\|_a \Big\}. \end{aligned}$$

This is the desired result (4.2) and (4.3) follows immediately. □

Corollary 4.1 *Under the conditions of Theorem 3.1, we have the following error estimate:*

$$E(u_h) - E(u) \leq \frac{C_4(\delta_h(u) + \eta_a(h))}{1-\alpha(\delta_h(u)+\eta_a(h))} \eta(\lambda_h, u_h, \mathbf{p}), \quad \forall \mathbf{p} \in \mathbf{W}, \tag{4.5}$$

where

$$C_4 = C_3 + \frac{\zeta}{2} C_u C_\Omega^3 (\|u\|_a + \|u_h\|_a)^3.$$

Moreover, if h is such small that

$$\frac{C_4(\delta_h(u) + \eta_a(h))}{1-\alpha(\delta_h(u)+\eta_a(h))} \leq 1,$$

the following explicit and asymptotic result holds

$$E_h^L := E(u_h) - \eta(\lambda_h, u_h, \mathbf{p}) \leq E, \quad \forall \mathbf{p} \in \mathbf{W}, \tag{4.6}$$

where E_h^L denotes an asymptotically lower bound of the ground state energy E.

Proof From the definition of ground state energy, we have

$$E(u) = \lambda - \int_\Omega \frac{\zeta}{2} |u|^4 \mathrm{d}\Omega, \quad E(u_h) = \lambda_h - \int_\Omega \frac{\zeta}{2} |u_h|^4 \mathrm{d}\Omega.$$

Then, we have the following formulas

$$E(u_h) - E(u) = \underbrace{(\lambda_h - \lambda)}_{A_1} + \underbrace{\int_\Omega \frac{\zeta}{2}(|u|^4 - |u_h|^4) \mathrm{d}\Omega}_{A_2} =: A_1 + A_2. \tag{4.7}$$

Using (4.2), the following inequality holds

$$A_1 \le \frac{C_3\,(\delta_h(u)+\eta_a(h))}{1-\alpha\,(\delta_h(u)+\eta_a(h))}\eta(\lambda_h, u_h, \mathbf{p}), \quad \forall \mathbf{p} \in \mathbf{W}. \tag{4.8}$$

For A_2, using Lemmas 2.1 and (3.1), the Hölder inequality and the triangle inequality, we have following estimates

$$\begin{aligned}
A_2 &\le \frac{\zeta}{2}\int_\Omega (|u|+|u_h|)^3\,|u-u_h|\mathrm{d}\Omega \\
&\le \frac{\zeta}{2}\left(\int_\Omega \left((|u|+|u_h|)^3\right)^2\mathrm{d}\Omega\right)^{1/2}\left(\int_\Omega |u-u_h|^2\mathrm{d}\Omega\right)^{1/2} \\
&\le \frac{\zeta}{2}\||u|+|u_h|\|_{0,6}^3\|u-u_h\|_0 \le \frac{\zeta}{2}(\|u\|_{0,6}+\|u_h\|_{0,6})^3\|u-u_h\|_0 \\
&\le \frac{\zeta}{2}C_u C_\Omega^3(\|u\|_a+\|u_h\|_a)^3\eta_a(h)\|u-u_h\|_a \\
&\le \frac{\zeta}{2}\frac{C_u C_\Omega^3(\|u\|_a+\|u_h\|_a)^3\eta_a(h)}{1-\alpha(\delta_h(u)+\eta_a(h))}\eta(\lambda_h, u_h, \mathbf{p}), \quad \forall \mathbf{p} \in \mathbf{W}.
\end{aligned} \tag{4.9}$$

The combination of (4.7), (4.8) and (4.9) leads to

$$\begin{aligned}
E(u_h)-E(u) &\le \frac{C_3\delta_h(u)+\left(C_3+\frac{\zeta}{2}C_u C_\Omega^3(\|u\|_a+\|u_h\|_a)^3\right)\eta_a(h)}{1-\alpha\,(\delta_h(u)+\eta_a(h))}\eta(\lambda_h, u_h, \mathbf{p}) \\
&\le \frac{C_4(\delta_h(u)+\eta_a(h))}{1-\alpha\,(\delta_h(u)+\eta_a(h))}\eta(\lambda_h, u_h, \mathbf{p})
\end{aligned}$$

where

$$C_4 = C_3 + \frac{\zeta}{2}C_u C_\Omega^3(\|u\|_a+\|u_h\|_a)^3.$$

Hence we obtain the desired result (4.5) and (4.6) can be derived easily. □

Remark 4.1 Practically, Theorem 4.1 and Corollary 4.1 are used with $\eta(\lambda_h, u_h, \mathbf{p}) = \eta(\lambda_h, u_h, \mathbf{p}^*)$ where $\mathbf{p}^*$ is a numerical approximation of the dual problem (3.10) and that it is not necessary to know the exact auxiliary function $\mathbf{p}$.

5 Numerical Examples

In this section, two numerical examples are presented to validate the efficiency of the computable a posteriori error estimate, the upper bounds of the error estimates for the principal eigenvalue and ground state energy, the lower bounds of the principal eigenvalue and the ground state energy.

In order to give the asymptotically accurate a posteriori error estimate $\eta(\lambda_h, u_h, \mathbf{p})$, we need to solve the auxiliary problem (3.12) with enough accuracy by some type of numerical method. Here, the auxiliary problem (3.12) is solved by the finite element method on the same mesh $\mathcal{T}_h$ and the $H(\mathrm{div};\Omega)$ conforming finite element space $\mathbf{W}_h$ that is defined as follows [12]

$$\mathbf{W}_h^p = \left\{\mathbf{w} \in \mathbf{W} : \mathbf{w}|_K \in \mathrm{RT}_p, \forall K \in \mathcal{T}_h\right\},$$

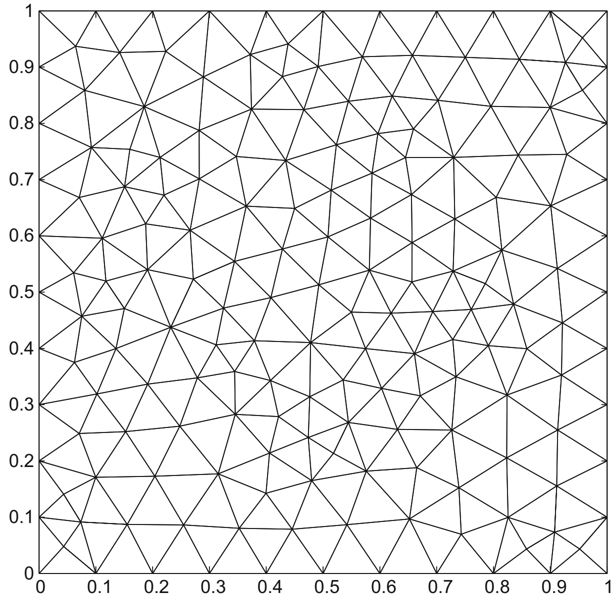

Fig. 1 The initial mesh for the unit square

where $\mathrm{RT}_p = (\mathcal{P}_p)^d + \mathbf{x}\mathcal{P}_p$ and $\mathcal{P}_p$ denotes the polynomial space with the degree no more than p. Then the approximate solution of the auxiliary problem (3.12) is defined as follows: Find $\mathbf{p}_h^* \in \mathbf{W}_h^p$ such that

$$a^*(\mathbf{p}_h^*, \mathbf{q}_h) = \mathcal{F}(\mathbf{q}_h), \quad \forall \mathbf{q}_h \in \mathbf{W}_h^p. \tag{5.1}$$

After obtaining $\mathbf{p}_h^*$, we can compute the a posteriori error estimate $\eta(\lambda_h, u_h, \mathbf{p}_h^*)$ as in (3.3). Based on λ_h and $\eta(\lambda_h, u_h, \mathbf{p}_h^*)$, we can obtain the asymptotically lower bound (4.3) with $\mathbf{p} = \mathbf{p}_h^*$ for the principal eigenvalue λ. Furthermore, we can also get an asymptotically lower bound of the ground state energy E_h^L.

Remark 5.1 In order to give an accurate a posteriori error estimator, it is a reasonable way to solve the auxiliary problem (5.1) with some type of numerical method. Of course, we can also use some simple local computing method to produce a function $\mathbf{p}_h$ to obtain an asymptotically upper bound of the error estimate for the eigenfunction approximation (cf. [4]).

Example 5.1 In this example, we consider the ground state solution of GPE (1.2) for BEC with $\zeta = 1$, $W(x) = x_1^2 + x_2^2$ and unit square $\Omega = (0, 1) \times (0, 1)$.

In this example, the initial mesh $\mathcal{T}_{h_1}$ with $h_1 = 1/10$ is showed in Fig. 1 which is generated by Delaunay method. Then we produce a sequence of meshes $\{\mathcal{T}_{h_i}\}_{i=2}^6$ by the regular refinement (connecting the midpoints of each edge) from $\mathcal{T}_{h_1}$ and then the mesh sizes are $h_2 = 1/20, \cdots, h_6 = 1/320$. Based on this sequence of meshes, a sequence of linear conforming finite element space $\{V_{h_i}\}_{i=1}^6$ and $H(\mathrm{div};\Omega)$ conforming finite element space $\{\mathbf{W}_{h_i}^1\}_{i=1}^6$ are built. Since the exact eigenvalue is not known, we choose an adequately accurate approximation obtained by the quadratic finite element method on the mesh $\mathcal{T}_{h_6}$ as the exact principal eigenpair for our numerical tests.

First we solve the GPE problem (2.1) in $\{V_{h_i}\}_{i=1}^6$ and the auxiliary problem (5.1) in $\{\mathbf{W}_{h_i}^1\}_{i=1}^6$, respectively. The corresponding numerical results are presented in Fig. 2 which

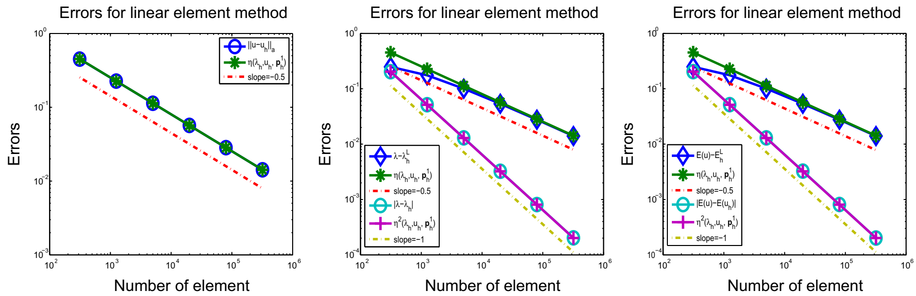

Fig. 2 The errors for the unit square domain when the eigenvalue problem is solved by the linear finite element method, where $\eta(\lambda_h, u_h, \mathbf{p}_h^1)$ denotes the a posteriori error estimator $\eta(\lambda_h, u_h, \mathbf{p}_h^*)$ when the auxiliary problem is solved in $\mathbf{W}_h^1$, λ_h^L denotes the asymptotically lower bound of the principal eigenvalue and E_h^L denotes the asymptotically lower bound of the ground state energy

shows that the a posteriori error estimate $\eta(\lambda_h, u_h, \mathbf{p}_h^*)$ is efficient when we solve the auxiliary problem in $\mathbf{W}_h^1$. In Fig. 2, we can find that the eigenvalue approximation λ_h^L and ground state energy approximation E_h^L are really asymptotically lower bounds for the principal eigenvalue λ and ground state energy $E(u)$, respectively. When the mesh has more than approximately 312 elements, the approximations λ_h^L and E_h^L are really below the exact principal eigenvalue λ and the exact ground state energy, respectively.

Example 5.2 In the second example, we solve the ground state solution of GPE (1.2) for BEC with $\zeta = 1$, $W(x) = x_1^2 + x_2^2$ on the L shape domain $\Omega = (-1, 1) \times (-1, 1)/[0, 1) \times (-1, 0]$.

Since Ω has a re-entrant corner, the singularity of the principal eigenfunction is expected. The convergence order for the eigenvalue approximation by the linear finite element method is less than 2 which is the order predicted by the theory for regular eigenfunctions. Since the exact eigenvalue is not known, we also choose an adequately accurate approximation obtained by the quadratic finite element method on the mesh which is refined by 16 times adaptively as the exact principal eigenpair for our numerical tests. In order to handle the singularity of the eigenfunction, the GPE (2.1) is solved by the adaptive finite element method (cf. [11]).

This example is presented to validate the results in this paper also hold on the adaptive meshes.

A standard adaptive mesh process can be described by the following one

$$\cdots \textbf{Solve} \rightarrow \textbf{Estimate} \rightarrow \textbf{Mark} \rightarrow \textbf{Refine} \cdots$$

More precisely, to get $T_{h_{k+1}}$ from T_{h_k} , we first solve the discrete equation on T_{h_k} to get the approximate solution and then calculate the a posteriori error estimator on each mesh element. Next, we mark the elements with big errors and these elements are refined in such a way that the triangulation is still shape regular and conforming.

For the computable-type a posteriori estimator can be defined as follows:

$$\eta_K(\lambda_h, u_h, \mathbf{p}) = \left(\|\lambda_h u_h - W u_h - \zeta u_h^3 + \mathrm{div}\mathbf{p}\|_{0,K}^2 + \|\mathbf{p} - \nabla u_h\|_{0,K}^2\right)^{1/2}, \qquad (5.2)$$

In order to compared with the effect of residual error estimator, we give the definition of the residual type a posteriori error estimator as follows: Define the element residual $\mathcal{R}_K(\lambda_h, u_h)$ and the jump residual $\mathcal{J}_E(u_h)$ as follows:

$$\mathcal{R}_K(\lambda_h, u_h) := \lambda_h u_h - \zeta |u_h|^2 u_h - W u_h + \Delta u_h, \quad \text{in } K \in \mathcal{T}_h,$$

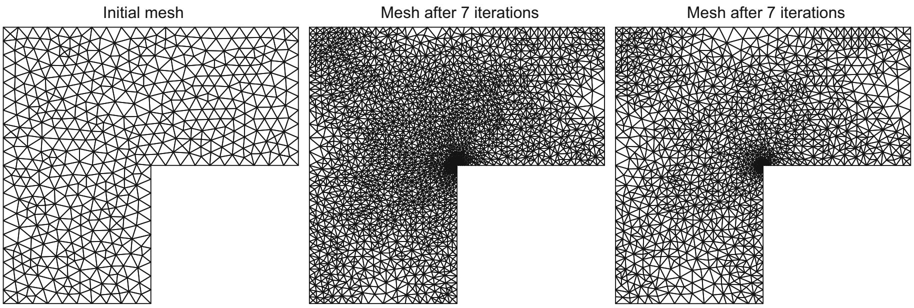

Fig. 3 The initial mesh of L-shape domain (left), the mesh after 7 adaptive refinements using the a posteriori error estimator $\eta_{ad}(\lambda_h, u_h)$ (middle) and the mesh after 7 adaptive refinements using the a posteriori error estimator $\eta(\lambda_h, u_h, \mathbf{p}_h)$ (right)

$$\mathcal{J}_e(u_h) := -\nabla u_h^+ \cdot \nu^+ - \nabla u_h^- \cdot \nu^- := [[\nabla u_h]]_e \cdot \nu_e, \quad \text{on } e \in \mathcal{E}_h,$$

where $\mathcal{E}_h$ denotes the interior edge set in the mesh $\mathcal{T}_h$, e is the common side of elements K^+ and K^- with unit outward normals ν^+ and ν^-, respectively, and $\nu_e = \nu^-$. For $K \in \mathcal{T}_h$, we define the local error indicator $\eta_h(\lambda_h, u_h, K)$ as follows

$$\eta_h^2(\lambda_h, u_h, K) := h_K^2 \|\mathcal{R}_K(\lambda_h, u_h)\|_{0,K}^2 + \sum_{e \in \mathcal{E}_h, e \subset \partial K} h_e \|\mathcal{J}_e(u_h)\|_{0,e}^2. \tag{5.3}$$

Then we define the global a posteriori error estimator $\eta_{ad}(\lambda_h, u_h)$ as

$$\eta_{ad}(\lambda_h, u_h) := \left(\sum_{K \in \mathcal{T}_h} \eta_h^2(\lambda_h, u_h, K) \right)^{1/2}. \tag{5.4}$$

In this example, we solve (2.5) in the linear conforming finite element space $V_{h,1}$ (or $V_{h,2}$) and solve the auxiliary problem (5.1) in the finite element space $\mathbf{W}_{h,1}^1$ (or $\mathbf{W}_{h,2}^1$), respectively. Here, $V_{h,1}$ and $\mathbf{W}_{h,1}^1$ denote the finite element spaces based on the meshes which are refined by using of the a posteriori error estimator $\eta_{ad}(\lambda_{h,1}, u_{h,1})$, $V_{h,2}$ and $\mathbf{W}_{h,2}^1$ denote the finite element spaces based on the meshes which are refined by using the a posteriori error estimator $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}_{h,2})$. Figure 3 shows the initial mesh (left), the adaptive meshes after 7 refinements by using the a posteriori error estimator $\eta_{ad}(\lambda_{h,1}, u_{h,1})$ (middle) and the a posteriori error estimator $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}_{h,2})$ (right), respectively. The corresponding numerical results are presented in Fig. 4 which shows that the a posteriori error estimate $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}_{h,2}^*)$ is more efficient than $\eta_{ad}(\lambda_{h,1}, u_{h,1})$ even on the adaptive meshes when the auxiliary problem is solved in $\mathbf{W}_{h,2}^1$. Figure 4 also shows λ_h^L and E_h^L are really asymptotically lower bounds for the principal eigenvalue λ and the ground state energy $E(u)$, respectively. When the meshes has more than approximately 982 elements, the approximations $\lambda_{h,1}^L$, $\lambda_{h,2}^L$, $E_{h,1}^L$ and $E_{h,2}^L$ are really below the exact principal eigenvalue λ and the exact ground state energy E, respectively.

Remark 5.2 In Fig. 4, we can see that the new a posteriori error estimator $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}_{h,2}^1)$ is smaller than $\eta(\lambda_{h,1}, u_{h,1}, \mathbf{p}_{h,1}^1)$ and both smaller than the residual type a posteriori error estimator $\eta_{ad}(\lambda_{h,1}, u_{h,1})$. Thus the error estimator $\eta(\lambda_h, u_h, \mathbf{p}_h^1)$ is more efficient than the residual type one $\eta_{ad}(\lambda_h, u_h)$. In addition, we can adjust the efficiency of $\eta(\lambda_h, u_h, \mathbf{p}_h^p)$ by solving the auxiliary problem (3.12) in different spaces $\mathbf{W}_h^p$.

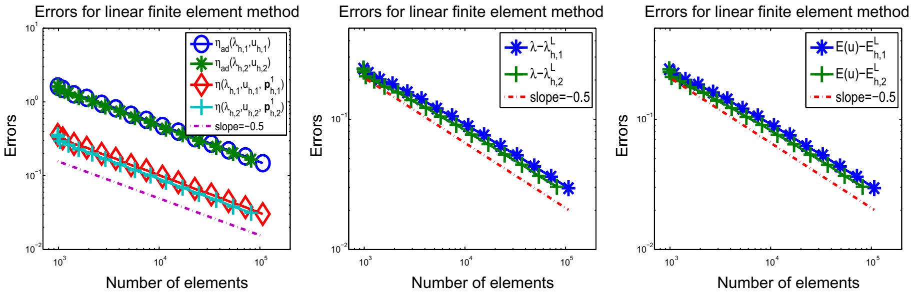

Fig. 4 The errors for the L shape domain when the eigenvalue problem is solved by the linear finite element method. Here, $\eta(\lambda_{h,1}, u_{h,1}, \mathbf{p}^1_{h,1})$ denotes $\eta(\lambda_{h,1}, u_{h,1}, \mathbf{p}^*_{h,1})$ when the auxiliary problem is solved in $\mathbf{W}^1_{h,1}$ on the meshes which are generated by adaptive refinement with the a posteriori error estimator $\eta_{ad}(\lambda_{h,1}, u_{h,1})$, $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}^1_{h,2})$ denotes $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}^*_{h,2})$ when the auxiliary problem is solved in $\mathbf{W}^1_{h,2}$ on the meshes which are generated by using the a posteriori error estimator $\eta(\lambda_{h,2}, u_{h,2}, \mathbf{p}^1_{h,2})$

6 Concluding Remarks

In this paper, we give a computable error estimate of the general conforming finite element methods of the GPE for the ground state of BEC on general meshes. Furthermore, the asymptotically lower bounds of the principal eigenvalue and ground state energy can be obtained by the computable error estimate. Some numerical examples are provided to demonstrate the validation of the efficiency of the computable error estimator and the asymptotically lower bounds for the principal eigenvalue and ground state energy. The method here can be extended to many other semilinear eigenvalue problems such as the Kohn-Sham model for Schrödinger equation. Moreover, we can adopt the efficient numerical methods to obtain these lower bounds, such as multilevel correction and multigrid method (cf. [26,37]). We can also adopt some efficient postprocessing methods (cf. [3,4,34]) to get the approximations of the auxiliary problem (5.1).

From the Definition (4.3), (4.6) and numerical examples, we find the accuracy of λ_h^L and E_h^L is not optimal. How to produce the lower bounds with the optimal accuracy will be our future work.

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